

Ian Chivers · Jane Sleighholme

Introduction to Programming with Fortran

With Coverage of Fortran 90, 95, 2003,
2008 and 77

Third Edition



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*The Yorkshire connection dedicates
the book to Steve, Mark and Jonathan.
The Welsh connection dedicates the book
to Joan, Martin and Jenny.*

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 - King’s College, IDC (1986–2002) and JS (1985–2008)
 - Chelsea College, JS (1978–1985)
 - Imperial College, IDC (1978–1986)

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Our Fortran home page is:

<http://www.fortranplus.co.uk/>

All of the program examples can be found there.

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Contents

1	Overview	1
1.1	Introduction	1
1.2	Program Examples	4
1.3	Web Addresses	4
2	Introduction to Problem Solving	5
2.1	Introduction	6
2.2	Natural Language	6
2.3	Artificial Language	7
2.3.1	Notations	7
2.4	Resume	7
2.5	Algorithms	8
2.5.1	Top-Down	8
2.5.2	Bottom-Up	8
2.5.3	Stepwise Refinement	9
2.6	Modular Programming	10
2.7	Object Oriented Programming	10
2.8	Systems Analysis and Design	10
2.8.1	Problem Definition	10
2.8.2	Feasibility Study and Fact Finding	11
2.8.3	Analysis	11
2.8.4	Design	11
2.8.5	Detailed Design	11
2.8.6	Implementation	12
2.8.7	Evaluation and Testing	12
2.8.8	Maintenance	12
2.9	Unified Modeling Language—UML	13
2.10	Conclusions	13
2.11	Problems	14

3	Introduction to Programming Languages	17
3.1	Introduction	17
3.2	Some Early Theoretical Work	17
3.3	What Is a Programming Language?	18
3.4	Program Language Development and Engineering	18
3.5	The Early Days	18
3.5.1	Fortran's Origins	18
3.5.2	Fortran 77	19
3.5.3	Cobol	19
3.5.4	Algol	20
3.6	Chomsky and Program Language Development	20
3.7	Lisp	21
3.8	Snobol	21
3.9	Second-Generation Languages	22
3.9.1	PL/1 and Algol 68	22
3.9.2	Simula	22
3.9.3	Pascal	22
3.9.4	APL	23
3.9.5	Basic	23
3.9.6	C	23
3.10	Some Other Strands in Language Development	24
3.10.1	Abstraction, Stepwise Refinement and Modules	24
3.10.2	Structured Programming	24
3.10.3	Data Structuring and Procedural Programming	25
3.10.4	Standardisation	25
3.11	Ada	26
3.12	Modula	26
3.13	Modula 2	27
3.14	Other Language Developments	27
3.14.1	Logo	27
3.14.2	Postscript, TEX and L ^A T _E X	28
3.14.3	Prolog	28
3.14.4	SQL	28
3.14.5	ICON	29
3.15	Object Oriented Programming	29
3.15.1	Simula	30
3.15.2	Smalltalk	30
3.15.3	Oberon and Oberon 2	30
3.15.4	Eiffel	31
3.15.5	C++	31
3.15.6	Java	32
3.15.7	C#	33

3.16	Back to Fortran!	34
3.16.1	Fortran 90	34
3.16.2	Fortran 95	35
3.16.3	ISO Technical Reports TR15580 and TR15581	35
3.16.4	Fortran 2003	36
3.16.5	DTR 19767 Enhanced Module Facilities	37
3.16.6	Fortran 2008	37
3.16.7	TS 29113 Further Interoperability of Fortran with C	37
3.16.8	Fortran 2015	37
3.17	Fortran Discussion Lists	38
3.18	ACM Fortran Forum	39
3.19	Other Sources	39
3.20	Summary	39
4	Introduction to Programming	47
4.1	Introduction	47
4.2	Language Strengths and Weaknesses	48
4.3	Elements of a Programming Language	48
4.3.1	Data Description Statements	49
4.3.2	Control Structures	49
4.3.3	Data-Processing Statements	49
4.3.4	Input and Output (I/O) Statements	49
4.4	Example 1: Simple Text I/O	50
4.5	Variables—Name, Type and Value	51
4.6	Example 2: Simple Numeric I/O and Arithmetic	52
4.7	Some More Fortran Rules	54
4.8	Fortran Character Set	54
4.9	Good Programming Guidelines	55
4.10	Compilers Used	57
4.11	Compiler Documentation	58
4.11.1	Gfortran	58
4.11.2	IBM	58
4.11.3	Intel	59
4.11.4	Nag	60
4.11.5	Oracle/Sun	60
4.12	Program Development	60
4.13	Reference Text for the Fortran 2003 Standard	61
4.14	Problems	62
5	Arithmetic	63
5.1	Introduction	64
5.2	The Fortran Operators and the Arithmetic Assignment Statement	64

5.3	Example 1: Simple Arithmetic Expressions in Fortran	65
5.4	The Fortran Rules for Arithmetic	66
5.5	Expression Equivalence	68
5.6	Rounding and Truncation	69
5.7	Example 2: Type Conversion and Assignment	69
5.8	Example 3: Integer Division and Real Assignment	70
5.9	Example 4: Time Taken for Light to Travel from the Sun to Earth	71
5.10	The Parameter Attribute	72
5.11	Round Off Errors and Computer Arithmetic	73
5.12	Relative and Absolute Errors	74
5.13	Example 5: Relative and Absolute Error.	75
5.14	Range, Precision and Size of Numbers.	76
5.15	Overflow and Underflow	77
5.15.1	Example 6: Overflow.	77
5.15.2	Example 7: Underflow	78
5.16	Health Warning: Optional Reading, Beginners Are Advised to Leave Until Later	79
5.16.1	Positional Number Systems.	79
5.16.2	Fortran Representational Models	79
5.17	Testing the Numerical Representation of Different Kind Types on a System	81
5.18	Example 8: Using the Numeric Inquiry Functions with Integer Types	82
5.19	Example 9: Using the Numeric Inquiry Functions with Real Types	84
5.20	Example 10: Literal Real Constants in a Calculation	87
5.21	Summation and Finite Precision	88
5.21.1	Example 11: Rounding Problem	89
5.22	Example 12: Binary Representation of Different Integer Kind Type Numbers	89
5.23	Example 13: Binary Representation of a Real Number.	91
5.24	Example 14: Initialisation of Physical Constants, Version 1	92
5.25	Example 15: Initialisation of Physical Constants, Version 2	94
5.26	Example 16: Initialisation of Physical Constants, Version 3	94
5.27	Summary of How to Select the Appropriate Kind Type	95
5.28	Variable Status	96
5.29	Fortran and the IEEE 754 Standard	96
5.30	Summary	97
5.31	Problems	98

6 Arrays 1: Some Fundamentals	103
6.1 Tables of Data	103
6.1.1 Telephone Directory	104
6.1.2 Book Catalogue.	104
6.1.3 Examination Marks or Results.	104
6.1.4 Monthly Rainfall	105
6.2 Arrays in Fortran.	106
6.2.1 The Dimension Attribute	106
6.2.2 An Index	106
6.2.3 Control Structure.	106
6.3 Example 1: Monthly Rainfall	107
6.4 Possible Missing Data	109
6.5 Example 2: People's Weights and Setting the Array Size With a Parameter	110
6.6 Summary	112
6.7 Problems	113
7 Arrays 2: Further Examples	115
7.1 Varying the Array Size at Run Time	115
7.1.1 Example 1: Allocatable Arrays	116
7.2 Higher-Dimension Arrays.	117
7.2.1 Example 2: Two Dimensional Arrays and a Map	117
7.2.2 Example 3: Sensible Tabular Output	119
7.2.3 Example 4: Average of Three Sets of Values	120
7.2.4 Example 5: Booking Arrangements in a Theatre or Cinema	121
7.3 Additional Forms of the Dimension Attribute and Do Loop Statement	122
7.3.1 Example 6: Voltage from -20 to +20 Volts	122
7.3.2 Example 7: Longitude from -180 to +180	123
7.3.3 Notes.	123
7.4 The Do Loop and Straight Repetition	124
7.4.1 Example 8: Table of Liquid Conversion Measurements	124
7.4.2 Example 9: Means and Standard Deviations	124
7.5 Summary	125
7.6 Problems	127
8 Whole Array and Additional Array Features	131
8.1 Terminology	131
8.2 Array Element Ordering.	132
8.3 Whole Array Manipulation.	132
8.4 Assignment	132
8.5 Expressions	133

8.6	Example 1: Rank 1 Whole Arrays in Fortran	134
8.7	Example 2: Rank 2 Whole Arrays in Fortran	135
8.8	Array Sections	136
8.8.1	Example 3: Rank 1 Array Sections	136
8.8.2	Example 4: Rank 2 Array Sections	136
8.9	Array Constructors	138
8.9.1	Example 5: Rank 1 Array Initialisation—Explicit Values	138
8.9.2	Example 6: Rank 1 Array Initialisation Using An Implied do loop	139
8.9.3	Example 7: Rank 1 Arrays and the <code>dot_product</code> Intrinsic	140
8.9.4	Initialising Rank 2 Arrays	140
8.9.5	Example 8: Initialising a Rank 2 Array	141
8.10	Miscellaneous Array Examples	142
8.10.1	Example 9: Rank 1 Arrays and a Stride of 2	142
8.10.2	Example 10: Rank 1 Array and the <code>sum</code> Intrinsic Function	143
8.10.3	Example 11: Rank 2 Arrays and the <code>sum</code> Intrinsic Function	144
8.10.4	Example 12: Masked Array Assignment and the <code>where</code> Statement	145
8.10.5	Notes	146
8.11	The <code>forall</code> Statement and <code>forall</code> Construct	146
8.11.1	Syntax	146
8.12	Array Element Ordering in More Detail	147
8.12.1	Example 13: Array Element Ordering	147
8.13	Physical and Virtual Memory	148
8.14	Type Declaration Statement Summary	149
8.15	Summary	149
8.16	Problems	150
9	Output of Results	153
9.1	Introduction	153
9.2	Integers and the <code>i</code> Format or Edit Descriptor	154
9.2.1	Example 1: Twelve Times Table	154
9.2.2	Example 2: Integer Overflow and the <code>i</code> Edit Descriptor	155
9.3	Reals and the <code>f</code> Edit Descriptor	156
9.3.1	Example 3: Imperial Pints and US Pints	156
9.3.2	Example 4: Imperial Pints and Litres	157
9.3.3	Example 5: Narrow Field Widths and the <code>f</code> Edit Descriptor	158
9.3.4	Example 6: Overflow and the <code>f</code> Edit Descriptor	158

9.4	Reals and the <code>e</code> Edit Descriptor	159
9.4.1	Example 7: Simple <code>e</code> Edit Descriptor Example	159
9.5	Reals and the <code>g</code> Edit Descriptor	161
9.5.1	Example 8: Simple <code>g</code> Edit Descriptor Example	161
9.6	Spaces	162
9.6.1	Example 9: Three Ways of Generating Spaces	162
9.7	Characters—a Format or Edit Descriptor	163
9.7.1	Example 10: Character Output and the <code>a</code> Edit Descriptor.	163
9.7.2	Example 11: Character, Integer and Real Output in a Format Statement	164
9.8	Common Mistakes.	164
9.9	Files in Fortran	165
9.9.1	The <code>open</code> Statement	165
9.9.2	The <code>close</code> Statement	166
9.9.3	Example 12: Open and Close Usage	166
9.9.4	Example 13: Timing of Writing Formatted Files	167
9.9.5	Example 14: Timing of Writing Unformatted Files	169
9.10	Example 15: Implied Do Loops and Array Sections for Array Output	170
9.11	Example 16: Repetition and Whole Array Output	171
9.12	Example 17: Choosing the Decimal Symbol	172
9.13	Example 18: Alternative Format Specification Using a String	173
9.14	Example 19: Alternative Format Specification Using a Character Variable.	174
9.15	The Remaining Control and Data Edit Descriptors.	174
9.16	Summary	174
9.17	Problems	175
10	Reading in Data	179
10.1	Reading from Files	179
10.2	Example 1: Reading Integer Data	179
10.3	Example 2: Reading Real Data	182
10.4	Met Office Historic Station Data	183
10.5	Example 3: Reading One Column of Data from a File	184
10.6	Example 4: Skipping Lines in a File	186
10.7	Example 5: Reading from Several Files Consecutively	187
10.8	Example 6: Reading Using Array Sections	189
10.9	Example 7: Reading Using Internal Files	190
10.10	Example 8: Timing of Reading Formatted Files	192
10.11	Example 9: Timing of Reading Unformatted Files	193
10.12	Summary	194
10.13	Problems	194

11 Summary of I/O Concepts	197
11.1 I/O Concepts and Statements	197
11.2 Records	198
11.3 File Access.	198
11.4 The open Statement	198
11.5 Data Transfer Statements	200
11.6 The inquire Statement.	201
11.7 Error, End of Record and End of File	202
11.7.1 Error Conditions and the <code>err=</code> Specifier	202
11.7.2 End-of-file Condition and the <code>end=</code> Specifier	202
11.7.3 End-of-Record Condition and the <code>eor=</code> Specifier	202
11.7.4 <code>iostat=</code> Specifier	203
11.7.5 <code>iomsg=</code> Specifier	203
11.8 Examples	203
11.8.1 Example 1: Simple Use of the <code>read</code> , <code>write</code> , <code>open</code> , <code>close</code> , <code>unit</code> Features	203
11.8.2 Example 2: Using <code>iostat</code> to Test for Errors.	204
11.9 Example 3: Use of <code>newunit</code> and <code>lentrим</code>	205
11.10 Unit Numbering	207
11.11 Summary	207
11.12 Problems	207
12 Functions	209
12.1 Introduction	209
12.2 An Introduction to Predefined Functions and Their Use	210
12.2.1 Example 1: Simple Function Usage	210
12.3 Generic Functions	211
12.3.1 Example 2: The <code>abs</code> Generic Function	211
12.4 Elemental Functions	212
12.4.1 Example 3: Elemental Function Use	212
12.5 Transformational Functions.	212
12.5.1 Example 4: Simple Transformational Use	212
12.5.2 Example 5: Intrinsic <code>dot_product</code> Use.	213
12.6 Notes on Function Usage	213
12.7 Example 6: Easter	214
12.8 Intrinsic Procedures	216
12.9 Supplying Your Own Functions	216
12.9.1 Example 7: Simple User Defined Function	216
12.10 An Introduction to the Scope of Variables, Local Variables and Interface Checking	219
12.11 Recursive Functions	220
12.11.1 Example 8: Recursive Factorial Evaluation	220
12.12 Example 9: Recursive Version of GCD	222
12.13 Example 10: GCD After Removing Recursion	223

12.14	Internal Functions	223
12.14.1	Example 11: Stirling's Approximation	224
12.15	Pure Functions	224
12.15.1	Pure Constraints	225
12.16	Elemental Functions	226
12.17	Resume	227
12.18	Formal Syntax	227
12.19	Rules and Restrictions	228
12.20	Problems	229
13	Control Structures	231
13.1	Introduction	231
13.2	Selection Among Courses of Action	232
13.3	The Block if Statement	232
13.3.1	Example 1: Quadratic Roots	235
13.3.2	Example 2: Date Calculation.	236
13.4	The Case Statement.	237
13.4.1	Example 3: Simple Calculator.	237
13.4.2	Example 4: Counting Vowels, Consonants, etc.	238
13.5	The Three Forms of the do Statement	239
13.5.1	Example 5: Sentinel Usage	240
13.5.2	Cycle and Exit	241
13.5.3	Example 6: The Evaluation of $e^{**}x$	242
13.5.4	Example 7: Wave Breaking on an Offshore Reef.	243
13.6	Summary	245
13.6.1	Control Structure Formal Syntax	245
13.7	Problems	246
14	Characters	249
14.1	Introduction	249
14.2	Character Input	250
14.2.1	Example 1: The * Edit Descriptor	251
14.2.2	Example 2: The a Edit Descriptor	251
14.3	Character Operators	251
14.4	Character Substrings	253
14.4.1	Example 3: Stripping Blanks from a String.	253
14.5	Character Functions	254
14.5.1	Example 4: The index Character Function	254
14.5.2	The len and len_trim Functions	255
14.5.3	Example 5: Using len and len_trim.	255
14.6	Collating Sequence	256
14.7	Example 6: Finding Out About the Character Set Available.	257
14.8	The scan Function.	258
14.8.1	Example 7: Using the scan Function	258

14.9	Summary	260
14.10	Problems	260
15	Complex.	265
15.1	Introduction	265
15.2	Example 1: Use of <code>cmplx</code> , <code>aimag</code> and <code>conjg</code>	266
15.3	Example 2: Polar Coordinate Example.	266
15.4	Complex and Kind Type	268
15.5	Summary	268
15.6	Problems	268
16	Logical.	269
16.1	Introduction	269
16.2	I/O	272
16.3	Summary	273
16.4	Problems	273
17	Introduction to Derived Types.	275
17.1	Introduction	275
17.2	Example 1: Dates	276
17.3	Type Definition.	277
17.4	Variable Definition	277
17.4.1	Example 2: Variant of Example 1 Using Modules.	277
17.5	Example 3: Address Lists.	278
17.6	Example 4: Nested User Defined Types	280
17.7	Problems	282
18	An Introduction to Pointers.	283
18.1	Introduction	283
18.2	Example 1: Illustrating Some Basic Pointer Concepts	284
18.3	Example 2: The <code>associated</code> Intrinsic Function	285
18.4	Example 3: Referencing Pointer Variables Before Allocation or Pointer Assignment	286
18.4.1	<code>gfortran</code>	287
18.4.2	<code>Intel</code>	287
18.4.3	<code>Nag</code>	288
18.5	Example 4: Pointer Allocation and Assignment.	288
18.6	Memory Leak Examples	288
18.6.1	Example 5: Simple Memory Leak	289
18.6.2	Example 6: More Memory Leaks	289
18.7	Non-standard Pointer Example	290
18.7.1	Example 7: Using the C <code>loc</code> Function.	291
18.8	Problems	292

19	Introduction to Subroutines	293
19.1	Introduction	293
19.2	Example 1: Roots of a Quadratic Equation	294
19.2.1	Referencing a Subroutine	296
19.2.2	Dummy Arguments or Parameters and Actual Arguments	296
19.2.3	The <code>intent</code> Attribute	297
19.2.4	Local Variables	297
19.2.5	Local Variables and the <code>save</code> Attribute	297
19.2.6	Scope of Variables	298
19.2.7	Status of the Action Carried Out in the Subroutine	298
19.2.8	Modules ‘Containing’ Procedures	298
19.3	Why Bother with Subroutines?	299
19.4	Summary	299
19.5	Problems	299
20	Subroutines: 2	301
20.1	More on Parameter Passing	301
20.1.1	Assumed-Shape Array	301
20.1.2	Deferred-Shape Array	301
20.1.3	Automatic Arrays	302
20.1.4	Allocatable Dummy Arrays	302
20.1.5	Keyword and Optional Arguments	302
20.2	Example 1: Assumed Shape Parameter Passing	303
20.2.1	Notes	305
20.3	Example 2: Character Arguments and Assumed-Length Dummy Arguments	305
20.4	Example 3: Rank 2 and Higher Arrays as Parameters	306
20.4.1	Notes	308
20.5	Example 4: Automatic Arrays and Median Calculation	308
20.5.1	Internal Subroutines and Scope	311
20.6	Example 5: Recursive Subroutines—Quicksort	312
20.6.1	Note—Recursive Subroutine	315
20.6.2	Note—Flexible Design	315
20.7	Example 6: Allocatable Dummy Arrays	315
20.8	Example 7: Elemental Subroutines	318
20.9	Summary	319
20.10	Problems	320
20.11	Commercial Numerical and Statistical Subroutine Libraries	322
21	Modules	323
21.1	Introduction	323
21.2	Basic Module Syntax	324
21.3	Modules for Global Data	324

21.4	Example 1: Modules for Precision Specification and Constant Definition	325
21.5	Example 2: Modules for Globally Sharing Data	327
21.6	Modules for Derived Data Types.	329
21.7	Example 3: Person Data Type.	329
21.8	Example 4: A Module for Simple Timing of a Program	332
21.9	private, public and protected attributes.	333
21.10	The use statement	333
21.11	Notes on Module Usage and Compilation.	334
21.12	Formal Syntax	334
21.12.1	Interface	334
21.12.2	Implicit and Explicit Interfaces	334
21.12.3	Explicit Interface	335
21.13	Summary	335
21.14	Problems	336
22	Data Structuring in Fortran	337
22.1	Introduction	337
22.2	Example 1: Singly Linked List: Reading an Unknown Amount of Text	337
22.3	Example 2: Reading in an Arbitrary Number of Reals Using a Linked List and Copying to an Array	341
22.4	Example 3: Ragged Arrays.	342
22.5	Example 4: Ragged Arrays and Variable Sized Data Sets.	343
22.6	Example 5: Perfectly Balanced Tree	344
22.7	Example 6: Date class	346
22.7.1	Notes: DST in the USA	357
22.8	Problems	357
23	An Introduction to Algorithms and the Big O Notation	359
23.1	Introduction	359
23.2	Basic Background	360
23.3	Brief Explanation	360
23.4	Example 1	361
23.5	Sorting.	362
23.6	Basic Array and Linked List Performance	363
24	Operator Overloading.	365
24.1	Introduction	365
24.2	Other Languages.	365
24.3	Example 1: Overloading the Addition (+) Operator.	366
24.4	Problems	367

25 Generic Programming	369
25.1 Introduction	369
25.2 Generic Programming and Other Languages	369
25.3 Example 1: Sorting Reals and Integers.	370
25.3.1 Generic Quicksort in C++	377
25.3.2 Generic Quicksort in C#	379
25.4 Example 2: Generic Statistics Module	380
25.5 Problems	386
26 Mathematical Examples	387
26.1 Introduction	387
26.2 Example 1: Using Linked Lists for Sparse Matrix Problems	387
26.2.1 Inner Product of Two Sparse Vectors	388
26.3 Example 2: Solving a System of First-Order Ordinary Differential Equations Using Runge–Kutta–Merson	392
26.3.1 Note: Alternative Form of the Allocate Statement	399
26.3.2 Note: Automatic Arrays	399
26.3.3 Note: Subroutine as a Dummy Procedure Argument	400
26.3.4 Note: Compilation When Using Modules	400
26.3.5 Keyword and Optional Argument Variation	400
26.4 Example 3: A Subroutine to Extract the Diagonal Elements of a Matrix	402
26.5 Example 4: The Solution of Linear Equations Using Gaussian Elimination	403
26.5.1 Notes	407
26.6 Example 5: Allocatable Function Results	408
26.7 Example 6: Elemental $e^{**}x$ Function	410
26.8 Problems	411
27 Parameterised Derived Types (PDTs) in Fortran	413
27.1 Introduction	413
27.2 Example 1: Linked List Parameterised by Real Kind	414
27.3 Example 2: Ragged Array Parameterised by Real Kind Type	416
27.4 Example 3: Specifying <code>len</code> in a PDT	418
27.5 Problems	420
28 Object Oriented Programming	421
28.1 Introduction	421
28.2 Brief Review of the History of Object Oriented Programming	421
28.3 Background Technical Material	422

28.4	Type Declaration Statements	423
28.4.1	Type	423
28.4.2	Class	423
28.4.3	Attributes	423
28.4.4	Passed Object Dummy Arguments	424
28.4.5	Derived Types and Structure Constructors	425
28.4.6	Structure Constructors and Generic Names	425
28.4.7	Assignment	425
28.4.8	Intrinsic Assignment Statement	426
28.4.9	Defined Assignment Statement	426
28.4.10	Polymorphic Variables	426
28.4.11	Executable Constructs Containing Blocks	426
28.4.12	The associate Construct	426
28.4.13	The select Type Construct	427
28.5	Example 1: The Basic Shape Class	427
28.5.1	Key Points	429
28.5.2	Notes	432
28.5.3	Example 2: Base Class with Private Data	432
28.5.4	Example 3: Using an Interface to Use the Class Name for the Structure Constructor	433
28.5.5	Public and Private Accessibility	435
28.6	Example 4: Simple Inheritance	436
28.6.1	Base Shape Class	436
28.6.2	Circle—Derived Type 1	436
28.6.3	Rectangle—Derived Type 2	439
28.6.4	Simple Inheritance Test Program	441
28.7	Example 5: Polymorphism and Dynamic Binding	443
28.7.1	Base Shape Class	443
28.7.2	Circle—Derived Type 1	445
28.7.3	Rectangle—Derived Type 2	445
28.7.4	Shape Wrapper Module	445
28.7.5	Display Subroutine	445
28.7.6	Test Program for Polymorphism and Dynamic Binding	446
28.8	Summary	449
28.9	Problems	449
29	Introduction to Parallel Programming	451
29.1	Introduction	451
29.2	Parallel Computing Classification	452
29.3	Amdahl's Law	453
29.3.1	Amdahl's Law Graph 1–8 Processors or Cores	453
29.3.2	Amdahl's Law Graph 2–64 Processors or Cores	454

29.4	Gustafson's Law	454
29.4.1	Gustafson's Law Graph 1–64 Processors or Cores	455
29.5	Memory Access	455
29.6	Cache	455
29.7	Bandwidth and Latency	456
29.8	Flynn's Taxonomy	456
29.9	Consistency Models.	457
29.10	Threads and Threading.	457
29.11	Threads and Processes	457
29.12	Data Dependencies	457
29.13	Race Conditions	458
29.14	Mutual Exclusion-Mutex	458
29.15	Monitors	458
29.16	Locks	458
29.17	Synchronization	458
29.18	Granularity and Types of Parallelism	459
29.19	Partitioned Global Address Space—PGAS	459
29.20	Fortran and Parallel Programming	459
29.21	MPI	459
29.22	OpenMP	461
29.23	Coarray Fortran.	462
29.24	Other Parallel Options	462
29.24.1	PVM	463
29.24.2	HPF.	463
29.25	Top 500 Supercomputers	463
29.26	Summary	464
30	MPI—Message Passing Interface	465
30.1	Introduction	465
30.2	MPI Programming.	465
30.3	Compiler and Implementation Combination	466
30.4	Individual Implementation	466
30.4.1	MPICH2	466
30.4.2	Open MPI	466
30.5	Compiler and MPI Combinations Used in the Book	467
30.5.1	Cray Archer System.	467
30.6	The MPI Memory Model	467
30.7	Example: 1—Hello World	468
30.8	Example: 2—Hello World Using Send and Receive.	470
30.9	Example: 3—Serial Solution for Pi Calculation.	473
30.10	Example: 4—Parallel Solution for Pi Calculation.	478
30.11	Example: 5—Work Sharing Between Processes	483
30.12	Summary	487
30.13	Problems	487

31 OpenMP	489
31.1 Introduction	489
31.2 OpenMP Memory Model	490
31.3 Example 1: Hello World	491
31.4 Example 2: Hello World Using Default Variable Data Scoping	494
31.5 Example 3: Hello World with Private <code>thread_number</code> variable	495
31.6 Example 4: Parallel Solution for Pi Calculation	496
31.7 Summary	499
31.8 Problems	499
32 Coarray Fortran	501
32.1 Introduction	501
32.2 Coarray Terminology	502
32.3 Example 1: Hello World	503
32.4 Example 2: Broadcasting Data	504
32.5 Example 3: Parallel Solution for Pi Calculation	505
32.6 Example 4: Work Sharing	508
32.7 Summary	512
32.8 Problems	512
33 C Interop	513
33.1 Introduction	513
33.2 The <code>iso_c_binding</code> Module	513
33.3 Named Constants and Derived Types in the Module	513
33.4 Character Interoperability	514
33.5 Procedures in the Module	515
33.6 Interoperability of Intrinsic Types	515
33.7 Other Aspects of Interoperability	516
33.7.1 Interoperability with C Pointer Types	516
33.7.2 Interoperability of Scalar Variables	516
33.7.3 Interoperability of Array Variables	516
33.7.4 Interoperability of Procedures and Procedure Interfaces	516
33.7.5 Interoperation with C Global Variables	516
33.7.6 Binding Labels for Common Blocks and Variables	517
33.7.7 Interoperation with C Functions	517
33.8 Compilers Used in the Examples	517
33.9 Example 1: Kind Type Support	518
33.10 Example 2: Fortran Calling a C Function	520
33.11 Example 3: C Calling a Fortran Function	521
33.12 Example 4: C++ Calling a Fortran Function	522
33.13 Example 5: Passing an Array from Fortran to C	522
33.14 Example 6: Passing an Array from C to Fortran	524

33.15	Example 7: Passing an Array from C++ to Fortran	525
33.16	Example 8: Passing a Rank 2 Array from Fortran to C	526
33.17	Example 9: Passing a Rank 2 Array from C to Fortran	527
33.18	Example 10: Passing a Rank 2 Array from C++ to Fortran.	528
33.19	Example 11: Passing a Rank 2 Array from C++ to Fortran and Taking Care of Array Storage.	530
	33.19.1 Compiler Switches.	532
33.20	Example 12: Passing a Rank 2 Array from C to Fortran and Taking Care of Array Storage.	533
	33.20.1 Compiler Switches.	535
33.21	Acknowledgements	535
33.22	c_loc Examples on our Web Site	535
	33.22.1 c_loc(x) Description	536
33.23	Problems	537
34	IEEE Arithmetic.	539
34.1	Introduction	539
34.2	History	539
34.3	IEEE 754 Specifications.	541
	34.3.1 Single Precision Floating Point Format.	542
	34.3.2 Double Precision Floating Point Format.	543
	34.3.3 Two Classes of Extended Floating Point Formats.	543
	34.3.4 Accuracy Requirements	544
	34.3.5 Base Conversion—Converting Between Decimal and Binary Floating Point Formats and Vice Versa	544
	34.3.6 Exception Handling	544
	34.3.7 Rounding Directions	544
	34.3.8 Rounding Precisions	545
34.4	Resume	545
34.5	Fortran Support for IEEE Arithmetic	545
34.6	Derived Types and Constants Defined in the Modules	546
	34.6.1 ieee_exceptions	546
	34.6.2 ieee_arithmetic	546
	34.6.3 ieee_features	547
	34.6.4 Further Information	547
34.7	Example 1: Testing IEEE Support.	548
34.8	Example 2: Testing What Flags are Supported	549
34.9	Example 3: Overflow.	550
34.10	Example 4: Underflow.	551
34.11	Example 5: Inexact Summation.	552
34.12	Example 6: NAN and Other Specials.	554
34.13	Summary	556
34.14	Problems	559

35 Miscellaneous Examples	561
35.1 Example 1: Date Data Type with USA and ISO Support	561
35.2 Example 2: Binary Search Example.	566
35.3 Comparison of Three Sorting Methods.	569
35.4 Example 3: Generic Recursive Quicksort Example with Timing Details.	569
35.5 Example 4: Non Recursive Quicksort Example with Timing Details.	572
35.5.1 Notes—Version Control Systems.	577
35.6 Subroutine and Function Libraries.	577
35.7 Numerical Libraries.	578
35.8 Serial and Parallel Libraries	578
35.9 The Nag Library for SMP and Multicore	578
35.10 Example 5: Calling the Nag M01caf Sorting Routine.	579
35.11 Graphics Libraries	581
35.12 The Dislin Graphics Library	581
35.12.1 Dislin Example 1: Amdahl’s Law Graph 1–8 Processors or Cores	582
35.12.2 Dislin Example 2: Amdahl’s Law Graph 2–64 Processors or Cores	583
35.12.3 Dislin Example 3: Gustafson’s Law Graph 1–64 Processors or Cores	583
35.12.4 Dislin Example 4: The Display of Tsunami Events.	583
35.13 Problems	589
36 Converting from Fortran 77	591
36.1 Introduction	591
36.2 Deleted Features	592
36.3 Obsolescent Features	592
36.3.1 Arithmetic If.	592
36.3.2 Real and Double Precision Do Control Variables . . .	592
36.3.3 Shared do Termination and Non-enddo Termination	592
36.3.4 Alternate Return	592
36.3.5 Pause Statement	593
36.3.6 Assign and Assigned Goto Statements	593
36.3.7 Assigned Format Statements	593
36.3.8 H Editing	593
36.4 Better Alternatives.	593
36.5 Commercial Conversion Tools	594
36.5.1 Convert	594
36.5.2 Forcheck	594
36.5.3 Forstruct.	595

Contents	xxvii
36.5.4 Forstudy	595
36.5.5 Plusfort	595
36.5.6 VAST/77to90	595
36.6 Example of PlusFORT Capability from Polyhedron Software	595
36.6.1 Original Fortran 66	596
36.6.2 Fortran 77 Version	596
36.6.3 Fortran 90 Version	597
36.7 Summary	598
Appendix A: Glossary	599
Appendix B: Intrinsic Functions and Procedures	611
Appendix C: Text Extracts, English, Latin and coded	655
Appendix D: Formal Syntax	657
Appendix E: Compiler Options	661
Index	663

List of Tables

Table 3.1	C++ standardisation history	32
Table 3.2	Fortran standardisation history	38
Table 4.1	Variable name, type and value	52
Table 4.2	The Fortran character set	55
Table 4.3	ASCII character set	56
Table 5.1	Fortran operators	64
Table 5.2	Hierarchy or precedence of the Fortran operators	67
Table 5.3	Some commonly used physical constants	73
Table 5.4	Word size and integer numbers	76
Table 5.5	Word size and real numbers	76
Table 5.6	Kind inquiry functions	81
Table 5.7	Numeric inquiry functions	81
Table 5.8	Integer kind type parameter name and integer value	83
Table 5.9	Integer kind and huge comparison	84
Table 5.10	Extended real type comparison	86
Table 6.1	Fortran statement ordering	112
Table 8.1	Array element ordering in Fortran	147
Table 9.1	Summary of data edit descriptors	175
Table 9.2	Text edit descriptors	175
Table 11.1	Open statement options	199
Table 11.2	Data transfer statement options	200
Table 11.3	Inquire statement options	201
Table 12.1	Some of the intrinsic functions available in Fortran	211
Table 13.1	Fortran logical and relational operators	234
Table 14.1	String functions in Fortran	260
Table 16.1	Simple truth table	271
Table 16.2	Fortran operator hierarchy	271
Table 23.1	Big O notation and complexity	360
Table 23.2	Quicksort and insertion sort comparison	362
Table 23.3	Array and linked list performance	363
Table 29.1	Bandwidth and latency	456
Table 30.1	Intel I7 with hyperthreading	482
Table 33.1	<code>iso_c_binding</code> module—named constants	514

Table 33.2	C Interop character interoperability	515
Table 33.3	Compilers used.	517
Table 33.4	Basic C Interop table.	519
Table 34.1	Computer hardware and manufacturers	540
Table 34.2	Operating systems.	540
Table 34.3	Compiler IEEE support for various precisions	548
Table 35.1	Generic recursive quicksort timing	572
Table 35.2	Non recursive quicksort timing.	577
Table 35.3	Sixty four bit real sort timings	580
Table 35.4	Nag sort m01caf timing.	581

Chapter 1

Overview

*I don't know what the language of the year 2000 will look like,
but it will be called Fortran.*

C.A.R. Hoare

Aims

The aims of the chapter are to provide a background to the organisation of the book.

1.1 Introduction

The book aims to provide coverage of a reasonable working subset of the Fortran programming language. The subset chosen should enable you to solve quite a wide range of frequently occurring problems.

This book has been written for both complete beginners with little or no programming background and experienced Fortran programmers who want to update their skills and move to a modern version of the language.

Chapters 2 and 3 provide a coverage of problem solving and the history and development of programming languages. Chapter 2 is essential for the beginner as the concepts introduced there are used and expanded on throughout the rest of the book. Chapter 3 should be read at some point but can be omitted initially. Programming languages evolve and some understanding of where Fortran has come from and where it is going will prove valuable in the longer term.

- Chapter 2 looks at problem solving in some depth, and there is a coverage of the way we define problems, the role of algorithms, the use of both top-down and bottom-up methods, and the requirement for formal systems analysis and design for more complex problems.
- Chapter 3 looks at the history and development of programming languages. This is essential as Fortran has evolved considerably from its origins in the mid-1950s, through the first standard in 1966, the Fortran 77 standard, the Fortran 90 standard, the Fortran 95 standard, TR 15580 and TR 15581, Fortran 2003 and Fortran 2008.

It helps to put many of the current and proposed features of Fortran into context. Languages covered include Cobol, Algol, Lisp, Snobol, PL/1, Algol 68, Simula, Pascal, APL, Basic, C, Ada, Modula, Modula 2, Logo, Prolog, SQL, ICON, Oberon, Oberon 2, Smalltalk, C++, C# and Java.

Chapters 4–8 cover the major features provided in Fortran for numeric programming in the first instance and for general purpose programming in the second. Each chapter has a set of problems. It is essential that a reasonable range of problems are attempted and completed, as it is impossible to learn any language without practice.

- Chapter 4 provides an introduction to programming with some simple Fortran examples. For people with a knowledge of programming this chapter can be covered fairly quickly.
- Chapter 5 looks at arithmetic in some depth, with a coverage of the various numeric data types, expressions and assignment of scalar variables. There is also a thorough coverage of the facilities provided in Fortran to help write programs that work on different hardware platforms.
- Chapter 6 is an introduction to arrays and do loops. The chapter starts with some examples of tabular structures that one should be familiar with. There is then an examination of what concepts we need in a programming language to support manipulation of tabular data.
- Chapter 7 takes the ideas introduced in Chap. 6 and extends them to higher-dimensioned arrays, additional forms of the dimension attribute and corresponding form of the do loop, and the use of looping for the control of repetition and manipulation of tabular information without the use of arrays.
- Chapter 8 looks at more of the facilities offered for the manipulation of whole arrays and array sections, ways in which we can initialise arrays using constructors, look more formally at the concepts we need to be able to accurately describe and understand arrays, and finally look at the differences between the way Fortran allows us to use arrays and the mathematical rules governing matrices.

Chapters 9–11 look at input and output (I/O) and file handling in Fortran. An understanding of I/O is necessary for the development of so-called production, non interactive programs. These are essentially fully developed programs that are used repeatedly with a variety of data inputs and results.

- Chapter 9 looks at output of results and how to generate something that is more comprehensible and easy to read than what is available with free format output and also how to write the results to a file rather than the screen.
- Chapter 10 extends the ideas introduced in Chap. 9 to cover input of data, or reading data into a program and also considers file I/O.
- Chapter 11 provides a summary of input and output concepts introduced in Chaps. 9 and 10, and expands on them by introducing additional features of the read, write, open and close statements.

Chapter 12 introduces the first building block available in Fortran for the construction of programs for the solution of larger, more complex problems. It looks at

the functions available in Fortran, the so-called intrinsic functions and procedures (over 100 of them) and covers how you can define and use your own functions.

It is essential to develop an understanding of the functions provided by the language and when it is necessary to write your own.

Chapter 13 introduces more formally the concept of control structures and their role in structured programming. Some of the control structures available in Fortran are introduced in earlier chapters, but there is a summary here of those already covered plus several new ones that complete our coverage of a minimal working set.

Chapters 14–16 complete our coverage of the intrinsic facilities in Fortran for data typing.

- Chapter 14 looks at the character data type in Fortran. There is a coverage of I/O again, with the operators available—only one in fact.
- Chapter 15 looks at the last numeric data type in Fortran, the complex data type. This data type is essential to the solution of a small class of problems in mathematics and engineering.
- Chapter 16 looks at the logical data type. The material covered here helps considerably in increasing the power and sophistication of the way we use and construct logical expressions in Fortran. This proves invaluable in the construction and use of logical expressions in control structures.

Chapter 17 introduces derived or user defined types with a small number of examples.

Chapter 18 looks at the dynamic data-structuring facilities now available in Fortran with the addition of pointers. This chapter looks at the basic syntax of pointers. They are used in range of examples in later chapters in the book.

The next two chapters look at the second major building block in Fortran—the subroutine. Chapter 19 provides a gentle introduction to some of the fundamental concepts of subroutine definition and use and Chap. 20 extends these ideas.

Chapter 21 introduces one of modern Fortran’s major key features - the module. A Fortran module can be thought of as equivalent to a class in C++, Java and C#. This chapter looks at the basic syntax, with a couple of simple examples.

Chapter 22 looks at simple data structuring in Fortran, as we have now covered modules in a bit more depth.

Chapter 23 introduces algorithms and the big O notation.

Chapter 24 looks briefly at operator overloading, first introduced in Fortran 90.

Chapter 25 looks at generic programming.

Chapter 26 has a small set of mathematical examples.

Chapter 27 introduces parameterised derived types.

Chapter 28 introduces object oriented programming in Fortran.

Chapters 29–32 look at parallel programming in Fortran with coverage of MPI, OpenMP and Coarray Fortran.

Chapter 33 looks at C interoperability.

Chapter 34 looks at IEEE Arithmetic support in Fortran.

Chapter 35 looks at a number of miscellaneous Fortran features.

Chapter 36 looks at converting from Fortran 77 to more modern Fortran.

Some of the chapters have annotated bibliographies. These often have pointers and directions for further reading. The coverage provided cannot be seen in isolation. The concepts introduced are by intention brief, and fuller coverage must be sought where necessary. There are several appendices:

- Appendix A—This is a glossary which provides coverage of both the new concepts provided by Fortran and a range of computing terms and ideas.
- Appendix B—Contains a list of some of the more commonly used intrinsic procedures in Fortran and includes an explanation of each procedure with a coverage of the rules and restrictions that apply and examples of use where appropriate.
- Appendix C—Contains the English and Latin text extracts used in one of the problems in the chapter on characters, and the coded text extract used in one of the problems in Chap. 14.
- Appendix D—Formal syntax.
- Appendix E—Sample compiler options.

This book is not and cannot possibly be completely self-contained and exhaustive in its coverage of the Fortran language. Our first intention has been to produce a coverage of the features that will get you started with Fortran and enable you to solve a range of problems successfully. All in all Fortran is an exciting language, and it has caught up with language developments of the last 50 years.

1.2 Program Examples

All of the program examples are available on line at

<http://www.fortranplus.co.uk/>

All examples have been reformatted using the Nag compiler *polish* option. This makes the programs have a consistent style. The examples in the book have been formatted to have a line length of 48 characters to fit the printed page. They were then manually edited to improve where the lines broke. The examples on the web site have been formatted to have a line length of 132 characters.

1.3 Web Addresses

Web addresses are used throughout the book. As some of these are likely to change over the lifetime of the book our web site will have up to date addresses. We have organised them by chapter.

Chapter 2

Introduction to Problem Solving

They constructed ladders to reach to the top of the enemy's wall, and they did this by calculating the height of the wall from the number of layers of bricks at a point which was facing in their direction and had not been plastered. The layers were counted by a lot of people at the same time, and though some were likely to get the figure wrong the majority would get it right...Thus, guessing what the thickness of a single brick was, they calculated how long their ladder would have to be.

Thucydides, The Peloponnesian War

'When I use a word', Humpty Dumpty said, in a rather scornful tone, 'it means just what I choose it to mean—neither more nor less'.

'The question is', said Alice, 'whether you can make words mean so many different things'.

Lewis Carroll, Through the Looking Glass and What Alice Found There

It is possible to invent a single machine which can be used to compute any computable sequence.

Alan Turing

Aims

The aims of this chapter are:

- To examine some of the ideas and concepts involved in problem solving.
- To introduce the concept of an algorithm.
- To introduce two ways of approaching algorithmic problem solving.
- To introduce the ideas involved with systems analysis and design, i.e., to show the need for pencil and paper study before using a computer system.
- To introduce the Unified Modeling Language - UML, a general purpose modeling language used in the field of software engineering.

2.1 Introduction

It is informative to consider some of the dictionary definitions of problem:

- A matter difficult of settlement or solution, Chambers.
- A question or puzzle propounded for solution, Chambers.
- A source of perplexity, Chambers.
- Doubtful or difficult question, Oxford.
- Proposition in which something has to be done, Oxford.
- A question raised for inquiry, consideration, or solution, Webster's.
- An intricate unsettled question, Webster's.

A common thread seems to be a question that we would like answered or solved. So one of the first things to consider in problem solving is how to pose the problem. This is often not as easy as it seems. Two of the most common methods to use here are:

- In natural language.
- In artificial or stylised language.

Both methods have their advantages and disadvantages.

2.2 Natural Language

Most people use natural language and are familiar with it, and the two most common forms are the written and spoken word. Consider the following language usage:

- The difference between a 3-year-old child and an adult describing the world.
- The difference between the way an engineer and a physicist would approach the design of a car engine.
- The difference between a manager and a worker considering the implications of the introduction of new technology.

Great care must be taken when using natural language to define a problem and a solution. It is possible that people use the same language to mean completely different things, and one must be aware of this when using natural language whilst problem solving.

Natural language can also be ambiguous: Old men and women eat cheese. Are both the men and women old?

2.3 Artificial Language

The two most common forms of artificial language are technical terminology and notations. Technical terminology generally includes both the use of new words and alternate use of existing words. Consider some of the concepts that are useful when examining the expansion of gases in both a theoretical and practical fashion:

- Temperature.
- Pressure.
- Mass.
- Isothermal expansion.
- Adiabatic expansion.

Now look at the following:

- A chef using a pressure cooker.
- A garage mechanic working on a car engine.
- A doctor monitoring blood pressure.
- An engineer designing a gas turbine.

Each has a particular problem to solve, and all will approach their problem in their own way; thus they will each use the same terminology in slightly different ways.

2.3.1 Notations

Some examples of notations are:

- Algebra.
- Calculus.
- Logic.

All of the above have been used as notations for describing both problems and their solutions.

2.4 Resume

We therefore have two ways of describing problems and they both have a learning phase until we achieve sufficient understanding to use them effectively. Having arrived at a satisfactory problem statement we next have to consider how we get the solution. It is here that the power of the algorithmic approach becomes useful.

2.5 Algorithms

An algorithm is a sequence of steps that will solve part or all of a problem. One of the most easily understood examples of an algorithm is a recipe. Most people have done some cooking, if only making toast and boiling an egg.

A recipe is made up of two parts:

- A check list of things you need.
- The sequence or order of steps.

Problems can occur at both stages, e.g., finding out halfway through the recipe that you do not have an ingredient or utensil; finding out that one stage will take an hour when the rest will be ready in ten minutes. Note that certain things can be done in any order—it may not make any difference if you prepare the potatoes before the carrots.

There are two ways of approaching problem solving when using a computer. They both involve algorithms, but are very different from one another. They are called top-down and bottom-up.

The name algorithm is derived from the name of a ninth century Persian mathematician Abu Ja'far Mohammed ibn Musa al-Kuwarizmi (father of Ja'far Mohammed, son of Moses, native of Kuwarizmi), and has been corrupted in western culture as Al-Kuwarizmi.

2.5.1 Top-Down

In a top-down approach the problem is first specified at a high or general level: prepare a meal. It is then refined until each step in the solution is explicit and in the correct sequence, e.g., peel and slice the onions, then brown in a frying pan before adding the beef. One drawback to this approach is that it is very difficult to teach to beginners because they rarely have any idea of what primitive tools they have at their disposal. Another drawback is that they often get the sequencing wrong, e.g., now place in a moderately hot oven is frustrating because you may not have lit the oven (sequencing problem) and secondly because you may have no idea how hot moderately hot really is. However, as more and more problems are tackled, top-down becomes one of the most effective methods for programming.

2.5.2 Bottom-Up

Bottom-up is the reverse to top-down! As before you start by defining the problem at a high level, e.g., prepare a meal. However, now there is an examination of what tools, etc. you have available to solve the problem. This method lends itself to teaching

since a repertoire of tools can be built up and more complicated problems can be tackled. Thinking back to the recipe there is not much point in trying to cook a six course meal if the only thing that you can do is boil an egg and open a tin of beans. The bottom-up approach thus has advantages for the beginner. However, there may be a problem when no suitable tool is available. A colleague and friend of the authors learned how to make Bechamel sauce, and was so pleased by his success that every other meal had a course with a Bechamel sauce. Try it on your eggs one morning. Here is a case of specifying a problem, prepare a meal, and using an inappropriate but plausible tool, Bechamel sauce.

The effort involved in tackling a realistic problem, introducing the constructs as and when they are needed and solving it is considerable. This approach may not lead to a reasonably comprehensive coverage of the language, or be particularly useful from a teaching point of view. Case studies do have great value, but it helps if you know the elementary rules before you start on them. Imagine learning French by studying Balzac, before you even look at a French grammar book. You can learn this way but even when you have finished, you may not be able to speak to a Frenchman and be understood. A good example of the case study approach is given in the book Software Tools, by Kernighan and Plauger.

In this book our aim is to gradually introduce more and more tools until you know enough to approach the problem using the top-down method, and also realise from time to time that it will be necessary to develop some new tools.

2.5.3 Stepwise Refinement

Both of the above techniques can be combined with what is called stepwise refinement. The original ideas behind this approach are well expressed in a paper by Wirth, entitled “Program Development by Stepwise Refinement”, published in 1971. It means that you start with a global problem statement and break the problem down in stages, into smaller and smaller subproblems that become more and more amenable to solution. When you first start programming the problems you can solve are quite simple, but as your experience grows you will find that you can handle more complex problems.

When you think of the way that you solve problems you will probably realise that unless the problem is so simple that you can answer it straightaway some thinking and pencil and paper work are required. An example that some may be familiar with is in practical work in a scientific discipline, where coming unprepared to the situation can be very frustrating and unrewarding. It is therefore appropriate to look at ways of doing analysis and design before using a computer.

2.6 Modular Programming

As the problems we try solving become more complex we need to look at ways of managing the construction of programs that comprise many parts. Modula 2 was one of the first languages to support this methodology and we will look at modular programming in more depth in a subsequent chapter.

2.7 Object Oriented Programming

There is a class of problems that are best solved by the treatment of the components of these problems as objects. We will look at the concepts involved in object oriented programming and object oriented languages in the next chapter.

2.8 Systems Analysis and Design

When one starts programming it is generally not apparent that one needs a methodology to follow to become successful as a programmer. This is usually because the problems are reasonably simple, and it is not necessary to be explicit about all of the stages one has gone through in arriving at a solution. As the problems become more complex it is necessary to become more rigorous and thorough in one's approach, to keep control in the face of the increasing complexity and to avoid making mistakes. It is then that the benefit of systems analysis and design becomes obvious. Broadly we have the following stages in systems analysis and design:

- Problem definition.
- Feasibility study and fact finding.
- Analysis.
- Initial system design.
- Detailed design.
- Implementation.
- Evaluation.
- Maintenance.

and each problem we address will entail slightly different time spent in each of these stages. Let us look at each stage in more detail.

2.8.1 *Problem Definition*

Here we are interested in defining what the problem really is. We should aim at providing some restriction on both the scope of the problem, and the objectives we

set ourselves. We can use the methods mentioned earlier to help us out. It is essential that the objectives are:

- Clearly defined.
- Understood and agreed to by all people concerned, when more than one person is involved.
- Realistic.

2.8.2 Feasibility Study and Fact Finding

Here we look to see if there is a feasible solution. We would try and estimate the cost of solving the problem and see if the investment was warranted by the benefits, i.e., cost-benefit analysis.

2.8.3 Analysis

Here we look at what must be done to solve the problem. Note that we are interested in finding out what we need to do, but that we do not actually do it at this stage.

2.8.4 Design

Once the analysis is complete we know what must be done, and we can proceed to the design. We may find there are several alternatives, and we thus examine alternate ways in which the problem can be solved. It is here that we use the techniques of top-down and bottom-up problem solving, combined with stepwise refinement to generate an algorithm to solve the problem. We are now moving from the logical to the physical side of the solution. This stage ends with a choice among several alternatives. Note that there is generally not one ideal solution, but several, each with its own advantages and disadvantages.

2.8.5 Detailed Design

Here we move from the general to the specific, The end result of this stage should be a specification that is sufficiently tightly defined to generate actual program code.

It is at this stage that it is useful to generate pseudocode. This means writing out in detail the actions we want carried out at each stage of our overall algorithm.

We gradually expand each stage (stepwise refinement) until it becomes Fortran—or whatever language we want.

2.8.6 Implementation

It is at this stage that we actually use a computer system to create the program(s) that will solve the problem. It is here that we actually need to know enough about a programming language to use it effectively to solve our problem. This is only one stage in the overall process, and mistakes at any of the stages can create serious difficulties.

2.8.7 Evaluation and Testing

Here we try to see if the program(s) we have produced will actually do what they are supposed to. We need to have data sets that enable us to say with confidence that the program really does work. This may not be an easy task, as quite often we only have numeric methods to solve the problem, which is why we are using the computer in the first place—hence we are relying on the computer to provide the proof; i.e., we have to use a computer to determine the veracity of the programs—and as Heller says, Catch 22.

2.8.8 Maintenance

It is rare that a program is run once and never used again. This means that there will be an ongoing task of maintaining the program, generally to make it work with different versions of the operating system or compiler, and to incorporate new features not included in the original design. It often seems odd when one starts programming that a program will need maintenance, as we are reluctant to regard a program in the same way as a mechanical object like a car that will eventually fall apart through use. Thus maintenance means keeping the program working at some tolerable level, often with a high level of investment in manpower and resources. Research in this area has shown that anything up to 80 % of the manpower investment in a program can be in maintenance.

2.9 Unified Modeling Language—UML

UML is a general purpose modeling language used in the field of software engineering. It was developed by Grady Booch, Ivar Jacobson and James Rumbaugh whilst working at Rational Software in the 1990s. They were three of the leading exponents of object oriented software methodologies at the time and decided to unify the various approaches that each had developed.

UML combines techniques from data modeling (entity relationship diagrams), business modeling (work flows), object modeling, and component modeling. It can be used with all processes, throughout the software development life cycle, and across different implementation technologies.

It tends to be used more in business computing than scientific computing.

2.10 Conclusions

A drawback, inherent in all approaches to programming and to problem solving in general, is the assumption that a solution is indeed possible. There are problems which are simply insoluble—not only problems like balancing a national budget, weather forecasting for a year, or predicting which radioactive atom will decay, but also problems which are apparently computationally solvable.

Knuth gives the example of a chess problem—determining whether the game is a forced victory for white. Although there is an algorithm to achieve this, it requires an inordinately long time to complete. For practical purposes it is unsolvable.

Other problems can be shown mathematically to be undecidable. The work of Gödel in this area has been of enormous importance, and the bibliography contains a number of references for the more inquisitive and mathematically orientated reader. The Hofstader coverage is the easiest, and least mathematical.

As far as possible we will restrict ourselves to solvable problems, like learning a programming language.

Within the formal world of Computer Science our description of an algorithm would be considered a little lax. For our introductory needs it is sufficient, but a more rigorous approach is given by Hopcroft and Ullman in Introduction to Automata Theory, Languages and Computation, and by Beckman in Mathematical Foundations of programming.

2.11 Problems

2.1 What is an algorithm?

2.2 What distinguishes top-down from bottom-up approaches to problem solving? Illustrate your answer with reference to the problem of a car, motor-cycle or bicycle having a flat tire.

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Chapter 3

Introduction to Programming Languages

We have to go to another language in order to think clearly about the problem.

Samuel R. Delany, Babel-17

Aims

The primary aim of this chapter is to provide a short history of program language development and give some idea as to the concepts that have had an impact on Fortran. It concentrates on some but not all of the major milestones of the last 40 years, in roughly chronological order. The secondary aim is to show the breadth of languages available. The chapter concludes with coverage of a small number of more specialised languages.

3.1 Introduction

It is important to realise that programming languages are a recent invention. They have been developed over a relatively short period—60 years—and are still undergoing improvement. Time spent gaining some historical perspective will help you understand and evaluate future changes. This chapter starts right at the beginning and takes you through some, but not all, of the developments during this 55 year span. The bulk of the chapter describes languages that are reasonably widely available commercially, and therefore ones that you are likely to meet. The chapter concludes with a coverage of some more specialised and/or recent developments.

3.2 Some Early Theoretical Work

Some of the most important early theoretical work in computing was that of Turing and von Neumann. Turing's work provided the base from which it could be shown that it was possible to get a machine to solve problems. The work of von Neumann

added the concept of storage and combined with Turing's work to provide the basis for most computers designed to this day.

3.3 What Is a Programming Language?

For a large number of people a programming language provides the means of getting a digital computer to solve a problem. There is a wide range of problems and an equally wide range of programming languages, with particular languages being suited to a particular class of problems, all of which often appears bewildering to the beginner.

3.4 Program Language Development and Engineering

There is much in common between the development of programming languages and the development of anything from the engineering world. Consider the car: old cars offer much of the same functionality as more modern ones, but most people prefer driving newer models. The same is true of programming languages, where you can achieve much with the older languages, but the newer ones are easier to use.

3.5 The Early Days

A concept that proves very useful when discussing programming languages is that of the level of a machine. By this is meant how close a language is to the underlying machine that the program runs on. In the early days of programming (up to 1954) there were only two broad categories: machine languages and assemblers. The language that digital machines use is that of 0 and 1, i.e., they are binary devices. Writing a program in terms of patterns of 0 and 1 was not particularly satisfactory and the capability of using more meaningful mnemonics was soon introduced. Thus it was realised quite quickly that one of the most important aspects of programming languages is that they have to be read and understood by both machines and humans.

3.5.1 *Fortran's Origins*

The next stage was the development of higher-level languages. The first of these was Fortran and it was developed over a 3 year period from 1954 to 1957 by an IBM team led by John Backus. This group achieved considerable success, and helped to prove that the way forward lay with high-level languages for computer-based problem solving. Fortran stands for formula translation and was used mainly by people with a

scientific background for solving problems that had a significant arithmetic content. It was thus relatively easy, for the time, to express this kind of problem in Fortran.

By 1966 and the first standard Fortran:

- Was widely available.
- Was easy to teach.
- Had demonstrated the benefits of subroutines and independent compilation.
- Was relatively machine independent.
- Often had very efficient implementations.

Possibly the single most important fact about Fortran was, and still is, its widespread usage in the scientific community.

3.5.2 Fortran 77

The next standard in 1977 (actually 1978, and thus out by one—a very common programming error, more of this later!) added character handling, but little else in the way of major new features, really tidying up some of the deficiencies of the 1966 standard. One important feature sometimes overlooked was backwards compatibility. This meant that the standard did not invalidate any standard conformant Fortran 66 program. This protected investment in old code.

3.5.3 Cobol

The business world also realised that computers were useful and several languages were developed, including FLOWMATIC, AIMACO, Commercial Translator and FACT, leading eventually to Cobol—Common Business Orientated Language. There is a need in commercial programming to describe data in a much more complex fashion than for scientific programming, and Cobol had far greater capability in this area than Fortran. The language was unique at the time in that a group of competitors worked together with the objective of developing a language that would be useful on machines used by other manufacturers.

The contributions made by Cobol include:

- Firstly the separation among:
- The task to be undertaken.
- The description of the data involved.
- The working environment in which the task is carried out.
- Secondly a data description mechanism that was largely machine independent.
- Thirdly its effectiveness for handling large files.
- Fourthly the benefit to be gained from a programming language that was easy to read.

Modern developments in computing—of report generators, file-handling software, fourth-generation development tools, and especially the increasing availability of commercial relational database management systems—are gradually replacing the use of Cobol, except where high efficiency and/or tight control are required.

3.5.4 *Algol*

Another important development of the 1950s was Algol. It had a history of development from Algol 58, the original Algol language, through Algol 60 eventually to the Revised Algol 60 Report. Some of the design criteria for Algol 58 were:

- The language should be as close as possible to standard mathematical notation and should be readable with little further explanation.
- It should be possible to use it for the description of computing processes in publications.
- The new language should be mechanically translatable into machine programs.

A sad feature of Algol 58 was the lack of any input/output facilities, and this meant that different implementations often had incompatible features in this area.

The next important step for Algol occurred at a UNESCO-sponsored conference in June 1959. There was an open discussion on Algol and the outcome was Algol 60, and eventually the Revised Algol 60 Report.

It was at this conference that John Backus gave his now famous paper on a method for defining the syntax of a language, called Backus Normal Form, or BNF. The full significance of the paper was not immediately recognised. However, BNF was to prove of enormous value in language definition, and helped provide an interface point with computational linguistics.

The contributions of Algol to program language development include:

- Block structure.
- Scope rules for variables because of block structure.
- The BNF definition by Backus—most languages now have a formal definition.
- The support of recursion.
- Its offspring.

Thus Algol was to prove to make a contribution to programming languages that was never reflected in the use of Algol 60 itself, in that it has been the parent of one of the main strands of program language development.

3.6 Chomsky and Program Language Development

Programming languages are of considerable linguistic interest, and the work of Chomsky in 1956 in this area was to prove of inestimable value. Chomsky's system of transformational grammar was developed in order to give a precise mathematical

description to certain aspects of language. Simplistically, Chomsky describes grammars, and these grammars in turn can be used to define or generate corresponding kinds of languages. It can be shown that for each type of grammar and language there is a corresponding type of machine. It was quickly realised that there was a link with the earlier work of Turing.

This link helped provide a firm scientific base for programming language development, and modern compiler writing has come a long way from the early work of Backus and his team at IBM. It may seem unimportant when playing a video game at home or in an arcade, but for some it is very comforting that there is a firm theoretical basis behind all that fun.

3.7 Lisp

There were also developments in very specialized areas. List processing was proving to be of great interest in the 1950s and saw the development of IPLV between 1954 and 1958. This in turn led to the development of Lisp at the end of the 1950s. Lisp has proved to be of considerable use for programming in the areas of artificial intelligence, playing chess, automatic theorem proving and general problem solving. It was one of the first languages to be interpreted rather than compiled. Whilst interpreted languages are invariably slower and less efficient in their use of the underlying computer systems than compiled languages, they do provide great opportunities for the user to explore and try out ideas whilst sitting at a terminal. The power that this gives to the computational problem solver is considerable.

Possibly the greatest contribution to program language development made by Lisp was its functional notation. One of the major problems for the Lisp user has been the large number of Lisp flavours, and this has reduced the impact that the language has had and deserved.

3.8 Snobol

Snobol was developed to aid in string processing, which was seen as an important part of many computing tasks, e.g., parsing of a program. Probably the most important thing that Snobol demonstrated was the power of pattern matching in a programming language, e.g., it is possible to define a pattern for a title that would include Mr, Mrs, Ms, Miss, Rev, etc., and search for this pattern in a text using Snobol. Like Lisp it is generally available as an interpreter rather than a compiler, but compiled versions do exist, and are often called Spitbol. Pattern-matching capabilities are now to be found in many editors and this makes them very powerful and useful tools. It is in the area of text manipulation that Snobol's greatest contribution to program language development lies.

3.9 Second-Generation Languages

3.9.1 PL/I and Algol 68

It is probably true that Fortran, Algol 60 and Cobol are the three main first-generation high-level languages. The 1960s saw the emergence of PL/1 and Algol 68. PL/1 was a synthesis of features of Fortran, Algol 60 and Cobol. It was soon realised that whilst PL/1 had great richness and power of expression this was in some ways offset by the greater difficulties involved in language definition and use.

These latter problems were also true of Algol 68. The report introduced its own syntactic and semantic conventions and thus forced another stage in the learning process on the prospective user. However, it has a small but very committed user population who like the very rich facilities provided by the language.

3.9.2 Simula

Another strand that makes up program language development is provided by Simula, a general purpose programming language developed by Dahl, Myhrhaug and Nygaard of the Norwegian Computing Centre. The most important contribution that Simula makes is the provision of language constructs that aid the programming of complex, highly interactive problems. It is thus heavily used in the areas of simulation and modelling. It was effectively the first language to offer the opportunity of object orientated programming, and we will come back to this very important development in programming languages later in this chapter.

3.9.3 Pascal

The designer of Pascal, Niklaus Wirth, had participated in the early stages of the design of Algol 68 but considered that the generality and complexity of Algol 68 was a move in the wrong direction. Pascal (like Algol 68) had its roots in Algol 60 but aimed at providing expressive power through a small set of straightforward concepts. This set is relatively easy to learn and helps in producing readable and hence more comprehensible programs.

It became the language of first choice within the field of computer science during the 1970s and 1980s, and the comment by Wirth sums up the language very well: “although Pascal had no support from industry, professional societies, or government agencies, it became widely used. The important reason for this success was that many people capable of recognising its potential actively engaged themselves in its promotion. As crucial as the existence of good implementations is the availability of documentation. The conciseness of the original report made it attractive

for many teachers to expand it into valuable textbooks. Innumerable books appeared between 1977 and 1985, effectively promoting Pascal to become the most widespread language used in introductory programming courses. Good course material and implementations are the indispensable prerequisites for such an evolution.”

3.9.4 APL

APL is another interesting language of the early 1960s. It was developed by Iverson early in the decade and was available by the mid to late 1960s. It is an interpretive vector and matrix based language with an extensive set of operators for the manipulation of vectors, arrays, etc., of whatever data type. As with Algol 68 it has a small but dedicated user population. A possibly unfair comment about APL programs is that you do not debug them, but rewrite them!

3.9.5 Basic

Basic stands for Beginners All Purpose Symbolic Instruction Code, and was developed by Kemeny and Kurtz at Dartmouth during the 1960s. Its name gives a clue to its audience and it is very easy to learn. It is generally interpreted, though compiled versions do exist. It has proved to be well suited to the rapid development of small programs. It is much criticised because it lacks features that encourage or force the adoption of sound programming techniques.

3.9.6 C

There is a requirement in computing to be able to access the underlying machine directly or at least efficiently. It is therefore not surprising that computer professionals have developed high-level languages to do this. This may well seem a contradiction, but it can be done to quite a surprising degree. Some of the earliest published work was that of Martin Richards on the development of BCPL.

This language directly influenced the work of Ken Thompson and can be clearly seen in the programming languages B and C. The UNIX operating system is almost totally written in C and demonstrates very clearly the benefits of the use of high-level languages wherever possible.

With the widespread use of UNIX within the academic world C gained considerable ground during the 1970s and 1980s. UNIX systems also offered much to the professional software developer, and became widely used for large-scale software development and as Ritchie says: “C is quirky, flawed, and an enormous success. while accidents of history surely helped, it evidently satisfied a need for a system

implementation language efficient enough to displace assembly language, yet sufficiently abstract and fluent to describe algorithms and interactions in a wide variety of environments.”

There have been several versions of C. Before the language was standardised most people relied on an informal specification contained in the book by Dennis Ritchie and Brian Kernighan, and this version is called K&R C. In 1989 the American National Standards Institute published the ANSI C or C89 standard. It became an ISO standard a year later. The second edition of the K&R book covers the ANSI C standard. ISO later released an extension to the internationalization support of the standard in 1995, and a revised standard (C99) in 1999.

C99 introduced several new features, including inline functions, several new data types (including long long int and a complex type to represent complex numbers), variable-length arrays, improved support for IEEE 754 floating point, support for variadic macros (macros of variable arity), and support for one-line comments beginning with // which are part of C++. This increased the compatibility of C and C++. Many of these had already been implemented as extensions in several C compilers.

The current version of the standard (C11) was approved in December 2011.

The C11 standard adds several new features to C and the library, including type generic macros, anonymous structures, improved Unicode support, atomic operations, multithreading, and bounds-checked functions. It improved compatibility with C++.

3.10 Some Other Strands in Language Development

There are many strands that make up program language development and some of them are introduced here.

3.10.1 Abstraction, Stepwise Refinement and Modules

Abstraction has proved to be very important in programming. It enables a complex task to be broken down into smaller parts concentrating on what we want to happen rather than how we want it to happen. This leads almost automatically to the ideas of stepwise refinement and modules, with collections of modules to perform specific tasks or steps.

3.10.2 Structured Programming

Structured programming in its narrowest sense concerns itself with the development of programs using a small but sufficient set of statements and, in particular, control statements. It has had a great effect on program language design, and most languages now support the minimal set of control structures.

In a broader sense structured programming subsumes other objectives, including simplicity, comprehensibility, verifiability, modifiability and maintenance of programs.

3.10.3 Data Structuring and Procedural Programming

By the 1970s languages started to emerge that offered the ability to organise data logically—so called data structuring, and we will look at two of these in the coverage below—C and Pascal.

C provided this facility via structs and Pascal did it via records. These languages also offered two ways of processing the data—directly or via procedures. The terms concrete and abstract data type are sometimes also used in the literature.

An example may help here. Consider a date. This is typically made up of three components, a day, a month and a year. In C we can create a user defined type called a date using structs. We can then create variables of this type. This is done in Pascal in a similar way using records.

Access to the components of a date (day, month and year) can then either be direct—an example of a concrete data types, or indirect (via procedures)—an abstract data types.

Simplistically direct access (or concrete data types) offer the benefit of efficiency, and the possibility of lack of data integrity. In our date example we may set a day to the value 31 when the month is February.

Indirect access (or abstract data types) are slightly less efficient as we now have the overhead of a procedure call to access the data, but better opportunity for data integrity as we can provide hidden code within the procedures to ensure that the day, month and year combinations are valid.

Fortran did not provide this facility until the Fortran 90 standard.

3.10.4 Standardisation

The purposes of a standard are quite varied and include:

- Investment in people: by this we mean that the time spent in learning a standard language pays off in the long term, as what one learns is applicable on any hardware/software platform that has a standard conformant compiler.
- Portability: one can take the code one has written for one hardware/software platform and move it to any hardware/software platform that has a standard conformant compiler.
- Known reference point: when making comparisons one starts with reference to the standard first, and then between the additional functionality of the various implementations.

These are some but not all of the reasons for the use of standards. Their importance is summed up beautifully by Ronald G. Ross in his introduction to the Cannan and Otten book on the SQL standard: “Anybody who has ever plugged in an electric cord into a wall outlet can readily appreciate the inestimable benefits of workable standards. Indeed, with respect to electrical power, the very fact that we seldom even think about such access (until something goes wrong) is a sure sign of just how fundamentally important a successful standard can be.”

3.11 Ada

Ada represents the culmination of many years of work in program language development. It was a collective effort and the main aim was to produce a language suitable for programming large-scale and real-time systems. Work started in 1974 with the formulation of a series of documents by the American Department of Defence (DoD), which led to the Steelman documents. It is a modern algorithmic language with the usual control structures and facilities for the use of modules, and allows separate compilation with type checking across modules.

Ada is a powerful and well-engineered language. Its widespread use is certain as it has the backing of the DoD. However, it is a large and complex language and consequently requires some effort to learn.

The latest version of the language is Ada 2012. The following url

<http://www.ada-europe.org/resources/online>

provides a good starting point. Visit this site if you want up to date details about Ada.

Another good source is

<http://www.adaic.org/ada-resources/standards/ada12>

Both sites have free electronic versions of the various Ada standards.

3.12 Modula

Modula was designed by Wirth during the 1970s at ETH, for the programming of embedded real-time systems. It has many of the features of Pascal, and can be taken for Pascal at a glance. The key new features that Modula introduced were those of processes and monitors.

As with Pascal it is relatively easy to learn and this makes it much more attractive than Ada for most people, achieving much of the capability without the complexity.

3.13 Modula 2

Wirth carried on developing his ideas about programming languages and the culmination of this can be seen in Modula 2. In his words: “In 1977, a research project with the goal to design a computer system (hardware and software) in an integrated approach, was launched at the Institut fur Informatik of ETH Zurich. This system (later to be called Lilith) was to be programmed in a single high level language, which therefore had to satisfy requirements of high level system design as well as those of low level programming of parts that closely interact with the given hardware. Modula 2 emerged from careful design deliberations as a language that includes all aspects of Pascal and extends them with the important module concept and those of multi-programming. Since its syntax was more in line with Modula than Pascal’s the chosen name was Modula 2.”

The language’s main additions with regard to Pascal are:

- The module concept, and in particular the facility to split a module into a definition part and an implementation part.
- A more systematic syntax which facilitates the learning process. In particular, every structure starting with a keyword also ends with a keyword, i.e., is properly bracketed.
- The concept of process as the key to multiprogramming facilities.
- So-called low-level facilities, which make it possible to breach the rigid type consistency rules and allow one to map data with Modula 2 structure onto a store without inherent structure.
- The procedure type, which allows procedures to be dynamically assigned to variables.

A sad feature of Modula 2 was the long time taken to arrive at a standard for the language.

3.14 Other Language Developments

The following is a small selection of language developments that the authors find interesting—they may well not be included in other people’s coverage.

3.14.1 Logo

Logo is a language that was developed by Papert and colleagues at the Artificial Intelligence Laboratory at MIT. Papert is a professor of both mathematics and education, and has been much influenced by the psychologist Piaget. The language is used to create learning environments in which children can communicate with a computer.

The language is primarily used to demonstrate and help children develop fundamental concepts of mathematics. Probably the turtle and turtle geometry are known by educationists outside of the context of Logo. Turtles have been incorporated into the Smalltalk computer system developed at Xerox Palo Alto Research Centre—Xerox PARC.

3.14.2 Postscript, TeX and L^AT_EX

The 1980s saw a rapid spread in the use of computers for the production of printed material. The 3 languages are each used quite extensively in this area.

Postscript is a low-level interpretive programming language with good graphics capabilities. Its primary purpose is to enable the easy production of pages containing text, graphical shapes and images. It is rarely seen by most end users of modern desktop publishing systems, but underlies many of these systems. It is supported by an increasing number of laser printers and typesetters.

TeX is a language designed for the production of mathematical texts, and was developed by Donald Knuth. It linearises the production of mathematics using a standard computer keyboard. It is widely used in the scientific community for the production of documents involving mathematical equations.

L^AT_EX is Leslie Lamport's version of TeX, and is regarded by many as more friendly. It is basically a set of macros that hide raw TeX from the end user. The TeX ratio is probably 1–9 (or so I'm reliably informed by a TeXie).

3.14.3 Prolog

Prolog was originally developed at Marseille by a group led by Colmerauer in 1972/1973. It has since been extended and developed by several people, including Pereira (L.M.), Pereira (F), Warren and Kowalski. Prolog is unusual in that it is a vehicle for logic programming. Most of the languages described here are basically algorithmic languages and require a specification of how you want something done. Logic programming concentrates on the what rather than the how. The language appears strange at first, but has been taught by Kowalski and others to 10-year-old children at schools in London.

3.14.4 SQL

SQL stands for Structured Query Language, and was originally developed by people mainly working for IBM in the San Jose Research Laboratory. It is a relational database language, and enables programmers to define, manipulate and control data

in a relational database. Simplistically, a relational database is seen by a user as a collection of tables, comprising rows and columns. It has become the most important language in the whole database field.

3.14.5 ICON

ICON is in the same family as Snobol, and is a high-level general purpose programming language that has most of the features necessary for efficient processing of nonnumeric data. Griswold (one of the original design team for Snobol) has learnt much since the design and implementation of Snobol, and the language is a joy to use in most areas of text manipulation.

It is available for most systems via anonymous FTP from a number of sites on the Internet.

3.15 Object Oriented Programming

Object oriented represents a major advance in program language development. The concepts that this introduces include:

- Classes.
- Objects.
- Messages.
- Methods.

These in turn draw on the ideas found in more conventional programming languages and correspond to

- Extensible data types.
- Instances of a class.
- Dynamically bound procedure calls.
- Procedures of a class.

Inheritance is a very powerful high-level concept introduced with object oriented programming. It enables an existing data type with its range of valid operations to form the basis for a new class, with more data types added with corresponding operations, and the new type is compatible with the original.

Fortran 2003 offered support for object oriented programming. This is achieved via the module facility rather than the class facility found in other languages like C++, Java and C#.

3.15.1 *Simula*

As was mentioned earlier, the first language to offer functionality in this area was Simula, and thus the ideas originated in the 1960s. The book Simula Begin by Birtwistle, Dahl, Myhrhaug and Nygaard is well worth a read as it represents one of the first books to introduce the concepts of object oriented programming.

3.15.2 *Smalltalk*

Language plus use of a computer system.

Smalltalk has been under development by the Xerox PARC Learning Research Group since the 1970s. In their words: “Smalltalk is a graphical, interactive programming environment. As suggested by the personal computer vision, Smalltalk is designed so that every component in the system is accessible to the user and can be presented in a meaningful way for observation and manipulation. The user interface issues in Smalltalk revolve around the attempt to create a visual language for each object. The preferred hardware system for Smalltalk includes a high resolution graphical display screen and a pointing device such as a graphics pen or mouse. With these devices the user can select information viewed on the screen and invoke messages in order to interact with the information.” Thus Smalltalk represents a very different strand in program language development. The ease of use of a system like this has long been appreciated and was first demonstrated commercially in the Macintosh microcomputers.

Wirth has spent some time at Xerox PARC and has been influenced by their work. In his own words “the most elating sensation was that after sixteen years of working for computers the computer now seemed to work for me.” This influence can be seen in the design of the Lilith machine, the original Modula 2 engine, and in the development of Oberon as both a language and an operating system.

3.15.3 *Oberon and Oberon 2*

As Wirth says: “The programming language Oberon is the result of a concentrated effort to increase the power of Modula-2 and simultaneously to reduce its complexity. Several features were eliminated, and a few were added in order to increase the expressive power and flexibility of the language.”

Oberon and Oberon 2 are thus developments beyond Modula 2. The main new concept added to Oberon was that of type extension. This enables the construction of new data types based on existing types and allows one to take advantage of what has already been done for that existing type.

Language constructs removed included:

- Variant records.
- Opaque types.
- Enumeration types.
- Subrange types.
- Local modules.
- With statement.
- Type transfer functions.
- Concurrency.

The short paper by Wirth provides a fuller coverage. It is available at ETH via anonymous FTP.

3.15.4 Eiffel

Eiffel was originally developed by Interactive Software Engineering Inc. (ISE) founded by Bertrand Meyer. Meyer's book Object-Oriented Software Construction contains a detailed treatment of the concepts and theory of the object technology that led to Eiffel's design.

The language first became available in 1986, and the first edition of Meyer's book was published in 1988. The following is a quote from the Wikipedia entry.

- The design goal behind the Eiffel language, libraries, and programming methods is to enable programmers to create reliable, reusable software modules. Eiffel supports multiple inheritance, genericity, polymorphism, encapsulation, type-safe conversions, and parameter covariance. Eiffel's most important contribution to software engineering is design by contract (DbC), in which assertions, preconditions, postconditions, and class invariants are employed to help ensure program correctness without sacrificing efficiency.

3.15.5 C++

Stroustrup did his PhD thesis at the Computing Laboratory, Cambridge University, England, and worked with Simula. He had previously worked with Simula at the University of Aarhus in Denmark. His comments are illuminating: “but was pleasantly surprised by the way the mechanisms of the Simula language became increasingly helpful as the size of the program increased. The class and co-routine mechanisms of Simula and the comprehensive type checking mechanisms ensured that problems and errors did not (as I—and I guess most people—would have expected) grow linearly with the size of the program. Instead, the total program acted like a collection of very small (and therefore easy to write, comprehend and debug) programs rather than a single large program.”

Table 3.1 C++ standardisation history

Year	C++ standard	Informal name
1998	ISO/IEC 14882:1998	C++98
2003	ISO/IEC 14882:2003	C++03
2007	ISO/IEC TR 19768:2007	C++TR1
2011	ISO/IEC 14882:2011	C++11

He designed C++ to provide Simula's functionality within the framework of C's efficiency, and he succeeded in this goal as C++ is one of the most widely used object oriented programming language.

The language began as enhancements to C, adding classes, virtual functions, operator overloading, multiple inheritance, templates and exception handling by the time of the first standard.

Its influence in the area of programming language design can be seen in Java and C#.

Table 3.1 summarises the C++ standardisation history.

The following are some of the guidelines used by the standards committee in the development of C++11.

- Maintain stability and compatibility with C++98 and possibly with C;
- Prefer introduction of new features through the standard library, rather than extending the core language;
- Prefer changes that can evolve programming technique;
- Improve C++ to facilitate systems and library design, rather than to introduce new features useful only to specific applications;
- Increase type safety by providing safer alternatives to earlier unsafe techniques;
- Increase performance and the ability to work directly with hardware;
- Provide proper solutions for real-world problems;
- Implement zero-overhead principle (additional support required by some utilities must be used only if the utility is used);
- Make C++ easy to teach and to learn without removing any utility needed by expert programmers.

Work is currently under way on the C++14 and C++17 standards.

3.15.6 Java

Bill Joy (of Sun fame) had by the late 1980s decided that C++ was too complicated and that an object oriented environment based upon C++ would be of use. At around about the same time James Gosling (mister emacs) was starting to get frustrated with the implementation of an SGML editor in C++. Oak was the outcome of Gosling's frustration.

Sun over the next few years ended up developing Oak for a variety of projects. It wasn't until Sun developed their own web browser, Hotjava, that Java as a language hit the streets. And as the saying goes the rest is history.

Java is a relatively simple object oriented language. Whilst it has its origins in C++ it has dispensed with most of the dangerous features. It is OO throughout. Everything is a class.

It is interpreted and the intermediate byte code will run on any machine that has a Java virtual machine for it. This is portability at the object code level, unlike portability at the source code level—which is what we expect with most conventional languages. Some of the safe features of the language include:

- Built in garbage collection.
- Array subscript checking.
- No pointers—everything is passed by reference.

It is multithreaded, which makes it a delight for many applications. It has an extensive windows toolkit, the so called AWT that was in the original release of the language and Swing that came in later.

It is under continual development and at the time of writing was in its eighth major release.

Sun was acquired by Oracle in 2010.

3.15.7 C#

C# is a recent language from Microsoft and is a key part of their .NET framework. It is a modern, well-engineered language in the same family of programming languages in terms of syntax as C, C++ and Java. If you have a knowledge of one of these languages it will look very familiar.

One of the design goals was to produce a component oriented language, and to build on the work that Microsoft had done with OLE, ActiveX and COM:

- ActiveX is a set of technologies that enables software components to interact with one another in a networked environment, regardless of the language in which they were created. ActiveX was built on the Component Object Model (COM).
- COM is the object model on which ActiveX Controls and OLE are built. COM allows an object to expose its functionality to other components and to host applications. It defines both how the object exposes itself and how this exposure works across processes and networks. COM also defines the object's life cycle.
- OLE is a mechanism that allows users to create and edit documents containing items or objects created by multiple applications. OLE was originally an acronym for Object Linking and Embedding. However, it is now referred to simply as OLE. Parts of OLE not related to linking and embedding are now part of Active technology.

Other design goals included creating a language:

- Where everything is an object—C# also has a mechanism for going between objects and fundamental types (integers, reals, etc.).
- Which would enable the construction of robust and reliable software — it has garbage collection, exception handling and type safety.
- Which would use a C/C++/Java syntax which is already widely known and thus help programmers converting from one of these languages to C#.

It has been updated three times since its original release. Some of the more important features added in C# 2 were Generics, Iterators, Partial Classes, Nullable Types and Static Classes. The major feature that C# 3 added for most people was LINQ, a mechanism for data querying. C# 4 was released in 2010 and added a number of additional features.

3.16 Back to Fortran!

We finish off with a coverage of the developments since the Fortran 77 standard. Practically all of the Fortran compilers available today support the Fortran 90 and 95 standards. Many also support several features of the 2003 standard, and some also implement one or more features from the Fortran 2008 standard. See the following document

http://www.fortranplus.co.uk/resources/fortran_2003_2008_compiler_support.pdf

for up to date information on what each compiler offers in terms of standard support.

3.16.1 Fortran 90

Almost as soon as the Fortran 77 standard was complete and published, work began on the next version. The language drew on many of the ideas covered in this chapter and these help to make Fortran 90 a very promising language. Some of the new features included:

- New source form, with blanks being significant and names being up to 31 characters.
- Implicit none.
- Better control structures.
- Control of the precision of numerical computation.
- Array processing.
- Pointers.
- User defined data types and operators.
- Procedures.

- Modules.
- Recursion.
- Dynamic storage allocation.

This was the major update that the Fortran community had been waiting a long time for. Backwards compatibility was again a key aim. This standard did not invalidate any standard conformant Fortran 77 program.

3.16.2 Fortran 95

Fortran was next standardised in 1996—yet again out by one! Firstly we have a clear up of some of the areas in the standard that had emerged as requiring clarification. Secondly Fortran 95 added the following major concepts:

- The `forall` construct.
- Pure and elemental procedures.
- Implicit initialisation of derived-type objects.
- Initial association status for pointers.

The first two help considerably in parallelization of code.

Minor features include amongst others:

- Automatic deallocation of allocatable arrays.
- Intrinsic `sign` function distinguishes between `-0` and `+0`.
- Intrinsic function `null` returns disconnected pointer.
- Intrinsic function `cpu_time` returns the processor time.
- References to some pure functions are allowed in specification statements.
- Nested `where` constructs.
- Masked `elsewhere` construct.
- Small changes to the `ceiling`, `floor`, `maxloc` and `minloc` intrinsic functions.

Some of these were added to keep Fortran in line with High Performance Fortran (HPF). More details are given later.

Part 2 of the standard (ISO/IEC 1539-2:1994) adds the functional specification for varying length character data type, and this extends the usefulness of Fortran for character applications very considerably.

3.16.3 ISO Technical Reports TR15580 and TR15581

There are two additional reports that have been published on Fortran. TR 15580 specifies three modules that provide access to IEEE floating point arithmetic and TR15581 allows the use of the allocatable attribute on dummy arguments, function results and structure components.

3.16.4 Fortran 2003

The language is known as Fortran 2003 even though the language did not make it through the standardisation process until 2004. It was a major revision.

- Derived type enhancements: parameterised derived types (allows the kind, length, or shape of a derived type's components to be chosen when the derived type is used), mixed component accessibility (allows different components to have different accessibility), public entities of private type, improved structure constructors, and finalisers.
- Object oriented programming support: enhanced data abstraction (allows one type to extend the definition of another type), polymorphism (allows the type of a variable to vary at run time), dynamic type allocation, select type construct (allows a choice of execution flow depending upon the type a polymorphic object currently has), and type-bound procedures.
- The associate construct (allows a complex expression or object to be denoted by a simple symbol).
- Data manipulation enhancements: allocatable components, deferred-type parameters, volatile attribute, explicit type specification in array constructors, intent specification of pointer arguments, specified lower bounds of pointer assignment and pointer rank remapping, extended initialisation expressions, max and min intrinsics for character type, and enhanced complex constants.
- Input/output enhancements: asynchronous transfer operations (allow a program to continue to process data while an input/output transfer occurs), stream access (allows access to a file without reference to any record structure), user specified transfer operations for derived types, user specified control of rounding during format conversions, the flush statement, named constants for preconnected units, regularisation of input/output keywords, and access to input/output error messages.
- Procedure pointers.
- Scoping enhancements: the ability to rename defined operators (supports greater data abstraction) and control of host association into interface bodies.
- Support for IEC 60559 (IEEE 754) exceptions and arithmetic (to the extent a processor's arithmetic supports the IEC standard).
- Interoperability with the C programming language (allows portable access to many libraries and the low-level facilities provided by C and allows the portable use of Fortran libraries by programs written in C).
- Support for international usage: (ISO 10646) and choice of decimal or comma in numeric formatted input/output.
- Enhanced integration with the host operating system: access to command line arguments and environment variables and access to the processor's error messages (improves the ability to handle exceptional conditions).

The earlier web address has details of Fortran compiler conformance to this standard.

3.16.5 DTR 19767 Enhanced Module Facilities

The module system in Fortran has a number of shortcomings and this DTR addresses some of the issues.

One of the major issues was the so-called recompilation cascade. Changes to one part of a module forced recompilation of all code that used the module. Modula 2 addressed this issue by distinguishing between the definition or interface and implementation. This can now be achieved in Fortran via submodules.

3.16.6 Fortran 2008

The most recent standard, ISO/IEC 1539-1:2010, commonly known as Fortran 2008, was approved in September 2010. The new features include:

- Submodules—Additional structuring facilities for modules; supersedes ISO/IEC TR 19767:2005
- Coarray Fortran—a parallel execution model
- The do concurrent construct—for loop iterations with no interdependencies
- The contiguous attribute—to specify storage layout restrictions
- The block construct—can contain declarations of objects with construct scope
- Recursive allocatable components—as an alternative to recursive pointers in derived types.

A more thorough coverage can be found in John Reid's paper.

<ftp://ftp.nag.co.uk/sc22wg5/N1851-N1900/N1891.pdf>

3.16.7 TS 29113 Further Interoperability of Fortran with C

This TS was published in 2012.

3.16.8 Fortran 2015

This standard has not been published at the time of going to press. Please visit the WG5 site for up to date information.

Table 3.2 summarises the Fortran standardisation history.

Table 3.2 Fortran standardisation history

Year	Fortran standard	Informal name
1966	Ansi x3.9-1966	Fortran 66
1978	Ansi x3.9-1977	Fortran 77
1978	ISO 1539-1980	Fortran 77
1991	ISO/IEC 1539:1991	Fortran 90
1997	ISO/IEC 1539-1:1997	Fortran 95
1998	ISO/IEC TR 15580:1998	Floating-point exception handling
1998	ISO/IEC TR 15581:1998	Enhanced data type facilities
1999	ISO/IEC 1539-3:1999	Conditional compilation
2000	ISO/TEC 1539-2:2000	Part 2: Varying length character strings
2001	ISO/TEC TR 15580:2001	Floating-point exception handling
2004	ISO/IEC 1539-1:2004	Fortran 2003
2009	ISO/IEC 1539-1	Module TSR
2010	1539-1:2010	Fortran 2008
2012	ISO/TEC TS 29113:2012	Further interoperability of Fortran with C
	ISO/TEC NP TS 18508	Additional parallel features in Fortran

3.17 Fortran Discussion Lists

The first to look at is the Fortran 90 list. Details can be found at

<http://www.jiscmail.ac.uk/lists/COMP-FORTRAN-90.html>

If you subscribe you will have access to people involved in Fortran standardisation, language implementors for most of the hardware and software platforms, people using Fortran in many very specialised areas, people teaching Fortran, etc.

There is also a comp.lang.fortran list available via USENET news. This provides access to people worldwide with enormous combined expertise in all aspects of Fortran. Invariably someone will have encountered your problem or one very much like it and have one or more solutions.

Here is an extract from Wikipedia.

Usenet is a worldwide distributed Internet discussion system. It was developed from the general purpose UUCP dial-up network architecture. Tom Truscott and Jim Ellis conceived the idea in 1979 and it was established in 1980. Users read and post messages (called articles or posts, and collectively termed news) to one or more categories, known as newsgroups. Usenet resembles a bulletin board system (BBS) in many respects, and is the precursor to Internet forums that are widely used today. Usenet can be superficially regarded as a hybrid between email and web forums. Discussions are threaded, as with web forums and BBSes, though posts are stored on the server sequentially.

One notable difference between a BBS or web forum and Usenet is the absence of a central server and dedicated administrator. Usenet is distributed among a large, constantly changing conglomeration of servers that store and forward messages to one another in so-called news feeds. Individual users may read messages from and post messages to a local server operated by a commercial usenet provider, their Internet service provider, university, employer, or their own server.

Another to consider is the Fortran group on ‘linkedin’ The address is

<https://www.linkedin.com/>

3.18 ACM Fortran Forum

Ian Chivers is also Editor of Fortran Forum, the SIGPLAN Special Interest Publication on Fortran, ACM Press. Visit

<http://portal.acm.org/citation.cfm?id=J286>

for more information.

3.19 Other Sources

The following URLs are very useful:

Our Fortran web site.

<http://www.fortranplus.co.uk>

The Fortran Market, maintained by Walt Brainerd.

<http://www.fortran.com/fortran/market.html>

3.20 Summary

It is hoped that you now have some idea about the wide variety of uses that programming languages are put to.

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Fortran 77 Standard

<ftp://ftp.nag.co.uk/sc22wg5/ARCHIVE/Fortran77.html>

Fortran 66 Standard

<ftp://ftp.nag.co.uk/sc22wg5/ARCHIVE/Fortran66.pdf>

The ISO home page is

<http://www.iso.org/>

The J3 home page is:

<http://j3-fortran.org>

The WG5 home page is:

<http://www.nag.co.uk/sc22wg5/>

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Mittelbach, F., Goossens, M., Braams, J., Carlisle, D., Rowley, C.: The L^AT_EX Companion. Addison Wesley (2005). ISBN 0201362996.

- The L^AT_EX book. It is required if you are setting a book using L^AT_EX.

Mossenbeck, H.: Object-Orientated programming in Oberon-2. Springer (1995)

- One of the best introductions to object oriented programming. Uses Oberon-2 as the implementation language. Highly recommended.

Papert, S.: Mindstorms—Children, Computers and Powerful Ideas. Harvester Press (1980)

- Very personal vision of the uses of computers by children. It challenges many conventional ideas in this area.

Sammet J., programming Languages: History and Fundamentals. Prentice-Hall (1969)

- Possibly the most comprehensive introduction to the history of program language development—ends unfortunately before the 1980s.

Sethi, R.: programming Languages: Concepts and Constructs. Addison-Wesley (1989)

- The annotated bibliographic notes at the end of each chapter and the extensive bibliography make it a useful book.

Reiser, M., Wirth, N.: programming in Oberon—Steps Beyond Pascal and Modula. Addison-Wesley (1992)

- Good introduction to Oberon. Revealing history of the developments behind Oberon.

Reiser, M.: The Oberon System: User Guide and programmer's Manual. Addison-Wesley (1991)

- How to use the Oberon system, rather than the language.

Stroustrup, B.: The C++ Programming Language, 3rd edn. 1997; 4th edn. 2014. Addison-Wesley (1997).

- The C++ book. Written by the designer of the language. The third edition is a massive improvement over the earlier editions. The fourth edition covers C++11. One of the best books on C++ and C++11 in particular.

- Young, S.J.: An Introduction to Ada, 2nd Edition. Ellis Horwood (1984)
- A readable introduction to Ada. Greater clarity than the first edition.
- Wexelblat, History of programming Languages, HOPL I, ACM Monograph Series. Academic Press (1978)
- Very thorough coverage of the development of programming languages up to June 1978. Sessions on Fortran, Algol, Lisp, Cobol, APT, Jovial, GPSS, Simula, JOSS, Basic, PL/I, Snobol and APL, with speakers involved in the original languages. Very highly recommended.
- Wiener, R.: Software development using Eiffel. Prentice Hall, 1995.
- The book's subtitle is *There can be life other than C++* The book gives a good introduction to object oriented analysis and design using the Booch 94 method using Eiffel.
- Wirth, N.: An Assessment of the Programming Language Pascal. IEEE Transactions on Software Engineering, 192–198 (June 1975)
- Short paper by Wirth on his experience with Pascal.
- Wirth, N.: History and Goals of Modula 2. Byte, 145–152 (August 1984)
- Straight from the horse's mouth!
- Wirth, N.: On the Design of programming Languages, Proc. IFIP Congress, vol. 74, pp. 386–393. North-Holland.
- Short paper given in 1974 on designing programming languages.
- Wirth, N.: The programming Language Pascal, Acta Informatica, vol. 1, pp. 35–63 (1971)
- Short paper on the development of Pascal from Algol 60.
- Wirth, N.: Modula: a language for modular multiprogramming, Softw. Pract. Exp. 7, 3–35 (1977)
- Short paper on Modula, the precursor of Modula 2.
- Wirth, N.: Programming in Modula 2, Springer (1983)
- The original definition of the language. Essential reading for anyone considering programming in Modula 2 on a long term basis.
- Wirth, N.: Type Extensions, ACM Trans. Prog. Lang. Syst. **10**(2):214–2004 (1988)
- Short paper on type extension.
- Wirth, N.: From modula 2 to oberon. Softw.—Pract. Exp. **18**(7):661–670 (1988).
- Brief paper on the move from Modula 2 to Oberon, looking at features that were removed and added.

Wirth, N., Gutknecht, J.: Project Oberon: The Design of an Operating System and Compiler. Addison-Wesley (1992)

- Fascinating background to the development of Oberon. Highly recommended for anyone involved in large scale program development, not only in the areas of programming languages and operating systems, but more generally.

Chapter 4

Introduction to Programming

Though this be madness, yet there is method in't
Shakespeare

*'Plenty of practice' he went on repeating, all the time that Alice
was getting him on his feet again. 'plenty of practice.'*
The White Knight, Through the Looking Glass and What Alice
Found There, Lewis Carroll

Aims

The aims of the chapter are:

- To introduce the idea that there is a wide class of problems that can be solved with a computer and, further, that there is a relationship between the kind of problem to be solved and the choice of programming language that is used.
- To give some of the reasons for the choice of Fortran.
- To introduce the fundamental components or kinds of statements to be found in a general purpose programming language.
- To introduce the three concepts of name, type and value.
- To illustrate the above with sample programs based on three of the five intrinsic data types:
 - character, integer and real
- To introduce some of the formal syntactical rules of Fortran.

4.1 Introduction

We have seen that an algorithm is a sequence of steps that will solve a part or the whole of a problem. A program is the realisation of an algorithm in a programming language, and there are at first sight a surprisingly large number of programming languages. The reason for this is that there is a wide range of problems that are solved using a computer, e.g., the telephone company generating itemised bills or the meteorological centre producing a weather forecast. These two problems make

different demands on a programming language, and it is unlikely that the same language would be used to solve both.

The range of problems that you want to solve will therefore strongly influence your choice of programming language. Fortran stands for FORmula TRANslation, which gives a hint of the expected range of problems for which it is suitable.

4.2 Language Strengths and Weaknesses

Some of the reasons for choosing Fortran are:

- It is a modern and expressive language;
- The language is suitable for a wide class of both numeric and nonnumeric problems;
- The language is widely available on a range of hardware and operating system platforms;
- A lot of software already exists that has been written in Fortran. Some 15% of code worldwide is estimated to be in Fortran.

There are a few warts, however. Given that there has to be backwards compatibility with earlier versions some of the syntax is clumsy to say the least. However, a considerable range of problems can now be addressed quite cleanly, if one sticks to a subset of the language and adopts a consistent style.

4.3 Elements of a Programming Language

As with ordinary (so-called natural) languages, e.g., English, French, Gaelic, German, etc., programming languages have rules of syntax, grammar and spelling. The application of these rules in a programming language is more strict. A program has to be unambiguous, since it is a precise statement of the actions to be taken. Many everyday activities are rather vaguely defined—Buy some bread on your way home—but we are generally sufficiently adaptable to cope with the variations which occur as a result. If, in a program to calculate wages, we had an instruction deduct some money for tax and insurance we could have an awkward problem when the program calculated completely different wages for the same person for the same amount of work every time it was run. One of the implications of the strict syntax of a programming language for the novice is that apparently silly error messages will appear when one first starts writing programs. As with many other new subjects you will have to learn some of the jargon to understand these messages.

Programming languages are made up of statements. We will look at the various kinds of statements briefly below.

4.3.1 Data Description Statements

These are necessary to describe the kinds of data that are to be processed. In the wages program, for example, there is obviously a difference between people's names and the amount of money they earn, i.e., these two things are not the same, and it would not make any sense adding your name to your wages. The technical term for this is data type—a wage would be of a different data type (a number) to a surname (a sequence of characters).

4.3.2 Control Structures

A program can be regarded as a sequence of statements to solve a particular problem, and it is common to find that this sequence needs to be varied in practice. Consider again the wages program. It will need to select among a variety of circumstances (say married or single, paid weekly or monthly, etc.), and also to repeat the program for everybody employed. So there is the need in a programming language for statements to vary and/or repeat a sequence of statements.

4.3.3 Data-Processing Statements

It is necessary in a programming language to be able to process data. The kind of processing required will depend on the kind or type of data. In the wages program, for example, you will need to distinguish between names and wages. Therefore there must be different kinds of statements to manipulate the different types of data, i.e., wages and names.

4.3.4 Input and Output (I/O) Statements

For flexibility, programs are generally written so that the data that they work on exist outside the program. In the wages example the details for each person employed would exist in a file somewhere, and there would be a record for each person in this file. This means that the program would not have to be modified each time a person left, was ill, etc., although the individual records might be updated. It is easier to modify data than to modify a program, and it is less likely to produce unexpected results. To be able to vary the action there must be some mechanism in a programming language for getting the data into and out of the program. This is done using input and output statements, sometimes shortened to I/O statements.

4.4 Example 1: Simple Text I/O

Let us now consider a simple program which will read in somebody's first name and print it out:

```
program ch0401
!
! This program reads in and prints out a name
!
implicit none
character *20 :: first_name

print *, ' type in your first name.'
print *, ' up to 20 characters'
read *, first_name
print *, first_name
end program ch0401
```

There are several very important points to be covered here, and they will be taken in turn:

- Each line is a statement.
- There is a sequence to the statements. The statements will be processed in the order that they are presented, so in this example the sequence is print, read, print.
- The first statement names the program. It makes sense to choose a name that conveys something about the purpose of the program.
- The next three lines are comment statements. They are identified by a !. Comments are inserted in a program to explain the purpose of the program. They should be regarded as an integral part of all programs. It is essential to get into the habit of inserting comments into your programs straightaway.
- The implicit none statement means that there has to be explicit typing of each and every data item used in the program. It is good programming practice to include this statement in every program that you write, as it will trap many errors, some often very subtle in their effect. Using an analogy with a play, where there is always a list of the persona involved before the main text of the play we can say that this statement serves the same purpose.
- The character*20 statement is a type declaration. It was mentioned earlier that there are different kinds of data. There must be some way of telling the programming language that these data are of a certain type, and that therefore certain kinds of operations are allowed and others are banned or just plain stupid! It would not make sense to add a name to a number, e.g., what does Fred + 10 mean? So this statement defines that the variable first_name is to be of type character and only character operations are permitted. The concept of a variable is covered in the next section. character variables of this type can hold up to 20 characters.

- The `print` statements print out an informative message to the screen—in this case a guide as to what to type in. The use of informative messages like this throughout your programs is strongly recommended.
- The `read` statement is one of the I/O statements. It is an instruction to read from the terminal or keyboard; whatever is typed in from the keyboard will end up being associated with the variable `first_name`. Input/output statements will be explained in greater detail in later sections.
- The `print` statement is another I/O statement. This statement will print out what is associated with the variable `first_name` and, in this case, what you typed in.
- The `end program` statement terminates this program. It can be thought of as being similar to a full stop in natural language, in that it finishes the program in the same way that a period (.) ends a sentence. Note the use of the name given in the program statement at the start of the program.
- Note also the use of the asterisk in three different contexts.
- Indentation has been used to make the structure of the program easier to determine. Programs have to be read by human beings and we will look at this in more depth later.
- Lastly, when you do run this program, character input will terminate with the first blank character.

The above program illustrates the use of some of the statements in the Fortran language. Let us consider the action of the `read *` statement in more detail—in particular, what is meant by a variable and a value.

4.5 Variables—Name, Type and Value

The idea of a variable is one that you are likely to have met before, probably in a mathematical context. Consider the following:

$$\text{circumference} = 2\pi r \quad (4.1)$$

This is an equation for the calculation of the circumference of a circle. The following represents a translation of this into Fortran:

```
circumference = 2 * pi * radius
```

There are a number of things to note about this equation:

- Each of the variables on the right-hand side of the equals sign (`pi` and `radius`) will have a value, which will allow the evaluation of the expression.
- When the expression is fully evaluated the value is assigned to the variable on the left-hand side of the equals sign.
- In mathematics the multiplication is implied. In Fortran we have to use the `*` operator to indicate that we want to multiply 2 by `pi` by the `radius`.
- We do not have access to mathematical symbols like π in Fortran but have to use variable names based on letters from the Roman alphabet.

Table 4.1 Variable name, type and value

Variable name	Data type	Value stored
Temperature	Real	28.55
Number_of_people	Integer	100
First_name	Character	Jane

The whole line is an example of an arithmetic assignment statement in Fortran.

The following arithmetic assignment statement illustrates clearly the concepts of name and value, and the difference in the equals sign in mathematics and computing:

$$i = i + 1 \quad (4.2)$$

In Fortran this reads as take the current value of the variable *i* and add one to it, store the new value back into the variable *i*, i.e., *i* takes the value *i*+1. Algebraically, *i* = *i* + 1 does not make any sense.

Variables can be of different types. Table 4.1 shows some of those available in Fortran.

Note the use of underscores to make the variable names easier to read.

The concept of data type seems a little strange at first, especially as we commonly think of integers and reals as numbers. However, the benefits to be gained from this distinction are considerable. This will become apparent after you have written several programs.

4.6 Example 2: Simple Numeric I/O and Arithmetic

Let us now consider another program, one that reads in three numbers, adds them up and prints out both the total and the average:

```
program ch0402
!
! This program reads in three numbers and sums
! and averages them
!
implicit none
real :: n1, n2, n3, average = 0.0, total = 0.0
integer :: n = 3

print *, ' type in three numbers.'
print *, ' Separated by spaces or commas'
read *, n1, n2, n3
total = n1 + n2 + n3
```

```
average = total/n
print *, 'Total of numbers is ', total
print *, 'Average of the numbers is ', average
end program ch0402
```

Here are some of the key points about this program.

- This program has declarations for numeric variables and Fortran (in common with most programming languages) discriminates between `real` and `integer` data types.
- The variables `average`, `total` and `n` are also given initial values within the type declaration. Variables are initially undefined in Fortran, so the variables `n1`, `n2`, `n3` fall into this category, as they have not been given values at the time that they are declared.
- The `print` statement makes a text message (in this case what is between the apostrophes) appear at the screen. As was noted earlier, it is good practice to put out a message like this so that you have some idea of what you are supposed to type in.
- The `read` statement looks at the input from the keyboard (i.e., what you type) and in this instance associates these values with the three variables. These values can be separated by commas (,), spaces (), or even by pressing the carriage return key, i.e., they can appear on separate lines.
- The next statement actually does some data processing. It adds up the values of the three variables (`n1`, `n2`, and `n3`) and assigns the result to the variable `total`. This statement is called an arithmetic assignment statement, and is covered more fully in the next chapter.
- The next statement is another data-processing statement. It calculates the average of the numbers entered and assigns the result to `average`. We could have actually used the value 3 here instead, i.e., written `average = total/3` and have exactly the same effect. This would also have avoided the type declaration for `n`. However, the original example follows established programming practice of declaring all variables and establishing their meaning unambiguously. We will see further examples of this type throughout the book.
- Indentation has been used to make the structure of the program easier to determine.
- The `sum` and `average` are printed out with suitable captions or headings. Do not write programs without putting captions on the results. It is too easy to make mistakes when you do this, or even to forget what each number means.
- Finally we have the end of the program and again we have the use of the name in the `program` statement.

4.7 Some More Fortran Rules

There are certain things to learn about Fortran which have little immediate meaning and some which have no logical justification at all, other than historical precedence. Why is a cat called a cat? At the end of several chapters there will be a brief summary of these rules or regulations when necessary. Here are a few:

- Source is free format.
- Lowercase letters are permitted, but not required to be recognised.
- Multiple statements may appear on one line and are separated by the semicolon character.
- There is an order to the statements in Fortran. Within the context of what you have covered so far, the order is:
 - Program statement.
 - Type declarations, e.g., implicit, integer, real or character
 - Processing and I/O statements.
 - End program statement.
- Comments may appear anywhere in the program, after program and before end; they are introduced with a ! character, and can be in line.
- Names may be up to 63 characters in length and include the underscore character.
- Lines may be up to 132 characters.
- Up to 39 continuation lines are allowed (using the ampersand (&) as the continuation character).
- The syntax of the read and print statement introduced in these examples is
 - read format, input-item-list.
 - print format, output-item-list.
 - where format is * in the examples and called list directed formatting.
 - and input-item-list is a list of variable names separated by commas.
 - and output-item-list is a list of variable names and/or a sequence of characters enclosed in either ' or ", again separated by commas.
- If the implicit none statement is not used, variables that are not explicitly declared will default to real if the first letter of the variable name is A-H or O-Z, and to integer if the first letter of the variable name is I-N.

4.8 Fortran Character Set

Table 4.2 has details of the Fortran character set.

The default character type shall support a character set that includes the Fortran character set. By supplying nondefault character types, the processor may support

Table 4.2 The Fortran character set

Graphic	Name of character	Graphic	Name of character
Alphanumeric characters			
A–Z	Uppercase letters	0–9	Digits
a–z	Lowercase letters	–	Underscore
Special characters			
	Blank	;	Semicolon
=	Equals	!	Exclamation mark
+	Plus	"	Quotation mark
-	Minus	%	Percent
*	Asterisk	&	Ampersand
/	Slash or oblique	~	Tilde
\	Backslash	<	Less than
(Left parenthesis	>	Greater than
)	Right parenthesis	?	Question mark
[Left square bracket	'	Apostrophe
Right square bracket	`	Grave accent	
{	Left curly bracket	^	Circumflex accent
}	Right curly bracket		Vertical bar or line
,	Comma	\$	Currency symbol
.	Period or decimal point	#	Number sign
:	Colon	@	Commercial at

additional character sets. The characters available in the ASCII and ISO 10646 character sets are specified by ISO/IEC 646:1991 (International Reference Version) and ISO/IEC 10646-1:2000 UCS-4, respectively; the characters available in other non default character types are not specified by the standard, except that one character in each nondefault character type shall be designated as a blank character to be used as a padding character.

Table 4.3 has details of the ASCII character set.

If you live and work outside of the USA and UK you may well have problems with your keyboard when programming. There is a very good entry in Wikipedia on keyboards, that is well worth a look at for the curious.

4.9 Good Programming Guidelines

The following are guidelines, and do not form part of the Fortran language definition:

- Use comments to clarify the purpose of both sections of the program and the whole program.

Table 4.3 ASCII character set

Decimal	Character	Decimal	Character	Decimal	Character	Decimal	Character
0	nul	32	&	64	@	96	'
1	soh	33	!	65	A	97	a
2	stx	34	"	66	B	98	b
3	etx	35	#	67	C	99	c
4	eot	36	\$	68	D	100	d
5	enq	37	%	69	E	101	e
6	ack	38	&	70	F	102	f
7	bel	39	,	71	G	103	g
8	bs	40	(72	H	104	h
9	ht	41)	73	I	105	i
10	lf	42	*	74	J	106	j
11	vt	43	+	75	K	107	k
12	ff	44	,	76	L	108	l
13	cr	45	-	77	M	109	m
14	so	46	.	78	N	110	n
15	si	47	/	79	O	111	o
16	dle	48	0	80	P	112	p
17	dc1	49	1	81	Q	113	q
18	dc2	50	2	82	R	114	r
19	dc3	51	3	83	S	115	s
20	dc4	52	4	84	T	116	t
21	nak	53	5	85	U	117	u
22	syn	54	6	86	V	118	v
23	etb	55	7	87	W	119	w
24	can	56	8	88	X	120	x
25	em	57	9	89	Y	121	y
26	sub	58	:	90	Z	122	z
27	esc	59	;	91	[123	{
28	fs	60	<	92	\	124	
29	gs	61	=	93]	125	}
30	rs	62	>	94	^	126	~
31	us	63	?	95	_	127	del

- Choose meaningful names in your programs.
- Use indentation to highlight the structure of the program. Remember that the program has to be read and understood by both humans and a computer.
- Use `implicit none` in all programs you write to minimise errors.
- Do not rely on the rules for explicit typing, as this is a major source of errors in programming.

4.10 Compilers Used

A number of hardware platforms, operating systems and compilers have been used when writing this book and earlier books. The following have been used in the production of this edition of the book:

- NAG Fortran Builder 6.0 for Windows
- NAG Fortran compiler 6.0 for Windows
- NAG Fortran Compiler 6.0 for Linux
- NAG Fortran Builder 5.3.1 for Windows
- Nag Fortran compiler 5.3.1 and 5.3.2 for Windows
- Intel Fortran 14.x, 15.x for Windows.
- Intel Fortran 15.x for Linux.
- gnu gfortran 4.8.x, 4.9.x, 4.10.x for Windows.
- gnu gfortran 4.8.x for Linux.
- Cray Fortran : Version 8.2.1 - Cray Archer service
- Oracle Solaris Studio 12.4 for Linux

Our recommendation is that you use at least two compilers in the development of your code. Moving code between compilers and platforms teaches you a lot.

The following have been used with earlier editions of the book:

- NAG Fortran Builder 5.1, 5.2, 5.3 for Windows
- NAG Fortran Compiler 5.1, 5.2, 5.3 for Linux.
- Intel Fortran 11.x, 12.x, 13.x for Windows.
- Intel Fortran 12.x for Linux.
- gnu gfortran 4.x for Windows.
- gnu gfortran 4.x for Linux.
- Cray Fortran : Version 7.3.1 - Cray Hector service
- g95 for Linux.
- pgi 10.x - Cray Hector service
- IBM XL Fortran for AIX, V13.1 (5724-X15), Version: 13.01.0000.0002
- Oracle Solaris Studio 12.0, 12.1, 12.2 for Linux

The following have been used with earlier books:

- DEC VAX under VMS and later OPEN VMS with the NAG Fortran 90 compiler.
- DEC Alpha under OPEN VMS using the DEC Fortran 90 compiler.
- Sun Ultra Sparc under Solaris:
- NAGACE F90 compiler.
- NAGWare F95 compiler.
- Sun (Release 1.x) F90 compiler.
- Sun (Release 2.x) F90 compiler.
- PCs under DOS and Windows:
- DEC/Compaq Fortran 90 and Fortran 95 compilers.
- Intel Compiler (7.x, 8.x).
- Lahey Fujitsu Fortran 95 (5.7).

- NAG Fortran 95 Compiler.
- NAG Salford Fortran 90 Compiler.
- Salford Fortran 95 Compiler.
- PCs under Linux:
- Intel Compiler.
- Lahey Fujitsu Fortran 95 Pro (6.1).
- NAG Fortran 95 (4.x, 5.x).

It is very illuminating to use more than one compiler whilst developing programs.

4.11 Compiler Documentation

The compiler may come with documentation. Here are some details for a number of compilers.

4.11.1 *Gfortran*

Manuals are available at

<http://gcc.gnu.org/wiki/GFortran\#manuals>

The following

[http://gcc.gnu.org/onlinedocs/
gcc-4.5.2/gfortran.pdf](http://gcc.gnu.org/onlinedocs/gcc-4.5.2/gfortran.pdf)

is a 236 page pdf.

4.11.2 *IBM*

Here is a starting point. The urls have been split as the lines are too long.

[http://www-03.ibm.com/software/
products/en/fortcompfami/](http://www-03.ibm.com/software/products/en/fortcompfami/)

Here is a starting point for the XLF for AIX system.

[http://www-01.ibm.com/support/
docview.wss?uid=swg27036673](http://www-01.ibm.com/support/docview.wss?uid=swg27036673)

and the starting point for the pdf version of the documentation is.

```
http://www-01.ibm.com/support/  
docview.wss?uid=swg27036673
```

They provide

- Getting Started with XL Fortran for AIX 15.1 This book introduces you to XL Fortran for Linux and its features, including features new for 15.1.
- Installation Guide - XL Fortran for AIX 15.1 This book contains information for installing XL Fortran and configuring your environment for basic compilation and program execution.
- Compiler Reference - XL Fortran for AIX 15.1 This book contains information about the many XL Fortran compiler options and environment variables that you can use to tailor the XL Fortran compiler to your application development needs.
- Language Reference - XL Fortran for AIX 15.1 This book contains information about the Fortran programming language as supported by IBM, including language extensions for portability and conformance to non-proprietary standards, compiler directives and intrinsic procedures.
- Optimization and Programming Guide - XL Fortran for AIX 15.1 This book contains information on advanced programming topics, such as application porting, interlanguage calls, floating-point operations, input/output, application optimization and parallelization, and the XL Fortran high-performance libraries.

4.11.3 Intel

Windows. The following will end up available after a complete install.

- Intel MKL
 - Release notes
 - Reference Manual
 - User Guide
- Parallel Debugger Extension
 - Release Notes
- Compiler
 - Reference Manual, Visual Studio Help files or html.
 - User Guide, Visual Studio Help files or html.

Intel also provide the following

```
http://software.intel.com/en-us/articles/  
intel-software-technical-documentation/
```

4.11.4 Nag

Windows

- Fortran Builder Help
 - Fortran Builder Tutorial - 44 pages
 - Fortran Builder Operation Guide - 67 pages
 - Fortran Language Guide - 115 pages
 - Compiler Manual - 149 pages
 - LAPACK Guide - 70 pages (440MB as PDF!)
 - GTK+ Library - 201 pages
 - OpenGL/GLUT Library - 38 pages
 - SIMDEM Library - 78 pages

4.11.5 Oracle/Sun

Oracle make available a range of documentation. From within Oracle Solaris Studio

- Help
 - Help Contents
 - Online Docs and Support
 - ..
 - ..
 - Quick Start Guide

and you will get taken to the Oracle site by some of these entries.

You can also download a 300+ MB zip file which contains loads of Oracle documentation. You should be able to locate (after some rummaging around)

- Sun Studio 12: Fortran Programming Guide - 174 pages
- Sun Studio 12: Fortran User's Guide - 216 pages
- Sun Studio 12: Fortran Library Reference - 144 pages
- Fortran 95 Interval Arithmetic Programming Reference - 166 pages

Happy reading :-)

4.12 Program Development

A number of ways of developing programs have been used, including:

- Using an integrated development environment, including
 - NAG Fortran Builder under Windows.

- Microsoft Visual Studio with the Intel compiler under Windows.
- Oracle Sunstudio under SuSe Linux.
- Using a DOS box and simple command line prompt under Windows.
- Using ssh to log in to the Archer service.
- Using a VPN, and SSH to log in to the IBM Power 7 system at Slovak Hydrometeorological Institute Jesnova 17
- Using a console or terminal window under SuSe Linux.
- Using X-Windows software to log into the SUN Ultra Sparc systems.
- Using terminal emulation software to log into the SUN Ultra Sparc.
- Using DEC terminals to log into the DEC VAX and DEC Alpha systems.
- Using PCs running terminal emulation software to log into the DEC VAX and DEC Alpha systems.

It is likely that you will end up doing at least one of the above and probably more. The key stages involved are:

- Creating and making changes to the Fortran program source.
- Saving the file.
- Compiling the program:
- If there are errors you must go back to the Fortran source and make the changes indicated by the compiler error messages.
- Linking if successful to generate an executable:
- Automatic link. This happens behind the scenes and the executable is generated for you immediately.
- Manual link. You explicitly invoke the linker to generate the executable.
- Running the program.
- Determining whether the program actually works and gives the results expected.

These steps must be taken regardless of the hardware platform, operating system and compiler you use. Some people like working at the operating system prompt (e.g., DOS, Linux and UNIX), and others prefer working within a development environment. Both have their strengths and weaknesses.

4.13 Reference Text for the Fortran 2003 Standard

Jeanne C. Adams, Walter S. Brainerd, Richard A. Hendrickson, Richard E. Maine, Jeanne T. Martin, Brian T. Smith. The Fortran 2003 Handbook: The Complete Syntax, Features and Procedures. Springer, 31 Oct 2008, ISBN-10: 1846283787, ISBN-13: 978-1846283789.

- It covers the whole of the Fortran 2003 standard in a lot of depth. The content and structure of the book follows that of the standard directly. A much easier read than the standard, and a lot cheaper.

4.14 Problems

4.1 Compile and run Example 1 in this chapter. Experiment with the following types of input.

Ian
Ian Chivers
“Jane Margaret Sleightholme”

4.2 Compile and run Example 2 in this chapter.

Think about the following points:

- Is there a difference between separating the input by spaces or commas?
- Do you need the decimal point?
- What happens when you type in too many data?
- What happens when you type in too few data?

If you have access to more than one compiler repeat the above and compare the results.

4.3 Write a program that will read in your name and address and print them out in reverse order.

Think about the following points:

- How many lines are there in your name and address?
- What is the maximum number of characters in the longest line in your name and address?
- What happens at the first blank character of each input line?
- Which characters can be used in Fortran to enclose each line of text typed in and hence not stop at the first blank character?
- If you use one of the two special characters to enclose text what happens if you start on one line and then press the return key before terminating the text?

The action here will vary between Fortran implementations.

Chapter 5

Arithmetic

Taking Three as the subject to reason about—A convenient number to state—We add Seven, and Ten, and then multiply out By One Thousand diminished by Eight. The result we proceed to divide, as you see, By Nine Hundred and Ninety and Two: then subtract Seventeen, and the answer must be Exactly and perfectly true.

Lewis Carroll, The Hunting of the Snark

Round numbers are always false.

Samuel Johnson

Aims

The aims of this chapter are to introduce:

- The Fortran rules for the evaluation of arithmetic expressions to ensure that they are evaluated as you intend;
- The idea of truncation and rounding;
- The use of the parameter attribute to define or set up constants;
- The use of Fortran's kind types to determine and control the precision by which arithmetic in Fortran is carried out;
- The concept of numeric models and positional number systems for integer and real arithmetic and their implementation on binary devices;
- Testing the numerical representation of different integer kind types on a system—8, 16, 32 and 64 bit integers;
- Testing the numerical representation of different real kind types on a system—32, 64, 80 and 128 bit reals;
- round off;
- relative error;
- absolute error.

5.1 Introduction

Most problems in the academic and scientific communities require arithmetic evaluation as part of the algorithm. The arithmetic performed by computers is not the same as the arithmetic you are familiar with in conventional mathematics and algebra.

There are two areas that we need to address

- computation involving finite precision—so called computer arithmetic
- the rules that apply in a programming language—different programming languages have different rules for the evaluation of expressions.

The outcome of the above means that $2 + 2$ is not necessarily 4 when using a computer!

5.2 The Fortran Operators and the Arithmetic Assignment Statement

In the previous chapter, we introduced the arithmetic assignment statement, emphasising the concepts of name, type and value. Here we will consider the way that arithmetic expressions are evaluated in Fortran.

Table 5.1 lists the five arithmetic operators available in Fortran.

Exponentiation is raising a number to a power. Note that the exponentiation operator is the * character twice.

The following are some examples of valid arithmetic assignment statements in Fortran:

```
taxable_income = gross_wage - personal_allowance
cost = bill + vat + service
delta = deltax/deltay
area = pi * radius * radius
cube = big ** 3
```

Table 5.1 Fortran operators

Mathematical operation	Fortran symbol or operator
Addition	+
Subtraction	-
Division	/
Multiplication	*
Exponentiation	**

These expressions are all simple, and there are no problems when it comes to evaluating them. However, now consider the following:

```
tax = gross_wage - personal_allowance * tax_rate
```

This is a poorly written arithmetic expression. There is a choice of doing the subtraction before or after the multiplication. Our everyday experience says that the subtraction should take place before the multiplication. However, if this expression were evaluated in Fortran the multiplication would be done before the subtraction.

5.3 Example 1: Simple Arithmetic Expressions in Fortran

A complete program to show the correct form in Fortran is as follow:

```
program ch0501
    implicit none
!
! Example of a Fortran program
! to calculate net pay
! given an employee's gross pay
!
! The UK personal allowance is
! correct as of 2014
!
real :: gross_wage, net_wage, tax
real :: tax_rate = 0.25
integer :: personal_allowance = 10000
character (len=60) :: their_name

print *, 'Input employees name'
read *, their_name
print *, 'Input Gross wage'
read *, gross_wage
tax = (gross_wage-personal_allowance)*tax_rate
net_wage = gross_wage - tax
print *, 'Employee: ', their_name
print *, 'Gross Pay: ', gross_wage
print *, 'Tax: ', tax
print *, 'Net Pay:', net_wage
end program ch0501
```

Let us look at some of the key points of this program.

- We have the `implicit none` statement which aids in detecting typing errors.
- We declare the variables `gross_wage`, `net_wage`, `tax` and `tax_rate` to be of type `real` as they will hold floating point values, i.e., numbers with a decimal point.
- The variable `their_name` is of type `character` and can hold up to 60 characters.
- The variable `personal_allowance` is of type `integer` as it holds integer values.
- We then have some i/o statements to prompt the user for input and read in their name and gross pay.
- We then calculate the tax payable and net income using two simple arithmetic assignment statements.
- We then print out the results.

This example illustrates some basic arithmetic in Fortran.

5.4 The Fortran Rules for Arithmetic

We need to look at three areas here:

- The rules for forming expressions—the syntax.
- The rules for interpreting expressions—the semantics.
- The rules for evaluating expressions—optimisation.

The syntax rules determine which expressions are valid. The semantics determine a valid interpretation, and once this has been done the compiler can replace the expression with any other one that is mathematically equivalent, generally in the interests of optimisation.

Here is the section of the Fortran 2008 standard on expression evaluation.

- 7.1.5.2.4 Evaluation of numeric intrinsic operations
 - 1 - Once the interpretation of a numeric intrinsic operation is established, the processor may evaluate any mathematically equivalent expression, provided that the integrity of parentheses is not violated.
 - 2 - Two expressions of a numeric type are mathematically equivalent if, for all possible values of their primaries, their mathematical values are equal. However, mathematically equivalent expressions of numeric type may produce different computational results.

The rules for the evaluation of expressions in Fortran are as follows:

- Brackets are used to define priority in the evaluation of an expression.
- Operators have a hierarchy of priority—a precedence. The hierarchy of operators is:
- Exponentiation: when the expression has multiple exponentiation, the evaluation is from right to left. For example,

```
l = i ** j ** k
```

is evaluated by first raising j to the power k , and then using this result as the exponent for i ; more explicitly,

```
l = i ** (j ** k)
```

Although this is similar to the way in which we might expect an algebraic expression to be evaluated, it is not consistent with the rules for multiplication and division, and may lead to some confusion. When in doubt, use brackets.

- Multiplication and division: within successive multiplications and divisions, the rules regarding any mathematically equivalent expression means that you must use brackets to ensure the evaluation you want. For example, with

```
a = b * c / d * e
```

for real and complex numeric types the compiler does not necessarily evaluate in a left to right manner, i.e., evaluate b times c , then divide the result by d and finally take that result and multiply by e .

- Addition and subtraction: as for multiplication and division the rules regarding any equivalent expression apply. However, it is seldom that the order of addition and subtraction is important, unless other operators are involved.

Table 5.2 summarises the hierarchy of the operators.

Table 5.2 Hierarchy or precedence of the Fortran operators

Mathematical operation	Fortran symbol or operator
Exponentiation	$**$
Division	$/$
Multiplication	$*$
Addition	$+$
Subtraction	$-$

The following are all examples of valid arithmetic expressions in Fortran:

```
Slope = (y1-y2) / (x1-x2)
x1 = (-b+((b*b-4*a*c)**0.5))/(2*a)
Q = Mass_D/2*(Mass_A*Veloc_A/Mass_D)**2 + &
  ((Mass_A * Veloc_A)**2)/2
```

Note that brackets have been used to make the order of evaluation more obvious. It is often possible to write involved expressions without brackets, but, for the sake of clarity, it is often best to leave the brackets in, even to the extent of inserting a few extra ones to ensure that the expression is evaluated correctly. The expression will be evaluated just as quickly with the brackets as without. Also note that none of the expressions is particularly complex. The last one is about as complex as you should try: with more complexity than this it is easy to make a mistake.

5.5 Expression Equivalence

The rule regarding any equivalent expression means if a , b and c are numeric then the following are true:

$$\begin{aligned} a + b &= b + a \\ -a + b &= b - a \\ a + b + c &= a + (b + c) \end{aligned}$$

The last is nominally evaluated left to right, as the additions are of equal precedence:

$$\begin{aligned} a * b &= b * a \\ a * b * c &= a * (b * c) \end{aligned}$$

and again the last is nominally evaluated left to right, as the multiplications are of equal precedence:

$$\begin{aligned} a * b - a * c &= a * (b - c) \\ a / b / c &= a / (b * c) \end{aligned}$$

The last is true for real and complex numeric types only.

Problems arise when the value that a faulty expression yields lies within the range of expected values and the error may well go undetected. This may appear strange at first, but a computer does exactly what it is instructed to do. If, through a misunderstanding on the part of a programmer, the program is syntactically correct but logically wrong from the point of view of the problem definition, then this will not

be spotted by the compiler. If an expression is complex, break it down into successive statements with elements of the expression on each line, e.g.,

```
temp = b * b - 4 * a * c
x1 = ( - b + ( temp ** 0.5 ) ) / ( 2 * a )
```

and

```
Moment = Mass_A * Veloc_A
Q = Mass_D / 2 * ( Moment / Mass_D ) **2 + &
( Moment **2 ) / 2
```

5.6 Rounding and Truncation

Computer arithmetic can be subject to truncation and rounding.

- Truncation. This operation involves throwing away part of the number, e.g., with 14.6 truncating the number to two figures leaves 14.
- Rounding. Consider 14.6 again. This is rounded to 15. Basically, the number is changed to the nearest whole number. It is still a real number. What do you think will happen with 14.5; will this be rounded up or down?

You must be aware of these two operations. They may occasionally cause problems in division and in expressions with more than one data type.

5.7 Example 2: Type Conversion and Assignment

To see some of the problems that can occur consider the examples below:

```
program ch0502
    implicit none
    real :: a, b, c
    integer :: i

    a = 1.5
    b = 2.0
    c = a/b
    i = a/b
    print *, a, b
    print *, c
    print *, i
end program ch0502
```

After executing these statements `c` has the value 0.75, and `i` has the value zero! This is an example of type conversion across the `=` sign. The variables on the right are all real, but the last variable on the left is an integer. The value is therefore made into an integer by truncation. In this example, 0.75 is real, so `i` becomes zero when truncation takes place.

5.8 Example 3: Integer Division and Real Assignment

Consider now an example where we assign into a real variable (so that no truncation due to the assignment will take place), but where part of the expression on the right-hand side involves integer division:

```
program ch0503
    implicit none
    integer :: i, j, k
    real :: answer

    i = 5
    j = 2
    k = 4
    answer = i/j*k
    print *, i
    print *, j
    print *, k
    print *, answer
end program ch0503
```

The value of `answer` is 8, because the `i / j` term involves integer division. The expected answer of 10 is not that different from the actual one of 8, and it is cases like this that cause problems for the unwary, i.e., where the calculated result may be close to the actual one. In complicated expressions it would be easy to miss something like this.

To recap, truncation takes place in Fortran:

- Across an `=` sign, when a real is assigned to an integer.
- In integer division.

It is very important to be careful when attempting mixed mode arithmetic—that is, when mixing reals and integers. If a real and an integer are together in a division or multiplication, the result of that operation will be real; when addition or subtraction takes place in a similar situation, the result will also be real. The problem arises when some parts of an expression are calculated using integer arithmetic and other parts

with real arithmetic:

$$c = a + b - i / j$$

The integer division is carried out before the addition and subtraction; hence the result of i/j is integer, although all the other parts of the expression will be carried out with real arithmetic.

5.9 Example 4: Time Taken for Light to Travel from the Sun to Earth

How long does it take for light to reach the Earth from the Sun? Light travels 9.46×10^{12} km in 1 year. We can take a year as being equivalent to 365.25 days. (As all school children know, the astronomical year is 365 days, 5 h, 48 min and 45.9747 s—hardly worth the extra effort.) The distance between the Earth and Sun is about 150,000,000 km. There is obviously a bit of imprecision involved in these figures, not least since the Earth moves in an elliptical orbit, not a circular one. One last point to note before presenting the program is that the elapsed time will be given in minutes and seconds. Few people readily grasp fractional parts of a year:

```
program ch0504
    implicit none
    real :: light_minute, distance, elapse
    integer :: minute, second
    real, parameter :: light_year = 9.46*10**12
! Light_year      : Distance travelled by light
!                      in one year in km
! Light_minute   : Distance travelled by light
!                      in one minute in km
! Distance       : Distance from sun to earth in
!                      km
! Elapse         : Time taken to travel a
!                      distance (Distance) in minutes
! Minute         : integer number part of elapse
! Second         : integer number of seconds
!                      equivalent to fractional
!                      part of elapse
!
light_minute = light_year/(365.25*24.0*60.0)
distance = 150.0*10**6
elapse = distance/light_minute
minute = elapse
second = (elapse-minute)*60
```

```

print *, ' Light takes ', minute, ' Minutes'
print *, ' ', second, ' Seconds'
print *, ' To reach the earth from the sun'
end program ch0504

```

The calculation is straightforward; first we calculate the distance travelled by light in 1 min, and then use this value to find out how many minutes it takes for light to travel a set distance. Separating the time taken in minutes into whole-number minutes and seconds is accomplished by exploiting the way in which Fortran will truncate a real number to an integer on type conversion. The difference between these two values is the part of a minute which needs to be converted to seconds. Given the inaccuracies already inherent in the exercise, there seems little point in giving decimal parts of a second.

It is worth noting that some structure has been attempted by using comment lines to separate parts of the program into fairly distinct chunks. Note also that the comment lines describe the variables used in the program.

Can you see any problems with this example?

5.10 The Parameter Attribute

This attribute is used to provide a way of associating a meaningful name with a constant in a program. Consider a program where π was going to be used a lot. It would be silly to have to type in 3.14159265358 every time. There would be a lot to type and it is likely that a mistake could be made typing in the correct value. It therefore makes sense to set up `pi` once and then refer to it by name. However, if `pi` was just a variable then it would be possible to do the following:

```

real :: li,pi
.
pi=4.0*atan(1.0)
.
pi=4*alpha/beta
.

```

The `pi=4*alpha/beta` statement should have been `li=4*alpha/beta`. What has happened is that, through a typing mistake (`p` and `l` are close together on a keyboard), an error has crept into the program. It will not be spotted by the compiler. Fortran provides a way of helping here with the parameter attribute, which should be added to or combined with a type declaration.

Table 5.3 has details of some commonly used physical constants.

The data has been taken from

<http://physics.nist.gov/cuu/index.html>

Table 5.3 Some commonly used physical constants

Atomic mass constant	m_u	$1.660\,538\,921 \times 10^{-27} \text{ kg}$
Avogadro constant	N_A, L	$6.022\,141\,29 \times 10^{23} \text{ mol}^{-1}$
Boltzmann constant	k	$1.380\,6488 \times 10^{-23} \text{ JK}^{-1}$
Electron mass	m_e	$9.109\,382\,91 \times 10^{-31} \text{ kg}$
Elementary charge	e	$1.602\,176\,565 \times 10^{-19} \text{ C}$
Proton mass	m_p	$1.672\,621\,777 \times 10^{-27} \text{ kg}$
Speed of light in vacuum	c, c_0	$299\,792\,458 \text{ m s}^{-1}$
Newtonian constant of gravitation	G	$6.673\,84 \times 10^{-11} \text{ m}^3 \text{ kg}^{-1} \text{ s}^{-2}$

A type statement with a parameter attribute may contain an arithmetic expression, so that some relatively simple arithmetic may be performed in setting up these constants. The evaluation must be confined to addition, subtraction, multiplication, division and integer exponentiation.

The following are some examples of the parameter attribute for some of the physical constants.

```
real , parameter :: pi = &
  4.0*atan(1.0)
real , parameter :: c  = &
  299792458 * 10.0 ** (-1)
real , parameter :: e  = &
  1.602176565 * 10.0 ** (-19)
```

We have introduced the Fortran intrinsic function `atan` in this example, and for further details see appendix B. We will also be covering intrinsic functions in a later chapter. The advantage of the parameter attribute is that you could not then assign another value to `pi`, `c` or `charge`. If you tried to do this, the compiler would generate an error message.

5.11 Round Off Errors and Computer Arithmetic

Precision is not the same as accuracy. In this age of digital timekeeping, it is easy to provide an extremely precise answer to the question What time is it? This answer need not be accurate, even though it is reported to tenths (or even hundredths!) of a second. Do not be fooled into believing that an answer reported to ten places of decimals must be accurate to ten places of decimals. The computer can only retain a limited precision. When calculations are performed, this limitation will tend to generate

inaccuracies in the result. The estimation of such inaccuracies is the domain of the branch of mathematics known as Numerical Analysis.

To give some idea of the problems, consider an imaginary decimal computer which retains two significant digits in its calculations. For example, 1.2, 12.0, 120.0 and 0.12 are all given to two-digit precision. Note therefore that 1234.5 would be represented as 1200.0 in this device. When any arithmetic operation is carried out, the result (including any intermediate calculations) will have two significant digits. Thus:

$$130 + 12 = 140 \text{ (rounding down from 142)}$$

and similarly:

$$17 / 3 = 5.7 \text{ (rounding up from 5.666666...)}$$

and:

$$16 * 16 = 260$$

where there are more involved calculations, the results can become even less attractive. Assume we wish to evaluate

$$(16 * 16) / 0.14$$

We would like an answer in the region of 1828.5718, or, to two significant digits, 1800.0. if we evaluate the terms within the brackets first, the answer is 260/0.14, or 1857.1428; 1900.0 on the two-digit machine. Thinking that we could do better, we could rewrite the fraction as

$$(16 / 0.14) * 16$$

Which gives a result of 1800.0.

Algebra shows that all these evaluations are equivalent if unlimited precision is available.

A round-off error, also called rounding error, is the difference between the calculated approximation of a number and its exact mathematical value. We will look at this issue in more depth later in this chapter.

5.12 Relative and Absolute Errors

When we are calculating numerical approximations to a solution we often need to measure how accurate our estimated solution is. If we are using an iterative method

we could look at the difference between successive calculations, or our algorithm may have an expression for estimating errors.

Either way there are two types of errors, absolute and relative.

Looking at relative errors is a better way of measuring accuracy than absolute errors because an absolute error depends on the size of the number being approximated.

If p' is an approximation to p then the relative error is $|p - p'|/|p|$ and the absolute error is $|p - p'|$.

Here is an example to illustrate the above.

5.13 Example 5: Relative and Absolute Error

```
program ch0505
    implicit none
    real :: p = 0.4e-4, papprox = 0.41e-4
    real :: abs_error, rel_error
    integer :: i

    do i = 1, 3
        abs_error = abs(p-papprox)
        rel_error = abs(p-papprox)/abs(p)
        print 100, p, papprox
        100 format ('p          = ', e11.4,&
                   '/papprox = ', e11.4)
        print 110, abs_error, rel_error
        110 format ('abs error:', 12x, e11.4,&
                   '/rel error:', 12x, e11.4/)
        p = p*1.0e5
        papprox = papprox*1.0e5
    end do
end program ch0505
```

This program introduces the intrinsic `abs` function and a new statement, the `format` statement and the `(e)` edit descriptor. For the moment just concentrate on the output. We will look at the `format` statement and `(e)` edit descriptor in more depth in a later chapter. See appendix B for more information on the `abs` intrinsic.

Here is the output from the Nag compiler.

```
p          = 0.4000E-04
approx to p = 0.4100E-04
abs error:           0.1000E-05
rel error:           0.2500E-01
```

```

p = 0.4000E+01
approx to p = 0.4100E+01
abs error: 0.1000E+00
rel error: 0.2500E-01

p = 0.4000E+06
approx to p = 0.4100E+06
abs error: 0.1000E+05
rel error: 0.2500E-01

```

This example shows that the same relative error of $0.25 * 10^{-1}$ occurs for widely varying absolute errors, therefore the absolute error can be misleading.

The relative error is more meaningful because it takes into consideration the size of the number.

5.14 Range, Precision and Size of Numbers

The range of integer numbers and the precision and the size of floating point numbers in computing are directly related to the number of bits allocated to their internal representation. Tables 5.4 and 5.5 summarise this information for the two most common bit sizes in use for integers and reals—32 bits and 64 bits, as defined in the IEEE standard. Most hardware in use today supports these standards to a greater or lesser extent.

We will look at IEEE 754 in later sections and in a separate chapter.

Table 5.4 looks at integer numbers and Table 5.5 looks at real numbers.

For practical purposes all compilers support the information contained in these two tables.

Table 5.4 Word size and integer numbers

Number of bits	Power of 2	Power of 10	Maximum integer
32	$(2 * 31) - 1$	$O(10 * 9)$	2,147,483,647
64	$(2 * 63) - 1$	$O(10 * 18)$	9,223,372,036,854,774,807

Table 5.5 Word size and real numbers

Number of bits	Precision	Smallest real	Largest real
32	6–9	$\approx 0.3E-38$	$\approx 1.7E38$
64	15–18	$\approx 0.5E-308$	$\approx 0.8E+308$

5.15 Overflow and Underflow

Care should also be taken when one is near the numerical limits of the machine. Consider the following:

$$z = b * c / d$$

where b , c and d are all $O(10^{30})$ and we are using 32-bit floating point numbers where the maximum real is $O(10^{38})$. Here the product $b * c$ generates a number of $O(10^{60})$ —beyond the limits of the machine. This is called overflow as the number is too large. Note that we could avoid this problem by retying this as

$$z = b * (c / d)$$

where the bracketed expression c/d would now be $O(10^{30})/O(10^{30})$, and is within machine limits.

5.15.1 Example 6: Overflow

Here is a sample program that illustrates the above.

```
program ch0506
    implicit none
    real :: z = 0.0
    real :: b = 1.0e30
    real :: c = 1.0e30
    real :: d = 1.0e30

    z = b*c/d
    print *, z
    z = b*(c/d)
    print *, z
end program ch0506
```

Here is the output from the Intel compiler.

```
      Infinity
1.0000000E+30
```

Here is the output from the Nag compiler.

```
nagfor ch0506.f90
NAG Fortran Compiler
Error: ch0506.f90, line 7:
Floating-point overflow in single-precision
multiplication
[NAG Fortran Compiler error termination, 1 error]
```

So the Nag compiler diagnoses the problem at compile time.

5.15.2 Example 7: Underflow

There is an inverse called underflow when the number is too small, which is illustrated below:

```
z = b * c * d
```

where b and c are $O(10^{-30})/O(10^{30})$. The intermediate result of $b * c$ is $O(10^{-60})$ —again beyond the limits of the machine. This problem could have been overcome by retying as

```
z = b * (c * d)
```

Here is a simple program that illustrates underflow.

```
program ch0507
    implicit none
    real :: z = 0.0
    real :: b = 1.0e-30
    real :: c = 1.0e-30
    real :: d = 1.0e30

    z = b*c*d
    print *, z
    z = b*(c*d)
    print *, z
end program ch0507
```

Here is the output from running the program with the Nag and Intel compilers.

```
0.0000000E+00
```

1.000000E-30

We will look at underflow in more detail in the chapter on IEEE arithmetic.

5.16 Health Warning: Optional Reading, Beginners Are Advised to Leave Until Later

Most people take arithmetic completely for granted and rarely think much about the subject. It is necessary to look at it in a bit more depth if we are to understand what the computer is doing in this area.

5.16.1 Positional Number Systems

Our way of working with numbers is essentially a positional one. When we look at the number 1024, for example, we rarely think of it in terms of $1 * 1000 + 0 * 100 + 2 * 10 + 4 * 1$. Thus the normal decimal system we use in everyday life is a positional one, with a base of 10.

We are probably aware that we can use other number bases, and 2, 8 and 16 are fairly common alternate number bases. As the computer is a binary device it uses base 2.

We are also reasonably familiar with a mantissa exponent or floating point combination when the numbers get very large or very small, e.g., a parsec is commonly expressed as $3.08 * 10 * 16$, and here the mantissa is 3.08, and the exponent is $10 * 16$.

The above information will help in understanding the way in which integers and reals are represented on computer systems.

5.16.2 Fortran Representational Models

Fortran has three representational models for data

- the bit model
- the integer number system model
- the real number system model

and these models (and the corresponding intrinsic functions) return values related to the models. We look at each in turn below.

5.16.2.1 Bit Data Type and Representation Model

The model is only defined for positive integers (or cardinal numbers), where they are represented as a sequence of binary digits, and is based on the model:

$$i = \sum_{k=0}^{n-1} b_k 2^k$$

where i is the integer value, n is the number of bits, and b_k is a bit value of 0 or 1, with bit numbering starting at 0, and reading right to left. Thus the integer 43 and bit pattern 101011 is given by:

$$43 = (1 * 32) + (0 * 16) + (1 * 8) + (0 * 4) + (1 * 2) + (1 * 1)$$

or

$$43 = (1 * 2^5) + (0 * 2^4) + (1 * 2^3) + (0 * 2^2) + (1 * 2^1) + (1 * 2^0)$$

5.16.2.2 Integer Data Type and Representation Model

The integer data type is based on the model

$$i = s \sum_{k=1}^q l_k r^{k-1}$$

where i is the integer value, s is the sign, q is the number of digits (always positive), r is the radix or base (integer greater than 1), and l_k is a positive integer (less than r).

A base of 2 is typical so 1023 is

$$1023 = (1 * 2^9) + (1 * 2^8) + (1 * 2^7) + (1 * 2^6) + (1 * 2^5) + (1 * 2^4) + (1 * 2^3) + (1 * 2^2) + (1 * 2^1) + (1 * 2^0)$$

5.16.2.3 Real Data Type and Representation Model

The real data type is based on the model

$$x = sb^e \sum_{k=1}^m f_k b^{-k}$$

where x is the real number, s is the sign, b is the radix or base (greater than 1), m is the number of bits in the mantissa, e is an integer in the range e_{\min} to e_{\max} , and f_k is a positive number less than b .

This means that with, for example, a 32-bit real there would be 8 bits allocated to the exponent and 24 to the mantissa. One of the bits in each part would be used to represent the sign and is called the sign bit. This reduces the number of bits that can actually be used to represent the mantissa and exponent to 31 and 7, respectively.

There is also the concept of normalisation, where the exponent is adjusted so that the most significant bit is in position 22—bits are typically numbered 0–22, rather than 1–23. This form of representation is not new, and is first documented around 1750 BC, when Babylonian mathematicians used a sexagesimal (radix 60) positional notation. It is interesting that the form they used omitted the exponent!

This is the theoretical basis of the representation of these three data types in Fortran.

This information together with the following provide a good basis for writing portable code across a range of hardware.

5.17 Testing the Numerical Representation of Different Kind Types on a System

Fortran 90 introduced the concept of a `kind` parameter for the intrinsic types. Each of the intrinsic types has a `kind` parameter that selects a processor dependent representation of objects of that type and kind.

Table 5.6 provides details of the kind query functions and Table 5.7 provides details of the numeric query functions.

The next set of programs test out the kinds of the intrinsic types supported by compilers.

Table 5.6 Kind inquiry functions

Function name	Simple explanation
<code>kind</code>	Kind parameter
<code>selected_char_kind</code>	Kind parameter of a specified character set
<code>selected_int_kind</code>	Kind parameter of an integer data type
<code>selected_real_kind</code>	Kind parameter of a real data type

Table 5.7 Numeric inquiry functions

Function name	Simple explanation
<code>digits</code>	Number of digits in the model number
<code>epsilon</code>	Smallest difference between two reals
<code>huge</code>	Returns the largest number
<code>maxexponent</code>	Maximum value for the model exponent
<code>minexponent</code>	Minimum value for the model exponent
<code>precision</code>	Returns the decimal precision
<code>radix</code>	Base of a model number
<code>range</code>	Decimal exponent range of a model number
<code>tiny</code>	Returns the smallest number

5.18 Example 8: Using the Numeric Inquiry Functions with Integer Types

This program looks at using the kind intrinsics with integer types.

```
program ch0508

implicit none

! example of the use of the kind function
! and the numeric inquiry functions
! for integer kind types

! 8 bit           -128  to
!                      127   10**2

! 16 bit          -32768 to
!                      32767  10**4

! 32 bit          -2147483648 to
!                      2147483647  10**9

! 64 bit          -9223372036854775808 to
!                      9223372036854775807  10**18

integer :: i
integer, parameter :: i8 = &
                     selected_int_kind( 2)
integer, parameter :: i16 = &
                     selected_int_kind( 4)
integer, parameter :: i32 = &
                     selected_int_kind( 9)
integer, parameter :: i64 = &
                     selected_int_kind(18)

integer (i8) :: i1
integer (i16) :: i2
integer (i32) :: i3
integer (i64) :: i4

print *, ' '
print *, ' integer kind support'
print *, ' kind          huge'
print *, ' '
```

```

print *, ' ', kind(i), ' ', huge(i)
print *, ''
print *, ' ', kind(i1), ' ', huge(i1)
print *, ' ', kind(i2), ' ', huge(i2)
print *, ' ', kind(i3), ' ', huge(i3)
print *, ' ', kind(i4), ' ', huge(i4)
print *, ''
end program ch0508

```

In this example we introduce parameters for each of the supported integer kind types.

Table 5.8 has details of the names we have given to the integer kind types as the kind type parameter has some information about the underlying representation.

Section 13.8.2.10 of the Fortran 2008 standard introduces the following named constants

- `int8`
- `int16`
- `int32`
- `int64`

where the values correspond to an integer type whose storage size expressed in bits is 8, 16, 32, and 64 respectively.

They are available via the `ISO_FORTRAN_ENV` intrinsic module.

As only one compiler supports the whole of the Fortran 2008 standard at the time of writing the book we will use `i8`, `i16`, `i32` and `i64` in the examples.

Table 5.9 has details of `huge` for each of the integer types.

As can be seen from the output for these three compilers they all support the same 4 integer kind types, namely 8 bit, 16 bit, 32 bit and 64 bit.

Run this program on whatever system you have access to and compare the output with the above examples.

Table 5.8 Integer kind type parameter name and integer value

Parameter	Integer type
<code>i8</code>	8 bit value
<code>i16</code>	16 bit value
<code>i32</code>	32 bit value
<code>i64</code>	64 bit value

Table 5.9 Integer kind and huge comparison

gfortran		Intel		Nag	
Kind	Huge	Kind	Huge	Kind	Huge
4	2147483647	4	2147483647	3	2147483647
1	127	1	127	1	127
2	32767	2	32767	2	32767
4	2147483647	4	2147483647	3	2147483647
8	9223372036854775807	8	9223372036854775807	4	9223372036854775807

5.19 Example 9: Using the Numeric Inquiry Functions with Real Types

```

program ch0509
  implicit none
! real arithmetic
!
! 32 and 64 bit reals are normally available.
! The IEEE format is as described below.
!
! 32 bit reals 8 bit exponent, 24 bit mantissa
! 64 bit reals 11 bit exponent, 53 bit mantissa
!
real :: r
integer, parameter :: sp = &
                     selected_real_kind( 6, 37)
integer, parameter :: dp = &
                     selected_real_kind(15, 307)
integer, parameter :: qp = &
                     selected_real_kind(30, 291)
real (sp) :: rsp
real (dp) :: rdp
real (qp) :: rqp

print *, '          ======'
print *, '          Real kind information'
print *, '          ======'
print *, ' kind number'
print *, '      ', kind(r), ' ', kind(rsp), ' ', &
         kind(rdp), ' ', kind(rqp)
print *, ' digits details'
print *, '      ', digits(r), ' ', digits(rsp), &
         digits(rdp)

```

```

      ', digits(rdp), ', digits(rqp)
print *, ' epsilon details'
print *, ', epsilon(r)
print *, ', epsilon(rsp)
print *, ', epsilon(rdp)
print *, ', epsilon(rqp)
print *, ' huge value'
print *, ', huge(r)
print *, ', huge(rsp)
print *, ', huge(rdp)
print *, ', huge(rqp)
print *, ' maxexponent value'
print *, ', maxexponent(r)
print *, ', maxexponent(rsp)
print *, ', maxexponent(rdp)
print *, ', maxexponent(rqp)
print *, ' minexponent value'
print *, ', minexponent(r)
print *, ', minexponent(rsp)
print *, ', minexponent(rdp)
print *, ', minexponent(rqp)
print *, ' precision details'
print *, ', precision(r), ', &
precision(rsp), ', precision(rdp), ', &
precision(rqp)
print *, ' radix details'
print *, ', radix(r), ', radix(rsp), &
', radix(rdp), ', radix(rqp)
print *, ' range details'
print *, ', range(r), ', range(rsp), &
', range(rdp), ', range(rqp)
print *, ' tiny details'
print *, ', tiny(r)
print *, ', tiny(rsp)
print *, ', tiny(rdp)
print *, ', tiny(rqp)
end program ch0509

```

In the above example we use a naming convention used by LAPACK95, which is a Fortran 95 interface to LAPACK.

For the real numeric kind types, where we have

- sp—single precision
- dp—double precision
- qp—quad precision

LAPACK is written in Fortran 90 and provides routines for solving systems of simultaneous linear equations, least-squares solutions of linear systems of equations, eigenvalue problems, and singular value problems. The associated matrix factorizations (LU, Cholesky, QR, SVD, Schur, generalized Schur) are also provided, as are related computations such as reordering of the Schur factorizations and estimating condition numbers. Dense and banded matrices are handled, but not general sparse matrices. In all areas, similar functionality is provided for real and complex matrices, in both single and double precision.

Their address is

<http://www.netlib.org/lapack95/>

Section 13.8.2.18 of the Fortran 2008 standard introduces `real32`, `real64`, and `real128`, where the values of these default integer scalar named constants shall be those of the kind type parameters that specify a `real` type whose storage size expressed in bits is 32, 64, and 128 respectively.

They are available via the `ISO_FORTRAN_ENV` intrinsic module.

As only one compiler supports the whole of the Fortran 2008 standard at the time of writing the book we will use `sp`, `dp` and `qp` in the examples.

Table 5.10 is a summary of the details of an extended type.

As can be seen all four compilers support the same 32 and 64 bit real types. They all support an extended 128 bit type, and Cray, gfortran and Intel are the same, but Nag is different.

Here are the details for `epsilon`, `huge` and `tiny` for these compilers.

Epsilon	
Cray	
1.92592994438723585305597794258492732E-34	
gfortran	
1.92592994438723585305597794258492732E-0034	
Intel	
1.925929944387235853055977942584927E-0034	

Table 5.10 Extended real type comparison

Function name	Cray	gfortran	Intel	Nag
<code>digits</code>	113	113	113	106
<code>maxexponent</code>	16384	16384	16384	1023
<code>minexponent</code>	-16381	-16381	-16381	-968
<code>precision</code>	33	33	33	31
<code>radix</code>	2	2	2	2
<code>range</code>	4931	4931	4931	291

```

Nag
2.46519032881566189191165177E-32
Huge
Cray
1.18973149535723176508575932662800702E+4932
gfortran
1.18973149535723176508575932662800702E+4932
Intel
1.189731495357231765085759326628007E+4932
Nag
8.98846567431157953864652595E+307
Tiny
Cray
3.3621031431120935062626778173217526E-4932
gfortran
3.36210314311209350626267781732175260E-4932
Intel
3.362103143112093506262677817321753E-4932
Nag
2.00416836000897277799610805E-292

```

Run this program on whatever system you have access to with your compiler(s) and compare the output with the above examples.

5.20 Example 10: Literal Real Constants in a Calculation

We have seen how to specify integer and real variables of different kind types but we also need to be able to do the same for literal constants. Examples of literal constants are 1.23, 5.643E-2 (default reals) and 400, -3 (default integers). To declare a literal constant to be of a different kind you need to specify the constant followed by an underscore and the kind type parameter. The following are two examples of 64 bit real literal constants: 1.23_dp, 5.643E-2_dp

You should be careful when writing programs using variables that are not the default kind making sure that any literal constants are also of the same kind. For example if you are using 64 bit real variables then make sure all your real literal constants are 64 bit. Here is a program where the variables and constants pi, area and r are 32 bit reals and pid, aread and rd are 64 bit reals. Try compiling and running the program. Do you get the same results as us?

```

program ch0510
implicit none
integer, parameter :: dp = &
selected_real_kind(15, 307)

```

```

real, parameter :: pi = 3.1415926535897931
real (dp), parameter :: pid = &
  3.1415926535897931_dp
real :: area, r = 2.0
real (dp) :: aread, rd = 2.0_dp

area = pi*r*r
aread = pid*rd*rd
print 100, r, rd
100 format ('r      = ', f22.18,/, 'rd      = ', &
f22.18)
print 110, area, aread
110 format ('area   = ', f22.18,/, 'aread   = ', &
f22.18,/, 16x, ' #####')
end program ch0510

```

Here is the Nag compiler output.

```
C:\fortran\fortran_book_edition3\chapter5>a
r      = 2.00000000000000000000
rd     = 2.00000000000000000000
area   = 12.566370964050292969
aread  = 12.566370614359172464
#####
```

Now edit the program and remove the `_dp` from the literal constant assigned to `pid`. You will see that the results for `area` (32 bit real) and `aread` (64 bit real) are the same. This is because the literal constant for `pid` reverts to a default 32 bit real.

```
C:\fortran\fortran_book_edition3\chapter5>a
r      = 2.00000000000000000000
rd     = 2.00000000000000000000
area   = 12.566370964050292969
aread  = 12.566370964050292969
#####
```

5.21 Summation and Finite Precision

The next example look at some of the problems that occur with the summation of floating point numbers. We will look at more summation problems in later chapters.

5.21.1 Example 11: Rounding Problem

Consider the following program.

```
program ch0511
    implicit none
    real :: x1 = 1.0
    real :: x2 = 0.1
    integer i

    print *, ' x1 = ', x1
    print *, ' x2 = ', x2
    do i = 1, 990
        x1 = x1 + x2
    end do
    print *, ' x1 = ', x1
end program ch0511
```

Here is the output from the Intel compiler.

```
x1 =      1.000000
x2 =      0.1000000
x1 =      99.99905
```

Here is the output from the Nag compiler.

```
x1 =      1.0000000
x2 =      0.1000000
x1 =      99.9990463
```

In both cases the summation is inexact, due to rounding errors.

5.22 Example 12: Binary Representation of Different Integer Kind Type Numbers

For those who wish to look at the internal binary representation of integer numbers with a variety of kinds, we have included the following program

`selected_int_kind(2)` means provide at least an integer representation with numbers between -10^2 and $+10^2$.

`selected_int_kind(4)` means provide at least an integer representation with numbers between -10^4 and $+10^4$.

`selected_int_kind(9)` means provide at least an integer representation with numbers between -10^9 and $+10^9$.

We use the `int` function to convert from one integer representation to another.

We use the logical function `btest` to determine whether the binary value at that position within the number is a zero or a one, i.e., if the bit is set.

`i_in_bits` is a character string that holds a direct mapping from the internal binary form of the integer and a text string that prints as a sequence of zeros or ones:

```

program ch0512
!
! use the bit functions in Fortran to write out
! a
! 32 bit integer number as a sequence of
! zeros and ones
!
implicit none
integer :: j
integer :: i
integer, parameter :: i8 = &
                     selected_int_kind( 2 )
integer, parameter :: i16 = &
                     selected_int_kind( 4 )
integer, parameter :: i32 = &
                     selected_int_kind( 9 )

integer (i8) :: i1
integer (i16) :: i2
integer (i32) :: i3
character (len=32) :: i_in_bits

print *, ' type in an integer '
read *, i
i1 = int(i, kind(2))
i2 = int(i, kind(4))
i3 = int(i, kind(9))
i_in_bits = ' '
do j = 0, 7
  if (btest(i1,j)) then
    i_in_bits(8-j:8-j) = '1'
  else
    i_in_bits(8-j:8-j) = '0'
  end if
end do
print *, '           1           2           3'

```

```

print *, '12345678901234567890123456789012'
print *, i1
print *, i_in_bits
do j = 0, 15
  if (btest(i2,j)) then
    i_in_bits(16-j:16-j) = '1'
  else
    i_in_bits(16-j:16-j) = '0'
  end if
end do
print *, i2
print *, i_in_bits
do j = 0, 31
  if (btest(i3,j)) then
    i_in_bits(32-j:32-j) = '1'
  else
    i_in_bits(32-j:32-j) = '0'
  end if
end do
print *, i3
print *, i_in_bits
end program ch0512

```

The do loop indices follow the convention of an 8-bit quantity starting at bit 0 and ending at bit 7, 16-bit quantities starting at 0 and ending at 15, etc.

The numbers written out follow the conventional mathematical notation of having the least significant quantity at the right-hand end of the digit sequence, i.e., with 127 in decimal we have $1 * 100, 2 * 10$ and $7 * 1$, so 00100001 in binary means $1 * 32 + 1 * 1$ decimal.

Try running this program on the system you are using. Does it produce the results you expect? Experiment with a variety of numbers. Try at least the following 0, +1, -1, -128, 127, 128, -32768, 32767, 32768.

5.23 Example 13: Binary Representation of a Real Number

The following program is a simple variant of the previous one, but we now look at a floating point number:

```

program ch0513
!
! use the bit functions in Fortran to write out
! a
! 32 bit integer number equivalenced to a real

```

```

! using the transfer intrinsic as a sequence of
! zeros and ones
!
implicit none
integer :: i, j
character (len=32) :: i_in_bits = ''
real :: x = 1.0

print *, '          1          2          3'
print *, '12345678901234567890123456789012'
print *, i_in_bits
i = transfer(x, i)
do j = 0, 31
  if (bttest(i,j)) then
    i_in_bits(32-j:32-j) = '1'
  else
    i_in_bits(32-j:32-j) = '0'
  end if
end do
print *, x
print *, i_in_bits
end program ch0513

```

We use the intrinsic function `transfer` to help out here. The `bttest` intrinsic takes an integer argument, so we need to copy the bit pattern of the real number into an integer variable.

5.24 Example 14: Initialisation of Physical Constants, Version 1

This is the first of three examples that uses the physical constant data in an earlier table to initialise parameters in a Fortran program.

```

program ch0514
  implicit none
  real, parameter :: atomic_mass_constant = &
    1.660538921*10**(-27)
  real, parameter :: avogadro_constant = &
    6.02214129*10**23
  real, parameter :: boltzmann_constant = &
    1.3806488*10**(-23)

```

```

real, parameter :: electron_mass = &
  9.10938291* 10**(-31)
real, parameter :: elementary_charge = &
  1.602176565*10**(-19)
real, parameter :: proton_mass = &
  1.672621777* 10**(-27)
real, parameter :: speed_of_light_in_vacuum = &
  299792458
real, parameter :: &
  newtonian_constant_of_gravitation = &
  6.67384* 10**(-11)

print *, atomic_mass_constant
print *, avogadro_constant
print *, boltzmann_constant
print *, electron_mass
print *, elementary_charge
print *, proton_mass
print *, speed_of_light_in_vacuum
print *, newtonian_constant_of_gravitation
end program ch0514

```

Here is the output from the Intel compiler.

```

0.0000000E+00
1.2066952E+18
0.0000000E+00
0.0000000E+00
0.0000000E+00
0.0000000E+00
0.0000000E+00
2.9979245E+08
0.0000000E+00

```

Here is the output from the Nag compiler.

```

nagfor ch0514.f90
NAG Fortran Compiler
Error: ch0514.f90, line 6:
Integer overflow for exponentiation 10**23
Errors in declarations,
no further processing for CH0514
[NAG Fortran Compiler error termination, 1 error]

```

5.25 Example 15: Initialisation of Physical Constants, Version 2

This is the second of three examples that uses the physical constant data in an earlier table to initialise parameters in a Fortran program.

```
program ch0515
    implicit none
    real, parameter :: atomic_mass_constant = &
        1.660538921e-27
    real, parameter :: avogadro_constant = &
        6.02214129e23
    real, parameter :: boltzmann_constant = &
        1.3806488e-23
    real, parameter :: electron_mass = &
        9.10938291e-31
    real, parameter :: elementary_charge = &
        1.602176565e-19
    real, parameter :: proton_mass = &
        1.672621777e-27
    real, parameter :: speed_of_light_in_vacuum = &
        299792458
    real, parameter :: &
        newtonian_constant_of_gravitation = &
        6.67384e-11

    print *, atomic_mass_constant
    print *, avogadro_constant
    print *, boltzmann_constant
    print *, electron_mass
    print *, elementary_charge
    print *, proton_mass
    print *, speed_of_light_in_vacuum
    print *, newtonian_constant_of_gravitation
end program ch0515
```

5.26 Example 16: Initialisation of Physical Constants, Version 3

This is the third of three examples that uses the physical constant data in an earlier table to initialise parameters in a Fortran program.

```

program ch0516
    implicit none
    real, parameter :: atomic_mass_constant = &
        1.660538921*10.0**(-27)
    real, parameter :: avogadro_constant = &
        6.02214129*10.0**23
    real, parameter :: boltzmann_constant = &
        1.3806488*10.0**(-23)
    real, parameter :: electron_mass = &
        9.10938291* 10.0**(-31)
    real, parameter :: elementary_charge = &
        1.602176565*10.0**(-19)
    real, parameter :: proton_mass = &
        1.672621777* 10.0**(-27)
    real, parameter :: speed_of_light_in_vacuum = &
        299792458
    real, parameter :: &
        newtonian_constant_of_gravitation = &
        6.67384* 10.0**(-11)

    print *, atomic_mass_constant
    print *, avogadro_constant
    print *, boltzmann_constant
    print *, electron_mass
    print *, elementary_charge
    print *, proton_mass
    print *, speed_of_light_in_vacuum
    print *, newtonian_constant_of_gravitation
end program ch0516

```

5.27 Summary of How to Select the Appropriate Kind Type

To write programs that will perform arithmetically in a similar fashion on a variety of hardware requires an understanding of:

- The integer data representation model and in practice the word size of the various integer kind types.
- The real data representation model and in practice the word size of the various real kind types and the number of bits in both the mantissa and exponent.

Armed with this information we can then choose a kind type that will ensure minimal problems when moving from one platform to another. End of health warning!

5.28 Variable Status

Fortran has two concepts regarding the status of a variable: defined and undefined. If a program does not provide an initial value (in a type statement) for a variable then its status is said to be undefined. Consider the following code segment taken from the earlier example that calculated the sum and average of three numbers:

```
real :: n1, n2, n3, average=0.0, total=0.0
integer :: n = 3
```

In the above the variables average, total and n all have a defined status. However, n1, n2 and n3 are said to be undefined. The use of undefined values is implementation dependent and therefore not portable. Care must be taken when writing programs to ensure that your variables have a defined status wherever possible. We will look at this area again in subsequent chapters.

5.29 Fortran and the IEEE 754 Standard

The ISO TR 15580 introduced IEEE Arithmetic support to Fortran.

IEEE 754-2008 governs binary floating-point arithmetic. It specifies number formats, basic operations, conversions, and exceptional conditions. The 2008 edition superseded both the

- 754-1985

standard and the related

- IEEE 854-1987

which generalized 754-1985 to cover decimal arithmetic as well as binary. The first standard IEEE 754: 1985 covered binary floating point arithmetic. The later IEEE 754: 1987 standard added decimal arithmetic.

The latest version of the standard is ISO/IEC/IEEE 60559:2011.

A considerable amount of hardware now offers support for the IEEE 754 standard. The standard can be purchased from

http://www.iso.org/iso/iso_catalogue/

The following is a useful site.

<http://grouper.ieee.org/groups/754/>

There are quite a lot of good links.

There is a separate chapter in the book on IEEE arithmetic and Fortran.

5.30 Summary

The following are some practical rules and guidelines:

- Learn the rules for the evaluation of arithmetic expressions.
- Break expressions down where necessary to ensure that the expressions are evaluated in the way you want.
- Take care with truncation owing to integer division in an expression. Note that this will only be a problem where both parts of the division are integer.
- Take care with truncation owing to the assignment statement when there is an integer on the left-hand side of the statement, i.e., assigning a real into an integer variable.
- When you want to set up constants which will remain unchanged throughout the program, use the parameter attribute.
- Do not confuse precision and accuracy.
- Learn what the default kinds are for the numeric types you work with, what the maximum and minimum values and precision are for real data, and what the maximum and minimum are for integer data.
- You have been introduced to the use of several intrinsic functions.

Bibliography

Some understanding of floating point arithmetic and numerical analysis is essential for successful use of Fortran when programming. As Froberg says “numerical analysis is a science—computation is an art.” The separate chapter on IEEE arithmetic also has several references.

The following are some of the more accessible books available.

Burden R.L., Faires J.D., Numerical Analysis, Brooks Cole, 2010.

- The first section of the book covers some of the mathematical preliminaries including a review of calculus, roundoff errors and computer arithmetic, algorithms and convergence. They provide programs or software to solve the problems in C, Fortran, Maple, Mathematica, Matlab and Pascal.

Froberg C.E., Introduction to Numerical Analysis, Addison-Wesley, 1969.

- The short chapter on numerical computation is well worth a read; it covers some of the problems of conversion between number bases and some of the errors that are introduced when we compute numerically. The Samuel Johnson quote owes its inclusion to Froberg!

Goldberg D., What Every Computer Scientist Should Know About Floating-Point Arithmetic, Computing Surveys, March 1991.

- The paper is a very good introduction to floating point arithmetic. It is available on line.

Higham Nicholas J., Accuracy and Stability of Numerical Algorithms, SIAM, 2002.

- The first four chapters cover finite precision computation, floating point arithmetic, error analysis and summation methods.

Knuth D., Seminumerical Algorithms, Addison-Wesley, 1969.

- A more thorough and mathematical coverage than Wakerly. The chapter on positional number systems provides a very comprehensive historical coverage of the subject. As Knuth points out the floating point representation for numbers is very old, and is first documented around 1750 B.C. by Babylonian mathematicians. Very interesting and worthwhile reading.

Wakerly J.F., Microcomputer Architecture and programming, Wiley, 1981.

- The chapter on number systems and arithmetic is surprisingly easy. There is a coverage of positional number systems, octal and hexadecimal number system conversions, addition and subtraction of nondecimal numbers, representation of negative numbers, two's complement addition and subtraction, one's complement addition and subtraction, binary multiplication, binary division, bcd or binary coded decimal representation and fixed and floating point representations. There is also coverage of a number of specific hardware platforms, including DEC PDP-11, Motorola 68000, Zilog Z8000, TI 9900, Motorola 6809 and Intel 8086. A little old but quite interesting nevertheless.

5.31 Problems

5.1 Compile and run examples 1 through 3 in this chapter.

5.2 Have another look at example 4. Compile and run it. It will generate an error on some systems. Can you see where the error is?

5.3 Write a program to calculate the period of a pendulum. This is given mathematically as

$$t = 2\pi \sqrt{\text{length}/9.81}$$

use the following Fortran arithmetic assignment statement:

```
t = 2 * pi * (length / 9.81) ** .5
```

The length `length` is in metres, and the time `t` in seconds, and `pi` was given a value earlier in this chapter.

Repeat the above using two other methods. Try a hand-held calculator and a spreadsheet. Do you get the same answers?

5.4 Base conversion.

In this chapter you have seen a brief coverage of base conversion. The following program illustrates some of the problems that can occur when going from base 10 to base 2 and back again. Which numbers will convert without loss?

```
program base_conversion
    implicit none
    real :: x1 = 1.0
    real :: x2 = 0.1
    real :: x3 = 0.01
    real :: x4 = 0.001
    real :: x5 = 0.0001

    print *, ' ', x1
    print *, ' ', x2
    print *, ' ', x3
    print *, ' ', x4
    print *, ' ', x5
end program base_conversion
```

Which do you think will provide the same number as originally entered?

5.5 Simple subtraction.

In this chapter we looked at representing floating point numbers in a finite number of bits.

Try the following program:

```
program subtract
    implicit none
    real :: a = 1.0002
    real :: b = 1.0001
    real :: c

    c = a - b
    print *, a
    print *, b
    print *, c
end program subtract
```

5.6 Expression equivalence.

We introduced some of the rules that apply in Fortran for expression evaluation. In mathematics the following is true:

$$x^2 - y^2 = (x * x - y * y) = (x - y) * (x + y)$$

Try the following program:

```
program expression_equivalence
!
! simple evaluation of x*x-y*y
```

```

! when x and y are similar
!
! we will evaluate in three ways.
!
implicit none
real :: x = 1.002
real :: y = 1.001
real :: t1, t2, t3, t4, t5

t1 = x - y
t2 = x + y
print *, t1
print *, t2
t3 = t1*t2
t4 = x**2 - y**2
t5 = x*x - y*y
print *, t3
print *, t4
print *, t5
end program expression_equivalence

```

Solve the problem with pencil and paper, calculator and Excel.

The last three examples show that you must be careful when using a computer to solve problems.

5.7 The following is a simple variant of ch0504. In this case we initialise light year in an assignment statement. Do you think you will get the same results as from running the earlier example?

```

program ch0504p
implicit none
real :: light_minute, distance, elapse
integer :: minute, second
real :: light_year
! Light_year : Distance travelled by light
! in one year in km
! Light_minute : Distance travelled by light
! in one minute in km
! Distance : Distance from sun to earth in km
! Elapse : Time taken to travel a
! distance (Distance) in minutes
! Minute : integer number part of elapse
! Second : integer number of seconds
! equivalent to fractional part of elapse
!
```

```
light_year = 9.46*10**12
light_minute = light_year/(365.25*24.0*60.0)
distance = 150.0*10**6
elapse = distance/light_minute
minute = elapse
second = (elapse-minute)*60
print *, ' Light takes ', minute, ' Minutes'
print *, ' ', second, ' Seconds'
print *, ' To reach the earth from sun'
end program ch0504p
```

- 5.8** Many communications satellites follow a geosynchronous orbit, some 35,870 km above the Earth's surface. What is the time lag incurred in using one such satellite for a telephone conversation?

This will also be the time delay for satellite based internet access.

You can use the above program as the basis for this problem. You will need to calculate the time in seconds (rather than minutes and seconds), as the distance is much smaller.

- 5.9** The Moon is about 384,400 km from the Earth on average. What implications does this have for control of experiments on the Moon? What is the time lag?

Chapter 6

Arrays 1: Some Fundamentals

Thy gifts, thy tables, are within my brain Full charactered with lasting memory.

William Shakespeare, The Sonnets
Here, take this book, and peruse it well: The iterating of these lines brings gold.

Christopher Marlowe, The Tragical History of Doctor Faustus

Aims

The aims of the chapter are to introduce the fundamental concepts of arrays and do loops, in particular:

- To introduce the idea of tables of data and some of the formal terms used to describe them:
 - Array.
 - Vector.
 - List and linear list.
- To discuss the array as a random access structure where any element can be accessed as readily as any other and to note that the data in an array are all of the same type.
- To introduce the twin concepts of data structure and corresponding control structure.
- To introduce the statements necessary in Fortran to support and manipulate these data structures.

6.1 Tables of Data

Consider the examples below.

6.1.1 Telephone Directory

A telephone directory consists of the following kinds of entries:

Name	Address	Number
Adcroft A.	61 Connaught Road, Roath, Cardiff	223309
Beale K.	14 Airedale Road, Balham	745 9870
Blunt R.U.	81 Stanlake Road, Shepherds Bush	674 4546
...		
...		
...		
Sims Tony	99 Andover Road, Twickenham	898 7330

This structure can be considered in a variety of ways, but perhaps the most common is to regard it as a table of data, where there are three columns and as many rows as there are entries in the telephone directory.

Consider now the way we extract information from this table. We would scan the name column looking for the name we are interested in, and then read along the row looking for either the address or telephone number, i.e., we are using the name to look up the item of interest.

6.1.2 Book Catalogue

A catalogue could contain:

Author(s)	Title	Publisher
Carroll L.	Alice through the looking glass	Penguin
Steinbeck J.	Sweet Thursday	Penguin
Wirth N.	Algorithms plus data structures = programs	Prentice-Hall

Again, this can be regarded as a table of data, having three columns and many rows. We would follow the same procedure as with the telephone directory to extract the information. We would use the Author to look up what books are available.

6.1.3 Examination Marks or Results

This could consist of:

Name	Physics	Maths	Biology	History	English	French
Fowler L.	50	47	28	89	30	46
Barron L.W.	37	67	34	65	68	98
Warren J.	25	45	26	48	10	36
Mallory D.	89	56	33	45	30	65
Codd S.	68	78	38	76	98	65

This can again be regarded as a table of data. This example has seven columns and five rows. We would again look up information by using the Name.

6.1.4 Monthly Rainfall

The following data are a sample of monthly average rainfall for London in inches:

Month	Rainfall
January	3.1
February	2.0
March	2.4
April	2.1
May	2.2
June	2.2
July	1.8
August	2.2
September	2.7
October	2.9
November	3.1
December	3.1

In this table there are two columns and twelve rows. To find out what the rainfall was in July, we scan the table for July in the Month column and locate the value in the same row, i.e., the rainfall figure for July.

These are just some of the many examples of problems where the data that are being considered have a tabular structure. Most general purpose languages therefore have mechanisms for dealing with this kind of structure. Some of the special names given to these structures include:

- Linear list.
- List.
- Vector.
- Array.

The term used most often here, and in the majority of books on Fortran programming, is array.

6.2 Arrays in Fortran

There are three key things to consider here:

- The ability to refer to a set or group of items by a single name.
- The ability to refer to individual items or members of this set, i.e., look them up.
- The choice of a control structure that allows easy manipulation of this set or array.

6.2.1 *The Dimension Attribute*

The dimension attribute defines a variable to be an array. This satisfies the first requirement of being able to refer to a set of items by a single name. Some examples are given below:

```
real , dimension(1:100) :: wages  
integer , dimension(1:10000) :: sample
```

For the variable `wages` it is of type `real` and an array of dimension or size 100, i.e., the variable array `wages` can hold up to 100 real items.

For the variable `sample` it is of type `integer` and an array of dimension or size 10,000, i.e., the variable `sample` can hold up to 10,000 integer items.

6.2.2 *An Index*

An index enables you to refer to or select individual elements of the array. In the telephone directory, book catalogue, exam marks table and monthly rainfall examples we used the name to index or look up the items of interest. We will give concrete Fortran code for this in the example of monthly rain fall.

6.2.3 *Control Structure*

The statement that is generally used to manipulate the elements of an array is the `do` statement. It is typical to have several statements controlled by the `do` statement, and the block of repeated statements is often called a `do loop`. Let us look at two complete programs that highlight the above.

6.3 Example 1: Monthly Rainfall

Let us look at this earlier example in more depth now. Consider the following:

Month	Associated integer representation	Array and index	Rainfall value
January	1	Rainfall (1)	3.1
February	2	Rainfall (2)	2.0
March	3	Rainfall (3)	2.4
April	4	Rainfall (4)	2.1
May	5	Rainfall (5)	2.2
June	6	Rainfall (6)	2.2
July	7	Rainfall (7)	1.8
August	8	Rainfall (8)	2.2
September	9	Rainfall (9)	2.7
October	10	Rainfall (10)	2.9
November	11	Rainfall (11)	3.1
December	12	Rainfall (12)	3.1

Most of you should be familiar with the idea of the use of an integer as an alternate way of representing a month, e.g., in a date expressed as 1/3/2000, for 1st March 2000 (Anglicised style) or January 3rd (Americanised style). Fortran, in common with other programming languages, only allows the use of integers as an index into an array. Thus when we write a program to use arrays we have to map between whatever construct we use in everyday life as our index (names in our examples of telephone directory, book catalogue, and exam marks) to an integer representation in Fortran. The following is an example of an assignment statement showing the use of an index:

```
rainfall(1)=3.1
```

We saw earlier that we could use the dimension attribute to indicate that a variable was an array. In the above example Fortran statement our array is called `rainfall`. In this statement we are assigning the value 3.1 to the first element of the array; i.e., the rainfall for the month of January is 3.1. We use the index 1 to represent the first month. Consider the following statement:

```
summeraverage = (rainfall(6) + rainfall(7) + &
                 rainfall(8))/3
```

This statement says take the values of the rainfall for June, July and August, add them up and then divide by 3, and assign the result to the variable `summeraverage`, thus providing us with the rainfall average for the three summer months—Northern Hemisphere of course!

The following program reads in the 12 monthly values from the terminal, computes the sum and average for the year, and prints the average out.

```

program ch0601
    implicit none
    real :: total = 0.0, average = 0.0
    real, dimension (1:12) :: rainfall
    integer :: month

    print *, ' type in the rainfall values'
    print *, ' one per line'
    do month = 1, 12
        read *, rainfall(month)
    end do
    do month = 1, 12
        total = total + rainfall(month)
    end do
    average = total/12
    print *, ' Average monthly rainfall was'
    print *, average
end program ch0601

```

`rainfall` is the array name. The variable `month` in brackets is the index. It takes on values from 1 to 12 inclusive, and is used to pick out or select elements of the array. The index is thus a variable and this permits dynamic manipulation of the array at run time. The general form of the `do` statement is

```
do counter = start, end, increment
```

The block of statements that form the loop is contained between the `do` statement, which marks the beginning of the block or loop, and the `enddo` statement, which marks the end of the block or loop.

In this program, the `do` loops take the form:

```

do month=1,12      start
    ...
    body
enddo            end

```

The body of the loop in the program above has been indented. This is not required by Fortran. However it is good practice and will make programs easier to follow.

The number of times that the `do` loop is executed is governed by the last part of the `do` statement, i.e., by the

```
counter = start, end, increment
```

`start` as it implies, is the initial value which the counter (or index, or control variable) takes. Each time the loop is executed, the value of the counter will be increased by the value of `increment`, until the value of `end` is reached. If `increment` is omitted, it is assumed to be 1. No other element of the `do` statement may be omitted. In order to execute the statements within the loop (the body) it must be possible to reach `end` from `start`. Thus zero is an illegal value of `increment`. In the event that

it is not possible to reach end, the loop will not be executed and control will pass to the statement after the end of the loop.

In the example above, both loops would be executed 12 times. In both cases, the first time around the loop the variable month would have the value 1, the second time around the loop the variable month would have the value 2, etc., and the last time around the loop month would have the value 12.

A summation:

$$\sum_{i=1}^{i=12} x_i$$

is often expressed in Fortran as a loop as in this example:

```
do month=1,12
    total = total + rainfall(month)
enddo
```

6.4 Possible Missing Data

The rainfall data in this example has been taken from the UK Met Office site. Visit

<http://www.metoffice.gov.uk/climate/uk/stationdata>

to see where some of the stations are. One of us was born in Wales, the other in Yorkshire so we have chosen stations accordingly. The urls have been split over two lines when too long.

The following is one of the mid Wales stations:

<http://www.metoffice.gov.uk/climate/>
[uk/stationdata/cwmystwythdata.txt](http://www.metoffice.gov.uk/stationdata/cwmystwythdata.txt)

Here is a sample of data from this site for 1965.

YYYY	mm	tmax degC	tmin degC	af days	rain mm	sun hours
1965	1	4.8	-0.2	17	214.8	38.8
1965	2	4.4	-1.2	17	25.1	33.3
1965	3	7.7	0.5	11	93.7	114.6
1965	4	9.9	2.4	9	146.9	134.3
1965	5	13.5	5.8	3	108.7	120.8
1965	6	15.9	8.3	0	115.0	140.4
1965	7	15.3	8.6	0	105.0	106.4
1965	8	---	9.6	0	155.7	140.2
1965	9	---	6.6	0	245.7	70.6
1965	10	13.5	7.0	0	92.5	134.3

1965	11	6.2	0.8	11	115.7	73.8
1965	12	7.0	1.6	8	417.3	31.4

Wales is relatively wet for the UK!

The following station is Whitby:

[http://www.metoffice.gov.uk/climate/
uk/stationdata/whitbydata.txt](http://www.metoffice.gov.uk/climate/uk/stationdata/whitbydata.txt)

Here is a sample of the Whitby data.

yyyy	mm	tmax	tmin	af	rain	sun
		degC	degC	days	mm	hours
1968	1	6.9	1.7	12	24.4	
1968	2	4.3	-0.7	16	45.1	
1968	3	9.4	3.4	2	34.5	
1968	4	10.8	1.6	9	28.8	
1968	5	10.6	2.8	2	37.1	
1968	6	16.7	6.8	0	58.5	
1968	7	15.0	8.1	0	81.4	
1968	8	16.3	9.6	0	28.0	
1968	9	15.7	---	---	66.0	
1968	10	14.7	---	---	35.2	
1968	11	8.5	5.1	1	35.1	
1968	12	5.7	1.5	9	---	

Bram Stoker found some of his inspiration for Dracula after staying in the town.

If you look at the data for some of these stations you will notice that data is missing for some months.

How do you think you could cope with missing data in Fortran?

The SQL standard has the concept of nulls or missing values, and missing data in a statistics package is commonly flagged by an exceptional value e.g., -999.

We will look at using this data in Chap. 10.

6.5 Example 2: People's Weights and Setting the Array Size With a Parameter

In the table we have ten people, with their names as shown. We associate each name with a number—in this case we have ordered the names alphabetically, and the numbers therefore reflect their ordering. `weight` is the array name. The number in brackets is called the index and it is used to pick out or select elements of the array. The table is read as the first element of the array `weight` has the value 85, the second element has the value 76, etc.

Person	Associated integer representation	Array and index	Associated value
Andy	1	Weight (1)	85
Barry	2	Weight (2)	76
Cathy	3	Weight (3)	85
Dawn	4	Weight (4)	90
Elaine	5	Weight (5)	69
Frank	6	Weight (6)	83
Gordon	7	Weight (7)	64
Hannah	8	Weight (8)	57
Ian	9	Weight (9)	65
Jatinda	10	Weight (10)	76

In the first example we so-called hard coded the number 12, which is the number of months, into the program. It occurred four times. Modifying the program to work with a different number of months would obviously be tedious and potentially error prone.

In this example we parameterise the size of the array and reduce the effort involved in modifying the program to work with a different number of people:

```

program ch0602
! The program reads up to number_of_people
! weights into the array Weight
! Variables used
! Weight, holds the weight of the people
! Person, an index into the array
! Total, total weight
! Average, average weight of the people
! Parameters used
! NumberOfPeople ,10 in this case.
! The weights are written out so that
! they can be checked
!
implicit none
integer, parameter :: number_of_people = 10
real :: total = 0.0, average = 0.0
integer :: person
real, dimension (1:number_of_people) :: weight

do person = 1, number_of_people
    print *, ' type in the weight for person ', &
    person
    read *, weight(person)
    total = total + weight(person)
end do

```

```

average = total/number_of_people
print *, ' The total of the weights is ', &
    total
print *, ' Average Weight is ', average
print *, ' ', number_of_people, &
    ' Weights were '
do person = 1, number_of_people
    print *, weight(person)
end do
end program ch0602

```

6.6 Summary

The dimension attribute declares a variable to be an array, and must come at the start of a program unit, with other declarative statements. It has two forms and examples of both of them are given below. In the first case we explicitly specify the upper and lower:

```
real , dimension(1:number_of_people) :: weight
```

In the second case the lower limit defaults to 1

```
real , dimension(number_of_people) :: weight
```

The latter form will be seen in legacy code, especially Fortran 77 code suites.

The parameter attribute declares a variable to have a fixed value that cannot be changed during the execution of a program. In our example above note that this statement occurs before the other declarative statements that depend on it. Table 6.1 summarises Fortran's statement ordering.

Table 6.1 Fortran statement ordering

Program	First statement	
integer	Declarative	In any order and the dimension and parameter attributes are added here
real		
character		
Arithmetic assignment	Executable	In any order
print *		
read *		
do		
enddo		
end program	Last statement	

We choose individual members using an index, and these are always of `integer` type in Fortran.

The do loop is a very convenient control structure for manipulating arrays, and we use indentation to clearly identify loops.

6.7 Problems

6.1 Compile and run example 1 from this chapter. If you live in the UK visit the Met Office site mentioned earlier and choose a site near you, and a year of interest, making sure that the data set is complete for that year.

If you don't live in the UK is there a site similar to the Met Office site that has data for the country you are from?

6.2 Compile and run program 2.

6.3 Using a do loop and an array rewrite the program which calculated the average of three numbers to ten.

6.4 Modify the program that calculates the total and average of people's weights to additionally read in their heights and calculate the total and average of their heights. Use the data given below, which have been taken from a group of first year undergraduates:

Height	Weight
1.85	85
1.80	76
1.85	85
1.70	90
1.75	69
1.67	83
1.55	64
1.63	57
1.79	65
1.78	76

6.5 Your body mass index is given by your weight (in kilos) divided by your height (in metres) squared. Calculate and print out the BMI for each person.

Grades of obesity according to Garrow as follows:

- Grade 0 (desirable) 20–24.9
- Grade 1 (overweight) 25–29.9
- Grade 2 (obese) 30–40
- Grade 3 (morbidly obese) >40
- Ideal BMI range,

- Men, Range 20.1–25 kg/m²
- Women, Range 18.7–23.8 kg/m²

6.6 When working on either a UNIX system or a PC in a DOS box it is possible to use the following characters to enable you to read data from a file or write output to a file when running your program:

character	Meaning
<	read from file
>	write to file

On a typical UNIX system we could use

```
a.out < data.txt > results.txt
```

to read the data from the file called data.txt and write the output to a file called results.txt.

On a PC in a DOS box the equivalent would be

```
program.exe < data.txt > results.txt
```

This is a quick and dirty way of developing programs that do simple I/O; we don't have to keep typing in the data and we also have a record of the behaviour of the program. Rerun the program that prints out the BMI values to write the output to a file called results.txt. Examine this file in an editor.

6.7 Modify the program that read in your name to read in ten names. Use an array and a do loop. When you have read the names into the array write them out in reverse order on separate lines.

Hint: Look at the formal syntax of the do statement.

6.8 Modify the rainfall program (which assumes that the measurement is in inches) to convert the values to centimetres. One inch equals 2.54 cm. Print out the two sets of values as a table.

Hint: use a second array to hold the metric measurements.

6.9 Combine the programs that read in and calculate the average weight with the one that reads in peoples names. The program should read the weights into one array and the names into another. Allow 20 characters for the length of a name. Print out a table linking names and weights.

6.10 In an earlier chapter we used the following formula to calculate the period of a pendulum:

```
t = 2 * pi * (length / 9.81) ** .5
```

write a program that uses a do loop to make the length go from 1 to 10 metres in 1-metre increments.

Produce a table with two columns, the first of lengths and the second of periods.

Chapter 7

Arrays 2: Further Examples

*Sir, In your otherwise beautiful poem (*The Vision of Sin*) there is a verse which reads Every moment dies a man, every moment one is born. Obviously this cannot be true and I suggest that in the next edition you have it read Every moment dies a man, every moment 1 1/16 is born. Even this value is slightly in error but should be sufficiently accurate for poetry.*

Charles Babbage in a letter to Lord Tennyson

Aims

The aims of the chapter are to extend the concepts introduced in the previous chapter and in particular:

- To set an array size at run time—allocatable arrays.
- To introduce the idea of an array with more than one dimension and the corresponding control structure to permit easy manipulation of higher-dimensioned arrays.
- To introduce an extended form of the dimension attribute declaration, and the corresponding alternative form to the do statement, to manipulate the array in this new form.
- To introduce the do loop as a mechanism for the control of repetition in general, not just for manipulating arrays.
- To formally define the block do syntax.

7.1 Varying the Array Size at Run Time

The earlier examples set the array size in the following two ways:

- Explicitly using a numeric constant
- Implicitly using a parameterised variable

In both cases we knew the size of the array at the time we compiled the program. We may not know the size of the array at compile time and Fortran provides the allocatable attribute to accommodate this kind of problem.

7.1.1 Example 1: Allocatable Arrays

Consider the following example.

```
program ch0701
!
! This program is a simple variant of ch0602.
! The array is now allocatable
! and the user is prompted for the
! number of people at run time.
!
implicit none
integer :: number_of_people
real :: total = 0.0, average = 0.0
integer :: person
real, dimension (:), allocatable :: weight

print *, ' How many people?'
read *, number_of_people
allocate (weight(1:number_of_people))
do person = 1, number_of_people
    print *, ' type in the weight for person ', &
    person
    read *, weight(person)
    total = total + weight(person)
end do
average = total/number_of_people
print *, ' The total of the weights is ', &
total
print *, ' Average Weight is ', average
print *, ' ', number_of_people, &
' Weights were '
do person = 1, number_of_people
    print *, weight(person)
end do
end program ch0701
```

The first statement of interest is the type declaration with the dimension and allocatable attributes, e.g.,

```
real , dimension(:) , allocatable :: weight
```

The second is the `allocate` statement

```
allocate(weight(1:number_of_people))
```

where the value of the variable `number_of_people` is not known until run time. This is known in Fortran as a deferred shape array.

7.2 Higher-Dimension Arrays

There are many instances where it is necessary to have arrays with more than one dimension. Consider the examples below.

7.2.1 Example 2: Two Dimensional Arrays and a Map

Consider the representation of the height of an area of land expressed as a two dimensional table of numbers e.g., we may have some information represented in a simple table as follows:

		Longitude		
		1	2	3
Latitude		1	2	3
1		10.0	40.0	70.0
2		20.0	50.0	80.0
3		30.0	60.0	90.0

The values in the array are the heights above sea level. The example is obviously artificial, but it does highlight the concepts involved. For those who have forgotten their geography, lines of latitude run east–west (the equator is a line of latitude) and lines of longitude run north–south (they go through the poles and are all of the same length). In the above table therefore the latitude values are ordered by row and the longitude values are ordered by column.

A program to manipulate this data structure would involve something like the following:

```
program ch0702
! Variables used
! Height - used to hold the heights above sea
! level
! Long - used to represent the longitude
! Lat - used to represent the latitude
! both restricted to integer values.
! Correct - holds the correction factor
implicit none
```

```

integer, parameter :: n = 3
integer :: lat, long
real, dimension (1:n, 1:n) :: height
real, parameter :: correct = 10.0

do lat = 1, n
    do long = 1, n
        print *, ' type in value at ', lat, ' ', &
                  long
        read *, height(lat, long)
    end do
end do
do lat = 1, n
    do long = 1, n
        height(lat, long) = height(lat, long) + &
                  correct
    end do
end do
print *, ' Corrected data is '
do lat = 1, n
    do long = 1, n
        print *, height(lat, long)
    end do
end do
end program ch0702

```

Note the way in which indentation has been used to highlight the structure in this example. Note also the use of a textual prompt to highlight which data value is expected. Running the program highlights some of the problems with the simple i/o used in the example above. We will address this issue in the next example.

The inner loop is said to be nested within the outer one. It is very common to encounter problems where nesting is a natural way to express the solution. Nesting is permitted to any depth. Here is an example of a valid nested do loop:

```

do      ! Start of outer loop
    do      ! Start of inner loop
        .
        .
        .
    enddo    ! End of inner loop
enddo    ! End of outer loop

```

This example introduces the concept of two indices, and can be thought of as a row and column data structure.

7.2.2 Example 3: Sensible Tabular Output

The first example had the values printed in a format that wasn't very easy to work with. In this example we introduce a so-called implied do loop, which enables us to produce neat and humanly comprehensible output:

```
program ch0703
! Variables used
! Height - used to hold the heights above sea
! level
! Long - used to represent the longitude
! Lat - used to represent the latitude
! both restricted to integer values.
implicit none
integer, parameter :: n = 3
integer :: lat, long
real, dimension (1:n, 1:n) :: height
real, parameter :: correct = 10.0

do lat = 1, n
    do long = 1, n
        read *, height(lat, long)
        height(lat, long) = height(lat, long) + &
            correct
    end do
end do
do lat = 1, n
    print *, (height(lat,long), long=1, n)
end do
end program ch0703
```

The key statement in this example is

```
print * , (height(lat,long),long=1,n)
```

This is called an implied do loop, as the `longitude` variable takes on values from 1 through 3 and will write out all three values on one line.

We will see other examples of this statement as we go on.

7.2.3 Example 4: Average of Three Sets of Values

This example extends the previous one. Now we have three sets of measurements and we are interested in calculating the average of these three sets. The two new data sets are:

9.5	39.5	69.5
19.5	49.5	79.5
29.5	59.5	89.5

and

10.5	40.5	70.5
20.5	50.5	80.5
30.5	60.5	90.5

and we have chosen the values to enable us to quickly check that the calculations for the averages are correct.

This program also uses implied do loops to read the data, as data in files are generally tabular:

```

program ch0704
! Variables used
! h1,h2,h3
! used to hold the heights above sea level
! h4
! used to hold the average of the above
! Long - used to represent the longitude
! Lat - used to represent the latitude
! both restricted to integer values.
implicit none
integer, parameter :: n = 3
integer :: lat, long
real, dimension (1:n, 1:n) :: h1, h2, h3, h4

do lat = 1, n
  read *, (h1(lat,long), long=1, n)
end do
do lat = 1, n
  read *, (h2(lat,long), long=1, n)
end do
do lat = 1, n
  read *, (h3(lat,long), long=1, n)
end do
do lat = 1, n

```

```

      do long = 1, n
        h4(lat, long) = (h1(lat,long)+h2(lat,long) &
                          +h3(lat,long)) /n
      end do
    end do
    do lat = 1, n
      print *, (h4(lat,long), long=1, n)
    end do
  end program ch0704

```

The original data was accurate to three significant figures. The output from the above has spurious additional accuracy. We will look at how to correct this in the later chapter on output.

7.2.4 Example 5: Booking Arrangements in a Theatre or Cinema

A theatre or cinema consists of rows and columns of seats. In a large cinema or a typical theatre there would also be more than one level or storey. Thus, a program to represent and manipulate this structure would probably have a 2-d or 3-d array. Consider the following program extract:

```

program ch0705
  implicit none
  integer, parameter :: nr = 5
  integer, parameter :: nc = 10
  integer, parameter :: nf = 3
  integer :: row, column, floor
  character *1, dimension (1:nr, 1:nc, 1:nf) :: &
    seats = ' '

```



```

  do floor = 1, nf
    do row = 1, nr
      read *, (seats(row,column,floor), column=1 &
                , nc)
    end do
  end do
  print *, ' Seat plan is'
  do floor = 1, nf
    print *, ' Floor = ', floor
    do row = 1, nr
      print *, (seats(row,column,floor), column= &
                1, nc)
    end do
  end do

```

```

    end do
end do
end program ch0705

```

Note here the use of the term `parameter` in conjunction with the integer declaration. This is called an entity orientated declaration. An alternative to this is an attribute-orientated declaration, e.g.,

```

integer :: nr,nc,nf
parameter :: nr=5,nc=10,nf=3

```

and we will be using the entity-orientated declaration method throughout the rest of the book. This is our recommended method as you only have to look in one place to determine everything that you need to know about an entity.

7.3 Additional Forms of the Dimension Attribute and Do Loop Statement

7.3.1 Example 6: Voltage from -20 to +20 Volts

Consider the problem of an experiment where the independent variable voltage varies from -20 to $+20$ volts and the current is measured at 1-volt intervals. Fortran has a mechanism for handling this type of problem:

```

program ch0706
implicit none
real, dimension (-20:20) :: current
real :: resistance
integer :: voltage

print *, ' type in the resistance'
read *, resistance
do voltage = -20, 20
    current(voltage) = voltage/resistance
    print *, voltage, ', ', current(voltage)
end do
end program ch0706

```

We appreciate that, due to experimental error, the voltage will not have exact integer values. However, we are interested in representing and manipulating a set of values, and thus from the point of view of the problem solution and the program this is a reasonable assumption. There are several things to note.

This form of the dimension attribute

```
dimension(first:last)
```

is of considerable use when the problem has an effective index which does not start at 1.

There is a corresponding form of the do statement which allows processing of problems of this nature. This is shown in the above program. The general form of the do statement statement is therefore:

```
do counter=start, end, increment
```

where start, end and increment can be positive or negative. Note that zero is a legitimate value of the dimension limits and of a do loop index.

7.3.2 Example 7: Longitude from -180 to +180

Consider the problem of the production of a table linking time difference with longitude. The values of longitude will vary from -180 to +180 degrees, and the time will vary from +12 hours to -12 hours. A possible program segment is:

```
program ch0707
    implicit none
    real, dimension (-180:180) :: time = 0
    integer :: degree, strip
    real :: value

    do degree = -180, 165, 15
        value = degree/15.
        do strip = 0, 14
            time(degree+strip) = value
        end do
    end do
    do degree = -180, 180
        print *, degree, ' ', time(degree)
    end do
end program ch0707
```

7.3.3 Notes

The values of the time are not being calculated at every degree interval.

The variable `time` is a real variable. It would be possible to arrange for the time to be an integer by expressing it in either minutes or seconds.

This example takes no account of all the wiggly bits separating time zones or of British Summer Time or Daylight Saving Time.

What changes would you make to the program to accommodate +180? What is the time at -180 and +180?

7.4 The Do Loop and Straight Repetition

7.4.1 Example 8: Table of Liquid Conversion Measurements

Consider the production of a table of liquid measurements. The independent variable is the litre value; the gallon and US gallon are the dependent variables. Strictly speaking, a program to do this does not have to have an array, i.e., the do loop can be used to control the repetition of a set of statements that make no reference to an array. The following shows a complete but simple conversion program:

```
program ch0708
    implicit none
!
! 1 us gallon = 3.7854118 litres
! 1 uk gallon = 4.545 litres
!
integer :: litre
real :: gallon, usgallon

do litre = 1, 10
    gallon = litre/4.545
    usgallon = litre/3.7854118
    print *, litre, ' ', gallon, ' ', usgallon
end do
end program ch0708
```

Note here that the do statement has been used only to control the repetition of a block of statements—there are no arrays at all in this program.

This is the other use of the do statement. The do loop thus has two functions—its use with arrays as a control structure and its use solely for the repetition of a block of statements.

7.4.2 Example 9: Means and Standard Deviations

In the calculation of the mean and standard deviation of a list of numbers, we can use the following formulae. It is not actually necessary to store the values, nor to

accumulate the sum of the values and their squares. In the first case, we would possibly require a large array, whereas in the second, it is conceivable that the accumulated values (especially of the squares) might be too large for the machine. The following example uses an updating technique which avoids these problems, but is still accurate. The do loop is simply a control structure to ensure that all the values are read in, with the index being used in the calculation of the updates:

```
program ch0709
! variables used are
! mean - for the running mean
! ssq - the running corrected sum of squares
! x - input values for which
! mean and sd required
! w - local work variable
! sd - standard deviation
! r - another work variable
implicit none
real :: mean = 0.0, ssq = 0.0, x, w, sd, r
integer :: i, n

print *, ' enter the number of readings'
read *, n
print *, ' enter the ', n, &
' values, one per line'
do i = 1, n
  read *, x
  w = x - mean
  r = i - 1
  mean = (r*mean+x)/i
  ssq = ssq + w*w*r/i
end do
sd = (ssq/r)**0.5
print *, ' mean is ', mean
print *, ' standard deviation is ', sd
end program ch0709
```

7.5 Summary

Arrays can have up to fifteen dimensions.

Do loops may be nested, but they must not overlap.

The dimension attribute allows limits to be specified for a block of information which is to be treated in a common way. The limits must be integer, and the second limit must exceed the first, e.g.,

```
real , dimension(-123:-10) :: list
real , dimension(0:100,0:100) :: surface
real , dimension(1:100) :: value
```

The last example could equally be written

```
real , dimension(100) :: value
```

where the first limit is omitted and is given the default value 1. The array `list` would contain 114 values, while `surface` would contain 10201.

A `do` statement and its corresponding `enddo` statement define a loop. The `do` statement provides a starting value, terminal value, and optionally, an increment for its index or counter.

The increment may be negative, but should never be zero. If it is not present, the default value is 1. It must be possible for the terminating value to be reached from the starting value.

The counter in a `do` loop is ideally suited for indexing an array, but it may be used anywhere that repetition is needed, and of course the index or counter need not be used explicitly.

The formal syntax of the block `do` construct is

```
[ do-construct-name : ] do [label] [ loop-control ]
  [execution-part-construct]
[ label ] end-do
```

where the forms of the loop control are

```
[ , ] scalar-variable-name =
scalar-numeric-expression ,
scalar-numeric-expression
[ , scalar-numeric-expression ]
```

and the forms of the `end-do` are

```
end do [ do-construct-name ]
continue
```

and `[]` identify optional components of the block `do` construct. This statement is looked at in much greater depth in Chap. 13.

We have introduced the concept of a deferred-shape array. Arrays do not need to have their shape specified at compile time, only their rank. Their actual shape is deferred until runtime. We achieve this by the combined use of the allocatable attribute on the variable declaration and the `allocate` statement, which makes Fortran a very flexible language for array manipulation.

7.6 Problems

7.1 Compile and run all the examples in this chapter, except example 5. This is covered in problem 7.8.

7.2 Modify the first example to convert the height in feet to height in metres. The conversion factor is one 1 ft equals 0.305 m.

Hint: You can either overwrite the height array or introduce a second array.

7.3 The following are two equations for temperature conversion

$$\begin{aligned}c &= 5 / 9 * (t - 32) \\f &= 32 + 9 / 5 * t\end{aligned}$$

Write a complete program where t is an integer do loop variable and loop from -50 to 250. Print out the values of c , t and f on one line. What do you notice about the c and f values?

7.4 Write a program to print out the 12 times table. Typical output would be of the form:

$$\begin{aligned}1 * 12 &= 12 \\2 * 12 &= 24 \\3 * 12 &= 36\end{aligned}$$

etc.

Hint: You don't need to use an array here.

7.5 Write a program to read the following data into a two-dimensional array:

$$\begin{matrix}1 & 2 & 3 \\4 & 5 & 6 \\7 & 8 & 9\end{matrix}$$

Calculate totals for each row and column and produce output similar to that shown below:

$$\begin{matrix}1 & 2 & 3 & 6 \\4 & 5 & 6 & 15 \\7 & 8 & 9 & 24 \\12 & 15 & 18 & \end{matrix}$$

Hint 1: Example ch0602 shows how to sum over a loop.

Hint 2: You need to introduce two one-dimensional arrays to hold the row and column totals. You need to index over the rows to get the column totals and over the columns to get the row totals.

7.6 Modify the above to produce averages for each row and column as well as the totals.

7.7 Using the following data from problem 6.4 in Chap. 6:

1.85	85
1.80	76
1.85	85
1.70	90
1.75	69
1.67	83
1.55	64
1.63	57
1.79	65
1.78	76

Use the program that evaluated the mean and standard deviation to do so for these heights and weights.

In the first case use the program as is and run it twice, first with the heights then with the weights.

What changes would you need to make to the program to read a height and a weight in a pair?

Hint: You could introduce separate scalar variables for the heights and weights.

7.8 Example 5 looked at seat bookings in a cinema or theatre. Here is an example of a sample data file for this program

```
P P P P P P P P P P  
P P P C C C C C P P P  
C C C E E P P P P P  
C C C C C C C C C C  
E E E P P P P P P P P  
C C E E P P C C E E  
P P P P P P P P P P P  
P P P C C C C P P P  
C C C E E P P P P P  
C C C C C C C C C C  
E E E P P P P P P P P  
C C E E P P C C E E  
P P P P P P P P P P P  
P P P C C C C P P P  
C C C E E P P P P P
```

The key for this is as follows:

C = Confirmed Booking
P = Provisional Booking
E = Seat Empty

Compile and run the program. The output would benefit from adding row and column numbers to the information displayed. We will come back to this issue in a subsequent chapter on output formatting.

The data are in a file on the web and the address is given below.

<http://www.fortranplus.co.uk>

Problem 6.6 in the last chapter shows how to read data from a file.

Chapter 8

Whole Array and Additional Array Features

A good notation has a subtlety and suggestiveness which at times make it seem almost like a live teacher.

Bertrand Russell

Aims

The aims of the chapter are:

- To look more formally at the terminology required to precisely describe arrays.
- To introduce ways in which we can manipulate whole arrays and parts of arrays (sections).
- To introduce the concept of array element ordering and physical and virtual memory.
- To introduce ways in which we can initialise arrays using array constructors.
- To introduce the `where` statement and array masking.
- To introduce the `forall` statement and construct.
- Physical and virtual memory
- Type declaration statement summary

8.1 Terminology

Fortran supports an abundance of array handling features. In order to make the description of these features more precise a number of additional terms have to be covered and these are introduced and explained below.

- Rank—The number of dimensions of an array is called its rank. A one dimensional array has rank 1, a two dimensional array has rank 2 and so on.
- Bounds—An array’s bounds are the upper and lower limits of the index in each dimension.
- Extent—The number of elements along a dimension of an array is called the extent.

```
integer, dimension(-10:15):: current
```

has bounds—10 and 15 and an extent of 26.

- **Size**—The total number of elements in an array is its size.
- **Shape**—The shape of an array is determined by its rank and its extents in each dimension.
- **Conformable**—Two arrays are said to be conformable if they have the same shape, that is, they have the same rank and the same extent in each dimension.

8.2 Array Element Ordering

Array element ordering states that the elements of an array, regardless of rank, form a linear sequence. The sequence is such that the subscripts along the first dimension vary most rapidly, and those along the last dimension vary most slowly. This is best illustrated by considering, for example, a rank 2 array *a* defined by

```
real , dimension(1:4,1:2) :: a
a has 8 real elements whose array element order is
a(1,1), a(2,1), a(3,1), a(4,1), a(1,2), a(2,2), a(3,2), a(4,2)
i.e., mathematically by column and not row.
```

We will look more formally at this later in this chapter.

8.3 Whole Array Manipulation

The examples of arrays so far have shown operations on arrays via array elements. One of the significant features of modern Fortran is its ability to manipulate arrays as whole objects. This allows arrays to be referenced not just as single elements but also as groups of elements. Along with this ability comes a whole host of intrinsic procedures for array processing. These procedures are mentioned in Chap. 12, and listed in alphabetical order with examples in Appendix B.

8.4 Assignment

An array name without any indices can appear on both sides of assignment and input and output statements. For example, values can be assigned to all the elements of an array in one statement:

```
real, dimension(1:12):: rainfall
rainfall=0.0
```

The elements of one array can be assigned to another:

```
integer, dimension(1:50) :: a,b
.
.
a=b
```

Arrays *a* and *b* must be conformable in order to do this.

The following example is illegal since *x* is rank 1 and extent 20, whilst *z* is rank 1 and extent 41.

```
real, dimension(1:20) :: x
real, dimension(1:41) :: z
x=50.0
z=x
```

But the following is legal because both arrays are now conformable, i.e., they are both of rank 1 and extent 41:

```
real , dimension (-20:20) :: x
real , dimension (1:41) :: y
x=50.0
y=x
```

8.5 Expressions

All the arithmetic operators available to scalars are available to arrays, but care must be taken because mathematically they may not make sense.

```
real , dimension (1:50) :: a,b,c,d,e
c=a+b
```

adds each element of *a* to the corresponding element of *b* and assigns the result to *c*.

```
e=c*d
```

multiplies each element of *c* by the corresponding element of *d*. This is not vector multiplication. To perform a vector dot product there is an intrinsic procedure *dot_product*, and an example of this is given in a subsequent section on array constructors.

For higher dimensions

```
real ,dimension (1:10,1:10) :: f,g,h
f=f**0.5
```

takes the square root of every element of f .

$h=f+g$

adds each element of f to the corresponding element of g .

$h=f*g$

multiples each element of f by the corresponding element of g . The last statement is not matrix multiplication. An intrinsic procedure `matmul` performs matrix multiplication; further details are given in Appendix B.

8.6 Example 1: Rank 1 Whole Arrays in Fortran

Consider the following example, which is a solution to a problem set earlier, but is now addressed using some of the whole array features of Fortran

```
program ch0801
    implicit none
    integer, parameter :: n = 12
    real, dimension (1:n) :: rainfall_ins = 0.0
    real, dimension (1:n) :: rainfall_cms = 0.0
    integer :: month

    print *, &
        ' Input the rainfall values in inches'
    read *, rainfall_ins
    rainfall_cms = rainfall_ins*2.54
    do month = 1, n
        print *, ' ', month, ' ', &
            rainfall_ins(month), ', ', rainfall_cms(month)
    end do
end program ch0801
```

The statements

```
real , dimension(1:n) :: rainfall_ins=0.0
real , dimension(1:n) :: rainfall_cms=0.0
```

are examples of whole array initialisation. Each element of the arrays is set to 0.0.
The statement

```
read *, rainfall_ins
```

is an example of whole array i/o, where we no longer have to use a do loop to read each element in.

Finally, we have the statement

```
rainfall_cms = rainfall_ins * 2.54
```

which is an example of whole array arithmetic and assignment.

8.7 Example 2: Rank 2 Whole Arrays in Fortran

Here is a two-dimensional example:

```
program ch0802
! This program reads in a grid of temperatures
! (degrees Fahrenheit) at 25 grid references
! and converts them to degrees Celsius
implicit none
integer, parameter :: n = 5
real, dimension (1:n, 1:n) :: fahrenheit, &
    celsius
integer :: long, lat
!
! read in the temperatures
!
do lat = 1, n
    print *, ' For Latitude= ', lat
    do long = 1, n
        print *, ' For Longitude', long
        read *, fahrenheit(lat, long)
    end do
end do
!
! Conversion applied to all values
!
celsius = 5.0/9.0*(fahrenheit-32.0)
print *, celsius
print *, fahrenheit
end program ch0802
```

Note the use of whole arrays in the print statements. The output does look rather messy though, and also illustrates array element ordering.

8.8 Array Sections

Often it is necessary to access part of an array rather than the whole, and this is possible with Fortran's powerful array manipulation features.

8.8.1 Example 3: Rank 1 Array Sections

Consider the following:

```
program ch0803
    implicit none
    integer, dimension (-5:5) :: x
    integer :: i

    x(-5:-1) = -1
    x(0) = 0
    x(1:5) = 1
    do i = -5, 5
        print *, ' ', i, ' ', x(i)
    end do
end program ch0803
```

The statement

```
x(-5:-1) = -1
```

is working with a section of an array. It assigns the value -1 to elements $x(-5)$ through $x(-1)$.

The statement

```
x(1:5) = 1
```

is also working with an array section. It assigns the value 1 to elements $x(1)$ through $x(5)$.

8.8.2 Example 4: Rank 2 Array Sections

In Chap. 6 we gave an example of a table of examination marks, and this is given again below:

Name	Physics	Maths	Biology	History	English	French
Fowler L.	50	47	28	89	30	46
Barron L.W.	37	67	34	65	68	98
Warren J.	25	45	26	48	10	36
Mallory D.	89	56	33	45	30	65
Codd S.	68	78	38	76	98	65

The following program reads the data in, scales column 3 by 2.5 as the Biology marks were out of 40 (the rest are out of 100), calculates the averages for each subject and for each person and prints out the results.

```

program ch0804
    implicit none
    integer, parameter :: nrow = 5
    integer, parameter :: ncol = 6
    real, dimension (1:nrow, 1:ncol) :: &
        exam_results = 0.0
    real, dimension (1:nrow) :: people_average = &
        0.0
    real, dimension (1:ncol) :: subject_average = &
        0.0
    integer :: r, c

    do r = 1, nrow
        read *, exam_results(r, 1:ncol)
    end do
    exam_results(1:nrow, 3) = 2.5* &
        exam_results(1:nrow, 3)
    do r = 1, nrow
        do c = 1, ncol
            people_average(r) = people_average(r) + &
                exam_results(r, c)
        end do
    end do
    people_average = people_average/ncol
    do c = 1, ncol
        do r = 1, nrow
            subject_average(c) = subject_average(c) + &
                exam_results(r, c)
        end do
    end do
    subject_average = subject_average/nrow
    print *, ' People averages'
    print *, people_average
    print *, ' Subject averages'
    print *, subject_average
end program ch0804

```

The statement

```
read *, exam_results(r,1:ncol)
```

uses sections to replace the implied do loop in the earlier example, takes column 3 of the two dimensional array `exam_results`, multiplies it by 2.5 (as a whole array) and overwrites the original values.

The statement

```
exam_results(1:nrow,3) = &
2.5 * exam_results(1:nrow,3)
```

uses array sections in the arithmetic and the assignment.

8.9 Array Constructors

Arrays can be given initial values in Fortran using array constructors. Some examples are given below.

8.9.1 Example 5: Rank 1 Array Initialisation—Explicit Values

```
program ch0805
    implicit none
    integer, parameter :: n = 12
    real :: total = 0.0, average = 0.0
    real, dimension (1:n) :: rainfall = &
        (/ 3.1, 2.0, 2.4, 2.1, 2.2, 2.2, &
        1.8, 2.2, 2.7, 2.9, 3.1, 3.1 /)
    integer :: month

    do month = 1, n
        total = total + rainfall(month)
    end do
    average = total/n
    print *, ' Average monthly rainfall was'
    print *, average
end program ch0805
```

The statement

```
real , dimension(1:n) :: rainfall = &
(/3.1,2.0,2.4,2.1,2.2,2.2,1.8,2.2,2.7,2.9,3.1,3.1/)
```

provides initial values to the elements of the array `rainfall`.

8.9.2 Example 6: Rank 1 Array Initialisation Using An Implied do loop

The next example uses a simple variant:

```
program ch0806
    implicit none
!
! 1 us gallon = 3.7854118 litres
! 1 uk gallon = 4.545 litres
!
integer, parameter :: n = 10
real, parameter :: us = 3.7854118
real, parameter :: uk = 4.545
integer :: i
integer, dimension (1:n) :: &
    litre = [ (i,i=1,n) ]
real, dimension (1:n) :: gallon, usgallon

gallon = litre/uk
usgallon = litre/us
print *, 'Litres Imperial USA'
print *, 'Gallon Gallon'
do i = 1, n
    print *, litre(i), ' ', gallon(i), ' ', &
        usgallon(i)
end do
end program ch0806
```

The statement

```
integer , dimension(1:n) :: litre=[(i,i=1,n)]
```

initialises the 10 elements of the `litre` array to the values 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 respectively.

8.9.3 Example 7: Rank 1 Arrays and the `dot_product` Intrinsic

This example uses an array constructor and the intrinsic procedure `dot_product`:

```
program ch0807
    implicit none
    integer, dimension (1:3) :: x, y
    integer :: result

    x = [ 1, 3, 5 ]
    y = [ 2, 4, 6 ]
    result = dot_product(x, y)
    print *, result
end program ch0807
```

and `result` has the value 44, which is obtained by the normal mathematical dot product operation, $1 * 2 + 3 * 4 + 5 * 6$.

The general form of the array constructor is `[list of expressions]` or `(/ a list of expressions /)` where each expression is of the same type.

8.9.4 Initialising Rank 2 Arrays

To construct arrays of higher rank than one the intrinsic function `reshape` must be used. An introduction to intrinsic functions is given in Chap. 12, and an alphabetic list with a full explanation of each function is given in Appendix B. To use it in its simplest form:

```
matrix = reshape ( source, shape)
```

where `source` is a rank 1 array containing the values of the elements required in the new array, `matrix`, and `shape` is a rank 1 array containing the shape of the new array `matrix`.

We consider the rank 1 array `b=(1, 3, 5, 7, 9, 11)`, and we wish to store these values in a rank 2 array `a`, such that `a` is the matrix:

$$a = \begin{pmatrix} 1 & 7 \\ 3 & 9 \\ 5 & 11 \end{pmatrix}$$

The following code extract is needed:

```
integer, dimension(1:6) :: b
integer, dimension(1:3, 1:2) :: a
b = (/1,3,5,7,9,11/)
a = reshape(b, (/3,2/))
```

Note that the elements of the source array `b` must be stored in the array element order of the required array `a`.

8.9.5 Example 8: Initialising a Rank 2 Array

The following example illustrates the additional forms of the `reshape` function that are used when the number of elements in the source array is less than the number of elements in the destination. The complete form is

```
reshape(source, shape, pad, order)
```

`pad` and `order` are optional. See Appendix B for a complete explanation of `pad` and `order`:

```
program ch0808
  implicit none
  integer, dimension (1:2, 1:4) :: x
  integer, dimension (1:8)      :: y = &
    (/ 1, 2, 3, 4, 5, 6, 7, 8 /)
  integer, dimension (1:6)      :: z = &
    (/ 1, 2, 3, 4, 5, 6 /)
  integer :: r, c

  print *, ' Source array y'
  print *, y
  print *, ' Source array z'
  print *, z
  print *, ' Simple reshape sizes match'
  x = reshape(y, (/2,4/))
  do r = 1, 2
    print *, (x(r,c), c=1, 4)
  end do
  print *, &
    ' Source 2 elements smaller pad with 0'
  x = reshape(z, (/2,4/), (/0,0/))
  do r = 1, 2
    print *, (x(r,c), c=1, 4)
```

```

end do
print *, &
' As previous now specify order as 1*2'
x = reshape(z, (/2,4/), (/0,0/), (/1,2/) )
do r = 1, 2
print *, (x(r,c), c=1, 4)
end do
print *, &
' As previous now specify order as 2*1'
x = reshape(z, (/2,4/), (/0,0/), (/2,1/) )
do r = 1, 2
print *, (x(r,c), c=1, 4)
end do
end program ch0808

```

8.10 Miscellaneous Array Examples

The following are examples of some of the flexibility of arrays in Fortran.

8.10.1 Example 9: Rank 1 Arrays and a Stride of 2

Consider the following example:

```

program ch0809
implicit none
integer :: i
integer, dimension (1:10) :: x = (/ (i,i=1,10) &
/)
integer, dimension (1:5) :: odd = (/ (i,i=1,10 &
,2) /)
integer, dimension (1:5) :: even

even = x(2:10:2)
print *, ' x'
print *, x
print *, ' odd'
print *, odd
print *, ' even'
print *, even
end program ch0809

```

The statement

```
integer , dimension(1:5) :: odd=(/(i,i=1,10,2)/)
```

steps through the array 2 at a time.

The statement

```
even=x(2:10:2)
```

shows an array section where we go from elements two through ten in steps of two. The 2:10:2 is an example of a subscript triplet in Fortran, and the first 2 is the lower bound, the 10 is the upper bound, and the last 2 is the increment. Fortran uses the term stride to mean the increment in a subscript triplet.

8.10.2 Example 10: Rank 1 Array and the sum Intrinsic Function

The following example is based on ch0805. It uses the `sum` intrinsic to calculate the sum of all the values in the `rainfall` array.

```
program ch0810
    implicit none
    real :: total = 0.0, average = 0.0
    real, dimension (12) :: rainfall = (/ 3.1, 2.0 &
        , 2.4, 2.1, 2.2, 2.2, 1.8, 2.2, 2.7, 2.9, &
        3.1, 3.1 /)

    total = sum(rainfall)
    average = total/12
    print *, ' Average monthly rainfall was'
    print *, average
end program ch0810
```

The statement

```
total = sum(rainfall)
```

replaces the statements below from the earlier example.

```
do month=1,n
    total = total + rainfall(month)
enddo
```

In this example the `sum` intrinsic function adds up all of the elements of the array `rainfall`.

So we have three ways of processing arrays:

- Element by element.
- Using sections.
- On a whole array basis.

The ability to use sections and whole arrays when programming is a major advance of the element by element processing supported by Fortran 77.

8.10.3 Example 11: Rank 2 Arrays and the sum Intrinsic Function

This example is based on the earlier exam results program:

```
program ch0811
    implicit none
    integer, parameter :: nrow = 5
    integer, parameter :: ncol = 6
    real, dimension (1:nrow*ncol) :: results = (/ &
        50, 47, 28, 89, 30, 46, 37, 67, 34, 65, 68, &
        98, 25, 45, 26, 48, 10, 36, 89, 56, 33, 45, &
        30, 65, 68, 78, 38, 76, 98, 65 /)
    real, dimension (1:nrow, 1:ncol) :: &
        exam_results = 0.0
    real, dimension (1:nrow) :: people_average = &
        0.0
    real, dimension (1:ncol) :: subject_average = &
        0.0

    exam_results = reshape(results, (/nrow,ncol/), &
        (/0.0,0.0/), (/2,1/) )
    exam_results(1:nrow, 3) = 2.5* &
        exam_results(1:nrow, 3)
    subject_average = sum(exam_results, dim=1)
    people_average = sum(exam_results, dim=2)
    people_average = people_average/ncol
    subject_average = subject_average/nrow
    print *, ' People averages'
    print *, people_average
    print *, ' Subject averages'
    print *, subject_average
end program ch0811
```

This example has several interesting array features:

- We initialise a rank 1 array with the values we want in our exam marks array. The data are laid out in the program as they would be in an external file in rows and columns.
- We use `reshape` to initialise our exam marks array. We use the fourth parameter `(/2, 1/)` to populate the rank 2 array with the data in row order.
- We use `sum` with a `dim` of 1 to compute the sums for the subjects.
- We use `sum` with a `dim` of 2 to compute the sums for the people.

8.10.4 Example 12: Masked Array Assignment and the `where` Statement

Fortran has array assignment both on an element by element basis and on a whole array basis. There is an additional form of assignment based on the concept of a logical mask.

Consider the example of time zones given in Chap. 7. The `time` array will have values that are both negative and positive. We can then associate the positive values with the concept of east of the Greenwich meridian, and the negative values with the concept of west of the Greenwich meridian e.g.:

```
program ch0812
  implicit none
  real, dimension (-180:180) :: time = 0
  integer :: degree, strip
  real :: value
  character (len=1), dimension (-180:180) :: &
    direction = ' '
  do degree = -180, 165, 15
    value = degree/15.
    do strip = 0, 14
      time(degree+strip) = value
    end do
  end do
  do degree = -180, 180
    print *, degree, ' ', time(degree)
  end do
  where (time>0.0)
    direction = 'E'
  elsewhere (time<0.0)
    direction = 'W'
  end where
```

```
print *, direction
end program ch0812
```

8.10.5 Notes

The arrays must be conformable, i.e., in our example `time` and `direction` are the same shape.

The selective assignment is achieved through the `where` construct.

Both the `where` and `elsewhere` blocks can be executed.

The formal syntax is:

```
where (array logical expression)
...
elsewhere (array logical expression)
...
end where
```

The first array assignment is executed where `time` is positive and the second is executed where `time` is negative. For further coverage of logical expressions see Chaps. 13 and 16.

8.11 The `forall` Statement and `forall` Construct

The `forall` statement and `forall` construct were introduced into Fortran to keep it inline with High Performance Fortran—HPF. They indicate to the compiler that the code can be optimised on a parallel processor. Consider the following example where a value is subtracted from the diagonal elements of a square matrix `A`:

```
forall (i=1:n)
  a(i,i) = a(i,i) - lamda
end forall
```

The `forall` construct allows the calculations to be carried out simultaneously in a multiprocessor environment.

8.11.1 Syntax

```
forall ( triplet [ , triplet ] ...
[ , mask ] ) variable = expression
forall ( triplet [ , triplet ] ...
[ , mask ] ) pointer => target
```

The triplet specifies a value set for an index variable. It has the following syntax:

```
index = first : last [ : stride ]
```

`first`, `last` and `stride` are scalar integer expressions.

`mask` is a scalar logical expression:

```
[ name : ] forall ( triplet [ , triplet ] ...
[ , mask ] ) end forall [ name ]
```

`name` is an optional name, which identifies the `forall` construct.

8.12 Array Element Ordering in More Detail

Fortran compilers will store arrays in memory according to the array element ordering scheme. Section 6.5.3.2 of the Fortran 2008 standard provides details of this. Table 8.1 summarises the information for rank 1, 2 and 3 arrays.

8.12.1 Example 13: Array Element Ordering

Here is a short program illustrating the above for a $2 * 5$ array.

```
program ch0813
  implicit none
  integer :: j1 = 1
  integer :: k1 = 2
  integer :: j2 = 1
  integer :: k2 = 5
  integer :: s1
```

Table 8.1 Array element ordering in Fortran

Rank	Subscript bounds	Subscript list	Subscript order value
1	j1:k1	s1	$1 + (s1 - j1)$
2	j1:k1, j2:k2	s1, s2	$1 + (s1 - j1)$
			$+(s2 - j2) * d1$
3	j1:k1, j2:k2, j3:k3	s1, s2, s3	$1 + (s1 - j1)$
			$+(s2 - j2) * d1$
			$+(s3 - j3) * d2 * d1$

```

integer :: s2
integer :: d1
integer :: position

d1 = k1 - j1 + 1
print *, ' Row Column Position'
do s1 = j1, k1
  do s2 = j2, k2
    position = 1 + (s1-j1) + (s2-j2)*d1
    print 100, s1, s2, position
  100 format (3x, i2, 6x, i2, 10x, i2)
  end do
end do

end program ch0813

```

If you run the program you will see that for rank 2 arrays the array element ordering is by column, not row.

8.13 Physical and Virtual Memory

There will be a limit to the amount of physical memory available on any computer system. To enable problems that require more than the amount of physical memory available to be solved, most implementations will provide access to virtual memory, which in reality means access to a portion of a physical disk.

Access to virtual memory is commonly provided by a paging mechanism of some description. Paging is a technique whereby fixed-sized blocks of data are swapped between real memory and disk as required.

In order to minimise paging (and hence reduce execution time) array operations should be performed according to the array element order.

Page sizes, past and present, include:

- Sun UltraSparc—4, 8 Kb.
- DEC Alpha—8, 16, 32, 64 Kb.
- Intel 80 × 86—4 Kb.
- Intel Pentium PIII—4 Kb, 2, 4 Mb.
- AMD64—4 Kb, 2, 4 Mb—legacy mode
- AMD64—4 Kb, 2 Mb, 1 Gb—64 bit mode
- Intel 64 and IA-32—4 Kb, 2 Mb, 1 Gb—depending on mode.

See the references at the end of the chapter for more details.

8.14 Type Declaration Statement Summary

A type declaration statement normally has three components

- a type declaration
- optional attributes
- variable list

A type declaration is one of

- intrinsic type specifier
- type (derived type specification)
- class (derived type specification)
- class (*)

The attribute specification is one of

- allocatable
- asynchronous
- bind
- dimension
- external
- intent
- intrinsic
- optional
- parameter
- pointer
- private
- protected
- public
- save
- target
- value
- volatile

8.15 Summary

We can now perform operations on whole arrays and partial arrays (array sections) without having to refer to individual elements. This shortens program development time and greatly clarifies the meaning of programs.

Array constructors can be used to assign values to rank 1 arrays within a program unit. The `reshape` function allows us to assign values to a two or higher rank array when used in conjunction with an array constructor.

8.16 Problems

8.1 Compile and run all the examples.

8.2 Give the rank, bounds, extent and size of the following arrays:

```
real , dimension(1:15) :: a
integer , dimension(1:3,0:4) :: b
real , dimension(-2:2,0:1,1:4) :: c
integer , dimension(0:2,1:5) :: d
```

Which two of these arrays are conformable?

8.3 Write a program to read in five rank 1 arrays, a, b, c, d, e and then store them as five columns in a rank 2 array table.

8.4 Take the first part of Problem 7 in Chap. 7 and rewrite it using the sum intrinsic function.

Bibliography

Alpha

Bhandarkar, D.P.: Alpha Implementation and Architecture: Complete Reference and Guide. Digital Press (1995)

AMD

Visit

<http://developer.amd.com/documentation/guides/pages/default.aspx>

for details of the AMD manuals. The following five manuals are available for download as pdf's from the above site.

- AMD64 Architecture Programmer's Manual Volume 1: Application Programming
- AMD64 Architecture Programmer's Manual Volume 2: System Programming
- AMD64 Architecture Programmer's Manual Volume 3: General Purpose and System Instructions
- AMD64 Architecture Programmer's Manual Volume 4: 128-bit and 256 bit media instructions

- AMD64 Architecture Programmer's Manual Volume 5: 64-Bit Media and x87 Floating-Point Instructions

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- Intel 64 and IA-32 Architectures Software Developer's Manual. Volume 1: Basic Architecture
- Intel 64 and IA-32 Architectures Software Developer's Manual. Combined Volumes 2A and 2B: Instruction Set Reference, A-Z.
- Intel 64 and IA-32 Architectures Software Developer's Manual. Combined Volumes 3A and 3B: System Programming Guide, Parts 1 and 2

Chapter 9

Output of Results

Why, sometimes I've believed as many as six impossible things before breakfast.

Lewis Carroll, Through the Looking-Glass and What Alice Found There

Aims

The aims here are to introduce some of the facilities for producing neat output using edit descriptors. There is also coverage of how to write the results to a file, rather than to the screen.

There are examples which will illustrate the use of

- The `i` edit descriptor for integer data
- The `f` edit descriptor for real data
- The `e` edit descriptor for real data
- The `g` edit descriptor for real data
- The `x` edit descriptor for spaces
- The `a` edit descriptor for character data
- Repetition of edit descriptors
- New lines
- Output using array sections
- Output using whole arrays
- The `open`, `write`, and `close` statements.

We will also provide a brief summary of the rest of the control and data edit descriptors, as people may see them in existing code.

9.1 Introduction

When you have used `print *` a few times it becomes apparent that it is not always as useful as it might be. The data are written out in a way which makes some sense, but may not be especially easy to read. Real numbers are generally written out with

all their significant places, which is very often rather too many, and it is often difficult to line up the columns for data which are notionally tabular. It is possible to be much more precise in describing the way in which information is presented by the program. To do this, we use `format` statements. Through the use of the `format` we can:

- Specify how many columns a number should take up.
- Specify where a decimal point should lie.
- Specify where there should be white space.
- Specify titles.

The `format` statement has a label associated with it; through this label, the `print` statement associates the data to be written with the form in which to write them.

9.2 Integers and the `i` Format or Edit Descriptor

Integer format (or edit descriptor) is reasonably straightforward, and offers clues for formats used in describing other numbers. `i3` is an integer taking three columns. The number is right justified, a bit of jargon meaning that it is written as far to the right as it will go, so that there are no trailing or following blanks. Consider the following example:

9.2.1 Example 1: Twelve Times Table

```
program ch0901
    implicit none
    integer :: t

    print *, ''
    print *, 'Twelve times table'
    print *, ''
    do t = 1, 12
        print 100, t, t*12
    end do
100 format (' ', i3, ' * 12 = ', i3)
end program ch0901
```

The first statement of interest is

```
print 100, t,t*12
```

The 100 is a statement label. There must be a format statement with this label in the program. The variables to be written out are *t* and *t*12*.

The second statement of interest is

```
100 format(' ',i3,' * 12 = ',i3)
```

Inside the brackets we have ' ' print out what occurs between the quote marks, in this case one space.

, the comma separates items in the format statement.

i3 print out the first variable in the print statement right justified in three columns
, item separator.

' * 12 = ' print out what occurs between the quote characters.
, item separator

i3 print out the second variable (in this case an expression) right justified in three columns.

All of the output will appear on one line.

9.2.1.1 Notes

The numbers are right justified in the field width.

If the edit descriptor has too few columns for the data we will get asterisks * displayed.

If the number to be displayed is negative we must allow one column for the minus sign.

9.2.2 Example 2: Integer Overflow and the *i* Edit Descriptor

Now consider the following example:

```
program ch0902
    implicit none
    integer :: big = 10
    integer :: i

    do i = 1, 40
        print 100, i, big
        big = big*10
    end do
100 format (' ', i3, ' ', i12)
end program ch0902
```

This program will loop and the variable `big` will overflow, i.e., go beyond the range of valid values for a 32-bit integer (2,147,483,647). Does the program crash or generate a run time error? This is the output from the NAG and Intel compilers.

```

1          10
2         100
3        1000
4       10000
5      100000
6     1000000
7    10000000
8   100000000
9  1000000000
10 1410065408
11 1215752192
12 -727379968
...
31 -2147483648
32          0
...
40          0

```

Is there a compiler switch to trap this kind of error?

9.3 Reals and the f Edit Descriptor

The `f` edit descriptor can be seen as an extension of the integer format, but here we have to deal with the decimal point. The general form is

- `fw.d`
- where `w` is the total width
- The `.` is decimal point
- `d` is the number of digits after the decimal point.
- as with the integer edit descriptor the number is right justified in the field width.

Let us look at some examples to illustrate the use of the `f` edit descriptor.

9.3.1 Example 3: Imperial Pints and US Pints

```

program ch0903
implicit none
integer :: fluid

```

```

real :: imperial_pint
real :: us_pint

print *, ' US           Imperial'
print *, ' pint(s)      pint(s)'
do fluid = 1, 10
    imperial_pint = fluid*1.20095
    us_pint = fluid/1.20095
    print 100, imperial_pint, fluid, us_pint
100 format (' ', f5.2, ' ', i3, ' ', f5.2)
end do
end program ch0903

```

The first two print statements are a heading for the subsequent output. Some experimentation is normally required to get a reasonable looking table. Note that in this example we used the f5.2 edit descriptor to print out both `imperial_pint` variable and the `us_pint` variable. That is an overall width of 5 spaces with 2 digits after the decimal point.

Note also that rounding has occurred, i.e. the real values are rounded to 2 digits after the decimal point.

9.3.2 Example 4: Imperial Pints and Litres

```

program ch0904
    implicit none
    integer :: fluid
    real :: litres
    real :: pints

    print *, ' Imperial      Litre(s)'
    print *, ' pint(s)      '
    do fluid = 1, 10
        litres = fluid/1.75
        pints = fluid*1.75
        print 100, pints, fluid, litres
    end do
100 format (' ', f6.2, ' ', i3, ' ', f5.2)
end program ch0904

```

Note that in this example we are using f6.2 to print out the `pints` variable, and f5.2 to print out the `litres` variable.

Note again that rounding is taking place, i.e. both variables are rounded to 2 digits after the decimal point.

9.3.3 Example 5: Narrow Field Widths and the **E** Edit Descriptor

Consider the following example.

```
program ch0905
    implicit none
    integer :: i
    real :: r1 = 9.9
    real :: r2 = 9.9
    real :: r3 = -9.9
    real :: r4 = -9.9

    do i = 1, 10
        print 100, i, r1, r2, r3, r4
100 format (' ', i3, ' ', f7.3, ' ', f7.3, &
           ' ', f7.3, ' ', f7.3)
        r1 = r1/10.0
        r2 = r2*10.0
        r3 = r3/10.0
        r4 = r4*10.0
    end do
end program ch0905
```

Here is the output.

When the number is too large for the field width asterisks are printed. Note also that space has to be allowed for the sign of the variable.

9.3.4 Example 6: Overflow and the **E** Edit Descriptor

Consider the following program:

```
program ch0906
    implicit none
    integer :: i
    real :: small = 1.0
    real :: big = 1.0

    do i = 1, 50
        print 100, i, small, big
100 format (' ', i3, ' ', f7.3, ' ', f7.3)
        small = small/10.0
```

```
big = big*10.0
end do
end program ch0906
```

In this program the variable `small` will underflow and `big` will overflow. The output from the Intel compiler is:

```
1    1.000    1.000
2    0.100   10.000
3    0.010  100.000
4    0.001  *****
...
39   0.000  *****
40   0.000  Infini
...
50   0.000  Infini
```

When the number is too small for the format, the printout is what you would probably expect. When the number is too large, you get asterisks. When the number actually overflows the Intel compiler tells you that the number is too big and has overflowed. However the program ran to completion and did not generate a run time error.

9.4 Reals and the e Edit Descriptor

The exponential or scientific notation is useful in cases where we need to provide a format which may encompass a wide range of values. If likely results lie in a very wide range, we can ensure that the most significant part is given. This takes a form such as

```
e12.4
```

The 12 refers to the total width and the 4 to the number of significant digits.

9.4.1 Example 7: Simple e Edit Descriptor Example

Let's look at a simple example to see what the output is like and then go over some more about the rules that apply.

```

program ch0907
    implicit none
    integer :: i
    real :: r1 = 1.23456
    real :: r2 = 1.23456

    do i = 1, 10
        print 100, i, r1, r2
        r1 = r1/10.0
        r2 = r2*10.0
    end do
100 format (' ', i3, '   ', e12.4, '   ', e12.4)
end program ch0907

```

Here is the output

1	0.1235E+01	0.1235E+01
2	0.1235E+00	0.1235E+02
3	0.1235E-01	0.1235E+03
4	0.1235E-02	0.1235E+04
5	0.1235E-03	0.1235E+05
6	0.1235E-04	0.1235E+06
7	0.1235E-05	0.1235E+07
8	0.1235E-06	0.1235E+08
9	0.1235E-07	0.1235E+09
10	0.1235E-08	0.1235E+10

There are a number of things to note here

- all exponent format numbers are written so that the number is between 0.1 and 0.9999..., with the exponent taking care of scale shifts, this implies that the first four significant digits are to be printed out.
- rounding is taking place
- the numbers are right justified

There is a minimum size for an exponential format. Because of all the extra bits and pieces it requires:

- The decimal point.
- The sign of the entire number.
- The sign of the exponent.
- The magnitude of the exponent.
- The e.

The width of the number less the number of significant places should not be less than 6. In the example given above, e12.4 meets this requirement. When the exponent is in the range 0 to 99, the e will be printed as part of the number; when the exponent is greater, the e is dropped, and its place is taken by a larger value; however, the sign of the exponent is always given, whether it is positive or negative.

The sign of the whole number will usually only be given when it is negative. This means that if the numbers are always positive, the rule of six given above can be modified to a rule of five. It is safer to allow six places over, since, if the format is insufficient, all you will get are asterisks.

The most common mistake with an e format is to make the edit descriptor too small, so that there is insufficient room for all the padding to be printed.

9.5 Reals and the g Edit Descriptor

This edit descriptor combines both the f and e edit descriptors, depending on the size of the number.

9.5.1 Example 8: Simple g Edit Descriptor Example

Here is a variant of the previous examples with the g edit descriptor replacing the e edit descriptor.

```
program ch0908
    implicit none
    integer :: i
    real :: r1 = 1.23456
    real :: r2 = 1.23456

    print 100
100 format (' ', &
             '1234567890123456789012345678901')
    print 110
110 format (' i3   g12.4           g12.4')
    do i = 1, 10
        print 120, i, r1, r2
        r1 = r1/10.0
        r2 = r2*10.0
    end do
120 format (' ', i3, ' ', g12.4, ' ', g12.4)
end program ch0908
```

Here is the output

```
1234567890123456789012345678901
i3   g12.4           g12.4
```

```

1      1.235      1.235
2      0.1235     12.35
3      0.1235E-01 123.5
4      0.1235E-02 1235.
5      0.1235E-03 0.1235E+05
6      0.1235E-04 0.1235E+06
7      0.1235E-05 0.1235E+07
8      0.1235E-06 0.1235E+08
9      0.1235E-07 0.1235E+09
10     0.1235E-08 0.1235E+10

```

Fortran provides quite a useful set of edit descriptors for real numbers. The `print *` is very useful when developing programs.

9.6 Spaces

Fortran provides a variety of ways of generating spaces in a format statement and these include using quotes ('), double quotes ("") and the x edit descriptor.

9.6.1 Example 9: Three Ways of Generating Spaces

```

program ch0909
  implicit none
  integer :: i

  do i = 1, 4
    print 100, i, i*i
    print 110, i, i*i
    print 120, i, i*i
  100 format (' ', i2, ' ', i4)
  110 format (" ", i2, " ", i4)
  120 format (1x, i2, 2x, i4)
  end do
end program ch0909

```

The output is the same from each format statement.

9.7 Characters—a Format or Edit Descriptor

This is perhaps the simplest output of all. Since you will already have declared the length of a character variable in your declarations,

```
character (10) :: b
```

when you come to write out b, the length is known—thus you need only specify that a character string is to be output:

```
print 100,b  
100 format(1x,a)
```

If you feel you need a little extra control, you can append an integer value to the a, like a10 (a9 or a1), and so on. if you do this, only the first 10 (9 or 1) characters are written out; the remainder are ignored. Do note that 10a1 and a10 are not the same thing. 10a1 would be used to print out the first character of ten character variables, while a10 would write out the first 10 characters of a single character variable. The general form is therefore just a, but if more control is required, this may be followed by a positive integer.

9.7.1 Example 10: Character Output and the a Edit Descriptor

The following program is a simple rewrite of one of the programs from Chap. 4.

```
program ch0910  
! This program reads in and prints out  
! your first name  
implicit none  
character (20) :: first_name  
  
print *, ' Type in your first name.'  
print *, ' up to 20 characters'  
read *, first_name  
print 100, first_name  
100 format (1x, a)  
end program ch0910
```

9.7.2 Example 11: Character, Integer and Real Output in a Format Statement

The following example shows how to mix and match character, integer and real output in one format statement:

```
program ch0911
    implicit none
    character (len=15) :: firstname
    integer :: age
    real :: weight
    character (len=1) :: gender

    print *, ' type in your first name '
    read *, firstname
    print *, ' type in your age in years'
    read *, age
    print *, ' type in your weight in kilos'
    read *, weight
    print *, ' type in your gender (f/m)'
    read *, gender
    print *, ' your personal details are'
    print *
    print 100
    print 110, firstname, age, weight, gender
100 format (4x, 'first name', 4x, 'age', 1x, &
            'weight', 2x, 'gender')
110 format (1x, a, 2x, i3, 2x, f5.2, 2x, a)
end program ch0911
```

Take care to match up the variables with the appropriate edit descriptors. You also need to count the number of characters and spaces when lining up the heading.

9.8 Common Mistakes

It must be stressed that an integer can only be printed out with an *i* format, and a real with an *f* (or *e*) format. You cannot use integer variables or expressions with *f*, *e* or *g* edit descriptors or real variables and expressions with *i* edit descriptors. If you do, unpredictable results will follow. There are (at least) two other sorts of errors you might make in writing out a value. You might try to write out something which has never actually been assigned a value; this is termed an indefinite value.

You might find that the letter `i` is written out. In passing, note that many loaders and link editors will preset all values to zero—i.e., unset (indefinite) values are actually set to zero. On better systems there is generally some way of turning this facility off, so that undefined is really indefinite. More often than not, indefinite values are the result of mistyping rather than of never setting values. It is not uncommon to type `O` for 0, or `I` for either `I` or 1. The other likely error is to try to print out a value greater than the machine can calculate—out of range values. Some machines will print out such values as `R`, but some will actually print out something which looks right, and such overflow and underflow conditions can go unnoticed. Be wary.

9.9 Files in Fortran

One of the particularly powerful features of Fortran is the way it allows you to manipulate files. Up to now, most of the discussion has centred on reading from the keyboard and writing to the screen. It is also possible to read and write to one or more files. This is achieved using the `open`, `write`, `read` and `close` statements. In a later chapter we will consider reading from files but here we will concentrate on writing.

9.9.1 *The open Statement*

This statement sets up a file for either reading or writing. A typical form is

```
open (unit=1,file='data.txt')
```

The file will be known to the operating system as `data.txt` and can be written to by using the unit number. This statement should come before you first read data from or write data to to the file.

You can also use a character variable to hold the filename. This is shown in the code segment below.

```
character*60 :: filename  
...  
...  
filename='data.txt'  
...  
...  
open (unit=1,file=filename)
```

It is not possible to write to the file `data.txt` directly; it must be referenced through its unit number. Within the Fortran program you write to this file using a statement such as

```
write(unit=1,fmt=100) x,y
```

or

```
write(1,100) x,y
```

These two statements are equivalent.

9.9.2 The `close` Statement

Besides opening a file, we really ought to close it when we have finished writing to it:

```
close(unit=1)
```

In fact, on many systems it is not obligatory to open and close all your files. Almost certainly, the terminal will not require this, since INPUT and OUTPUT units will be there by default. At the end of the job, the system will close all your files. Nevertheless, explicit open and close cannot hurt, and the added clarity generally assists in understanding the program.

9.9.3 Example 12: Open and Close Usage

The following program contains all of the above statements:

```
program ch0912
    implicit none
    integer :: fluid
    real :: litres
    real :: pints

    open (unit=1, file='ch0912.txt')
    write (unit=1, fmt=100)
    do fluid = 1, 10
        litres = fluid/1.75
        pints = fluid*1.75
```

```
      write (unit=1, fmt=110) pints, fluid, litres
    end do
    close (1)
100 format ('    Pints      Litres')
110 format (' ', f7.3, ' ', i3, ' ', f7.3)
end program ch0912
```

In this example the file will be created in the directory that the program executable runs in.

Using the following open statement

```
open (unit=1, file=&
      'c:\document\fortran\ch0912.txt')
```

creates the file in the

c:\document\fortran

directory under the Windows operating system.

Using the following open statement

```
open (unit=1, file=&
      '/home/ian/document/fortran/ch0912.txt')
```

creates the file in the

/home/ian/document/fortran

directory under a Linux operating system.

9.9.4 Example 13: Timing of Writing Formatted Files

The following example looks at the amount of time spent in different sections of a program with the main emphasis on formatted output:

```
program ch0913
  implicit none
  integer, parameter :: n = 10000000
  integer, dimension (1:n) :: x = 0
  real, dimension (1:n) :: y = 0.0
  integer :: i
  real :: t, t1, t2, t3, t4, t5
```

```
character *30 :: comment

open (unit=10, file='ch0913.txt')
call cpu_time(t)
t1 = t
comment = ' Program starts '
print 120, comment, t1
do i = 1, n
    x(i) = i
end do
call cpu_time(t)
t2 = t - t1
comment = ' Integer array initialised'
print 120, comment, t2
y = real(x)
call cpu_time(t)
t3 = t - t1 - t2
comment = ' Real      array initialised'
print 120, comment, t2
do i = 1, n
    write (10, 100) x(i)
end do
call cpu_time(t)
t4 = t - t1 - t2 - t3
comment = ' Integer write '
print 120, comment, t4
do i = 1, n
    write (10, 110) y(i)
end do
call cpu_time(t)
t5 = t - t1 - t2 - t3 - t4
comment = ' Real      write '
print 120, comment, t5
100 format (1x, i10)
110 format (1x, f10.0)
120 format (1x, a, 2x, f7.3)

end program ch0913
```

There is a call to the built-in intrinsic `cpu_time` to obtain timing information. Try this example out with your compiler. Formatted output takes up a lot of time, as we are converting from an internal binary representation to an external decimal form.

Program starts	0.016
Integer array initialised	0.094
Real array initialised	0.094
Integer write	2.262
Real write	8.408

9.9.5 Example 14: Timing of Writing Unformatted Files

The following program is a variant of the above but now the output is in unformatted or binary form:

```
program ch0914
    implicit none
    integer, parameter :: n = 10000000
    integer, dimension (1:n) :: x = 0
    real, dimension (1:n) :: y = 0
    integer :: i
    real :: t, t1, t2, t3, t4, t5
    character *30 :: comment

    open (unit=10, file='ch0914.dat', &
          form='unformatted')
    call cpu_time(t)
    t1 = t
    comment = ' Program starts '
    print 100, comment, t1
    do i = 1, n
        x(i) = i
    end do
    call cpu_time(t)
    t2 = t - t1
    comment = ' Integer assignment '
    print 100, comment, t2
    y = real(x)
    call cpu_time(t)
    t3 = t - t1 - t2
    comment = ' Real     assignment '
    print 100, comment, t2
    write (10) x
    call cpu_time(t)
    t4 = t - t1 - t2 - t3
    comment = ' Integer write '
```

```

print 100, comment, t4
write (10) y
call cpu_time(t)
t5 = t - t1 - t2 - t3 - t4
comment = ' Real      write '
print 100, comment, t5
100 format (1x, a, 2x, f7.3)
end program ch0914

```

Try this example out with your compiler. Unformatted is very efficient in terms of time. It also has the benefit for real or floating point numbers of no information loss.

Program starts	0.016
Integer assignment	0.078
Real assignment	0.078
Integer write	0.078
Real write	0.031

Note that binary or unformatted files are not necessarily portable between different compilers and different hardware platforms. You should consult your compiler documentation for help in this area.

9.10 Example 15: Implied Do Loops and Array Sections for Array Output

The following program shows how to use both implied do loops and array sections to output an array in a neat fashion:

```

program ch0915
implicit none
integer, parameter :: nrow = 5
integer, parameter :: ncol = 6
real, dimension (1:nrow*ncol) :: results = (/ &
50, 47, 28, 89, 30, 46, 37, 67, 34, 65, 68, &
98, 25, 45, 26, 48, 10, 36, 89, 56, 33, 45, &
30, 65, 68, 78, 38, 76, 98, 65 /)
real, dimension (1:nrow, 1:ncol) :: &
exam_results = 0.0
real, dimension (1:nrow) :: people_average = &
0.0

```

```

real, dimension (1:ncol) :: subject_average = &
  0.0
integer :: r, c

exam_results = reshape(results, (/nrow,ncol/), &
  (/0.0,0.0/), (/2,1/) )
exam_results(1:nrow, 3) = 2.5* &
  exam_results(1:nrow, 3)
subject_average = sum(exam_results, dim=1)
people_average = sum(exam_results, dim=2)
people_average = people_average/ncol
subject_average = subject_average/nrow
do r = 1, nrow
  print 100, (exam_results(r,c), c=1, ncol), &
    people_average(r)
end do
print *, &
  ' ===== ===== ===== ===== ===== ====='
print 110, subject_average(1:ncol)
100 format (1x, 6(1x,f5.1), ' = ', f6.2)
110 format (1x, 6(1x,f5.1))
end program ch0915

```

The print 100 uses an implied do loop and the print 110 uses an array section. Here is the output.

```

50.0  47.0  70.0  89.0  30.0  46.0 =  55.33
37.0  67.0  85.0  65.0  68.0  98.0 =  70.00
25.0  45.0  65.0  48.0  10.0  36.0 =  38.17
89.0  56.0  82.5  45.0  30.0  65.0 =  61.25
68.0  78.0  95.0  76.0  98.0  65.0 =  80.00
===== ===== ===== ===== ===== =====
53.8  58.6  79.5  64.6  47.2  62.0

```

We are using repeat factors in this example in the format statement to repeat the use of one or more edit descriptors, e.g. 6 (1x, f5.1).

We have also added a print statement to make the output a bit more understandable.

9.11 Example 16: Repetition and Whole Array Output

Take care when using whole arrays. Consider the following program:

```

program ch0916
    real, dimension (10, 10) :: y
    integer :: nrows = 6
    integer :: ncols = 7
    integer :: i, j
    integer :: k = 0

    do i = 1, nrows
        do j = 1, ncols
            k = k + 1
            y(i, j) = k
        end do
    end do
    write (unit=*, fmt=100) y
100 format (1x, 10f10.4)
end program ch0916

```

There are several points to note with this example. Firstly, this is a whole array reference, and so the entire contents of the array will be written; there is no scope for fine control. Secondly, the order in which the array elements are written is according to Fortran's array element ordering, i.e., the first subscript varying 1 to 10 (the array bound), with the second subscript as 1, then 1 to 10 with the second subscript as 2 and so on; the sequence is

```

Y(1,1)Y(2,1)Y(3,1)Y(10,1)
Y(1,2)Y(2,2)Y(3,2)Y(10,2)
.
.
.
Y(1,10)Y(2,10)Y(10,10)

```

Thirdly we have defined values for part of the array.

Finally we have used `write(unit=*, fmt=100)` and this will print to the screen.

9.12 Example 17: Choosing the Decimal Symbol

Fortran provides a mechanism to choose the decimal symbol. The `dc` edit descriptor sets the decimal symbol to a comma. The `dp` edit descriptor sets the decimal symbol to a full stop or period.

The following example

```

program ch0917
    implicit none

```

```
integer :: fluid
real :: litres
real :: pints

open (unit=1, file='ch0917.txt')
write (unit=1, fmt=100)
do fluid = 1, 10
    litres = fluid/1.75
    pints = fluid*1.75
    write (unit=1, fmt=110) pints, fluid, litres
end do
close (1)
100 format ('    Pints      Litres')
110 format (dc, ' ', f7.3, ' ', i3, ' ', f7.3)
end program ch0917
```

produces the following output.

Pints	Litres
1,750	1 0,571
3,500	2 1,143
5,250	3 1,714
7,000	4 2,286
8,750	5 2,857
10,500	6 3,429
12,250	7 4,000
14,000	8 4,571
15,750	9 5,143
17,500	10 5,714

9.13 Example 18: Alternative Format Specification Using a String

Here is an example of an alternate format specification using a string.

```
program ch0918
implicit none
integer :: t

print *, ''
print *, 'Twelve times table'
print *, ''
```

```

do t = 1, 12
    print ('( '' ', i3, ' ' * 12 = ' ', i3)', t, &
           t*12
    end do
end program ch0918

```

9.14 Example 19: Alternative Format Specification Using a Character Variable

Here is an example of using a character variable in a format specification.

```

program ch0919
    implicit none
    integer :: t
    character *30 :: fmt_100 = &
        '( '' ', i3, ' ' * 12 = ' ', i3)'

    print *, ' '
    print *, ' Twelve times table'
    print *, ' '
    do t = 1, 12
        write (unit=*, fmt=fmt_100) t, t*12
    end do
end program ch0919

```

9.15 The Remaining Control and Data Edit Descriptors

Tables 9.1 and 9.2 summarise details of the control and data edit descriptors available in Fortran.

9.16 Summary

You have been introduced in this chapter to the use of format or layout descriptors which will give you greater control over output.

The main features are:

- The `i` format for integer variables.
- The `e`, `f` and `g` formats for real numbers.
- The `a` format for characters.
- The `x`, which allows insertion of spaces.

Table 9.1 Summary of data edit descriptors

Descriptor	Description: data conversion
A w	Character
B w[.m]	Integer to/from binary
D w.d	Real
DT [character literal constant][(v-list)]	Derived type
E w.d[Ee]	Real with exponent
EN w.d[Ee]	Real to engineering
ES w.d[Ee]	Real to scientific
F w.d	Real with no exponent
G w.d[Ee]	Any intrinsic type
I w[.m]	Integer
L w	Logical
O	Octal
Z	Hexadecimal
Symbol	Explanation
w	Width of the field
m	Number of digits in the field
d	Number of digits after the decimal symbol
e	Number of digits in the exponent field
v	Signed integer literal constant Interpretation depends on the user Supplied derived type io subroutine

Table 9.2 Text edit descriptors

Descriptor	Description: data conversion
'text'	Transfer of a character literal constant to output record
"text"	Transfer of a character literal constant to output record

Output can be directed to files as well as to the terminal through the write statement. The `write`, together with the `open` and `close` statements, also introduces the class of Fortran statements which use equated keywords, as well as positionally dependent parameters.

The format statement and its associated layout or edit descriptor are powerful and allow repetition of patterns of output (both explicitly and implicitly).

9.17 Problems

9.1 Rewrite the temperature conversion program which was problem 7.3 in Chap. 7 to produce neat tabular output. Pay attention to the number of significant decimal places.

9.2 Information on car fuel consumption is usually given in miles per gallon in Britain and the United States and in l/100 km in Europe. Just to add an extra problem US gallons are 0.8 imperial gallons.

Prepare a table which allows conversion from either US or imperial fuel consumption figures to the metric equivalent. Use the parameter statement where appropriate:

```
1 imperial gallon = 4.54596 litres  
1 mile = 1.60934 kilometres
```

9.3 The two most commonly used operating systems for Fortran programming are UNIX and DOS. It is possible to use the operating system file redirection symbols

< >

to read from a file and write to a file, respectively. Rerun the program in problem 1 to write to a file using the open statement. Examine the file using an editor.

9.4 Modify any of the above to write to a file rather than the screen or terminal.

9.5 What features of Fortran reveal its evolution from punched card input?

9.6 Try to create a real number greater than the maximum possible on your computer—write it out. Try to repeat this for an integer. You may have to exercise some ingenuity.

9.7 Check what a number too large for the output format will be printed as on your local system—is it all asterisks?

9.8 Write a program which stores litres and corresponding pints in arrays. You should now be able to control the output of the table (excluding headings—although this could be done too) in a single write or print statement. If you don't like litres and pints, try some other conversion (sterling to US dollars, leagues to fathoms, Scots miles to Betelgeusian pfnings). The principle remains the same.

9.9 Fortran is an old programming language and the text formatting functionality discussed in this chapter assumes very dumb printing devices.

The primary assumption is that we are dealing with so-called monospace fonts, i.e., that digits, alphabetic characters, punctuation, etc., all have the same width.

If you are using a PC try using:

- Notepad
- and
- Word

to open your programs and some of the files created in this chapter. What happens to the layout?

If you are using Notepad look at the Word wrap and set Font options under the edit menu.

What fonts are available? What happens to the layout when you choose another font?

If you are using Word what fonts are available? What happens when you make changes to your file and exit Word? Is it sensible to save a Fortran source file as a Word document?

Chapter 10

Reading in Data

Winnie-the-Pooh read the two notices very carefully, first from left to right, and afterwards, in case he had missed some of it, from right to left.

A.A Milne, Winnie-the-Pooh

Aims

The aims of this chapter are to introduce some of the ideas involved in reading data into a program. In particular, using the following:

- Reading from files
- Reading integer data
- Reading real data
- Skipping columns of data in a file
- Skipping lines in a file
- Reading from several files consecutively
- Reading using internal files
- Timing of formatted and unformatted reads

10.1 Reading from Files

In the examples so far we have been reading from the keyboard using what Fortran calls list directed input. In this chapter we will look at reading data from files where the data is generally in tabular form.

10.2 Example 1: Reading Integer Data

In this example we are interested in reading in people's heights and weights in imperial measurements (feet and inches and stones and pounds) from a file and converting to their metric equivalent (metres and kilograms). The data is taken from an undergraduate class of Mechanical Engineering students.

Here is the data.

```

6   1   13   5
5   11  11   13
6   1   13   5
5   7   14   2
5   9   10   12
5   6   13   1
5   1   10   1
5   4   8    13
5   10  10   3
5   10  11   13

```

The first two columns are the heights in feet and inches, and the second two columns are the weights in stones and pounds.

Here is the program.

```

program ch1001
    implicit none
    integer, parameter :: npeople = 10
    integer, dimension (1:npeople) :: height_feet, &
        height_inch, weight_stone, weight_pound
    real, dimension (1:npeople) :: weight_kg, &
        height_m
    integer :: i

    open (unit=10, file='ch1001.txt')
    do i = 1, npeople
        read (10, fmt=100) height_feet(i), &
            height_inch(i), weight_stone(i), &
            weight_pound(i)
100     format (i2, 2x, i2, 2x, i2, 2x, i2)
        weight_kg(i) = (weight_stone(i)*14+ &
            weight_pound(i))/2.2
        height_m(i) = (height_feet(i)*12+height_inch &
            (i))*2.54/100
        write (unit=*, fmt=110) height_m(i), &
            weight_kg(i)
110     format (1x, f5.2, 2x, f4.1)
    end do
    close (10)
end program ch1001

```

Here is the output.

```
1.85 85.0
1.80 75.9
1.85 85.0
1.70 90.0
1.75 69.1
1.68 83.2
1.55 64.1
1.63 56.8
1.78 65.0
1.78 75.9
```

The first statement of interest is

```
open(unit=10,file='ch1001.txt')
```

which links the Fortran unit number 10 with a file called ch1001.txt
The next statements of interest are

```
read(10,fmt=100)height_feet(i),height_inch(i), &
                 weight_stone(i),weight_pound(i)
100 format(i2,2x,i2,2x,i2,2x,i2)
```

which reads 4 integer values from a line with integer data in columns 1–2, 5–6, 9–10 and 13–14 with 2 spaces between each value.

At the end of the program we close the file.

```
close(10)
```

We write out the metric versions of the height and weight with the following statement.

```
write(unit=*,fmt=200)height_m(i),weight_kg(i)
200 format(1x,f5.2,2x,f4.1)
```

We recommend that when working with formatted files you use a text editor that displays the column and line details.

NotePad under Windows has a status bar option under the View menu. Gvim under Windows has line and column information available. Under Redhat, vim and gedit both display line and column information. Under SuSe Linux kedit and vim display line and column information. There should be an editor available on your system that has this option.

10.3 Example 2: Reading Real Data

This example reads in the height and weight data created by the previous program and calculates their BMI values. BMI stands for Body Mass Index and is calculated as $Weight/Height^2$

Here is the program.

```
program ch1002
    implicit none
    integer, parameter :: n = 10
    real, dimension (1:n) :: h
    real, dimension (1:n) :: w
    real, dimension (1:n) :: bmi
    integer :: i

    open (unit=100, file='ch1001.out')
    do i = 1, n
        read (100, fmt='(1x,f5.2, 2x, f4.1)') h(i), &
            w(i)
    end do
    close (100)
    bmi = w/(h*h)
    do i = 1, n
        write (unit=*, fmt='(1x,f4.1)') bmi(i)
    end do
end program ch1002
```

The following statement

```
open(unit=100,file='ch1001.out')
```

links the Fortran unit number 100 with the file ch1001.out.

The following statement

```
read (100,fmt='(1x,f5.2, 2x, f4.1)') h(i), w(i)
```

reads the height and weight data from the file. We skip the first space then read the height from the next 5 columns in f5.1 format. We skip two spaces and then read the weight from the next 4 columns in f4.1 format.

The following statement

```
close(100)
```

closes the file.

The following statement

```
write(unit=*, fmt='(1x,f4.1)') bmi(i)
```

writes out the BMI values in f4.1 format.

Here is the output.

```
24.8  
23.4  
24.8  
31.1  
22.6  
29.5  
26.7  
21.4  
20.5  
24.0
```

10.4 Met Office Historic Station Data

The UK Met Office makes historic station data available.

Visit

[http://www.metoffice.gov.uk/public/weather/
climate-historic/#?tab=climateHistoric](http://www.metoffice.gov.uk/public/weather/climate-historic/#?tab=climateHistoric)

to see the data. The line has been broken to fit the page width.

The data consists of

- Mean daily maximum temperature (tmax)
- Mean daily minimum temperature (tmin)
- Days of air frost (af)
- Total rainfall (rain)
- Total sunshine duration (sun)

Here is a sample of the Nairn data. Nairn is a town in Scotland on the North Sea. The first seven lines have had to be formatted to fit the page width.

```
Nairn      there is a site change in 1998  
Location before 1998 2869E 8568N 8m amsl  
          after 1998 2912E 8573N 23 m amsl  
Estimated data is marked with a * after the value.  
Missing data (more than 2 days missing in month)  
is marked by    ---.  
Sunshine data taken from an automatic Kipp &
```

Zonen sensor marked with a #, otherwise
sunshine data taken from a
Campbell Stokes recorder.

YYYY	mm	tmax	tmin	af	rain	sun
		degC	degC	days	mm	hours
1931	1	5.0	0.6	11	78.4	43.4
1931	2	6.7	0.7	7	48.9	63.6
1931	3	6.2	-1.5	19	37.6	145.4
1931	4	10.4	3.1	3	44.6	110.1
1931	5	13.2	6.1	1	63.7	167.4
1931	6	15.4	8.0	0	87.8	150.3
1931	7	17.3	10.6	0	121.4	111.2
1931	8	15.6	9.1	0	57.2	127.5
1931	9	15.0	8.4	0	38.1	122.3
1931	10	12.1	5.5	2	59.4	95.8
1931	11	10.3	3.9	3	43.7	61.5
1931	12	8.9	3.2	7	33.6	36.5

In the examples that follow we will be using this station's data.

10.5 Example 3: Reading One Column of Data from a File

Here is the file we will be reading the rainfall values from.

1931	1	5.0	0.6	11	78.4	43.4
1931	2	6.7	0.7	7	48.9	63.6
1931	3	6.2	-1.5	19	37.6	145.4
1931	4	10.4	3.1	3	44.6	110.1
1931	5	13.2	6.1	1	63.7	167.4
1931	6	15.4	8.0	0	87.8	150.3
1931	7	17.3	10.6	0	121.4	111.2
1931	8	15.6	9.1	0	57.2	127.5
1931	9	15.0	8.4	0	38.1	122.3
1931	10	12.1	5.5	2	59.4	95.8
1931	11	10.3	3.9	3	43.7	61.5
1931	12	8.9	3.2	7	33.6	36.5
12345678901234567890123456789012345678901234567890						
1	2	3	4	5		

We have added two additional lines at the end to indicate the columns where the data is. These lines are not read by the program.

Here is the program.

```
program ch1003
    implicit none
    character*20 :: file_name = &
        'nairndata_01.txt'
    integer, parameter :: nmonths = 12
    real, dimension (1:nmonths) :: rainfall
    real :: rain_sum
    real :: rain_average
    integer :: i

    open (unit=100, file=file_name)
    do i = 1, nmonths
        read (unit=100, fmt=100) rainfall(i)
100 format (37x, f5.1)
    end do
    close (100)
    rain_sum = sum(rainfall)/25.4
    rain_average = rain_sum/nmonths
    write (unit=*, fmt=110)
110 format (19x, 'Yearly      Monthly', /, 19x, &
        'Sum          Average')
    write (unit=*, fmt=120) rain_sum, rain_average
120 format ('Rainfall (inches) ', f7.2, 2x, &
        f7.2)
end program ch1003
```

The data file is called `nairndata_01.txt` and we open the file at the start of the program and associate the file with unit 100.

The following statements read the 12 monthly values from the file skipping the first 37 characters.

```
do i=1,nmonths
    read(unit=100,fmt=100) rainfall(i)
100 format(37x,f5.1)
end do
```

We then close the file and calculate the rainfall sums and average and print out the results. Here is the output.

	Yearly	Monthly
	Sum	Average
Rainfall (inches)	28.13	2.34

The format statement 110 uses a/ to move to the next line, so that the headings line up.

10.6 Example 4: Skipping Lines in a File

This program is a simple variant of the last one.

Now we are reading from the original Met Office Nairn data file, which has seven header lines.

```
program ch1004
    implicit none
    character*20 :: file_name = 'nairnrdat.txt'
    integer, parameter :: nmonths = 12
    real, dimension (1:nmonths) :: rainfall
    real :: rain_sum
    real :: rain_average
    integer :: i

    open (unit=100, file=file_name)
    do i = 1, 7
        read (unit=100, fmt=*)
    end do
    do i = 1, nmonths
        read (unit=100, fmt=100) rainfall(i)
100 format (37x, f5.1)
    end do
    close (100)
    rain_sum = sum(rainfall)/25.4
    rain_average = rain_sum/nmonths
    write (unit=*, fmt=110)
110 format (19x, ' Yearly Monthly', /, 19x, &
               ' Sum      Average')
    write (unit=*, fmt=120) rain_sum, rain_average
120 format ('Rainfall (inches) ', f7.2, 2x, &
               f7.2)
end program ch1004
```

The key statements are

```
do i=1,7
    read(unit=100,fmt=*)
end do
```

which skips the data on these lines. Fortran reads a record at a time in this example. The output is as before.

10.7 Example 5: Reading from Several Files Consecutively

In this example we read from eight of the Met Office data files for Cardiff, Eastbourne, Lerwick, Leuchars, Nairn, Paisley, Ross On Wye and Valley.

We skip the first seven lines, then read year, month rainfall and sunshine data, skipping the other columns.

We then calculate rainfall and sunshine yearly totals and averages for these eight stations.

We use a character array to hold the station file names.

Here is the program.

```
program ch1005
  implicit none
  character*20, dimension (8) :: file_name = (/ &
    'cardiffdata.txt' , 'eastbourne data.txt' &
    , 'lerwickdata.txt' , &
    'leucharsdata.txt' , 'nairndata.txt' &
    , 'paisleydata.txt' , &
    'rossonwyedata.txt' , 'valleydata.txt' &
    /)

  integer, parameter :: nmonths = 12
  integer, dimension (1:nmonths) :: year, month
  real, dimension (1:nmonths) :: rainfall, &
    sunshine
  real :: rain_sum
  real :: rain_average
  real :: sun_sum
  real :: sun_average
  integer :: i, j
  character *80 :: fmt1 = '(3x,i4,2x,i2,3x,4x,4x,&
  &4x,4x,4x,3x,f5.1,3x,f5.1)'

do j = 1, 8
  open (unit=100, file=file_name(j))
  do i = 1, 7
    read (unit=100, fmt='(a)')
  end do
  do i = 1, nmonths
    read (unit=100, fmt=fmt1) year(i), &
      month(i), rainfall(i), sunshine(i)
  end do
  close (100)
  rain_sum = sum(rainfall)/25.4
```

```

sun_sum = sum(sunshine)
rain_average = rain_sum/nmonths
sun_average = sun_sum/nmonths
write (unit=*, fmt='(//,"Station = ",a,/)' ) &
       file_name(j)
write (unit=*, fmt= &
       '(2x,''Start ',i4,2x,i2)') year(1), &
       month(1)
write (unit=*, fmt= &
       '(2x,''End   ',i4,2x,i2)') year(12), &
       month(12)
write (unit=*, fmt=100)
100 format (19x, ' Yearly    Monthly', /, 19x, &
            ' Sum        Average')
write (unit=*, fmt=110) rain_sum, &
       rain_average
110 format ('Rainfall  (inches) ', f7.2, 2x, &
            f7.2)
write (unit=*, fmt=120) sun_sum, sun_average
120 format ('Sunshine           ', f7.2, 2x, &
            f7.2)
end do

end program ch1005

```

Each time round the loop we open one of the data files.

```
open(unit=100,file=file_name(j))
```

We then skip the next seven lines.

```

do i=1,7
  read(unit=100,fmt='(a)')
end do

```

We then read the data.

```

do i=1,nmonths
  read(unit=100,fmt=fmt1) &
  year(i),month(i),&
  rainfall(i),sunshine(i)
end do

```

We then close the file.

```
close(100)
```

We then do the calculations and print out the sum and average data for each site. The format statement uses // to generate a blank line.

Programs that will download the latest versions of the Met Office station data files are available on our web site. The programs are available for both Windows and Linux.

10.8 Example 6: Reading Using Array Sections

Consider the following output, which is the exam results data from an earlier chapter after scaling.

50.0	47.0	70.0	89.0	30.0	46.0
37.0	67.0	85.0	65.0	68.0	98.0
25.0	45.0	65.0	48.0	10.0	36.0
89.0	56.0	82.5	45.0	30.0	65.0
68.0	78.0	95.0	76.0	98.0	65.0

A program to read this file using array sections is as follows:

```
program ch1006
    implicit none
    integer, parameter :: nrow = 5
    integer, parameter :: ncol = 6
    real, dimension (1:nrow, 1:ncol) :: &
        exam_results = 0.0
    real, dimension (1:nrow) :: people_average = &
        0.0
    real, dimension (1:ncol) :: subject_average = &
        0.0
    integer :: r, c

    open (unit=100, file='ch1006.txt')
    do r = 1, nrow
        read (unit=100, fmt=100) exam_results(r, &
            1:ncol)
        people_average(r) = sum(exam_results(r,1: &
            ncol))
    end do
    close (100)
```

```

people_average = people_average/ncol
do c = 1, ncol
    subject_average(c) = sum(exam_results(1:nrow &
        ,c))
end do
subject_average = subject_average/nrow
do r = 1, nrow
    print 120, (exam_results(r,c), c=1, ncol), &
        people_average(r)
end do
print *, &
    ' ===== ===== ===== ===== ===== ====='
print 130, subject_average(1:ncol)
100 format (1x, 6(1x,f5.1), 4x, f6.2)
110 format (1x, 6(1x,f5.1))
120 format (1x, 6(1x,f5.1), ' = ', f6.2)
130 format (1x, 6(1x,f5.1))
end program ch1006

```

Here is the output.

```

50.0  47.0  70.0  89.0  30.0  46.0 = 55.33
37.0  67.0  85.0  65.0  68.0  98.0 = 70.00
25.0  45.0  65.0  48.0  10.0  36.0 = 38.17
89.0  56.0  82.5  45.0  30.0  65.0 = 61.25
68.0  78.0  95.0  76.0  98.0  65.0 = 80.00
===== ===== ===== ===== ===== =====
53.8  58.6  79.5  64.6  47.2  62.0

```

10.9 Example 7: Reading Using Internal Files

Sometimes external data does not have a regular structure and it is not possible to use the standard mechanisms we have covered so far in this chapter. Fortran provides something called internal files that allow us to solve this problem. The following example is based on a problem encountered whilst working at the following site

<http://www.shmu.sk/sk/?page=1>

They have data that is in the following format

```
#xxxxxxxxxx yyyyYYYYYY
```

where x and y can vary between 1 and 10 digits. The key here is to read the whole line (a maximum of 22 characters) and then scan the line for the blank character between the x and y digits.

We then use the `index` intrinsic to locate the position of the blank character. We now have enough information to be able to read the x and y integer data into the variables `n1` and `n2`.

```
program ch1007
  implicit none
  integer :: ib1, ib2
  integer :: n1, n2
  character (len=22) :: buffer, buff1, buff2
! program to read a record of the form
! #xxxxxxxxxx yyyyyyyyyy
! so that integers n1 = xxxxxxxxxx n2 =
! yyyyyyyyyy
! where the number of digits varies from 1 to 10
!
! use internal files
print *, 'input micael''s numbers'
read (*, '(a)') buffer
ib1 = index(buffer, ' ')
ib2 = len_trim(buffer)
buff1 = buffer(2:ib1-1)
buff2 = buffer(ib1+1:ib2)
read (buff1, '(i10)') n1
read (buff2, '(i10)') n2
print *, 'n1 = ', n1
print *, 'n2 = ', n2
end program ch1007
```

The statement

```
read(buff1,'(i10}')n1
```

reads from the string `buff1` and extracts the x number into the variable `n1`, and the statement

```
read(buff2,'(i10}')n2
```

reads from the string `buff2` and extracts the y number into the variable `n2`.

This is a very powerful feature and allows you to manage quite widely varying external data formats in files. `buff1` and `buff2` are called internal files in Fortran terminology.

10.10 Example 8: Timing of Reading Formatted Files

A program to read a formatted file is shown below:

```
program ch1008
    implicit none
    integer, parameter :: n = 10000000
    integer, dimension (1:n) :: x
    real, dimension (1:n) :: y
    integer :: i
    real :: t, t1, t2, t3
    character *15 :: comment

    call cpu_time(t)
    t1 = t
    comment = ' Program starts '
    print 120, comment, t1
    open (unit=10, file='ch0913.txt', &
          status='old')
    do i = 1, n
        read (10, 100) x(i)
    end do
    call cpu_time(t)
    t2 = t - t1
    comment = ' Integer read '
    print 120, comment, t2
    do i = 1, n
        read (10, 110) y(i)
    end do
    call cpu_time(t)
    t3 = t - t1 - t2
    comment = ' Real read '
    print 120, comment, t3
    do i = 1, 10
        print 130, x(i), y(i)
    end do
100 format (1x, i10)
110 format (1x, f10.0)
120 format (1x, a, 2x, f7.3)
130 format (1x, i4, 2x, f10.7)

end program ch1008
```

Here is some sample timing.

```
Program starts      0.016
Integer read       2.964
Real read          4.072
 1   1.0000000
 2   2.0000000
  ...
  ...
 9   9.0000000
10  10.0000000
```

10.11 Example 9: Timing of Reading Unformatted Files

The following is a program to read from an unformatted file:

```
program ch1009
  implicit none
  integer, parameter :: n = 10000000
  integer, dimension (1:n) :: x
  real, dimension (1:n) :: y
  integer :: i
  real :: t, t1, t2, t3
  character *15 :: comment

  call cpu_time(t)
  t1 = t
  comment = ' Program starts '
  print 100, comment, t1
  open (unit=10, file='ch0914.dat', &
        form='unformatted')
  read (10) x
  call cpu_time(t)
  t2 = t - t1
  comment = ' Integer read '
  print 100, comment, t2
  read (10) y
  call cpu_time(t)
  t3 = t - t1 - t2
  comment = ' Real read '
  print 100, comment, t3
  do i = 1, 10
    print 110, x(i), y(i)
  end do
100 format (1x, a, 2x, f7.3)
```

```
110 format (1x, i10, 2x, f10.6)
end program ch1009
```

Here is some sample timing.

```
Program starts      0.031
Integer read        0.016
Real read           0.031
      1      1.000000
      2      2.000000
      ...
      9      9.000000
     10     10.000000
```

10.12 Summary

This chapter has provided a coverage of some of the basics of reading data into a program in Fortran. We have seen examples that have

- Read integer data
- Read real data
- Skipped lines in a file
- Skipped columns of data in a file
- Read from files
- Used the open and close statements
- Associated unit numbers with files
- Read using fixed format data files
- Shown the time difference between using formatted files and unformatted files
- Used internal files

The above coverage should enable you make effective use of reading data in Fortran.

We would recommend not using edit descriptors when reading numeric data entered via the keyboard as it is difficult to see if the data matches what the edit descriptors expect.

10.13 Problems

10.1 Compile and run the examples in this chapter.

Note that you will have to run ch0913.f90 and ch0914.f90 to create the data files that are needed by ch1008.f90 and ch1009.f90

10.2 Write a program to read in and write out a real number using the following:

```
format(f7.2)
```

What is the largest number that you can read in and write out with this format? What is the largest negative number that you can read in and write out with this format? What is the smallest number, other than zero, that can be read in and written out?

10.3 Rewrite two of the earlier programs that used `read`, * and `print`, * to use `format` statements.

10.4 Write a program to read the file created by either the temperature conversion program or the litres and pints conversion program. Make sure that the programs ignore any header and title information. This kind of problem is very common in programming (writing a program to read and possibly manipulate data created by another program).

10.5 Demonstrate that input and output formats are not symmetric—i.e., what goes in does not necessarily come out.

10.6 What happens at your computer when you enter faulty data, inappropriate for the formats specified? We will look at how we address this problem in Chap. 18.

Chapter 11

Summary of I/O Concepts

It is a capital mistake to theorise before one has data.
Sir Arthur Conan Doyle

Aims

This chapter covers more formally some of the concepts introduced in Chaps. 9 and 10. There is a coverage of

- I/O concepts and I/O statements
- Files, records and streams
- Sequential, direct and stream access
- Options or specifiers on the `open` statement
- Options or specifiers on the `close` statement
- Options or specifiers on the `write` statement
- Options or specifiers on the `read` statement

11.1 I/O Concepts and Statements

Fortran input and output statements provide the means of transferring data from external media to internal storage or from an internal file to internal storage and vice versa.

The input/output statements are the `open`, `close`, `read`, `write`, `print`, `backspace`, `endfile`, `rewind`, `flush`, `wait`, and `inquire` statements.

The `inquire` statement is a file inquiry statement.

The `backspace`, `endfile`, and `rewind` statements are file positioning statements.

Data is commonly organised in either record files or stream files. In a record type file transfers are done a record at a time. In a stream type file transfers are done in file storage units.

11.2 Records

A record is a sequence of values or a sequence of characters. There are three kinds of records:

- formatted
- unformatted
- end of file

A record in Fortran is commonly called a logical record.

A formatted record is typically a sequence of printable characters. You have seen examples in earlier chapters.

You saw examples of unformatted i/o in the previous chapters.

11.3 File Access

The three file access methods are:

- sequential
- direct
- stream

The examples so far have shown sequential access.

Direct access is a method of accessing the records of an external record file in arbitrary order.

Stream access is a method of accessing the file storage units of an external stream file. The properties of an external file connected for stream access depend on whether the connection is for unformatted or formatted access.

11.4 The `open` Statement

An `open` statement initiates or modifies the connection between an external file and a specified unit. The `open` statement can do a number of things including

- connect an existing file to a unit;
- create a file that is preconnected;
- create a file and connect it to a unit;
- change certain modes of a connection between a file and a unit.

The only keyword option that can be omitted is the `unit` specifier. This is assumed to be the first parameter of the `open` statement.

Table 11.1 summarises the `open` statement options:

Table 11.1 Open statement options

<code>unit =</code>	file-unit-number
<code>access =</code>	sequential, direct or stream
<code>action =</code>	read, write or readwrite
<code>asynchronous =</code>	yes or no
<code>blank =</code>	null or zero
<code>decimal =</code>	comma or point
<code>delim =</code>	apostrophe, quote or none
<code>encoding =</code>	utf8 or default
<code>err =</code>	statement label
<code>file =</code>	file name
<code>form =</code>	formatted or unformatted
<code>iomsg =</code>	iomsg-variable
<code>iostat =</code>	scalar-int-variable
<code>newunit =</code>	scalar-int-variable
<code>pad =</code>	yes or no
<code>position =</code>	asis, rewind, append
<code>recl =</code>	record length, positive integer
<code>round =</code>	up, down, zero, nearest, compatible or processor defined
<code>sign =</code>	plus, suppress or processor defined
<code>status =</code>	old, new, scratch, replace or unknown

11.5 Data Transfer Statements

The `read`, `write` and `print` statements are used to transfer data to and from files.

Table 11.2 summarises the options of the data transfer statements.

Table 11.2 Data transfer statement options

<code>unit =</code>	<code>io-unit</code>
<code>fmt =</code>	<code>format</code>
<code>nml =</code>	<code>namelist-group-name</code>
<code>advance =</code>	<code>yes</code> or <code>no</code>
<code>asynchronous =</code>	<code>yes</code> or <code>no</code>
<code>blank =</code>	<code>null</code> or <code>zero</code>
<code>decimal =</code>	<code>comma</code> or <code>point</code>
<code>delim =</code>	<code>apostrophe</code> , <code>quote</code> or <code>none</code>
<code>end =</code>	<code>label</code>
<code>eor =</code>	<code>label</code>
<code>err =</code>	<code>label</code>
<code>id =</code>	<code>scalar-int-variable</code>
<code>iomsg =</code>	<code>iomsg-variable</code>
<code>iostat =</code>	<code>scalar-int-variable</code>
<code>pad =</code>	<code>yes</code> or <code>no</code>
<code>pos =</code>	file position in file storage units
<code>rec =</code>	record number to be read or written
<code>round =</code>	<code>up</code> , <code>down</code> , <code>zero</code> , <code>nearest</code> , <code>compatible</code> or processor defined
<code>sign =</code>	<code>plus</code> , <code>suppress</code> or processor defined
<code>size =</code>	<code>scalar-int-variable</code>

11.6 The inquire Statement

Table 11.3 summarises the options on the inquire statement.

Table 11.3 Inquire statement options

unit =	file-unit-number
file =	file name
access =	sequential, direct, stream
action =	read, write, readwrite, undefined
asynchronous =	yes, no
blank =	zero, null
decimal =	comma, point
delim =	apostrophe, quote, none
direct =	yes, no, unknown
encoding =	utf8, default
err =	label
exist =	true, false
form =	formatted, unformatted, undefined
formatted =	yes, no, unknown
id =	scalar-int-expr
iomsg =	iomsg-variable
iostat =	scalar-int-variable
name =	file name
named =	scalar-logical-variable
nextrec =	scalar-int-variable
number =	unit number, -1 if unassigned
opened =	true, false
pad =	yes, no
pending =	scalar-logical-variable
pos =	scalar-int-variable
position =	scalar-default-char-variable
read =	yes, no, unknown
readwrite =	yes, no, unknown
recl =	scalar-int-variable
round =	up, down, zero, nearest, compatible or processor defined
sequential =	yes, no, unknown
sign =	plus, suppress, processor defined
size =	scalar-int-variable
stream =	yes, no, unknown
unformatted =	yes, no, unknown
write =	yes, no, unknown

11.7 Error, End of Record and End of File

The set of input/output error conditions is processor dependent.

An end-of-record condition occurs when a non-advancing input statement attempts to transfer data from a position beyond the end of the current record, unless the file is a stream file and the current record is at the end of the file (an end-of-file condition occurs instead). An end-of-file condition occurs when

- an endfile record is encountered during the reading of a file connected for sequential access,
- an attempt is made to read a record beyond the end of an internal file, or
- an attempt is made to read beyond the end of a stream file.

An end-of-file condition may occur at the beginning of execution of an input statement. An end-of-file condition also may occur during execution of a formatted input statement when more than one record is required by the interaction of the input list and the format. An end-of-file condition also may occur during execution of a stream input statement.

11.7.1 *Error Conditions and the **err=** Specifier*

The set of error conditions which are detected is processor dependent. The standard does not specify any i/o errors. Compilers will vary in the errors they detect and how they treat them. The **err=** option provides one way of catching errors and taking the appropriate action.

11.7.2 *End-of-file Condition and the **end=** Specifier*

An end of file occurs may occur during an input transfer. The **end=** option provides a way of handling the end of file in a program.

11.7.3 *End-of-Record Condition and the **eor=** Specifier*

An end of record may occur during an input transfer. The **eor=** option provides a way of handling this in a program.

11.7.4 iostat=Specifier

Execution of an input/output statement containing the `iostat=` specifier causes the scalar-int-variable in the `iostat=` specifier to become defined with one of a set of values. Normally

- 0 if no errors occur
- a processor dependent negative value if end-of-file occurs
- a processor dependent negative value if an end-of-record occurs

If you use `iostat_inquire_internal_unit` from the intrinsic module `iso_fortran_env` you will get a processor-dependent positive integer value if a unit number in an inquire statement identifies an internal file.

When using `iostat_inquire_internal_unit` you will get a processor-dependent positive integer value which is different from the above if any other error condition occurs.

11.7.5 iomsg=Specifier

If an error, end-of-file, or end-of-record condition occurs during execution of an input/output statement, the processor shall assign an explanatory message to `iomsg`-variable. If no such condition occurs, the processor shall not change the value of `iomsg`-variable.

11.8 Examples

Here are three examples using the `iostat=` option. Examples illustrating some of the other options can be found throughout the rest of the book.

11.8.1 Example 1: Simple Use of the `read`, `write`, `open`, `close`, `unit` Features

This example shows the use of several of the i/o features including

- the `write` statement
- the `read` statement
- the use of `unit=6` on a write statement
- the use of `unit=5` on a read statement
- several `fmt=` variations
- the `open` statement

- the `file=` option on the `open` statement
- the `iostat=` option on the `open` statement
- the `close` statement

```

program ch1101
    implicit none
    integer :: filestat
    real :: x
    character (len=20) :: which

    do

        write (unit=6, fmt= &
            ('("data file name,or end")'))
        read (unit=5, fmt='(a)') which
        if (which=='end') exit
        open (unit=1, file=which, iostat=filestat, &
            status='old')
        if (filestat>0) then
            print *, &
                'error opening file, please check'
            stop
        end if
        read (unit=1, fmt=100) x
        write (unit=6, fmt=110) which, x
        close (unit=1)

    end do

100 format (f6.0)
110 format ('from file ', a, ' x = ', f8.2)
end program ch1101

```

It is common for compilers to associate units 5 and 6 with the keyboard and screen.

11.8.2 Example 2: Using `iostat` to Test for Errors

```

program ch1102
    implicit none
    integer :: io_stat_number = -1
    integer :: i

    do
        print *, 'input integer i:'

```

```

read (unit=*, fmt=100, iostat=io_stat_number &
      ) i
print *, ' iostat=' , io_stat_number
if (io_stat_number==0) exit
end do
print *, 'i = ', i, ' read successfully'
100 format (i3)
end program ch1102

```

11.9 Example 3: Use of **newunit** and **lentrim**

This example illustrates the use of the following:

- the `len_trim` function
- the `newunit` option on the `read` statement to get an unused `unit` number
- the use of `iostat=` to test whether a file was opened correctly
- the use of the `cycle` control statement to go back to the start of the `do` and try reading the file name again
- the use of the `iostat` option to test if the read was successful

```

program ch1103
  implicit none
  character (len=20) :: station, file_name
  integer :: i, io_stat_number, filestat,flen, &
             uno
  integer, parameter :: nmonths = 12
  integer, dimension (1:nmonths) :: year, month
  real, dimension (1:nmonths) :: &
    rainfall, sunshine
  real :: rain_sum
  real :: rain_average
  real :: sun_sum
  real :: sun_average

  do
    print *, 'input weather station'
    print *, ' or "end" to stop program'
    read '(a)', station
    if (station=='end') exit
   flen = len_trim(station)
    file_name = station(1:flen) // 'data.txt'
    open (newunit=uno, file=file_name, &
          iostat=filestat, status='old')
    if (filestat/=0) then

```

```
print *, 'error opening file ', file_name
print *, 'Retype the file name'
cycle
end if
do i = 1, 7
  read (unit=uno, fmt='(a)')
end do
do i = 1, nmonths
  read (unit=uno, fmt=100, iostat= &
        io_stat_number) year(i), month(i), &
        rainfall(i), sunshine(i)
  100 format (3x, i4, 2x, i2, 27x, f4.1, 3x, &
              f5.1)
  if (io_stat_number/=0) then
    print *, ' error reading record ', &
    i + 8, &
    ' so following results incorrect:'
    exit
  end if
end do
close (unit=uno)
rain_sum = sum(rainfall)/25.4
sun_sum = sum(sunshine)
rain_average = rain_sum/nmonths
sun_average = sun_sum/nmonths
write (unit=*, fmt=110) station
  110 format (//, 'Station = ', a, '/')
write (unit=*, fmt=120) year(1), month(1)
  120 format (2x, 'Start ', i4, 2x, i2)
write (unit=*, fmt=130) year(12), month(12)
  130 format (2x, 'Start ', i4, 2x, i2)
write (unit=*, fmt=140)
  140 format (19x, ' Yearly Monthly', /, 19x, &
              ' Sum Average')
write (unit=*, fmt=150) rain_sum, &
  rain_average
  150 format ('Rainfall (inches) ', f7.2, 2x, &
              f7.2)
write (unit=*, fmt=160) sun_sum, sun_average
  160 format ('Sunshine ', f7.2, 2x, f7.2)
end do
end program ch1103
```

In this program based on an earlier example in Chap. 10, we have use of the `newunit` option on the `open` statement. A unique negative number is returned, which cannot clash with any user specified unit number, which are always positive. We are also using the character intrinsic function `len_trim` and the character operator

```
//
```

We also introduce the `do end do` and `cycle` statements. These are covered in more detail in Chap. 13.

11.10 Unit Numbering

Care must be taken with unit numbering as firstly they must always be positive, and secondly many compilers have conventions that apply, for example unit 5 is often associated with the `read *` statement and unit 6 is often associated with the `print *` statement.

11.11 Summary

This chapter has listed most of the i/o options available in Fortran. There are a small number of examples that illustrate some of their use.

Later chapters provide additional examples.

11.12 Problems

The Whitby data and Cardiff data are on our web pages.

11.1 Compile and run the examples in this chapter.

11.2 With the Whitby or Cardiff data make a mistake, e.g., a non-numeric character in the last column. Test program `ch1103.f90` to see that it picks this up.

Chapter 12

Functions

*I can call spirits from the vasty deep. Why so can I, or so can
any man; but will they come when you do call for them?*

William Shakespeare, King Henry IV, part 1

Aims

The aims of this chapter are:

- To consider some of the reasons for the inclusion of functions in a programming language.
- To introduce, with examples, some of the predefined functions available in Fortran.
- To introduce a classification of intrinsic functions, generic, elemental, transformational.
- To introduce the concept of a user defined function.
- To introduce the concept of a recursive function.
- To introduce the concept of user defined elemental and pure functions.
- To briefly look at scope rules in Fortran for variables and functions.
- To look at internal user defined functions.

12.1 Introduction

The role of functions in a programming language and in the problem-solving process is considerable and includes:

- Allowing us to refer to an action using a meaningful name, e.g., `sine(x)` a very concrete use of abstraction.
- Providing a mechanism that allows us to break a problem down into parts, giving us the opportunity to structure our problem solution.
- Providing us with the ability to concentrate on one part of a problem at a time and ignore the others.

- Allowing us to avoid the replication of the same or very similar sections of code when solving the same or a similar subproblem which has the secondary effect of reducing the memory requirements of the final program.
- Allowing us to build up a library of functions or modules for solving particular subproblems, both saving considerable development time and increasing our effectiveness and productivity.

Some of the underlying attributes of functions are:

- They take parameters or arguments.
- The parameter(s) can be an expression.
- A function will normally return a value and the value returned is normally dependent on the parameter(s).
- They can sometimes take arguments of a variety of types.

Most languages provide both a range of predefined functions and the facility to define our own. We will look at the predefined functions first.

12.2 An Introduction to Predefined Functions and Their Use

Fortran provides over a hundred intrinsic functions and subroutines. For the purposes of this chapter a subroutine can be regarded as a variation on a function. Subroutines are covered in more depth in a later chapter. They are used in a straightforward way. If we take the common trigonometric functions, sine, cosine and tangent, the appropriate values can be calculated quite simply by:

```
x=sin(y)
z=cos(y)
a=tan(y)
```

This is in rather the same way that we might say that x is a function of y , or x is sine y . Note that the argument, y , is in radians not degrees.

12.2.1 Example 1: Simple Function Usage

A complete example is given below:

```
program ch1201
    implicit none
    real :: x
    print *, ' type in an angle (in radians)'
    read *, x
    print *, ' Sine of ', x, ' = ', sin(x)
end program ch1201
```

Table 12.1 Some of the intrinsic functions available in Fortran

Function	Action	Example
int	Conversion to integer	j = int(x)
real	Conversion to real	x = real(j)
abs	Absolute value	x = abs(x)
mod	Remaindering Remainder when I divided by j	k = mod(i,j)
sqrt	Square root	x = sqrt(y)
exp	Exponentiation	y = exp(x)
log	Natural logarithm	x = log(y)
log10	Common logarithm	x = log10(y)
sin	Sine	x = sin(y)
cos	Cosine	x = cos(y)
tan	Tangent	x = tan(y)
asin	Arcsine	y = asin(x)
acos	Arcosine	y = acos(x)
atan	Arctangent	y = atan(x)
atan2	Arctangent(a/b)	y = atan2(a,b)

These functions are called intrinsic functions. Table 12.1 has details of some of the intrinsic functions available in Fortran.

A more complete list is given in Appendix B.

12.3 Generic Functions

All but four of the intrinsic functions and procedures are generic, i.e., they can be called with arguments of one of a number of kind types.

12.3.1 Example 2: The **abs** Generic Function

The following short program illustrates this with the **abs** intrinsic function:

```
program ch1202
  implicit none
  complex :: c = cmplx(1.0, 1.0)
  real :: r = 10.9
  integer :: i = -27
  print *, abs(c)
```

```

print *, abs(r)
print *, abs(i)
end program ch1202

```

Type this program in and run it on the system you use.

It is now possible with Fortran for the arguments to the intrinsic functions to be arrays. It is convenient to categorise the functions into either elemental or transformational, depending on the action performed on the array elements.

12.4 Elemental Functions

These functions work with both scalar and array arguments, i.e., with arguments that are either single or multiple valued.

12.4.1 Example 3: Elemental Function Use

Taking the earlier example with the evaluation of sine as a basis, we have:

```

program ch1203
    implicit none
    real, dimension (5) :: x = (/ 1.0, 2.0, 3.0, &
        4.0, 5.0 /)
    print *, ' sine of ', x, ' = ', sin(x)
end program ch1203

```

In the above example the sine function of each element of the array x is calculated and printed.

12.5 Transformational Functions

Transformational functions are those whose arguments are arrays, and work on these arrays to transform them in some way.

12.5.1 Example 4: Simple Transformational Use

To highlight the difference between an element-by-element function and a transformational function consider the following examples:

```

program ch1204
    implicit none
    real, dimension (5) :: x = (/ 1.0, 2.0, 3.0, &
        4.0, 5.0 /)
! elemental function
    print *, ' sine of ', x, ' = ', sin(x)
! transformational function
    print *, ' sum of ', x, ' = ', sum(x)
end program ch1204

```

The `sum` function adds each element of the array and returns the sum as a scalar, i.e., the result is single valued and not an array.

12.5.2 Example 5: Intrinsic dot_product Use

The following program uses the transformational function `dot_product`:

```

program ch1205
    implicit none
    real, dimension (5) :: x = (/ 1.0, 2.0, 3.0, &
        4.0, 5.0 /)

    print *, ' dot product of x with x is'
    print *, ' ', dot_product(x, x)
end program ch1205

```

Try typing these examples in and running them to highlight the differences between elemental and transformational functions.

12.6 Notes on Function Usage

You should not use variables which have the same name as the intrinsic functions; e.g., what does `sin(x)` mean when you have declared `sin` to be a real array?

When a function has multiple arguments care must be taken to ensure that the arguments are in the correct position and of the appropriate kind type.

You may also replace arguments for functions by expressions, e.g.,

```
x = log(2.0)
or
x = log(abs(y))
or
x = log(abs(y)+z/2.0)
```

12.7 Example 6: Easter

This example uses only one function, mod (or modulus). It is used several times, helping to emphasise the usefulness of a convenient, easily referenced function. The program calculates the date of Easter for a given year. It is derived from an algorithm by Knuth, who also gives a fuller discussion of the importance of its algorithm. He concludes that the calculation of Easter was a key factor in keeping arithmetic alive during the Middle Ages in Europe. Note that determination of the Eastern churches' Easter requires a different algorithm:

```
program ch1206
implicit none
integer :: year, metcyc, century, error1, &
           error2, day
integer :: epact, luna, temp
! a program to calculate the date of easter
print *, ' input the year for which easter'
print *, ' is to be calculated'
print *, ' enter the whole year, e.g. 1978 '
read *, year
! calculating the year in the 19 year
! metonic cycle using variable metcyc
metcyc = mod(year, 19) + 1
if (year<=1582) then
  day = (5*year)/4
  epact = mod(11*metcyc-4, 30) + 1
else
  ! calculating the century-century
  century = (year/100) + 1
!  accounting for arithmetic inaccuracies
!  ignores leap years etc.
  error1 = (3*century/4) - 12
  error2 = ((8*century+5)/25) - 5
!  locating Sunday
```

```

    day = (5*year/4) - error1 - 10
!   locating the epact(full moon)
    temp = 11*metcyc + 20 + error2 - error1
    epact = mod(temp, 30)
    if (epact<=0) then
        epact = 30 + epact
    end if
    if ((epact==25 .and. metcyc>11) .or. &
        epact==24) then
        epact = epact + 1
    end if
    end if
! finding the full moon
    luna = 44 - epact
    if (luna<21) then
        luna = luna + 30
    end if
! locating easter Sunday
    luna = luna + 7 - (mod(day+luna,7))
! locating the correct month
    if (luna>31) then
        luna = luna - 31
        print *, ' for the year ', year
        print *, ' easter falls on April ', luna
    else
        print *, ' for the year ', year
        print *, ' easter falls on march ', luna
    end if
end program ch1206

```

We have introduced a new statement here, the `if then endif`, and a variant the `if then else endif`. A more complete coverage is given in the chapter on control structures. The main point of interest is that the normal sequential flow from top to bottom can be varied. In the following case,

```

if (expression) then
    block of statements
endif

```

If the expression is true the block of statements between the `if then` and the `endif` is executed. If the expression is false then this block is skipped, and execution proceeds with the statements immediately after the `endif`.

In the following case,

```
if (expression) then
    block 1
else
    block 2
endif
```

if the expression is true block 1 is executed and block 2 is skipped. If the expression is false then block 2 is executed and block 1 is skipped. Execution then proceeds normally with the statement immediately after the `endif`.

As well as noting the use of the `mod` generic function in this program, it is also worth noting the structure of the decisions. They are nested, rather like the nested do loops we met earlier.

12.8 Intrinsic Procedures

An alphabetical list of all intrinsic functions and subroutines is given in appendix B. This list provides the following information:

- Function name.
- Description.
- Argument name and type.
- Result type.
- Classification.
- Examples of use.

This appendix should be consulted for a more complete and thorough understanding of intrinsic procedures and their use in Fortran.

12.9 Supplying Your Own Functions

There are two stages here: firstly, to define the function and, secondly, to reference or use it. Consider the calculation of the greatest common divisor of two integers.

12.9.1 Example 7: Simple User Defined Function

The following defines a function to achieve this:

```
module gcd_module
contains
```

```
integer function gcd(a, b)
    implicit none
    integer, intent (in) :: a, b
    integer :: temp

    if (a<b) then
        temp = a
    else
        temp = b
    end if
    do while ((mod(a,temp)/=0) .or. (mod(b, &
        temp)/=0))
        temp = temp - 1
    end do
    gcd = temp
end function gcd

end module gcd_module
```

To use this function, you reference or call it with a form like:

```
program ch1207

use gcd_module

implicit none
integer :: i, j, result

print *, ' type in two integers'
read *, i, j
result = gcd(i, j)
print *, ' gcd is ', result

end program ch1207
```

We will start by talking about the actual function and then cover the following statements

```
module gcd_module
contains
  ..
  ..
end module gcd_module
```

later.

The first line of the function

```
integer function gcd(a,b)
```

has a number of items of interest:

- Firstly the function has a type, and in this case the function is of type integer, i.e., it will return an integer value.
- The function has a name, in this case `gcd`.
- The function takes arguments or parameters, in this case `a` and `b`.

The structure of the rest of the function is the same as that of a program, i.e., we have declarations, followed by the executable part. This is because both a program and a function can be regarded as a program unit in Fortran terminology. We will look into this more fully in later chapters.

In the declaration we also have a new attribute for the integer declaration. The two parameters `a` and `b` are of type integer, and the `intent(in)` attribute means that these parameters will NOT be altered by the function. It is good programming practice for functions not to have side effects, i.e. not modify their arguments, and do no i/o.

The value calculated is returned through the function name somewhere in the body of the executable part of the function. In this case `gcd` appears on the left-hand side of an arithmetic assignment statement at the bottom of the function. The end of the function is signified in the same way as the end of a program:

```
end function gcd
```

We then have the program which actually uses the function `gcd`. In the program the function is called or invoked with `i` and `j` as arguments. The variables are called `a` and `b` in the function, and references to `a` and `b` in the function will use the values that `i` and `j` have respectively in the main program. We cover the area of argument association in the next section.

Note also a new control statement, the `do while enddo`. In the following case,

```
do while (expression)
    block of statements
enddo
```

the block of statements between the `do while` and the `enddo` is executed whilst the expression is true. There is a more complete coverage in Chap. 13.

We have two options here regarding compilation. Firstly, to make the function and the program into one file, and invoke the compiler once. Secondly, to make the function and program into separate files, and invoke the compiler twice, once

for each file. With large programs comprising one program and several functions it is probably worthwhile to keep the component parts in different files and compile individually, whereas if it consists of a simple program and one function then keeping things together in one file makes sense.

12.10 An Introduction to the Scope of Variables, Local Variables and Interface Checking

One of the major strengths of Fortran is the ability to work on parts of a problem at a time. This is achieved by the use of program units (a main program, one or more functions and one or more subroutines) to solve discrete subproblems. Interaction between them is limited and can be isolated, for example, to the arguments of the function. Thus variables in the main program can have the same name as variables in the function and they are completely separate variables, even though they have the same name. Thus we have the concept of a local variable in a program unit.

In the example above `i`, `j`, `result`, are local to the main program. The declaration of `gcd` is to tell the compiler that it is an integer, and in this case it is an external function.

`a` and `b` in the function `gcd` do not exist in any real sense; rather they will be replaced by the actual variable values from the calling routine, in this case by whatever values `i` and `j` have. `temp` is local to `gcd`.

A common programming error in Fortran 66 and 77 was mismatches between actual and dummy arguments. Problems caused by this were often very subtle and hard to find.

Fortran 90 introduced a solution to the problem via the use of modules and contains statements. We have added

```
module gcd_module
contains
  ...
end module gcd_module
```

around the function definition, which contains the function in a module and the following statement in the main program

```
use gcd_module
```

provides an explicit interface (in Fortran terminology) that requires the compiler to check at compile time that the call is correct, i.e. that there are the correct number of parameters, they are of the correct type and in this case that the function return type is correct. We will cover this area in greater depth in later chapters.

12.11 Recursive Functions

There is an additional form of the function header that must be used when the function is recursive. Recursion means the breaking down of a problem into a simpler but identical subproblem. The concept is best explained with reference to an actual example. Consider the evaluation of a factorial, e.g., $5!$. From simple mathematics we know that the following is true:

$$\begin{aligned}5! &= 5 * 4! \\4! &= 4 * 3! \\3! &= 3 * 2! \\2! &= 2 * 1! \\1! &= 1\end{aligned}$$

and thus $5! = 5 * 4 * 3 * 2 * 1$ or 120.

12.11.1 Example 8: Recursive Factorial Evaluation

Let us look at a program with recursive function to solve the evaluation of factorials.

```
module factorial_module
    implicit none

    contains
        recursive integer function factorial(i) &
            result (answer)
        implicit none
        integer, intent (in) :: i

        if (i==0) then
            answer = 1
        else
            answer = i*factorial(i-1)
        end if
    end function factorial
end module factorial_module

program ch1208
    use factorial_module
    implicit none
    integer :: i, f
```

```

print *, ' type in the number, integer only'
read *, i
do while (i<0)
    print *, ' factorial only defined for '
    print *, ' positive integers: re-input'
    read *, i
end do
f = factorial(i)
print *, ' answer is', f
end program ch1208

```

What additional information is there? Firstly, we have an additional attribute on the function header that declares the function to be recursive. Secondly, we must return the result in a variable, in this case `answer`. Let us look now at what happens when we compile and run the whole program (both function and main program). If we type in the number 5 the following will happen:

- The function is first invoked with argument 5. The else block is then taken and the function is invoked again.
- The function now exists a second time with argument 4. The else block is then taken and the function is invoked again.
- The function now exists a third time with argument 3. The else block is then taken and the function is invoked again.
- The function now exists a fourth time with argument 2. The else block is then taken and the function is invoked again.
- The function now exists a fifth time with argument 1. The else block is then taken and the function is invoked again.
- The function now exists a sixth time with argument 0. The if block is executed and `answer=1`. This invocation ends and we return to the previous level, with `answer=1*1`.
- We return to the previous invocation and now `answer=2*1`.
- We return to the previous invocation and now `answer=3*2`.
- We return to the previous invocation and now `answer=4*6`.
- We return to the previous invocation and now `answer=5*24`.

The function now terminates and we return to the main program or calling routine. The answer 120 is the printed out.

Add a `print *, i` statement to the function after the last declaration and type the program in and run it. Try it out with 5 as the input value to verify the above statements.

Recursion is a very powerful tool in programming, and remarkably simple solutions to quite complex problems are possible using recursive techniques. We will look at recursion in much more depth in the later chapters on dynamic data types, and subroutines and modules.

12.12 Example 9: Recursive Version of GCD

The following is another example of the earlier gcd function but with the algorithm in the function replaced with an alternate recursive solution:

```

module gcd_module
    implicit none

contains
    recursive integer function gcd(i, j) &
        result (answer)
    implicit none
    integer, intent (in) :: i, j

    if (j==0) then
        answer = i
    else
        answer = gcd(j, mod(i,j))
    end if
end function gcd
end module gcd_module

program ch1209
    use gcd_module
    implicit none
    integer :: i, j, result

    print *, ' type in two integers'
    read *, i, j
    result = gcd(i, j)
    print *, ' gcd is ', result
end program ch1209

```

Try this program out on the system you work with, look at the timing information provided, and compare the timing with the previous example. The algorithm is a much more efficient algorithm than in the original example, and hence should be much faster. On one system there was a twentyfold decrease in execution time between the two versions.

Recursion is sometimes said to be inefficient, and the following example looks at a nonrecursive version of the second algorithm.

12.13 Example 10: GCD After Removing Recursion

The following is a variant of the above, with the same algorithm, but with the recursion removed:

```
module gcd_module
    implicit none

contains
    integer function gcd(i, j)
        implicit none
        integer, intent (inout) :: i, j
        integer :: temp

        do while (j /= 0)
            temp = mod(i, j)
            i = j
            j = temp
        end do
        gcd = i
    end function gcd
end module gcd_module

program ch1210
    use gcd_module
    implicit none
    integer :: i, j, result

    print *, ' type in two integers'
    read *, i, j
    result = gcd(i, j)
    print *, ' gcd is ', result
end program ch1210
```

12.14 Internal Functions

An internal function is a more restricted and hidden form of the normal function definition.

Since the internal function is specified within a program segment, it may only be used within that segment and cannot be referenced from any other functions or subroutines, unlike the intrinsic or other user defined functions.

12.14.1 Example 11: Stirling's Approximation

In this example we use Stirling's approximation for large n,

$$n! = \sqrt{2\pi n} (n/e)^n$$

and a complete program to use this internal function is given below:

```
program ch1211
    implicit none
    real :: result, n, r

    print *, ' type in n and r'
    read *, n, r
! number of possible combinations that can
! be formed when
! r objects are selected out of a group of n
! n!/r!(n-r)!
    result = stirling(n)/(stirling(r)*stirling(n-r &
        ))
    print *, result
    print *, n, r
contains
    real function stirling(x)
        real, intent (in) :: x
        real, parameter :: pi = 3.1415927, &
            e = 2.7182828

        stirling = sqrt(2.*pi*x)*(x/e)**x
    end function stirling
end program ch1211
```

The difference between this example and the earlier ones lies in the contains statement. The function is now an integral part of the program and could not, for example, be used elsewhere in another function. This provides us with a very powerful way of information hiding and making the construction of larger programs more secure and bug free.

12.15 Pure Functions

We mentioned earlier that functions should not have side effects. If your functions do have side effects and are running the code on parallel systems we have the additional problem that it may not actually work! We would also like to be able to take advantage

of automatic parallelisation if possible. In the following example we show how to do this using the pure prefix specification.

```

module gcd_module
    implicit none

contains
    pure integer function gcd(a, b)
        implicit none
        integer, intent (in) :: a, b
        integer :: temp

        if (a<b) then
            temp = a
        else
            temp = b
        end if
        do while ((mod(a,temp)/=0) .or. (mod(b, &
            temp)/=0))
            temp = temp - 1
        end do
        gcd = temp
    end function gcd
end module gcd_module

program ch1212
    use gcd_module
    implicit none
    integer :: i, j, result

    print *, ' type in two integers'
    read *, i, j
    result = gcd(i, j)
    print *, ' gcd is ', result
end program ch1212

```

Subroutines can also be made pure.

12.15.1 Pure Constraints

The following are some of the constraints on pure procedures

- a dummy argument must be `intent(in)`
- local variables may not have the `save` attribute

- no i/o must be done in the procedure
- any procedures referenced must be pure
- you cannot have a stop statement in a pure procedure

The above information should be enough to write simple pure functions.

12.16 Elemental Functions

Fortran 77 introduced the concept of generic intrinsic functions. Fortran 90 added elemental intrinsic functions and the ability to write generic user defined functions. Fortran 95 squared the circle and enabled us to write elemental user defined functions. Here is an example to illustrate this.

```
module reciprocal_module

contains

  real elemental function reciprocal(a)
    implicit none
    real, intent (in) :: a

    reciprocal = 1.0/a
  end function reciprocal
end module reciprocal_module

program ch1213
  use reciprocal_module
  implicit none
  real :: x = 10.0
  real, dimension (5) :: y = [ 1.0, 2.0, 3.0, &
    4.0, 5.0 ]

  print *, ' reciprocal of x is ', reciprocal(x)
  print *, ' reciprocal of y is ', reciprocal(y)
end program ch1213
```

Here is the output from one compiler.

```
reciprocal of x is 0.1000000
reciprocal of y is 0.9999999
0.5000000 0.3333333
0.2500000 0.2000000
```

Hence we can call our own elemental functions with both scalar and array arguments.

Elemental functions require the use of explicit interfaces, and we have therefore used modules to achieve this.

12.17 Resume

There are a large number of Fortran supplied functions and subroutines (intrinsic functions) which extend the power and scope of the language. Some of these functions are of generic type, and can take several different types of arguments. Others are restricted to a particular type of argument. Appendix B should be consulted for a fuller coverage concerning the rules that govern the use of the intrinsic functions and procedures.

When the intrinsic functions are inadequate, it is possible to write user defined functions. Besides expanding the scope of computation, such functions aid in problem visualisation and logical subdivision, may reduce duplication, and generally help in avoiding programming errors.

In addition to separately defined user functions, internal functions may be employed. These are functions which are used within a program segment.

Although the normal exit from a user defined function is through the `end` statement, other, abnormal, exits may be defined through the `return` statement.

Communication with nonrecursive functions is through the function name and the function arguments. The function must contain a reference to the function name on the left-hand side of an assignment. Results may also be returned through the argument list.

We have also covered briefly the concept of scope for a variable, local variables, and argument association. This area warrants a much fuller coverage and we will do this after we have covered subroutines and modules.

12.18 Formal Syntax

The syntax of a function is:

```
{ [function prefix] function_statement &
[result (result_name) ]
[specification part]
[execution_part]
[internal sub program part]
end [function [function name]] }
```

and prefix is:

```
[type specification] recursive
```

or

```
[recursive] type specification
```

and the function_statement is:

```
function function_name ([dummy argument name list])
```

[] represent optional parts to the specification.

The simple syntax for a module as we have used them in this chapter is

```
module module_name  
...  
end module_name
```

and

```
use module_name
```

in the calling routine.

12.19 Rules and Restrictions

The type of the function must only be specified once, either in the function statement or in a type declaration.

The names must match between the function header and end function function name statement.

If there is a result clause, that name must be used as the result variable, so all references to the function name are recursive calls.

The function name must be used to return a result when there is no result clause.

We will look at additional rules and restrictions in later chapters.

12.20 Problems

12.1 Find out the action of the `mod` function function when one of the arguments is negative. Write your own modulus function to return only a positive remainder. Don't call it `mod`!

12.2 Create a table which gives the sines, cosines and tangents for -1 to 91° in 1° intervals. Remember that the arguments have to be in radians. What value will you give `pi`? One possibility is `pi=4*atan(1.0)`. Pay particular attention to the following angle ranges:

`-1, 0, +1`

`29, 30, 31`

`44, 45, 46`

`59, 60, 61`

`89, 90, 91`

What do you notice about sine and cosine at 0 and 90° ? What do you notice about the tangent of 90° ? Why do you think this is?

Use a calculator to evaluate the sine, cosine at 0 and 90° . do the same for the tangent at 90° . Does this surprise you?

Repeat using a spreadsheet, e.g., Excel.

Are you surprised?

Repeat the Fortran program using one or more real kind types.

12.3 Write a program that will read in the lengths `a` and `b` of a right-angled triangle and calculate the hypotenuse `c`. Use the Fortran `sqr`t intrinsic.

12.4 Write a program that will read in the lengths `a` and `b` of two sides of a triangle and the angle between them θ (in degrees). Calculate the length of the third side `c` using the cosine rule: $c^2 = a^2 + b^2 - 2ab\cos(\theta)$

12.5 Write a function to convert an integer to a binary character representation. It should take an integer argument and return a character string that is a sequence of zeros and ones. Use the program in Chap. 5 as a basis for the solution.

Bibliography

Abramowitz M., Stegun I., Handbook of Mathematical Functions, Dover, 1968.

- This book contains a fairly comprehensive collection of numerical algorithms for many mathematical functions of varying degrees of obscurity.

It is a widely used source.

Association of Computing Machinery (ACM)

- Collected Algorithms, 1960–1974
- Transactions on Mathematical Software, 1975—

A good source of more specialised algorithms. Early algorithms tended to be in Algol, Fortran now predominates.

Recursion and Problem Solving

The following are a number of books that look at the role of recursion in problem solving and algorithms.

Hofstader D. R., Gödel, Escher, Bach—an Eternal Golden Braid, Harvester Press.

- The book provides a stimulating coverage of the problems of paradox and contradiction in art, music and mathematics using the works of Escher, Bach and Gödel, and hence the title. There is a whole chapter on recursive structures and processes. The book also covers the work of Church and Turing, both of whom have made significant contributions to the theory of computing.

Kruse R.L., Data Structures and Program Design, Prentice-Hall, 1994.

- Quite a gentle introduction to the use of recursion and its role in problem solving. Good choice of case studies with explanations of solutions. Pascal is used.

Sedgewick R., Algorithms in Modula 3, Addison-Wesley, 1993.

- Good source of algorithms. Well written. The gcd algorithm was taken from this source.

Vowels R.A., Algorithms and data Structures in F and Fortran, Unicomp, 1998.

- The only book currently that uses Fortran 90/95 and F. Visit the Fortran web site for more details. They are the publishers. Sadly no longer available. We found one at over 100 on Abebooks!

<http://www.fortran.com/fortran/market.html>

Wirth N., Algorithms + Data Structures = Programs, Prentice-Hall, 1976.

- In the context of this chapter the section on recursive algorithms is a very worthwhile investment in time.

Wood D., Paradigms and Programming in Pascal, Computer Science Press.

- contains a number of examples of the use of recursion in problem solving. Also provides a number of useful case studies in problem solving.

Chapter 13

Control Structures

Summarizing: as a slow-witted human being I have a very small head and I had better learn to live with it and to respect my limitations and give them full credit, rather than try to ignore them, for the latter vain effort will be punished by failure.

Edsger W. Dijkstra, Structured Programming

Aims

The aims of this chapter are to introduce:

- Selection among various courses of action as part of the algorithm.
- The concepts and statements in Fortran needed to support the above:
 - Logical expressions and logical operators.
 - One or more blocks of statements.
- The `if then endif` construct.
- The `if then else if endif` construct.
- To introduce the `case` statement with examples.
- To introduce the `do loop`, in three forms with examples, in particular:
 - The iterative `do loop`.
 - The `do while` form.
 - The `do ... if then exit end do` or `repeat until` form.
 - The `cycle` statement.
 - The `exit` statement.

13.1 Introduction

When we look at this area it is useful to gain some historical perspective concerning the control structures that are available in a programming language.

At the time of the development of Fortran in the 1950s there was little theoretical work around and the control structures provided were very primitive and closely related to the capability of the hardware.

At the time of the first standard in 1966 there was still little published work regarding structured programming and control structures. The seminal work by Dahl, Dijkstra and Hoare was not published until 1972.

By the time of the second standard there was a major controversy regarding languages with poor control structures like Fortran which essentially were limited to the `goto` statement. The facilities in the language had led to the development and continued existence of major code suites that were unintelligible, and the pejorative term spaghetti was applied to these programs. Developing an understanding of what a program did became an almost impossible task in many cases.

Fortran missed out in 1977 on incorporating some of the more modern and intelligible control structures that had emerged as being of major use in making code easier to understand and modify.

It was not until the 1990 standard that a reasonable set of control structures had emerged and became an accepted part of the language. The more inquisitive reader is urged to read at least the work by Dahl, Dijkstra and Hoare to develop some understanding of the importance of control structures and the role of structured programming. The paper by Knuth is also highly recommended as it provides a very balanced coverage of the controversy of earlier times over the `goto` statement.

13.2 Selection Among Courses of Action

In most problems you need to choose among various courses of action, e.g.,

- If overdrawn, then do not draw money out of the bank.
- If Monday, Tuesday, Wednesday, Thursday or Friday, then go to work.
- If Saturday, then go to watch Queens Park Rangers.
- If Sunday, then lie in bed for another two hours.

As most problems involve selection between two or more courses of action it is necessary to have the concepts to support this in a programming language. Fortran has a variety of selection mechanisms, some of which are introduced below.

13.3 The Block if Statement

The following short example illustrates the main ideas:

```

    . wake up
    .
    . check the date and time
if (Today == Sunday) then
    .
    . lie in bed for another two hours
.
endif
```

```

.
. get up
. make breakfast
.
```

If today is Sunday then the block of statements between the `if` and the `endif` is executed. After this block has been executed the program continues with the statements after the `endif`. If today is not Sunday the program continues with the statements after the `endif` immediately. This means that the statements after the `endif` are executed whether or not the expression is true. The general form is:

```

if (logical expression) then
.
block of statements
.
endif
```

The logical expression is an expression that will be either true or false; hence its name. Some examples of logical expressions are given below:

```

(alpha >= 10.1)
  test if alpha is greater than or equal to 10.1
(balance <= 0.0)
  test if overdrawn
(( today == saturday).or.( today == sunday))
  test if today is saturday or sunday
((actual - calculated) <= 1.0e-6)
  test if actual minus calculated
    is less than or equal to 1.0e-6
```

Table 13.1 lists the Fortran logical and relational operators.

The first six should be self-explanatory. They enable expressions or variables to be compared and tested. The last three enable the construction of quite complex comparisons, involving more than one test; in the example given earlier there was a test to see whether `today` was Saturday or Sunday.

Use of logical expressions and logical variables (something not mentioned so far) is covered again in a later chapter on logical data types.

The `if expression then statements endif` is called a block if construct. There is a simple extension to this provided by the `else` statement. Consider the following example:

```

if (balance > 0.0) then
  . draw money out of the bank
else
  . borrow money from a friend
endif
buy a round of drinks.
```

Table 13.1 Fortran logical and relational operators

Operator	Meaning	Type
<code>==</code>	Equal	Relational
<code>/ =</code>	Not equal	Relational
<code>>=</code>	Greater than or equal	Relational
<code><=</code>	Less than or equal	Relational
<code><</code>	Less than	Relational
<code>></code>	Greater than	Relational
<code>.AND.</code>	and	Logical
<code>.OR.</code>	or	Logical
<code>.NOT.</code>	not	Logical

In this instance, one or other of the blocks will be executed. Then execution will continue with the statements after the `endif` statement (in this case buy a round).

There is yet another extension to the block if which allows an `elseif` statement. Consider the following example:

```

if (today == monday) then
    .
elseif (today == tuesday) then
    .
elseif (today == wednesday) then
    .
elseif (today == thursday) then
    .
elseif (today == friday) then
    .
elseif (today == saturday) then
    .
elseif (today == sunday) then
    .
else
    there has been an error.
    the variable today has
    taken on an illegal value.
endif

```

Note that as soon as one of the logical expressions is true, the rest of the test is skipped, and execution continues with the statements after the `endif`. This implies that a construction like

```

if(i < 2)then
  ...
elseif(i < 1)then
  ...
else
  ...
endif

```

is inappropriate. If i is less than 2, the latter condition will never be tested. The `else` statement has been used here to aid in trapping errors or exceptions. This is recommended practice. A very common error in programming is to assume that the data are in certain well-specified ranges. The program then fails when the data go outside this range. It makes no sense to have a day other than Monday, Tuesday, Wednesday, Thursday, Friday, Saturday or Sunday.

13.3.1 Example 1: Quadratic Roots

A quadratic equation is:

$$ax^2 + bx + c = 0$$

This program has a simple structure. The roots of the quadratic are either real, equal and real, or complex depending on the magnitude of the term $b^{**} 2 - 4 * a * c$. The program tests for this term being greater than or less than zero: it assumes that the only other case is equality to zero (from the mechanics of a computer, floating point equality is rare, but we are safe in this instance):

```

program ch1301
  implicit none
  real :: a, b, c, term, a2, root1, root2

  ! a b and c are the coefficients of the terms
  ! a*x**2+b*x+c
  ! find the roots of the quadratic, root1 and
  ! root2

  print *, ' give the coefficients a, b and c'
  read *, a, b, c
  term = b*b - 4.*a*c
  a2 = a*2.

  ! if term < 0, roots are complex
  ! if term = 0, roots are equal
  ! if term > 0, roots are real and different
  if (term<0.0) then

```

```

    print *, ' roots are complex'
else if (term>0.0) then
    term = sqrt(term)
    root1 = (-b+term)/a2
    root2 = (-b-term)/a2
    print *, ' roots are ', root1, ' and ', &
        root2
else
    root1 = -b/a2
    print *, ' roots are equal, at ', root1
end if
end program ch1301

```

Given the understanding you now have about real arithmetic and finite precision will the `else` block above ever be executed?

13.3.2 Example 2: Date Calculation

This next example is also straightforward. It demonstrates that, even if the conditions on the `if` statement are involved, the overall structure is easy to determine. The comments and the names given to variables should make the program self-explanatory. Note the use of integer division to identify leap years:

```

program ch1302
    implicit none
    integer :: year, n, month, day, t

! calculates day and month from year and
! day-within-year
! t is an offset to account for leap years.
! Note that the first criteria is division by 4
! but that centuries are only
! leap years if divisible by 400
! not 100 (4 * 25) alone.

    print *, ' year, followed by day within year'
    read *, year, n
! checking for leap years
    if ((year/4)*4==year) then
        t = 1
        if ((year/400)*400==year) then
            t = 1
        else if ((year/100)*100==year) then

```

```

        t = 0
    end if
else
    t = 0
end if
! accounting for February
if (n>(59+t)) then
    day = n + 2 - t
else
    day = n
end if
month = (day+91)*100/3055
day = (day+91) - (month*3055)/100
month = month - 2
print *, ' calendar date is ', day, month, &
year
end program ch1302

```

13.4 The Case Statement

The case statement provides a very clear and expressive selection mechanism between two or more courses of action. Strictly speaking it could be constructed from the if then else if endif statement, but with considerable loss of clarity. Remember that programs have to be read and understood by both humans and compilers!

13.4.1 Example 3: Simple Calculator

```

program ch1303
    implicit none
! Simple case statement example
    integer :: i, j, k
    character :: operator

    do
        print *, ' type in two integers'
        read *, i, j
        print *, ' type in operator'
        read '(a)', operator

        calculator: select case (operator)
            case ('+') calculator

```

```

      k = i + j
      print *, ' Sum of numbers is ', k
      case ('-') calculator
      k = i - j
      print *, ' Difference is ', k
      case ('/') calculator
      k = i/j
      print *, ' Division is ', k
      case ('*') calculator
      k = i*j
      print *, ' Multiplication is ', k
      case default calculator
      exit
end select calculator

end do
end program ch1303

```

The user is prompted to type in two integers and the operation that they would like carried out on those two integers. The `case` statement then ensures that the appropriate arithmetic operation is carried out. The program terminates when the user types in any character other than `+`, `-`, `*` or `/`.

The `case default` option introduces the `exit` statement. This statement is used in conjunction with the `do` statement. When this statement is executed control passes to the statement immediately after the matching `end do` statement. In the example above the program terminates, as there are no executable statements after the `end do`.

13.4.2 Example 4: Counting Vowels, Consonants, etc.

This example is more complex, but again is quite easy to understand. The user types in a line of text and the program produces a summary of the frequency of the characters typed in:

```

program ch1304
implicit none

! Simple counting of vowels, consonants,
! digits, blanks and the rest

integer :: vowels = 0, consonants = 0, &
           digits = 0
integer :: blank = 0, other = 0, i

```

```

character :: letter
character (len=80) :: line

read '(a)', line
do i = 1, 80
  letter = line(i:i)
!   the above extracts one character
!   at position i
  select case (letter)
    case ('A', 'E', 'I', 'O', 'U', 'a', 'e', &
          'i', 'o', 'u')
      vowels = vowels + 1
    case ('B', 'C', 'D', 'F', 'G', 'H', 'J', &
          'K', 'L', 'M', 'N', 'P', 'Q', 'R', 'S', &
          'T', 'V', 'W', 'X', 'Y', 'Z', 'b', 'c', &
          'd', 'f', 'g', 'h', 'j', 'k', 'l', 'm', &
          'n', 'p', 'q', 'r', 's', 't', 'v', 'w', &
          'x', 'y', 'z')
      consonants = consonants + 1
    case ('1', '2', '3', '4', '5', '6', '7', &
          '8', '9', '0')
      digits = digits + 1
    case (' ')
      blank = blank + 1
    case default
      other = other + 1
    end select
  end do
  print *, ' Vowels = ', vowels
  print *, ' Consonants = ', consonants
  print *, ' Digits = ', digits
  print *, ' Blanks = ', blank
  print *, ' Other characters = ', other
end program ch1304

```

13.5 The Three Forms of the do Statement

You have already been introduced in the chapters on arrays to the iterative form of the do loop, i.e.,

```

do variable = start, end, increment
  block of statements
end do

```

A complete coverage of this form is given in the three chapters on arrays.

There are two additional forms of the block do that complete our requirements:

```
do while (logical expression)
    block of statements
enddo
```

and

```
do
    block of statements
    if (logical expression) exit
end do
```

The first form is often called a while loop as the block of statements executes whilst the logical expression is true, and the second form is often called a repeat until loop as the block of statements executes until the statement is true.

Note that the while block of statements may never be executed, and the repeat until block will always be executed at least once.

13.5.1 Example 5: Sentinel Usage

The following example shows a complete program using this construct:

```
program ch1305
    implicit none
! this program picks up the first occurrence
! of a number in a list.
! a sentinel is used, and the array is 1 more
! than the max size of the list.
    integer, allocatable, dimension(:) :: a
    integer :: mark
    integer :: i, howmany

    open (unit=1, file='data.txt')
    print *, ' What number are you looking for?'
    read *, mark
    print *, ' How many numbers to search?'
    read *, howmany
    allocate (a(1:howmany+1))
    read (unit=1, fmt=*) (a(i), i=1, howmany)
    i = 1
    a(howmany+1) = mark
    do while (mark/=a(i))
        i = i + 1
    end do
```

```

if (i==(howmany+1)) then
    print *, ' item not in list'
else
    print *, ' item is at position ', i
end if
end program ch1305

```

The repeat until construct is written in Fortran as:

```

do
  ...
  ...
  if (logical expression) exit
end do

```

There are problems in most disciplines that require a numerical solution. The two main reasons for this are either that the problem can only be solved numerically or that an analytic solution involves too much work. Solutions to this type of problem often require the use of the repeat until construct. The problem will typically require the repetition of a calculation until the answers from successive evaluations differ by some small amount, decided generally by the nature of the problem. A program extract to illustrate this follows:

```

real , parameter :: tol=1.0e-6
.
do
  ...
  change=
  ...
  if (change <= tol) exit
end do

```

Here the value of the tolerance is set to 1.0E-6. Note again the use of the `exit` statement. The `do end do` block is terminated and control passes to the statement immediately after the matching `end do`.

13.5.2 Cycle and Exit

These two statements are used in conjunction with the block do statement. You have seen examples above of the use of the `exit` statement to terminate the block `do`, and pass control to the statement immediately after the corresponding `end do` statement.

The `cycle` statement can appear anywhere in a block `do` and will immediately pass control to the start of the block `do`. Examples of `cycle` and `exit` are given in the next two examples, and later chapters in the book.

13.5.3 Example 6: The Evaluation of $e^{**}x$

The function `etox` illustrates one use of the repeat until construct. The function evaluates e^x . This may be written as

$$1 + x/1! + x^2/2! + x^3/3! \dots$$

or

$$1 + \sum_{n=1}^{\infty} \frac{x^{n-1}}{(n-1)!} x/n$$

Every succeeding term is just the previous term multiplied by x/n . At some point the term x/n becomes very small, so that it is not sensibly different from zero, and successive terms add little to the value. The function therefore repeats the loop until x/n is smaller than the tolerance. The number of evaluations is not known beforehand, since this is dependent on x :

```
module etox_module
    implicit none

contains
    real function etox(x)
        implicit none
        real :: term
        real, intent (in) :: x
        integer :: nterm
        real, parameter :: tol = 1.0e-6

        etox = 1.0
        term = 1.0
        nterm = 0
        do
            nterm = nterm + 1
            term = (x/nterm)*term
            etox = etox + term
            if (abs(term)<=tol) exit
        end do
    end function etox
end module etox_module

program ch1306
    use etox_module
    implicit none
```

```

real, parameter :: x = 1.0
real :: y

print *, ' Fortran intrinsic ', exp(x)
y = etox(x)
print *, ' User defined etox ', y
end program ch1306

```

The whole program compares the user defined function with the Fortran intrinsic `exp` function.

13.5.4 Example 7: Wave Breaking on an Offshore Reef

This example is drawn from a situation where a wave breaks on an offshore reef or sand bar, and then reforms in the near-shore zone before breaking again on the coast. It is easier to observe the heights of the reformed waves reaching the coast than those incident to the terrace edge.

Both types of loops are combined in this example. The algorithm employed here finds the zero of a function. Essentially, it finds an interval in which the zero must lie; the evaluations on either side are of different signs. The while loop ensures that the evaluations are of different signs, by exploiting the knowledge that the incident wave height must be greater than the reformed wave height (to give the lower bound). The upper bound is found by experiment, making the interval bigger and bigger. Once the interval is found, its mean is used as a new potential bound. The zero must lie on one side or the other; in this fashion, the interval containing the zero becomes smaller and smaller, until it lies within some tolerance. This approach is rather plodding and unexciting, but is suitable for a wide range of problems.

Here is the program:

```

program ch1307
implicit none
real :: hi, hr, hlow, high, half, xl
real :: xh, xm, d
real, parameter :: tol = 1.0e-6
! problem - find hi from expression given
! in function f
! F=A*(1.0-0.8*EXP(-0.6*C/A))-B
! The above is a Fortran 77
! statement function.
! hi is incident wave height (c)
! hr is reformed wave height (b)
! d is water depth at terrace edge (a)

```

```

print *, ' Give reformed wave height, &
&and water depth'
read *, hr, d

! for hlow - let hlow=hr
! for high - let high=hlow*2.0

! check that signs of function
! results are different

hlow = hr
high = hlow*2.0
x1 = f(hlow, hr, d)
xh = f(high, hr, d)

do while ((x1*xh)>=0.0)
    high = high*2.0
    xh = f(high, hr, d)
end do

do
    half = (hlow+high)*0.5
    xm = f(half, hr, d)
    if ((x1*xm)<0.0) then
        xh = xm
        high = half
    else
        x1 = xm
        hlow = half
    end if
    if (abs(high-hlow)<=tol) exit
end do
print *, ' Incident Wave Height Lies Between'
print *, hlow, ' and ', high, ' metres'
contains
real function f(a, b, c)
implicit none
real, intent (in) :: a
real, intent (in) :: b
real, intent (in) :: c

f = a*(1.0-0.8*exp(-0.6*c/a)) - b
end function f
end program ch1307

```

13.6 Summary

You have been introduced in this chapter to several control structures and these include:

- The block if.
- The if then else if.
- The case construct.
- The block do in three forms.
- The iterative do or do variable=start, end, increment ... end do.
- The while construct, or do while ... end do.
- The repeat until construct, or do ... if then exit end do.
- The cycle and exit statements, which can be used with the do statement.

These constructs are sufficient for solving a wide class of problems. There are other control statements available in Fortran, especially those inherited from Fortran 66 and Fortran 77, but those covered here are the ones preferred. We will look in Chap. 35 at one more control statement, the so-called goto statement, with recommendations as to where its use is appropriate.

13.6.1 Control Structure Formal Syntax

```
case
select case ( case variable )
  [ case case selector
    [executable construct] ... ] ...
  [ case default
    [executable construct] ]
end select
do
do [ label ]
  [executable construct] ...
do termination
do [ label ] [ , ] loop variable =
  initial value , final value , [
increment ]
  [executable construct] ...
do termination
do [ label ] [ , ] while
  (scalar logical expression)
  [executable construct] ...
do termination
if
if ( scalar logical expression ) then
```

```

[executable construct] ...
[else if ( scalar logical expression    then
  [executable construct] ... ] ...]
[else
  [executable construct] ...]
end if

```

13.7 Problems

13.1 Rewrite the program for the period of a pendulum. The new program should print out the length of the pendulum and period, for pendulum lengths from 0 to 100 cm in steps of 0.5 cm. The program should incorporate a function for the evaluation of the period.

13.2 Write a program to read an integer that must be positive.

Hint: use a `do while` to make the user re-enter the value.

13.3 Using functions, do the following:

- Evaluate $n!$ from $n = 0$ to $n = 10$.
- Calculate $76!$
- Now calculate $(x^n)/n!$, with $x = 13.2$ and $n = 20$.
- Now do it another way.

13.4 The program ch1307 is taken from a real example. In the particular problem, the reformed wave height was 1 m, and the water depth at the reef edge was 2 m. What was the incident wave height? Rather than using an absolute value for the tolerance, it might be more realistic to use some value related to the reformed wave height. These heights are unlikely to be reported to better than about 5 % accuracy. Wave energy may be taken as proportional to wave height squared for this example. What is the reduction in wave energy as a result of breaking on the reef or bar for this particular case.

13.5 What is the effect of using `int` on negative real numbers? Write a program to demonstrate this.

13.6 How would you find the nearest integer to a real number? Now do it another way. Write a program to illustrate both methods. Make sure you test it for negative as well as positive values.

13.7 The function `etox` has been given in this chapter. The standard Fortran function `exp` does the same job. Do they give the same answers? Curiously the Fortran standard does not specify how a standard function should be evaluated, or even how accurate it should be.

The physical world has many examples in which processes require that some threshold be overcome before they begin operation: critical mass in nuclear reactions, a given slope to be exceeded before friction is overcome, and so on. Unfortunately, most of these sorts of calculations become rather complex and not really appropriate here. The following problem tries to restrict the range of calculation, whilst illustrating the possibilities of decision making.

13.8 If a cubic equation is expressed as

$$ax^3 + bx^2 + cx + d = 0$$

and we let

$$\Delta = 18abcd - 4b^3d + b^2c^2 - 4ac^3 - 27a^2d^2$$

We can determine the nature of the roots as follows

$\Delta > 0$: three distinct real roots

$\Delta = 0$: has a multiple root and all roots are real

$\Delta < 0$: 1 real root and 2 non real complex conjugate roots.

Incorporate this into a program, to determine the nature of the roots of a cubic from suitable input.

13.9 The form of breaking waves on beaches is a continuum, but for convenience we commonly recognise three major types: surging, plunging and spilling. These may be classified empirically by reference to the wave period, T (seconds), the breaker wave height, H_b (metres), and the beach slope, m . These three variables are combined into a single parameter, B , where

$$B = H_b / (gmT^2)$$

g is the gravitational constant (981 cm s^{-2}). If B is less than 0.003, the breakers are surging; if B is greater than 0.068, they are spilling, and between these values, plunging breakers are observed.

(i) On the east coast of New Zealand, the normal pattern is swell waves, with wave heights of 1–2 m and wave periods of 10–15 s. During storms, the wave period is generally shorter, say 6–8 s, and the wave heights higher, 3–5 m. The beach slope may be taken as about 0.1. What changes occur in breaker characteristics as a storm builds up?

(ii) Similarly, many beaches have a concave profile. The lower beach generally has a very low slope, say less than 1° ($m = 0.018$), but towards the high-tide mark, the slope increases dramatically, to say 10° or more ($m = 0.18$). What changes in wave type will be observed as the tide comes in?

Bibliography

Dahl, O.J., Dijkstra, E.W., Hoare, C.A.R.: Structured Programming. Academic Press (1972)

- This is the original text, and a must. The quote at the start of the chapter by Dijkstra summarises beautifully our limitations when programming and the discipline we must have to master programming successfully.

Knuth, D.E.: Structured programming with goto statements. Current Trends in Programming Methodology, vol 1. Prentice-Hall (1977)

- The chapter by Knuth provides a very succinct coverage of the arguments for the adoption of structured programming, and dispels many of the myths concerning the use of the goto statement. Highly recommended.

Chapter 14

Characters

These metaphysics of magicians, And necromantic books are

heavenly; Lines, circles, letters and characters.

Christopher Marlowe, The Tragical History of Doctor Faustus

Aims

The aims of this chapter are:

- To extend the ideas about characters introduced in earlier chapters.
- To demonstrate that this enables us to solve a whole new range of problems in a satisfactory way.

14.1 Introduction

For each type in a programming language there are the following concepts:

- Values are drawn from a finite domain.
- There are a restricted number of operations defined for each type.

For the character data type the basic unit is an individual character. The complete Fortran character set is given in Sect. 4.8 in Chap. 4. This provides us with 95 printing characters. Other characters may be available. The Wikipedia entry

http://en.wikipedia.org/wiki/Character_encoding

has quite detailed information on how complex this area actually is.

As the most common current internal representation for the character data type uses 8 bits this should provide access to 256 characters. However, there is little agreement over the encoding of these 256 possible characters, and the best you can normally assume is access to the ASCII character set, which is given in Chap. 4. One of the problems at the end of this chapter looks at determining what characters one has available.

The only operations defined are concatenation (joining character strings together) and comparison.

We will look into the area of character sets in more depth later in this chapter.

We can declare our character variables:

```
character :: a, string, line
```

Note that there is no default typing of the character variable (unlike integer and real data types), and we can use any convenient name within the normal Fortran conventions. In the declaration above, each character variable would have been permitted to store one character. This is limiting, and, to allow character strings which are several units long, we have to add one item of information:

```
character (10) :: a
character (16) :: string
character (80) :: line
```

This indicates that `a` holds 10 characters, `string` holds 16, and `line` holds 80. If all the character variables in a single declaration contain the same number of characters, we can abbreviate the declaration to

```
character(80) :: list, string, line
```

But we cannot mix both forms in the one declaration. We can now assign data to these variables, as follows:

```
a='first one '
string='a longer one'
line='the quick brown fox jumps over the lazy dog'
```

The delimiter apostrophe (') or quotation mark ("") is needed to indicate that this is a character string (otherwise the assignments would have looked like invalid variable names).

14.2 Character Input

In an earlier chapter we saw how we could use the `read *` and `print *` statements to do both numeric and character input and output or I/O. When we use this form of the statement we have to include any characters we type within delimiters (either the apostrophe ' or the quotation mark ""). This is a little restricting and there is a slightly more complex form of the `read` statement that allows one to just type the string on its own.

14.2.1 Example 1: The * Edit Descriptor

The following two programs illustrate the differences:

```
program ch1401
!
! Simple character i/o
!
character (80) :: line

read *, line
print *, line
end program ch1401
```

This form requires enclosing the string with delimiters.

14.2.2 Example 2: The a Edit Descriptor

Consider the next form:

```
program ch1402
!
! Simple character i/o
!
character (80) :: line

read '(a)', line
print *, line
end program ch1402
```

With this form one can just type the string in and input terminates with the carriage return key. The additional syntax involves '(a)' where '(a)' is a character edit descriptor. The simple examples we have used so far have used implied format specifiers and edit descriptors. For each data type we have one or more edit descriptors to choose from. For the character data type only the a edit descriptor is available.

14.3 Character Operators

The first manipulator is a new operator—the concatenation operator // . With this operator we can join two character variables to form a third, as in

```

character (5) :: first, second
character (10) :: third
first='three'
second='blind'
...
third=first//second
.
third=first//mice'
```

where there is a discrepancy between the created length of the concatenated string and the declared lengths of the character strings, truncation will occur. For example,

```
third=first//' blind mice'
```

will only append the first five characters of the string ' blind mice' i.e., ' blin', and third will therefore contain 'three blin'.

What would happen if we assigned a character variable of length 'n' a string which was shorter than n? For example,

```

character (4) :: c2
c2='ab'
```

The remaining two characters are considered to be blank, that is, it is equivalent to saying

```
c2='ab      '
```

However, while the strings 'ab' and 'ab ' are equivalent, ' ab' and 'ab ' are not. In the jargon, the character strings are always left justified, and the unset characters are trailing blanks.

If we concatenate strings which have 'trailing blanks', the blanks, or spaces, are considered to be legitimate characters, and the concatenation begins after the end of the first string. Thus

```

character (4) :: c2,c3
character (8) :: jj
c2='a'
c3='man'
jj=c2//c3
print*, 'the concatenation of ',c2,' and ',c3,' is'
print*,jj
```

would appear as

```
the concatenation of a    man gives
a    man
```

at the terminal.

14.4 Character Substrings

Sometimes we need to be able to extract parts of character variables—substrings. The actual notation for doing this is a little strange at first, but it is very powerful. To extract a substring we must provide two items:

- The position in the string at which the substring begins.
- The position at which it ends.

In the examples that follow we will use the following

```
string='share and enjoy'
```

Substring	Characters
string(3:3)	a
string(3:5)	are
string(:3)	sha
string(11:)	enjoy

Character variables may also form arrays:

```
character (10) , dimension(20) :: a
```

sets up a character array of twenty elements, where each element contains ten characters. In order to extract substrings from these array elements, we need to know where the array reference and the substring reference are placed. The array reference comes first, so that

```
do i=1,20
  first=a(i)(1:1)
end
```

places the first character of each element of the array into the variable first. The syntax is therefore ‘position in array, followed by position within string’.

Any argument can be replaced by an integer variable or expression:

```
string(i:j)
```

14.4.1 Example 3: Stripping Blanks from a String

This offers interesting possibilities, since we can, for example, strip blanks out of a string:

```
program ch1403
  implicit none
```

```

character (80) :: string, strip
integer :: ipos, i, length = 80

ipos = 0
print *, ' type in a string'
read '(a)', string
do i = 1, length
    if (string(i:i)/=' ') then
        ipos = ipos + 1
        strip(ipos:ipos) = string(i:i)
    end if
end do
print *, string
print *, strip
end program ch1403

```

14.5 Character Functions

There are special functions available for use with character variables: `index` will give the starting position of a string within another string.

14.5.1 Example 4: The `index` Character Function

If, for example, we were looking for all occurrences of the string ‘Geology’ in a file, we could construct something like:

```

program ch1404
implicit none
character (80) :: line
integer :: i

do
    read '(a)', line
    i = index(line, 'Geology')
    if (i/=0) then
        print *, &
            ' String Geology found at position ', i
        print *, ' in line ', line
        exit
    end if
end program ch1404

```

```
    end do  
end program ch1404
```

There are two things to note about this program. Firstly the `index` function will only report the first occurrence of the string in the line; any later occurrences in any particular line will go unnoticed, unless you account for them in some way. Secondly, if the string does not occur, the result of the `index` function is zero, and given the infinite loop (`do enddo`) the program will crash at run time with an end of file error message. This isn't good programming practice.

14.5.2 The `len` and `len_trim` Functions

The `len` function provides the length of a character string. This function is not immediately useful, since you really ought to know how many characters there are in the string. However, as later examples will show, there are some cases where it can be useful. Remember that trailing blanks do count as part of the character string, and contribute to the length.

14.5.3 Example 5: Using `len` and `len_trim`

The following example illustrates the use of both `len` and `len_trim`:

```
program ch1405  
    implicit none  
    character (len=20) :: name  
    integer :: name_length  
  
    print *, ' type in your name'  
    read '(a)', name  
! show len first  
    name_length = len(name)  
    print *, ' name length is ', name_length  
    print *, ' ', name(1:name_length), &  
        '<-end is here'  
    name_length = len_trim(name)  
    print *, ' name length is ', name_length  
    print *, ' ', name(1:name_length), &  
        '<-end is here'  
end program ch1405
```

14.6 Collating Sequence

The next group of functions need to be considered together. They revolve around the concept of a collating sequence. In other words, each character used in Fortran is ordered as a list and given a corresponding weight. No two weights are equal. Although Fortran has only 63 defined characters, the machine you use will generally have more; 95 printing characters is a typical minimum number. On this type of machine the weights would vary from 0 to 94. There is a defined collating sequence, the ASCII sequence, which is likely to be the default. The parts of the collating sequence which are of most interest are fairly standard throughout all collating sequences.

In general, we are interested in the numerals (0–9), the alphabetics (A–Z, a–z) and a few odds and ends like the arithmetic operators (+ – / *), some punctuation (. and ,) and perhaps the prime ('). As you might expect, 0–9 carry successively higher weights (though not the weights 0–9), as do A–Z and a–z. The other odds and ends are a little more problematic, but we can find out the weights through the function `ichar`. This function takes a single character as argument and returns an integer value. The ASCII weights for the alphanumerics are as follows:

0–9	48–57
A–Z	65–90

One of the exercises is to determine the weights for other characters. The reverse of this procedure is to determine the character from its weighting, which can be achieved through the function `char`. `char` takes an integer argument and returns a single character. Using the ASCII collating sequence, the alphabet would be generated from

```
do i=65,90
    print*,char(i)
enddo
```

This idea of a weighting can then be used in four other functions:

function	Action
<code>lle</code>	lexically less than or equal to
<code>lge</code>	lexically greater than or equal to
<code>lgt</code>	lexically greater than
<code>llt</code>	lexically less than

In the sequence we have seen before, A is lexically less than B, i.e., its weight is less. Clearly, we can use `ichar` and get the same result. For example,

```
if(lgt('a','b')) then
```

is equivalent to

```
if(ichar('a') > ichar('b')) then
```

but these functions can take character string arguments of any length. They are not restricted to single characters.

These functions provide very powerful tools for the manipulation of characters, and open up wide areas of nonnumerical computing through Fortran. Text formatting and word processing applications may now be tackled (conveniently ignoring the fact that lower-case characters may not be available).

There are many problems that require the use of character variables. These range from the ability to provide simple titles on reports, or graphical output, to the provision of a natural language interface to one of your programs, i.e., the provision of an English-like command language. Software Tools by Kernighan and Plauger contains many interesting uses of characters in Fortran.

14.7 Example 6: Finding Out About the Character Set Available

The following program prints out the characters between 32 and 127.

```
program ch1406
    implicit none
    integer :: i

    do i = 32, 62
        print *, i, char(i), i + 32, char(i+32), &
                  i + 64, char(i+64)
    end do
    i = 63
    print *, i, char(i), i + 32, char(i+32), &
                  i + 64, 'del'
end program ch1406
```

This is the output from the Intel compiler under Windows.

32	64	@	96	'
33	65	A	97	a
34	66	B	98	b
35	67	C	99	c
36	68	D	100	d
37	69	E	101	e
38	70	F	102	f
39	71	G	103	g
40	72	H	104	h
41	73	I	105	i
42	74	J	106	j
43	75	K	107	k

44 ,	76 L	108 l
45 -	77 M	109 m
46 .	78 N	110 n
47 /	79 O	111 o
48 0	80 P	112 p
49 1	81 Q	113 q
50 2	82 R	114 r
51 3	83 S	115 s
52 4	84 T	116 t
53 5	85 U	117 u
54 6	86 V	118 v
55 7	87 W	119 w
56 8	88 X	120 x
57 9	89 Y	121 y
58 :	90 Z	122 z
59 ;	91 [123 {
60 <	92 \	124
61 =	93]	125 }
62 >	94 ^	126 ~
63 ?	95 _	127 del

Try this program out on the system you use. Do the character sets match?

14.8 The `scan` Function

The `scan` function scans a string for characters from a set of characters. The syntax is given below.

- `scan(string, set)`—Scans a string for any one of the characters in a set of characters.

14.8.1 Example 7: Using the `scan` Function

```
program ch1407
    implicit none
    character (1024) :: string01
    character (1) :: set = ' '
    integer :: i
    integer :: l
    integer :: start, end

    string01 = 'The important issue about &
```

```
&a language, is not so'
string01 = trim(string01) // ' ' // 'much &
&what features the language possesses, &
&but'
string01 = trim(string01) // ' ' // 'the &
&features it does possess, are sufficient, &
&to'
string01 = trim(string01) // ' ' // 'support &
&the desired programming styles, in &
&the'
string01 = trim(string01) // ' ' // '&
'desired application areas.'
l = len(trim(string01))
print *, ' Length of string is = ', l
print *, ' String is'
print *, trim(string01)
start = 1
end = l
print *, ' Blanks at positions '
do
  i = scan(string01(start:end), set)
  start = start + i
  if (i==0) exit
  write (*, 100, advance='no') start - 1
end do
100 format (i5)
end program ch1407
```

Note the use of the `trim` function when using the concatenation operator to initialise the string to the text we want.

The output from one compiler is given below. The text has been wrapped to fit the page

```
Length of string is =          217
String is
The important issue about a language, is not so much
what features the language possesses,
but the features it does possess, are sufficient,
to support the desired programming styles,
in the desired application areas.

Blanks at positions
  4   14   20   26   28   38   41   45   48   53   58
  67   71   80   91   95   99   108  111  116  125  129
141  144  152  156  164  176  184  187  191  199  211
```

The text in this program is used in two problems at the end of this chapter.

Table 14.1 String functions in Fortran

Function name	Explanation
achar	Return the character in the ASCII character set
adjustl	Adjust left, remove leading blanks, add trailing blanks
adjustr	Adjust right, remove trailing blanks, insert leading blanks
char	Return the character in the processor collating sequence
iachar	As above but in the ASCII character set
index	Locate one string in another
len	Character length including trailing blanks
len_trim	Character length without the trailing blanks
lle	Lexically less than or equal to
lge	Lexically greater than or equal to
lgtr	Lexically greater than
llt	Lexically less than
repeat	Concatenate several copies of a string
scan	Scans a string for anyone of the characters in the set
trim	Remove the trailing blanks
verify	Verify that a set of characters contains all the characters in a string

14.9 Summary

Characters represent a different data type to any other in Fortran, and as a consequence there is a restricted range of operations which may be carried out on them.

A character variable has a length which must be assigned in a character declaration statement.

Character strings are delimited by apostrophes (') or quotation marks ("). Within a character string, the blank is a significant character.

Character strings may be joined together (concatenated) with the // operator.

Substrings occurring within character strings may be also be manipulated. Table 14.1 has details of a number of functions especially for use with characters.

A detailed explanation is given in Appendix B.

14.10 Problems

14.1 Suggest some circumstances where PRIME="" might be useful. What other alternative is there and why do you think we use that instead?

14.2 Write a program to write out the weights for the Fortran character set. Modify this program to print out the weights of the complete implementation defined character set for your version of Fortran. Is it ASCII? if not, how does it differ?

14.3 Write a program that produces the following output.

```
!
"#
$%&
' ()*
+, -./
012345
6789: ;<
=>?@ABCD
EFGHIJKLMNOP
XYZ[\]^_`ab
cdefghijklmn
opqrstuvwxyz{
| }~
```

We assume the ASCII character set in this example.

14.4 Modify the above program to produce the following output.

```
!
"#$%
%&'()
*+, -./0
123456789
: ;<=>?@ABCD
EFGHIJKLMNOPQ
RSTUVWXYZ[\]^_`'
abcdefghijklmnopqrstuvwxyz{|}~
```

Again we assume the ASCII character set.

14.5 Modify program ch1407 to break the text into phrases, using the comma and full stop as breaking characters. The output expected is given below.

```
The important issue about a language
is not so much what features the language possesses
but the features it does possess
are sufficient
to support the desired programming styles
in the desired application areas
```

Modify the above to break the text into words and count the frequency of occurrence of words by length. The output should be similar to that given below.

1	a	1
2	is so it to in	5
3	The not the but the are the the	8
4	much what does	3
5	issue about areas	3
6	styles	1
7	possess support desired desired	4
8	language features language features	4
9	important possesses	2
10	sufficient	1
11	programming application	2

14.6 Use the `index` function in order to find the location of all the strings 'is' in the following data:

If a programmer is found to be indispensable, the best thing to do is to get rid of him as quickly as possible.

14.7 Find the 'middle' character in the following strings. Do you include blanks as characters? What about punctuation?

Practice is the best of all instructors. experience is a dear teacher, but fools will learn at no other.

14.8 In English, the order of occurrence of the letters, from most frequent to least is

E, T, A, O, N, R, I, S, H, D, L,
F, C, M, U, G, Y, P, W, B, V, K,
X, J, Q, Z

Use this information to examine the two files given in Appendix C (one is a translation of the other) to see if this is true for these two extracts of text. The second text is in medieval Latin (c. 1320). Note that a fair amount of compression has been achieved by expressing the passage in Latin rather than modern English. Does this provide a possible model for information compression?

14.9 A very common cypher is the substitution cypher, where, for example, every letter A is replaced by (say) an M, every B is replaced by (say) a Y, and so on. These enciphered messages can be broken by reference to the frequency of occurrence of the letters (given in the previous question).

Since we know that (in English) E is the most commonly occurring letter, we can assume that the most commonly occurring letter in the enciphered message represents an E; we then repeat the process for the next most common and so on. Of course,

these correspondences may not be exact, since the message may not be long enough to develop the frequencies fully.

However, it may provide sufficient information to break the cypher.

The file given in Appendix C contains an encoded message. Break it.

Clue—Pg+Fybdjuvef jo Tdjfodf, Jorge Luis Borges.

14.10 Write a program that counts the total number of vowels in a sentence or text. Output the frequency of occurrence of each vowel.

Chapter 15

Complex

Make it as simple as possible, but no simpler.
Albert Einstein

Aims

The aims of this chapter are:

- To introduce the last predefined numeric data type in Fortran.
- To illustrate with examples how to use this type.

15.1 Introduction

This variable type reflects an extension of the real data type available in Fortran—the complex data type, where we can store and manipulate complex variables. Problems that require this data type are restricted to certain branches of mathematics, physics and engineering. Complex numbers are defined as having a real and imaginary part, i.e., $a = x + iy$ where i is the square root of -1 .

They are not supported in many programming languages as a base type which makes Fortran the language of first choice for many people.

To use this variable type we have to write the number as two parts, the real and imaginary elements of the number, for example,

```
complex :: u  
u=cmplx(1.0,2.0)
```

represents the complex number $1 + i2$. Note that the complex number is enclosed in brackets. We can do arithmetic on variables like this, and most of the intrinsic functions such as `log`, `sin`, `cos`, etc., accept a complex data type as argument.

All the usual rules about mixing different variable types, like reals and integers, also apply to complex. Complex numbers are read in and written out in a similar way to real numbers, but with the provision that, for each single complex value, two

format descriptors must be given. You may use either E or F formats (or indeed, mix them), as long as there are enough of them. Although you use brackets around the pairs of numbers in a program, these must not appear in any input, nor will they appear on the output.

15.2 Example 1: Use of **cmplx**, **aimag** and **conjg**

There are a number of intrinsic functions to enable complex calculations to be performed. The program below uses some of them:

```
program ch1501
    implicit none
    complex :: z, z1, z2, z3, zbar
    real :: x,y,zmod
    real :: x2 = 3.0 , y2 = 4.0
    real :: x3 = -2.0 , y3 = -3.0

    z1 = cmplx(1.0, 2.0) ! 1 + i 2
    z2 = cmplx(x2, y2)   ! x2 + i y2
    z3 = cmplx(x3, y3)   ! x3 + i y3
    z = z1*z2/z3
    x = real(z)           ! real part of z
    y = aimag(z)          ! imaginary part of z
    zmod = abs(z)          ! modulus of z
    zbar = conjg(z)         ! complex conjugate of z
    print 100, z1, z2, z3
    100 format (3(1x,f4.1,' + i ',f4.1/))
    print 110, z, zmod, zbar
    110 format (1x, f4.1, ' + i ', f4.1, /1x, f4.1, &
                /, 1x, f4.1, ' + i ', f4.1)
    print 120, x, y
    120 format (2(1x,f4.1/))
end program ch1501
```

15.3 Example 2: Polar Coordinate Example

The second order differential equation:

$$\frac{d^2y}{dt^2} + 2\frac{dy}{dt} + y = x(t)$$

could describe the behaviour of an electrical system, where $x(t)$ is the input voltage and $y(t)$ is the output voltage and dy/dt is the current. The complex ratio

$$\frac{y(w)}{x(w)} = 1/(-w^2 + 2jw + 1)$$

is called the frequency response of the system because it describes the relationship between input and output for sinusoidal excitation at a frequency of w and where j is $\sqrt(-1)$. The following program reads in a value of w and evaluates the frequency response for this value of w together with its polar form (magnitude and phase):

```

program ch1502
implicit none

! program to calculate frequency
! response of a system
! for a given omega
! and its polar form (magnitude and phase).

real :: omega, real_part, imag_part, &
         magnitude, phase
complex :: frequency_response

! Input frequency omega

print *, 'Input frequency'
read *, omega

frequency_response = 1.0/cmplx(-omega*omega+ &
        1.0, 2.0*omega)
real_part = real(frequency_response)
imag_part = aimag(frequency_response)

! Calculate polar coordinates
! (magnitude and phase)

magnitude = abs(frequency_response)
phase = atan2(imag_part, real_part)

print *, ' at frequency ', omega
print *, 'response = ', real_part, ' + i ', &
        imag_part
print *, 'in polar form'
print *, ' magnitude = ', magnitude
print *, ' phase = ', phase
end program ch1502

```

15.4 Complex and Kind Type

The standard requires that there be a minimum of two kind types for real numbers and this is also true of the complex data type. Chapter 5 must be consulted for a full coverage of real kind types. We would therefore use something like the following to select a complex kind type other than the default:

```
integer , parameter :: &
    dp = selected_real_kind(15,307)
complex (dp) :: z
```

Chapter 21 includes a good example of how to use modules to define and use precision throughout a program and subprogram units.

15.5 Summary

Complex is used to store and manipulate complex numbers: those with a real and an imaginary part. There are standard functions which allow conversion between the numerical data types—`cmplx`, `real` and `int`.

15.6 Problems

15.1 The program used in Chap. 13 which calculated the roots of a quadratic had to abandon the calculation if the roots were complex. You should now be able to remedy this, remembering that it is necessary to declare any complex variables. Instead of raising the expression to the power 0.5 in order to take its square root, use the function `sqrt`. The formulae for the complex roots are

$$\frac{-b}{2a} \pm i \frac{\sqrt{-(b^2 - 4ac)}}{2a}$$

If you manage this to your satisfaction, try your skills on the roots of a cubic (see the problems in Chap. 13).

Chapter 16

Logical

*A messenger yes/no semaphore her black/white keys in/out whirl
of morse hoopoe signals salvation deviously.*

Nathaniel Tarn, The Laurel Tree

Aims

The aims of this chapter are:

- To examine the last predefined type available in Fortran: logical.
- To introduce the concepts necessary to use logical expressions effectively:
 - Logical variables.
 - Logical operators.
 - The hierarchy of operations.
 - Truth tables.

16.1 Introduction

Often we have situations where we need on or off, true or false, yes or no switches, and in such circumstances we can use logical type variables, e.g.,

```
logical :: flag
```

Logicals may take only two possible values, as shown in the following:

```
flag=.true.  
or  
flag=.false.
```

Note the full stops, which are essential. With a little thought you can see why they are needed. You will already have met some of the ideas associated with logical variables from `if` statements:

```

if(a == b) then
.
else
.
endif

```

The logical expression (a == b) returns a value true or false, which then determines the route to be followed; if the quantity is true, then we execute the next statement, else we take the other route.

Similarly, the following example is also legitimate:

```

logical :: answer
answer=.true.
...
if (answer) then
...
else
...
endif

```

Again the expression `if (answer)` is evaluated; here the variable `answer` has been set to `.true.`, and therefore the statements following the `then` are executed. Clearly, conventional arithmetic is inappropriate with logicals. What does 2 times true mean? (very true?). There are a number of special operators for logicals:

- `.not.` which negates a logical value (i.e., changes true to false or vice versa).
- `.and.` logical intersection.
- `.or.` logical union.

To illustrate the use of these operators, consider the following program extract:

```

logical :: a,b,c
a=.true.
b=.not.a  !(b now has the value 'false')
c=a.or.b !(c has the value 'true')
c=a.and.b !(c now has the value 'false')

```

Table 16.1 shows the effect of these operators on logicals in a simple case.

As with arithmetic operators, there is an order of precedence associated with the logical operators:

- `.and.` is carried out before
- `.or.` and `.not.`

In dealing with logicals, the operations are carried out within a given level, from left to right. Any expressions in brackets would be dealt with first. The logical

Table 16.1 Simple truth table

x1	x2	.not.x1	x1.and.x2	x1.or.x2
True	True	False	True	True
True	False	False	False	True
False	True	True	False	True
False	False	True	False	False

Table 16.2 Fortran operator hierarchy

Expressions within brackets
Exponentiation
Multiplication and division
Addition and subtraction
Relational and logical
.and.
.or. and .not

operators are a lower order of precedence than the arithmetic operators, i.e., they are carried out later. Table 16.2 shows a more complete operator hierarchy.

Although you can build up complicated expressions with mixtures of operators, these are often difficult to comprehend, and it is generally more straightforward to break ‘big’ expressions down into smaller ones whose purpose is more readily appreciated.

Historically, logicals have not been in evidence extensively in Fortran programs, although clearly there are occasions on which they are of considerable use. Their use often aids significantly in making programs more modular and comprehensible. They can be used to make a complex section of code involving several choices much more transparent by the use of one logical function, with an appropriate name. Logicals may be used to control output; e.g.,

```
logical :: debug
...
debug=.true.
...
if(debug)then
...
print *, 'lots of printout'
...
endif
```

ensures that, while debugging a program you have more output then, when the program is correct, run with `debug=.false.`.

Note that Fortran does try to protect you while you use logical variables. You cannot do the following:

```
logical :: up, down
up=down+.false.
```

or

```
logical :: a2
real , dimension(10):: omega
.
a2=omega(3)
```

The compiler will note that this is an error, and will not permit you to run the program. This is an example of strong typing, since only a limited number of pre-determined operations are permitted. The `real`, `integer` and `complex` variable types are much more weakly typed (which helps lead to the confusion inherent in mixing variable types in arithmetic assignments).

16.2 I/O

Since logicals may take only the values `.true.` and `.false.`, the possibilities in reading and writing logical values are clearly limited. The `1` edit descriptor or format allows logicals to be input and output. On input, if the first nonblank characters are either `T` or `.T`, the logical value `.true.` is stored in the corresponding list item; if the first nonblank characters are `F` or `.F`, then `.false.` is stored. (Note therefore that reading, say, `ted` and `fahr` in an `14` format would be acceptable.) If the first nonblank character is not `F`, `T`, `.F` or `.T`, then an error message will be generated. On output, the value `T` or `F` is written out, right justified, with blanks (if appropriate). Thus,

```
logical :: flag
flag=.true.
print 100, flag, .not.flag
100 format(2L3)
```

would produce

`T F`

at the terminal.

Assigning a logical variable to anything other than a `.true.` or `.false.` value in your program will result in errors. The ‘shorthand’ forms of `.T`, `.F`, `F` and `T` are not acceptable in the program.

16.3 Summary

Another type of data—logical—is also recognised. A logical variable may take one of two values—true or false.

- There are special operators for manipulating logicals:
 - .not.
 - .and.
 - .or.
- Logical operators have a lower order of precedence than any others.

16.4 Problems

16.1 Why are the full stops needed in a statement like `A = .true.?`

16.2 Generate a truth table like the one given in this chapter.

16.3 Write a program which will read in numerical data from the terminal, but will flag any data which is negative, and will also turn these negative values into positive ones.

Chapter 17

Introduction to Derived Types

Russell's theory of types leads to certain complexities in the foundations of mathematics...Its interesting features for our purposes are that types are used to prevent certain erroneous expressions from being used in logical and mathematical formulae; and that a check against violation of type constraints can be made purely by scanning the text, without any knowledge of the value which a particular symbol might happen to have.

C.A.R. Hoare, Structured Programming

Aims

The aim of this chapter is to introduce the concepts and ideas involved in using the facilities offered in modern Fortran for the construction and use of derived or user defined types;

- defining our own types.
- declaring variables to be of a user defined type.
- manipulating variables of our own types.
- nesting types within types.

The examples are simple and are designed to highlight the syntax. More complex and realistic examples of the use of user defined data types are to be found in later chapters.

17.1 Introduction

In the coverage so far we have used the intrinsic types provided by Fortran. The only data structuring technique available has been to construct arrays of these intrinsic types. Whilst this enables us to solve a reasonable variety of problems, it is inadequate for many purposes. In this chapter we look at the facilities offered by Fortran for the construction of our own types and how we manipulate data of these new, user defined types.

With the ability to define our own types we can now construct aggregate data types that have components of a variety of base types. These are given a variety of names including

- Record in the Pascal family of languages and in many older books on computing and data structuring;
- Structs in C;
- Classes in C++, Java, C# and Eiffel;
- Cartesian product is often used in mathematics and this is the terminology adopted by Hoare;

Chapter 3 has details of some books for further reading:

- Dahl O.J., Dijkstra E.W., Hoare C.A.R., Structured Programming;
- Wirth N., Algorithms + Data Structures = Programs;
- Wirth N., Algorithms + Data Structures.

We will use the term user defined type and derived types interchangeably.

There are two stages in the process of creating and using our own data types: we must first define the type, and then create variables of this type.

17.2 Example 1: Dates

```
program ch1701

implicit none

type date

    integer :: day = 1
    integer :: month = 1
    integer :: year = 2000

end type date

type (date) :: d

print *, d%day, d%month, d%year
print *, ' type in the date, day, month, year'
read *, d%day, d%month, d%year
print *, d%day, d%month, d%year

end program ch1701
```

This complete program illustrates both the definition and use of the type. It also shows how you can define initial values within the type definition.

17.3 Type Definition

The type `date` is defined to have three component parts, comprising a day, a month and a year, all of integer type. The syntax of a type construction comprises:

```
type typename
    data type :: component_name
    etc
end type typename
```

Reference can then be made to this new type by the use of a single word, `date`, and we have a very powerful example of the use of abstraction.

17.4 Variable Definition

This is done by

```
type (typename) :: variablename
```

and we then define a variable `d` to be of this new type. The next thing we do is have a `read *` statement that prompts the user to type in three integer values, and the data are then echoed straight back to the user. We use the notation

```
variablename%component_name
```

to refer to each component of the new data type.

17.4.1 Example 2: Variant of Example 1 Using Modules

The following is a variant on the above and achieves the same result with a small amount of additional syntax.

```
module date_module

type date

    integer :: day = 1
    integer :: month = 1
    integer :: year = 2000
```

```

end type date

end module date_module

program ch1702

use date_module

implicit none
type (date) :: d

print *, d%day, d%month, d%year
print *, ' type in the date, day, month, year'
read *, d%day, d%month, d%year
print *, d%day, d%month, d%year

end program ch1702

```

The key here is that we have embedded the type declaration inside a module, and then used the module in the main program. Modules are covered in more detail in a later chapter.

If you are only using the type within one program unit then the first form is satisfactory, but if you are going to use the type in several program units the second is the required form.

We will use the second form in the examples that follow.

17.5 Example 3: Address Lists

```

module address_module

type address

character (len=40) :: name
character (len=60) :: street
character (len=60) :: district
character (len=60) :: city
character (len=8) :: post_code

end type address

end module address_module

program ch1703

```

```
use address_module

implicit none

integer :: n_of_address

type (address), dimension (:), &
allocatable :: addr

integer :: i

print *, 'input number of addresses'
read *, n_of_address

allocate (addr(1:n_of_address))

open (unit=1, file='address.txt')

do i = 1, n_of_address

    read (unit=1, fmt='(a40)') addr(i)%name
    read (unit=1, fmt='(a60)') addr(i)%street
    read (unit=1, fmt='(a60)') addr(i)%district
    read (unit=1, fmt='(a60)') addr(i)%city
    read (unit=1, fmt='(a8)')  addr(i)%post_code

end do

do i = 1, n_of_address

    print *, addr(i)%name
    print *, addr(i)%street
    print *, addr(i)%district
    print *, addr(i)%city
    print *, addr(i)%post_code

end do

end program ch1703
```

In this example we define a type `address` which has components that one would expect for a person's address. We then define an array `addr` of this type. Thus we are now creating arrays of our own user defined types. We index into the array in the way we would expect from our experience with integer, real and character arrays.

The complete example is rather trivial in a sense in that the program merely reads from one file and prints the file out to the screen. However, it highlights many of the important ideas of the definition and use of user defined types.

17.6 Example 4: Nested User Defined Types

The following example builds on the two data types already introduced. Here we construct nested user defined data types based on them and construct a new data type containing them both plus additional information.

```
module personal_module

type address

    character (len=60) :: street
    character (len=60) :: district
    character (len=60) :: city
    character (len=8) :: post_code

end type address

type date_of_birth

    integer :: day
    integer :: month
    integer :: year

end type date_of_birth

type personal
    character (len=20) :: first_name
    character (len=20) :: other_names
    character (len=40) :: surname
    type (date_of_birth) :: dob
    character (len=1) :: sex
    type (address) :: addr

end type personal

end module personal_module
```

```
program ch1704

use personal_module

implicit none

integer :: n_people
integer :: i

type (personal), dimension (:), &
allocatable :: p

print *, 'input number of people'
read *, n_people

allocate (p(1:n_people))

open (unit=1, file='person.txt')

do i = 1, n_people

read (1, fmt=100) p(i)%first_name, &
p(i)%other_names, p(i)%surname, &
p(i)%dob%day, p(i)%dob%month, &
p(i)%dob%year, p(i)%sex, p(i)%addr%street, &
p(i)%addr%district, p(i)%addr%city, &
p(i)%addr%post_code

end do

do i = 1, n_people

write (*, fmt=110) p(i)%first_name, &
p(i)%other_names, p(i)%surname, &
p(i)%dob%day, p(i)%dob%month, &
p(i)%dob%year, p(i)%sex, p(i)%addr%street, &
p(i)%addr%district, p(i)%addr%city, &
p(i)%addr%post_code

end do

100 format (a20, /, a20, /, a40, /, i2, 1x, i2, &
1x, i4, /, a1, /, a60, /, a60, /, a60, /, &
a8)
```

```
110 format (a20, a20, a40, /, i2, 1x, i2, 1x, &
           i4, /, a1, /, a60, /, a60, /, a60, /, a8)

end program ch1704
```

Here we have a date of birth data type (`date_of_birth`) based on the `date` data type from the first example, plus a slightly modified address data type, incorporated into a new data type comprising personal details. Note the way in which we reference the component parts of this new, aggregate data type.

17.7 Problems

17.1 Modify the last example to include a more elegant printed name. The current example will pad with blanks the `first_name`, `other_names` and `surname` and span 80 characters on one line, which looks rather ugly.

Add a new variable name which will comprise all three subcomponents and write out this new variable, instead of the three subcomponents.

Chapter 18

An Introduction to Pointers

Not to put too fine a point on it.

Charles Dickens, Bleak House.

Aims

The primary aim of the chapter is to introduce some of the key concepts of pointers in Fortran.

18.1 Introduction

All of the data types introduced so far, with the exception of the allocatable array, have been static. Even with the allocatable array a size has to be set at some stage during program execution. The facilities provided in Fortran by the concept of a pointer combined with those offered by a user defined type enable us to address a completely new problem area, previously extremely difficult to solve in Fortran. There are many problems where one genuinely does not know what requirements there are on the size of a data structure. Linked lists allow sparse matrix problems to be solved with minimal storage requirements, two-dimensional spatial problems can be addressed with quad-trees and three-dimensional spatial problems can be addressed with oct-trees. Many problems also have an irregular nature, and pointer arrays address this problem.

First we need to cover some of the technical aspects of pointers. A pointer is a variable that has the pointer attribute. A pointer is associated with a target by allocation or pointer assignment. A pointer becomes associated as follows:

- The pointer is allocated as the result of the successful execution of an allocate statement referencing the pointer
 - or
- The pointer is pointer-assigned to a target that is associated or is specified with the target attribute and, if allocatable, is currently allocated.

A pointer may have a pointer association status of associated, disassociated, or undefined. Its association status may change during execution of a program. Unless a pointer is initialised (explicitly or by default), it has an initial association status of undefined. A pointer may be initialised to have an association status of disassociated.

A pointer shall neither be referenced nor defined until it is associated. A pointer is disassociated following execution of a `deallocate` or `nullify` statement, following pointer association with a disassociated pointer, or initially through pointer initialisation.

Let us look at some examples to clarify these points.

18.2 Example 1: Illustrating Some Basic Pointer Concepts

With the introduction of pointers as a data type into Fortran we also have the introduction of a new assignment statement—the pointer assignment statement. Consider the following example:

```
program ch1801
    implicit none
    integer, pointer :: a => null(), b => null()
    integer, target :: c
    integer :: d

    c = 1
    a => c
    c = 2
    b => c
    d = a + b
    print *, a, b, c, d
end program ch1801
```

The following

```
integer , pointer :: a=>null(),b=>null()
```

is a declaration statement that defines `a` and `b` to be variables, with the `pointer` attribute. This means we can use `a` and `b` to refer or point to integer values. We also use the `null` intrinsic to set the status of the pointers `a` and `b` to disassociated. Using the `null` intrinsic means that we can test the status of a pointer variable and avoid making a number of common pointer programming errors. Note that in this case no space is set aside for the pointer variables `a` and `b`, i.e. `a` and `b` should not be referenced in this state.

The second declaration defines `c` to be an integer, with the `target` attribute, i.e., we can use pointers to refer or point to the value of the variable `c`.

The last declaration defines `d` to be an ordinary integer variable.

In the case of the last two declarations space is set aside to hold two integers.

Let us now look at the various executable statements in the program, one at a time:

```
c = 1
```

This is an example of the normal assignment statement with which we are already familiar. We use the variable name `c` in our program and whenever we use that name we get the value of the variable `c`.

```
a => c
```

This is an example of a pointer assignment statement. This means that both `a` and `c` now refer to the same value, in this case 1. `a` becomes associated with the target `c`. `a` can now be referenced.

```
c = 2
```

Conventional assignment statement, and `c` now has the value 2.

```
b => c
```

Second example of pointer assignment. `b` now points to the value that `c` has, in this case 2. `b` becomes associated with the target `c`. `b` can now be referenced.

```
d = a + b
```

Simple arithmetic assignment statement. The value that `a` points to is added to the value that `b` points to and the result is assigned to `d`.

The last statement prints out the values of `a`, `b`, `c` and `d`.

The output is

```
2 2 4
```

18.3 Example 2: The `associated` Intrinsic Function

The `associated` intrinsic returns the association status of a pointer variable. Consider the following example which is a simple variant on the first.

```
program ch1802
    implicit none
    integer, pointer :: a => null(), b => null()
    integer, target :: c
    integer :: d
```

```

print *, associated(a)
print *, associated(b)
c = 1
a => c
c = 2
b => c
d = a + b
print *, a, b, c, d
print *, associated(a)
print *, associated(b)
end program ch1802

```

The output from running this program is shown below

```

F
F
2 2 2 4
T
T

```

and as you can see we therefore have a mechanism to test pointers to see if they are in a valid state before use.

18.4 Example 3: Referencing Pointer Variables Before Allocation or Pointer Assignment

Consider the following example:

```

program ch1803
    implicit none
    integer, pointer :: a => null(), b => null()
    integer, target :: c
    integer :: d

    print *, a
    print *, b
    c = 1
    a => c
    c = 2
    b => c
    d = a + b
    print *, a, b, c, d
end program ch1803

```

Here we are actually referencing the pointers `a` and `b`, even though their status is disassociated. Most compilers generate a run time error with this example with the default compiler options, and the error message tends to be a little cryptic. It is recommended that you look at the diagnostic compilation switches for your compiler. We include some sample output below from gfortran, Intel and Nag. The error messages are now much more meaningful.

18.4.1 gfortran

Switches are

```
gfortran -W -Wall -fbounds-check -pedantic-errors
         -std=f2003 -Wunderflow
         -O -fbacktrace -ffpe-trap=zero,
         overflow,underflow -g
```

The program runs to completion with no error message. Here is the output.

```
ch1803.out
          0
          0
          2           2           4
```

18.4.2 Intel

Switches are

```
/check:all /traceback
```

Here is the output.

```
D:\document\fortran\newbook\examples\ch18>>
ch1803
forrtl: severe (408): fort: (7):
Attempt to use pointer A when it
is not associated with a target
Image          PC          Routine Line
Source
ch1803.exe    000000013F0AC598  Unknown Unknown
Unknown
...
ntdll.dll     0000000077096611  Unknown Unknown
Unknown
```

18.4.3 Nag

Switches are

```
-C=all -C=undefined -info -g -gline
```

Here is the output.

```
Runtime Error: ch1803.f90, line 5:
Reference to disassociated POINTER A
Program terminated by fatal error
ch1803.f90, line 5: Error occurred in CH1803
```

18.5 Example 4: Pointer Allocation and Assignment

Consider the following example:

```
program ch1804
    implicit none
    integer, pointer :: a => null(), b => null()
    integer, target :: c
    integer :: d

    allocate (a)
    a = 1
    c = 2
    b => c
    d = a + b
    print *, a, b, c, d
    deallocate (a)
end program ch1804
```

In this example we allocate `a` and then can do conventional assignment. If we had not allocated `a` the assignment would be illegal. Try out Problem 18.2 to see what will happen with your compiler.

Our simple recommendation when using pointers is to nullify them when declaring them and to explicitly allocate them before conventional assignment.

18.6 Memory Leak Examples

Dynamic memory brings greater versatility but requires greater responsibility.

18.6.1 Example 5: Simple Memory Leak

```
program ch1805
    implicit none
    integer, pointer :: a => null(), b => null()
    integer, target :: c
    integer :: d

    allocate (a)
    allocate (b)
    a = 100
    b = 200
    print *, a, b
    c = 1
    a => c
    c = 2
    b => c
    d = a + b
    print *, a, b, c, d
end program ch1805
```

What has happened to the memory allocated to a and b?

18.6.2 Example 6: More Memory Leaks

Now consider the following example.

```
program ch1806
    implicit none
    integer :: allocate_status = 0
    integer, parameter :: n1 = 100000000
    integer, parameter :: n2 = 5
    integer, dimension (:), pointer :: x
    integer, dimension (1:n2), target :: y
    integer :: i

    do
        allocate (x(1:n1), stat=allocate_status)
        if (allocate_status>0) then
            print *, ' allocate failed. program ends.'
            stop
        end if
        do i = 1, n1
```

```

        x(i) = i
end do
do i = 1, n2
    print *, x(i)
end do
do i = 1, n2
    y(i) = i*i
end do
do i = 1, n2
    print *, y(i)
end do
!   x now points to y
!   x => y !                                x now points
!                                         to y
do i = 1, n2
    print *, x(i)
end do
!   what has happened to the memory that x
!   used to point to?
end do
end program ch1806

```

Before running the above example we recommend starting up a memory monitoring program.

Under Microsoft Windows holding [CTRL] + [ALT] + [DEL] will bring up the Windows Task Manager. Choose the [Performance] tab to get a screen which will show CPU usage, PF Usage, CPU Usage History and Page File Usage History. You will also get details of Physical and Kernel memory usage.

Under Linux type

`top`

in a terminal window.

In these examples we also see the recommended form of the `allocate` statement when working with arrays. This enables us to test if the allocation has worked and take action accordingly. A positive value indicates an allocation error, zero indicates OK.

The second program can require a power off on a Windows operating system with a compiler that will remain anonymous!

18.7 Non-standard Pointer Example

Some Fortran compilers provide a non-standard `loc` intrinsic. This can be used to print out the address of the variable passed as an argument.

18.7.1 Example 7: Using the C loc Function

Here is the program.

```
program ch1807
    implicit none
    integer, pointer :: a => null(), b => null()
    integer, target :: c
    integer :: d

    allocate (a)
    allocate (b)
    a = 100
    b = 200
    print *, a, b
    print *, loc(a)
    print *, loc(b)
    print *, loc(c)
    print *, loc(d)
    c = 1
    a => c
    c = 2
    b => c
    d = a + b
    print *, a, b, c, d
    print *, loc(a)
    print *, loc(b)
    print *, loc(c)
    print *, loc(d)
end program ch1807
```

Here is the output from a compiler with loc support.

100	200		
13803552			
13803600			
2948080			
2948084			
2	2	2	4
2948080			
2948080			
2948080			
2948084			

This program clearly shows the memory leak.

18.8 Problems

18.1 Compile and run all of the example programs in this chapter with your compiler and examine the output.

18.2 Compile and run example 4 without the `allocate(a)` statement. See what happens with your compiler.

Here is the output from the Nag compiler. The first run is with the default options.

```
nagfor ch1804p.f90
NAG Fortran Compiler:
[NAG Fortran Compiler normal termination]
a.exe
```

There is no meaningful output.

The following adds the `-C=all` compilation option.

```
nagfor ch1804p.f90 -C=all
NAG Fortran Compiler:
[NAG Fortran Compiler normal termination]
a.exe
Runtime Error: ch1804p.f90, line 5:
Reference to disassociated POINTER
A
Program terminated by fatal error
```

We now get a meaningful error message.

Chapter 19

Introduction to Subroutines

A man should keep his brain attic stacked with all the furniture he is likely to use, and the rest he can put away in the lumber room of his library, where he can get at it if he wants.

Sir Arthur Conan Doyle, Five Orange Pips

Aims

The aims of this chapter are:

- To consider some of the reasons for the inclusion of subroutines in a programming language.
- To introduce with a concrete example some of the concepts and ideas involved with the definition and use of subroutines.
 - Arguments or parameters.
 - The `intent` attribute for parameters.
 - The `call` statement.
 - Scope of variables.
 - Local variables and the `save` attribute.
 - The use of parameters to report on the status of the action carried out in the subroutine.
- Module procedures to provide interfaces.

19.1 Introduction

In the earlier chapter on functions we introduced two types of function

- Intrinsic functions—which are part of the language.
- User defined functions—by which we extend the language.

We now introduce subroutines which collectively with functions are given the name procedures. Procedures provide a very powerful extension to the language by:

- Providing us with the ability to break problems down into simpler more easily solvable subproblems.
- Allowing us to concentrate on one aspect of a problem at a time.
- Avoiding duplication of code.
- Hiding away messy code so that a main program is a sequence of calls to procedures.
- Providing us with the ability to put together collections of procedures that solve commonly occurring subproblems, often given the name libraries, and generally compiled.
- Allowing us to call procedures from libraries written, tested and documented by experts in a particular field. There is no point in reinventing the wheel!

There are a number of concepts required for the successful use of subroutines and we met some of them in Chap. 12 when we looked at user defined functions. We will extend the ideas introduced there of parameters and introduce the additional concept of an interface via the use of modules. The ideas are best explained with a concrete example.

Note that we use the terms parameters and arguments interchangeably.

19.2 Example 1: Roots of a Quadratic Equation

This example is one we met earlier that solves a quadratic equation, i.e., solves

$$ax^2 + bx + c = 0$$

The program to do this originally was just one program. In the example below we break that problem down into smaller parts and make each part a subroutine. The components are:

- Main program or driving routine.
- Interaction with user to get the coefficients of the equation.
- Solution of the quadratic.

Let us look now at how we do this with the use of subroutines:

```
module interact_module
contains
  subroutine interact(a, b, c, ok)
    implicit none
    real, intent (out) :: a
    real, intent (out) :: b
    real, intent (out) :: c
```

```
logical, intent (out) :: ok
integer :: io_status = 0

print *, &
  ' type in the coefficients a, b and c'
read (unit=*, fmt=*, iostat=io_status) a, b, &
  c
if (io_status==0) then
  ok = .true.
else
  ok = .false.
end if
end subroutine interact
end module interact_module

module solve_module
contains
  subroutine solve(e, f, g, root1, root2, ifail)
    implicit none
    real, intent (in) :: e
    real, intent (in) :: f
    real, intent (in) :: g
    real, intent (out) :: root1
    real, intent (out) :: root2
    integer, intent (inout) :: ifail
! local variables
    real :: term
    real :: a2

    term = f*f - 4.*e*g
    a2 = e*2.0
! if term < 0, roots are complex
    if (term<0.0) then
      ifail = 1
    else
      term = sqrt(term)
      root1 = (-f+term)/a2
      root2 = (-f-term)/a2
    end if
  end subroutine solve
end module solve_module

program ch1901
  use interact_module
  use solve_module
```

```

implicit none
! simple example of the use of a main program
! and two subroutines.
! one interacts with the user and the
! second solves a quadratic equation,
! based on the user input.
real :: p, q, r, root1, root2
integer :: ifail = 0
logical :: ok = .true.

call interact(p, q, r, ok)
if (ok) then
    call solve(p, q, r, root1, root2, ifail)
    if (ifail==1) then
        print *, ' complex roots'
        print *, ' calculation abandoned'
    else
        print *, ' roots are ', root1, ' ', root2
    end if
else
    print *, ' error in data input program ends'
end if
end program ch1901

```

19.2.1 Referencing a Subroutine

To reference a subroutine you use the `call` statement:

```
call subroutine_name(optional actual argument list)
```

and from the earlier example the call to subroutine `interact` was of the form:

```
call interact(p,q,r,ok)
```

When a subroutine returns to the calling program unit control is passed to the statement following the `call` statement.

19.2.2 Dummy Arguments or Parameters and Actual Arguments

Procedures and their calling program units communicate through their arguments. We often use the terms parameter and arguments interchangeably through out this

text. The subroutine statement normally contains a list of dummy arguments, separated by commas and enclosed in brackets. The dummy arguments have a type associated with them; for example, in subroutine `solve` `x` is of type `real`, but no space is put aside for this in memory. When the subroutine is referenced e.g., `call solve(p,q,r,root1,root2,ifail)`, then the dummy argument points to the actual argument `p`, which is a variable in the calling program unit. The dummy argument and the actual argument must be of the same type—in this case `real`.

19.2.3 The `intent` Attribute

It is recommended that dummy arguments have an `intent` attribute. In the earlier example subroutine `solve` has a dummy argument `e` with `intent(in)`, which means that when the subroutine is referenced or called it is expecting `e` to have a value, but its value cannot be changed inside the subroutine. This acts as an extra security measure besides making the program easier to understand. For each parameter it may have one of three attributes:

- `intent(in)`, where the parameter already has a value and cannot be altered in the called routine.
- `intent(out)`, where the parameter does not have a value, and is given one in the called routine.
- `intent(inout)`, where the parameter already has a value and this is changed in the called routine.

19.2.4 Local Variables

We saw with functions that variables could be essentially local to the function and unavailable elsewhere. The concept of local variables also applies to subroutines. In the example above `term` and `a2` are both local variables to the subroutine `solve`.

19.2.5 Local Variables and the `save` Attribute

Local variables are usually created when a procedure is called and their value lost when execution returns to the calling program unit. To make sure that a local variable retains its values between calls to a subprogram the `save` attribute can be used on a type statement; e.g.,

```
integer , save :: i
```

means that when this statement appears in a subprogram the value of the local variable `i` is saved between calls.

19.2.6 Scope of Variables

In most cases variables are only available within the program unit that defines them. The introduction of argument lists to procedures immediately opens up the possibility of data within one program unit becoming available in one or more other program units.

In the main program we declare the variables `p`, `q`, `r`, `root1`, `root2`, `ifail` and `ok`.

Subroutine `interact` has no variables locally declared. It works on the arguments `a`, `b`, `c` and `ok`; which map onto `p`, `q`, `r` and `ok` from the main program, i.e., it works with those variables.

Subroutine `solve` has two locally defined variables, `term` and `a2`. It works with the variables `e`, `f`, `g`, `root1`, `root2` and `ifail`, which map onto `p`, `q`, `r`, `root1`, `root2` and `ifail` from the main program.

19.2.7 Status of the Action Carried Out in the Subroutine

It is also useful to use parameters that carry information regarding the status of the action carried out by the subroutine. With the subroutine `interact` we use a logical variable `ok` to report on the status of the interaction with the user. In the subroutine `solve` we use the status of the integer variable `ifail` to report on the status of the solution of the equation.

19.2.8 Modules 'Containing' Procedures

At the same time as introducing procedures we have 'contained' them in a module and then the main program 'uses' the module in order to make the procedure available. Procedures 'contained' in modules are called module procedures.

With the `use` statement the interface to the procedure is available to the compiler so that the types and positions of the actual and dummy arguments can be checked. This was a major source of errors with Fortran 77.

The `use` statement must be the first statement in the main program or calling unit, also the modules must be compiled before the program or calling unit.

We will cover modules in more depth in later chapters.

There are times when an interface is mandatory in Fortran so it's good practice to use module procedures from the start. There are other ways of providing explicit interfaces and we will cover them later.

19.3 Why Bother with Subroutines?

Given the increase in the complexity of the overall program to solve a relatively straightforward problem, one must ask why bother. The answer lies in our ability to manage the solution of larger and larger problems. We need all the help we can get if we are to succeed in our task of developing large-scale reliable programs.

We need to be able to break our problems down into manageable subcomponents and solve each in turn. We are now in a very good position to be able to do this. Given a problem that requires a main program, one or more functions and one or more subroutines we can work on each subcomponent in relative isolation, and know that by using features like module procedures we will be able to glue all of the components together into a stable structure at the end. We can independently compile the main program and the modules containing the functions and subroutines and use the linker to generate the overall executable, and then test that. Providing we keep our interfaces the same we can alter the actual implementations of the functions and subroutines and just recompile the changed procedures.

19.4 Summary

We now have the following concepts for the use of subroutines:

- Module procedures providing interfaces.
- Intent attribute for parameters.
- Dummy parameters.
- The use of the call statement to invoke a subroutine.
- The concepts of variables that are local to the called routines and are unavailable elsewhere in the over all program.
- Communication between program units via the argument list.
- The concept of parameters on the call that enable us to report back on the status of the called routine.

19.5 Problems

19.1 Type the program and module procedures for example 1 into one file. Compile, link and run providing data for complex roots to test this part of the code.

19.2 Split the main program and modules up into three separate files. Compile the modules and then compile the main program and link the object files to create one executable. Look at the file size of the executable and the individual object files. What do you notice?

The development of large programs is eased considerably by the ability to compile small program units and eradicate the compilation errors from one unit at a time. The linker obviously also has an important role to play in the development process.

19.3 Write a subroutine to calculate new coordinates (x', y') from (x, y) when the axes are rotated counter clockwise through an angle of a radians using:

$$\begin{aligned}x' &= x \cos a + y \sin a \\y' &= -x \sin a + y \cos a\end{aligned}$$

Hint:

The subroutine would look some thing like

```
subroutine ChangeCoordinate(x, y, a, xd, yd)
```

Write a main program to read in values of x, y and a and then call the subroutine and print out the new coordinates. Use a module procedure.

Chapter 20

Subroutines: 2

It is one thing to show a man he is in error, and another to put him in possession of the truth.

John Locke

Aims

The aims of this chapter are to extend the ideas in the earlier chapter on subroutines and look in more depth at parameter passing, in particular using a variety of ways of passing arrays.

20.1 More on Parameter Passing

So far we have seen scalar parameters of type real, integer and logical. We will now look at numeric array parameters and character parameters. We need to introduce some technical terminology first. Don't panic if you don't fully understand the terminology as the examples should clarify things.

20.1.1 Assumed-Shape Array

An assumed-shape array is a nonpointer dummy argument array that takes its shape from the associated actual argument array.

20.1.2 Deferred-Shape Array

A deferred-shape array is an allocatable array or an array pointer. An allocatable array is an array that has the allocatable attribute and a specified rank, but its bounds, and hence shape, are determined by allocation or argument association.

20.1.3 Automatic Arrays

An automatic array is an explicit-shape array that is a local variable. Automatic arrays are only allowed in function and subroutine subprograms, and are declared in the specification part of the subprogram. At least one bound of an automatic array must be a nonconstant specification expression. The bounds are determined when the subprogram is called.

20.1.4 Allocatable Dummy Arrays

Fortran provides the ability to declare an array in the main program and allocate in a subroutine.

20.1.5 Keyword and Optional Arguments

Fortran provides the ability to supply the actual arguments to a procedure by keyword, and hence in any order.

To do this the name of the dummy argument is referred to as the keyword and is specified in the actual argument list in the form

```
dummy-argument = actual-argument
```

A number of points need to be noted when using keyword and optional arguments:

- If all the actual arguments use keywords, they may appear in any order.
- When only some of the actual arguments use keywords, the first part of the list must be positional followed by keyword arguments in any order.
- When using a mixture of positional and keyword arguments, once a keyword argument is used all subsequent arguments must be specified by keyword.
- If an actual argument is omitted the corresponding optional dummy argument must not be redefined or referenced, except as an argument to the present intrinsic function.
- If an optional dummy argument is at the end of the argument list then it can just be omitted from the actual argument list.
- Keyword arguments are needed when an optional argument not at the end of an argument list is omitted, unless all the remaining arguments are omitted as well.
- Keyword and optional arguments require explicit procedure interfaces, i.e., the procedure must be internal, a module procedure or have an interface block available in the calling program unit.

A number of the intrinsic procedures have optional arguments. Consult appendix B for details.

We look at a complete example in a later chapter.

20.2 Example 1: Assumed Shape Parameter Passing

We are going to use an example based on a main program and a subroutine that calculates the mean and standard deviation of an array of numbers. The subroutine has the following parameters:

- x —the array containing the real numbers.
- n —the number of elements in the array.
- mean —the mean of the numbers.
- std_dev —the standard deviation of the numbers.

Consider the following program and subroutine.

```
module statistics_module
    implicit none

    contains

        subroutine stats(x, n, mean, std_dev)
            implicit none
            integer, intent (in) :: n
            real, intent (in), dimension () :: x
            real, intent (out) :: mean
            real, intent (out) :: std_dev
            real :: variance
            real :: sumxi, sumxi2
            integer :: i

            variance = 0.0
            sumxi = 0.0
            sumxi2 = 0.0
            do i = 1, n
                sumxi = sumxi + x(i)
                sumxi2 = sumxi2 + x(i)*x(i)
            end do
            mean = sumxi/n
            variance = (sumxi2-sumxi*sumxi/n) / (n-1)
            std_dev = sqrt(variance)
        end subroutine stats
    end module statistics_module
```

```

program ch2001
  use statistics_module
  implicit none
  integer, parameter :: n = 10
  real, dimension (1:n) :: x
  real, dimension (-4:5) :: y
  real, dimension (10) :: z
  real, allocatable, dimension(:) :: t
  real :: m, sd
  integer :: i

  do i = 1, n
    x(i) = real(i)
  end do
  call stats(x, n, m, sd)
  print *, 'x'
  print 100, m, sd
100 format (' Mean = ', f7.3, ' Std Dev = ', &
             f7.3)
  y = x
  call stats(y, n, m, sd)
  print *, 'y'
  print 100, m, sd
  z = x
  call stats(z, 10, m, sd)
  print *, 'z'
  print 100, m, sd
  allocate (t(n))
  t = x
  call stats(t, 10, m, sd)
  print *, 't'
  print 100, m, sd
end program ch2001

```

A fundamental rule in modern Fortran is that the shape of an actual array argument and its associated dummy arguments are the same, i.e., they both must have the same rank and the same extents in each dimension. The best way to apply this rule is to use assumed-shape dummy array arguments as shown in the example above.

In the subroutine we have

```
real , intent(in) , dimension(:) :: x
```

where x is an assumed-shape dummy array argument, and it will assume the shape of the actual argument when the subroutine is called.

In two of the calls we have passed a variable n as the size of the array and used a literal integer constant (10) in the other two cases. Both parameter passing mechanisms work.

20.2.1 Notes

There are several restrictions when using assumed-shape arrays:

- The rank is equal to the number of colons, in this case 1.
- The lower bounds of the assumed-shape array are the specified lower bounds, if present, and 1 otherwise. In the example above it is 1 because we haven't specified a lower bound.
- The upper bounds will be determined on entry to the procedure and will be whatever values are needed to make sure that the extents along each dimension of the dummy argument are the same as the actual argument. In this case the upper bound will be n .
- An assumed-shape array must not be defined with the pointer or allocatable attribute in Fortran.
- When using an assumed-shape array an interface is mandatory. In this example it is provided by the the `stats` subroutine being a contained subroutine in a module, and the use of the module in the main program.

20.3 Example 2: Character Arguments and Assumed-Length Dummy Arguments

The types of parameters considered so far have been real, integer and logical. Character variables are slightly different because they have a length associated with them. Consider the following program and subroutine which, given the name of a file, opens it and reads values into the real array x :

```
module read_module
    implicit none

contains
    subroutine readin(name, x, n)
        implicit none
        integer, intent (in) :: n
        real, dimension (:), intent (out) :: x
        character (len=*), intent (in) :: name
        integer :: i
```

```

open (unit=10, status='old', file=name)
do i = 1, n
    read (10, *) x(i)
end do
close (unit=10)
end subroutine readin
end module read_module

program ch2002
use read_module
implicit none
real, allocatable, dimension(:) :: a
integer :: nos, i
character (len=20) :: filename

print *, ' Type in the name of the data file'
read '(a)', filename
print *, ' Input the number of items'
read *, nos
allocate (a(1:nos))
call readin(filename, a, nos)
print *, ' data read in was'
do i = 1, nos
    print *, ' ', a(i)
end do
end program ch2002

```

The main program reads the file name from the user and passes it to the subroutine that reads in the data. The dummy argument name is of type assumed-length, and picks up the length from the actual argument filename in the calling routine, which is in this case 20 characters. An interface must be provided with assumed-shape dummy arguments, and this is achieved in this case by the subroutine being in a module.

20.4 Example 3: Rank 2 and Higher Arrays as Parameters

The following example illustrates the modern way of passing rank 2 and higher arrays as parameters. We start with a simple rank 2 example.

```

module matrix_module
implicit none

contains
subroutine matrix_bits(a, b, c, a_t, n)

```

```
implicit none
integer, intent (in) :: n
real, dimension (:, :), intent (in) :: a, b
real, dimension (:, :), intent (out) :: c, &
a_t
integer :: i, j, k
real :: temp
! matrix multiplication c=ab
do i = 1, n
    do j = 1, n
        temp = 0.0
        do k = 1, n
            temp = temp + a(i, k)*b(k, j)
        end do
        c(i, j) = temp
    end do
end do
! calculate a_t transpose of a
! set a_t to be transpose matrix a
do i = 1, n
    do j = 1, n
        a_t(i, j) = a(j, i)
    end do
end do
end subroutine matrix_bits
end module matrix_module
```

```
program ch2003
use matrix_module
implicit none
real, allocatable, dimension (:, :) :: one, &
two, three, one_t
integer :: i, n

print *, 'input size of matrices'
read *, n
allocate (one(1:n,1:n))
allocate (two(1:n,1:n))
allocate (three(1:n,1:n))
allocate (one_t(1:n,1:n))
do i = 1, n
    print *, 'input row ', i, ' of one'
    read *, one(i, 1:n)
end do
do i = 1, n
```

```

print *, 'input row ', i, ' of two'
read *, two(i, 1:n)
end do
call matrix_bits(one, two, three, one_t, n)
print *, ' matrix three:'
do i = 1, n
    print *, three(i, 1:n)
end do
print *, ' matrix one_t:'
do i = 1, n
    print *, one_t(i, 1:n)
end do
end program ch2003

```

The subroutine is doing a matrix multiplication and transpose. There are intrinsic functions in Fortran called `matmul` and `transpose` that provide the same functionality as the subroutine. One of the problems at the end of the chapter is to replace the code in the subroutine with calls to the intrinsic functions.

20.4.1 Notes

The dummy array and actual array arguments look the same but there is a difference:

- The dummy array arguments `a`, `b`, `c`, `a_t` are all assumed-shape arrays and take the shape of the actual array arguments `one`, `two`, `three` and `one_t`, respectively.
- The actual array arguments `one`, `two`, `three` and `one_t` in the main program are allocatable arrays or deferred-shape arrays. An allocatable array is an array that has an allocatable attribute. Its bounds and shape are declared when the array is allocated, hence deferred-shape.

20.5 Example 4: Automatic Arrays and Median Calculation

This example looks at the calculation of the median of a set of numbers and also illustrates the use of an automatic array.

The median is the middle value of a list, i.e., the smallest number such that at least half the numbers in the list are no greater. If the list has an odd number of entries, the median is the middle entry in the list after sorting the list into ascending order. If the list has an even number of entries, the median is equal to the sum of the two middle (after sorting) numbers divided by two. One way to determine the median computationally is to sort the numbers and choose the item in the middle.

Wirth classifies sorting into simple and advanced, and his three simple methods are as follows:

- Insertion sorting—The items are considered one at a time and each new item is inserted into the appropriate position relative to the previously sorted item. If you have ever played bridge then you have probably used this method.
- Selection sorting—First the smallest (or largest) item is chosen and is set aside from the rest. Then the process is repeated for the next smallest item and set aside in the next position. This process is repeated until all items are sorted.
- Exchange sorting—if two items are found to be out of order they are interchanged. This process is repeated until no more exchanges take place.

Knuth also identifies the above three sorting methods. For more information on sorting the Knuth and Wirth books are good starting places. Knuth is a little old (1973) compared to Wirth (1986), but it is still a very good coverage. Knuth uses mix assembler to code the examples whilst the Wirth book uses Modula 2, and is therefore easier to translate into modern Fortran.

In the example below we use an exchange sort:

```
module statistics_module
    implicit none

contains
    subroutine stats(x, n, mean, std_dev, median)
        implicit none
        integer, intent (in) :: n
        real, intent (in), dimension () :: x
        real, intent (out) :: mean
        real, intent (out) :: std_dev
        real, intent (out) :: median
        real, dimension (1:n) :: y
        real :: variance
        real :: sumxi, sumxi2

        sumxi = 0.0
        sumxi2 = 0.0
        variance = 0.0
        sumxi = sum(x)
        sumxi2 = sum(x*x)
        mean = sumxi/n
        variance = (sumxi2-sumxi*sumxi/n) / (n-1)
        std_dev = sqrt(variance)
        y = x
        if (mod(n,2)==0) then
```

```

    median = (find(n/2)+find((n/2)+1))/2
else
    median = find((n/2)+1)
end if
contains
real function find(k)
implicit none
integer, intent (in) :: k
integer :: l, r, i, j
real :: t1, t2

l = 1
r = n
do while (l<r)
    t1 = y(k)
    i = l
    j = r
    do
        do while (y(i)<t1)
            i = i + 1
        end do
        do while (t1<y(j))
            j = j - 1
        end do
        if (i<=j) then
            t2 = y(i)
            y(i) = y(j)
            y(j) = t2
            i = i + 1
            j = j - 1
        end if
        if (i>j) exit
    end do
    if (j<k) then
        l = i
    end if
    if (k<i) then
        r = j
    end if
end do
find = y(k)
end function find
end subroutine stats
end module statistics_module

```

```

program ch2004
  use statistics_module
  implicit none
  integer :: n
  integer :: i
  real, allocatable, dimension () :: x
  real :: m, sd, median
  integer, dimension (8) :: timing

n = 1000000
do i = 1, 3
  print *, ' n = ', n
  allocate (x(1:n))
  call random_number(x)
  x = x*1000
  call date_and_time(values=timing)
  print *, ' initial '
  print *, timing(6), timing(7), timing(8)
  call stats(x, n, m, sd, median)
  print *, ' Mean = ', m
  print *, ' Standard deviation = ', sd
  print *, ' Median is = ', median
  call date_and_time(values=timing)
  print *, timing(6), timing(7), timing(8)
  n = n*10
  deallocate (x)
end do
end program ch2004

```

In the subroutine `stats` the array `y` is automatic. It will be allocated automatically when we call the subroutine. We use this array as a work array to hold the sorted data. We then use this sorted array to determine the median.

Note the use of the `sum` intrinsic in this example:

```

sumxi=sum(x)
sumxi2=sum(x*x)

```

These statements replace the do loop from the earlier example. A good optimising compiler would not make two passes over the data with these two statements.

20.5.1 Internal Subroutines and Scope

The `stats` subroutine contains the `find` subroutine. The `stats` subroutine has access to the following variables

- $x, n, \text{mean}, \text{std_dev}, \text{median}$ —these are made available as they are passed in as parameters.
- $y, \text{variance}, \text{sumxi}, \text{sumxi2}$ —are local to the subroutine `stats`.

The subroutine `find` has access to the above as it is contained within subroutine `stats`. It also has the following local variables that are only available within subroutine `selection`

- $i, j, k, \text{minimum}$

This program uses an algorithm developed by Hoare to determine the median. The number of computations required to find the median is approximately $2 * n$.

The limiting factor with this algorithm is the amount of installed memory. The program will crash on systems with a failure to allocate the automatic array. This is a drawback of automatic arrays in that there is no mechanism to handle this failure gracefully. You would then need to use allocatable local work arrays. The drawback here is that the programmer is then responsible for the deallocation of these arrays. Memory leaks are then possible.

20.6 Example 5: Recursive Subroutines—Quicksort

In Chap. 12 we saw an example of recursive functions. This example illustrates the use of a recursive subroutine. It uses a simple implementation of Hoare’s Quicksort. References are given in the bibliography. We took the algorithm from Wirth’s book for our example.

The program times the various components parts of the program

- dynamic allocation of the real array
- use the `random_number` subroutine to generate the numbers
- call the `sort_data` subroutine to sort the data
- print out the first 10 sorted elements
- deallocate the array

We also use the `date_and_time` intrinsic subroutine to provide the timing details.

```
module sort_data_module
    implicit none

contains
    subroutine sort_data(raw_data, how_many)
        implicit none
        integer, intent (in) :: how_many
```

```
real, intent (inout), dimension (: ) :: &
  raw_data

call quicksort(1, how_many)
contains
recursive subroutine quicksort(l, r)
  implicit none
  integer, intent (in) :: l, r
! local variables
  integer :: i, j
  real :: v, t

  i = l
  j = r
  v = raw_data(int((l+r)/2))
  do
    do while (raw_data(i)<v)
      i = i + 1
    end do
    do while (v<raw_data(j))
      j = j - 1
    end do
    if (i<=j) then
      t = raw_data(i)
      raw_data(i) = raw_data(j)
      raw_data(j) = t
      i = i + 1
      j = j - 1
    end if
    if (i>j) exit
  end do
  if (l<j) then
    call quicksort(l, j)
  end if
  if (i<r) then
    call quicksort(i, r)
  end if
end subroutine quicksort
end subroutine sort_data
end module sort_data_module

program ch2005
use sort_data_module
implicit none
integer, parameter :: n = 10000000
real, allocatable, dimension (:) :: x
```

```

integer, dimension (8) :: timing
real :: t1, t2
character *30, dimension (4) :: heading = [ &
  ' Allocate =           ', &
  ' Random number generation = ', &
  ' Sort =           ', &
  ' Deallocate =      ' ]

call date_and_time(values=timing)
print *, ' Program starts'
write (unit=*, fmt=100) timing(1:3), &
  timing(5:7)
100 format (2x, i4, 2(' '//,i2), ' ', 2(i2,:':'), &
  i2)
t1 = td()
allocate (x(n))
t2 = td()
write (unit=*, fmt=110) heading(1), (t2-t1)
110 format (a30, f8.3)
t1 = t2
heading = ' Random number generation = '
call random_number(x)
t2 = td()
write (unit=*, fmt=110) heading(2), (t2-t1)
t1 = t2
heading = ' Sort = '
call sort_data(x, n)
t2 = td()
write (unit=*, fmt=110) heading(3), (t2-t1)
print *, ' First 10 sorted numbers are'
write (unit=*, fmt=120) x(1:10)
120 format (2x, e12.6)
t1 = t2
heading = ' Deallocate = '
deallocate (x)
t2 = td()
write (unit=*, fmt=110) heading(4), (t2-t1)
call date_and_time(values=timing)
print *, ' Program terminates'
write (unit=*, fmt=100) timing(1:3), &
  timing(5:7)

contains

function td()

```

```
real :: td

call date_and_time(values=timing)
td = 60*timing(6) + timing(7) + &
     real(timing(8))/1000.0
end function td
end program ch2005
```

20.6.1 Note—Recursive Subroutine

The actual sorting is done in the recursive subroutine `QuickSort`. The actual algorithm is taken from the Wirth book. See the bibliography for a reference.

Recursion provides us with a very clean and expressive way of solving many problems. There will be instances where it is worthwhile removing the overhead of recursion, but the first priority is the production of a program that is correct. It is pointless having a very efficient but incorrect solution.

We will look again at recursion and efficiency in a later chapter and see under what criteria we can replace recursion with iteration.

20.6.2 Note—Flexible Design

The `QuickSort` recursive routine can be replaced with another sorting algorithm and we can maintain the interface to `sort_data`. We can thus decouple the implementation of the actual sorting routine from the defined interface. We would only need to recompile the `sort_data` routine and we could relink using the already compiled main routine.

A later chapter looks at a non recursive implementation of quicksort where we look at some of the ways of rewriting the above program by replacing the recursive quicksort with the non recursive version.

We call the `date_and_time` intrinsic subroutine to get timing information. The first three values are the year, month and day, and 5, 6 and 7 provide the hour minute and second. The last element of the array is milliseconds.

20.7 Example 6: Allocatable Dummy Arrays

In the examples so far allocation of arrays has taken place in the main program and the arrays have been passed into subroutines and functions.

In this example the allocation takes place in the `read_data` subroutine.

```
module read_data_module
    implicit none

contains
    subroutine read_data(file_name, raw_data, &
        how_many)
        implicit none
        character (len=*), intent (in) :: file_name
        integer, intent (in) :: how_many
        real, intent (out), allocatable, &
            dimension (: ) :: raw_data
!    local variables
    integer :: i

    allocate (raw_data(1:how_many))
    open (file=file_name, unit=1)
    do i = 1, how_many
        read (unit=1, fmt=*) raw_data(i)
    end do
end subroutine read_data
end module read_data_module

module sort_data_module
    implicit none

contains
    subroutine sort_data(raw_data, how_many)
        implicit none
        integer, intent (in) :: how_many
        real, intent (inout), dimension (: ) :: &
            raw_data

        call quicksort(1, how_many)
contains
    recursive subroutine quicksort(l, r)
        implicit none
        integer, intent (in) :: l, r
!    local variables
        integer :: i, j
        real :: v, t

        i = l
        j = r
        v = raw_data(int((l+r)/2))
        do
```

```
do while (raw_data(i)<v)
    i = i + 1
end do
do while (v<raw_data(j))
    j = j - 1
end do
if (i<=j) then
    t = raw_data(i)
    raw_data(i) = raw_data(j)
    raw_data(j) = t
    i = i + 1
    j = j - 1
end if
if (i>j) exit
end do
if (l<j) then
    call quicksort(l, j)
end if
if (i<r) then
    call quicksort(i, r)
end if
end subroutine quicksort
end subroutine sort_data
end module sort_data_module

module print_data_module
    implicit none

contains
    subroutine print_data(raw_data, how_many)
        implicit none
        integer, intent (in) :: how_many
        real, intent (in), dimension(:) :: raw_data
!       local variables
        integer :: i

        open (file='sorted.txt', unit=2)
        do i = 1, how_many
            write (unit=2, fmt=*) raw_data(i)
        end do
        close (2)
    end subroutine print_data
end module print_data_module
```

```

program ch2006
  use read_data_module
  use sort_data_module
  use print_data_module
  implicit none
  integer :: how_many
  character (len=20) :: file_name
  real, allocatable, dimension(:) :: raw_data
  integer, dimension(8) :: timing

  print *, ' how many data items are there?'
  read *, how_many
  print *, ' what is the file name?'
  read '(a)', file_name
  call date_and_time(values=timing)
  print *, ' initial'
  print *, timing(6), timing(7), timing(8)
  call read_data(file_name, raw_data, how_many)
  call date_and_time(values=timing)
  print *, ' allocate and read'
  print *, timing(6), timing(7), timing(8)
  call sort_data(raw_data, how_many)
  call date_and_time(values=timing)
  print *, ' sort'
  print *, timing(6), timing(7), timing(8)
  call print_data(raw_data, how_many)
  call date_and_time(values=timing)
  print *, ' print'
  print *, timing(6), timing(7), timing(8)
  print *, ''
  print *, ' data written to file sorted.txt'
end program ch2006

```

We now have a choice of where we do the allocation. This is more flexible than having to do the allocation in the main program, which is effectively a more Fortran 77 style of programming.

20.8 Example 7: Elemental Subroutines

We saw an example in Chap. 12 of elemental functions. Here is an example of an elemental subroutine.

```
module swap_module
    implicit none

contains
    elemental subroutine swap(x, y)
        integer, intent (inout) :: x, y
        integer :: temp

        temp = x
        x = y
        y = temp
    end subroutine swap
end module swap_module

program ch2007
    use swap_module
    implicit none
    integer, dimension (10) :: a, b
    integer :: i

    do i = 1, 10
        a(i) = i
        b(i) = i*i
    end do
    print *, a
    print *, b
    call swap(a, b)
    print *, a
    print *, b
end program ch2007
```

The subroutine is written as if the arguments are scalar, but work with arrays!
User defined elemental procedures came in with Fortran 95.

20.9 Summary

We now have a lot of the tools to start tackling problems in a structured and modular way, breaking problems down into manageable chunks and designing subprograms for each of the tasks.

20.10 Problems

20.1 Below is the random number program that was used to generate the data sets for the Quicksort example:

```
program ch2008
    implicit none
    integer :: n
    integer :: i
    real, allocatable, dimension(:) :: x

    print *, ' how many values ?'
    read *, n
    allocate (x(1:n))
    call random_number(x)
    x = x*1000
    open (unit=10, file='random.txt')
    do i = 1, n
        write (10, 100) x(i)
    end do
100 format (f8.3)
end program ch2008
```

Run the Quick_Sort program in this chapter with the data file as input. Obtain timing details.

What percentage of the time does the program spend in each subroutine? Is it worth trying to make the sort much more efficient given these timings?

20.2 Try using the operating system SORT command to sort the file. What timing figures do you get now?

Was it worth writing a program?

20.3 Consider the following program:

```
program ch2009
    ! program to test array subscript checking
    ! when the array is passed as an argument.

    implicit none
    integer, parameter :: array_size = 10
    integer :: i
    integer, dimension (array_size) :: a
```

```
do i = 1, array_size
    a(i) = i
end do
call sub01(a, array_size)
end program ch2009
subroutine sub01(a, array_size)
    implicit none
    integer, intent (in) :: array_size
    integer, intent (in), dimension (array_size) &
        :: a
    integer :: i
    integer :: atotal = 0
    integer :: rtotal = 0

    do i = 1, array_size
        rtotal = rtotal + a(i)
    end do
    do i = 1, array_size + 1
        atotal = atotal + a(i)
    end do
    print *, ' Apparent total is ', atotal
    print *, ' real total is ', rtotal
end subroutine sub01
```

The key thing to note is that we haven't used a module procedure (we haven't provided an interface for the subroutine) and we have an error in the subroutine where we go outside the array. Run this program. What answer do you get for the apparent total?

Are there any compiler flags or switches which will enable you to trap this error?

20.4 Use the intrinsic functions `matmul` and `transpose` to replace the current Fortran 77 style code in program ch2003.

Bibliography

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20.11 Commercial Numerical and Statistical Subroutine Libraries

There are two major suppliers of commercial numerical and statistical libraries:

- NAG: Numerical Algorithms Group
and
- Rogue Wave Software

They can be found at:

<http://www.nag.co.uk/>

and

<http://www.roguewave.com/>

respectively. Their libraries are written by numerical analysts, and are fully tested and well documented. They are under constant development and available for a wide range of hardware platforms and compilers. Parallel versions are also available. In a later chapter we look at using a sorting routine from the Nag SMP library.

Chapter 21

Modules

Common sense is the best distributed commodity in the world, for every man is convinced that he is well supplied with it.

Descartes

Aims

The aims of this chapter are to look at the facilities found in Fortran provided by modules, in particular:

- The use of a module to aid in the consistent definition of precision throughout a program and subprograms.
- The use of modules for global data.
- The use of modules for derived data types.
- Modules containing procedures
- A module for timing programs
- Public, private and protected attributes
- The use statement and its extensions

21.1 Introduction

We have now covered the major executable building blocks in Fortran and they are

- The main program unit
- Functions
- Subroutines

and these provide us with the tools to solve many problems using just a main program, and one or more external and internal procedures. Both external and internal procedures communicate through their argument lists, whilst internal procedures have access to data in their host program units.

We have also introduced modules. The first set of examples was in the chapter on functions. The second set were in the chapter on derived types and the third set were in the subroutine chapters.

We will now look at examples of modules in more detail for

- Precision definition.
- Global data
- Modules containing procedures
- Derived type definition
- Simple timing information of a program

Modules provide the code organisational mechanism in Fortran and can be thought of as the equivalent of classes in C++, Java and C#. They are one of the most important features of modern Fortran.

21.2 Basic Module Syntax

The form of a module is

```
module module_name
  ...
  ...
end module module_name
```

and the specifications and definitions contained within it is made available in the program units that need to access it by

```
use module_name
```

The `use` statement must be the first statement after the program, function or subroutine statement.

21.3 Modules for Global Data

So far the only way that a program unit can communicate with a procedure is through the argument list. Sometimes this is very cumbersome, especially if a number of procedures want access to the same data, and it means long argument lists. The problem can be solved using modules; e.g., by defining the precision to which you wish to work and any constants defined to that precision which may be needed by a number of procedures.

21.4 Example 1: Modules for Precision Specification and Constant Definition

In the chapter on arithmetic we introduced the features in Fortran that enable us to specify the precision of real numbers.

For the real numeric kind types, we used

- sp—single precision
- dp—double precision
- qp—quad precision

and here is the Fortran code segment from the program example.

```
integer, parameter :: &
    sp = selected_real_kind( 6, 37)
integer, parameter :: &
    dp = selected_real_kind(15, 307)
integer, parameter :: &
    qp = selected_real_kind(30, 291)
```

In this example we are going to package the above in a module, and then use the module to enable us to choose a working precision for the program and associated functions and subroutines. This module will be referred to in many examples in the book.

We will also have a second module with a set of physical and mathematical constants.

```
module precision_module
    implicit none
    integer, parameter :: sp &
        = selected_real_kind( 6, 37)
    integer, parameter :: dp &
        = selected_real_kind(15, 307)
    integer, parameter :: qp &
        = selected_real_kind(30, 291)
end module precision_module

module maths_module

    use precision_module, wp => dp

    implicit none
    real (wp), parameter :: c = 299792458.0_wp
    ! units m s-1
```

```
real (wp), parameter :: e = &
 2.7182818284590452353602874713526624977_wp

real (wp), parameter :: g = 9.812420_wp
! 9.780 356 m s-2 at sea level on the equator
! 9.812 420 m s-2 at sea level in london
! 9.832 079 m s-2 at sea level at the poles

real (wp), parameter :: pi = &
 3.141592653589793238462643383279502884_wp

end module maths_module

module sub1_module
  implicit none

contains

subroutine sub1(radius, area, circumference)

  use precision_module, wp => dp
  use maths_module
  implicit none
  real (wp), intent (in) :: radius
  real (wp), intent (out) :: area, &
    circumference

  area = pi*radius*radius
  circumference = 2.0_wp*pi*radius

end subroutine sub1

end module sub1_module

program ch2101

  use precision_module, wp => dp
  use sub1_module

  implicit none

  real (wp) :: r, a, c
```

```

print *, 'radius?'
read *, r
call sub1(r, a, c)
print *, ' for radius = ', r
print *, ' area = ', a
print *, ' circumference = ', c

end program ch2101

```

In our example we have

```
use precision_module , wp => dp
```

and the `wp => dp` is called a `rename-list` in Fortran terminology. We are using it in this example to make `wp` point to the `dp` precision in the module.

Thus we can chose the working precision of our program very easily.

The kind type parameter `wp` is then used with all the real type declaration e.g.,

```
real (wp):: r ,a,c
```

To make sure that all floating point calculations are performed to the working precision specified by `wp` any constants such as 2.0 in subroutine `Sub1` are specified as `const_wp` e.g.,

```
2.0_wp
```

We set `e` and `pi` to over 33 digits as this is the number in a 128 bit real. This ensures that all calculations are carried out accurately to the maximum precision.

21.5 Example 2: Modules for Globally Sharing Data

The following example uses a module to define a parameter and two arrays. The module also contains three subroutines that have access to the data in the module. The main program has the statement

```
use data_module
```

which interfaces to the three subroutines.

Note that in this example the calls to the subroutines have no parameters. They work with the data contained in the module.

```
module data_module
    implicit none
    integer, parameter :: n = 12
    real, dimension (1:n) :: rainfall
    real, dimension (1:n) :: sorted

contains
    subroutine readdata
        implicit none
        integer :: i
        character (len=40) :: filename

        print *, ' What is the filename ?'
        read *, filename
        open (unit=100, file=filename)
        do i = 1, n
            read (100, *) rainfall(i)
        end do
    end subroutine readdata

    subroutine sortdata
        implicit none

        sorted = rainfall
        call selection
contains
    subroutine selection
        implicit none
        integer :: i, j, k
        real :: minimum

        do i = 1, n - 1
            k = i
            minimum = sorted(i)
            do j = i + 1, n
                if (sorted(j)<minimum) then
                    k = j
                    minimum = sorted(k)
                end if
            end do
            sorted(k) = sorted(i)
            sorted(i) = minimum
        end do
    end subroutine selection
end subroutine sortdata
```

```
subroutine printdata
    implicit none
    integer :: i

    print *, ' original data is '
    do i = 1, n
        print 100, rainfall(i)
    end do
    print *, ' Sorted data is '
    do i = 1, n
        print 100, sorted(i)
    end do
100 format (1x, f7.1)
end subroutine printdata
end module data_module

program ch2102
use data_module
implicit none

call readdata
call sortdata
call printdata
end program ch2102
```

21.6 Modules for Derived Data Types

When using derived data types and passing them as arguments to procedures, both the actual arguments and dummy arguments must be of the same type, i.e., they must be declared with reference to the same type definition. The only way this can be achieved is by using modules. The user defined type is declared in a module and each program unit that requires that type uses the module.

21.7 Example 3: Person Data Type

In this example we have a user defined type person which we wish to use in the main program and pass arguments of this type to the subroutines `read_data` and `stats`. In order to have the type `person` available to two subroutines and the

main program we have defined `person` in a module `personal_module` and then made the module available to each program unit with the statement

```
use personal_module
```

Note that we have put both subroutines in one module.

```
module personal_module
    implicit none
    type person
        real :: weight
        integer :: age
        character :: sex
    end type person
end module personal_module
module subs_module
    use personal_module
    implicit none
contains
    subroutine read_data(data, no)
        implicit none
        type (person), dimension (:), allocatable, &
            intent (out) :: data
        integer, intent (out) :: no
        integer :: i

        print *, 'input number of patients'
        read *, no
        allocate (data(1:no))

        do i = 1, no
            print *, 'for person ', i
            print *, 'weight ?'
            read *, data(i)%weight
            print *, 'age ?'
            read *, data(i)%age
            print *, 'sex ?'
            read *, data(i)%sex
        end do
    end subroutine read_data
    subroutine stats(data, no, m_a, f_a)
        implicit none
        type (person), dimension (:), &
```

```
      intent (in) :: data
      real, intent (out) :: m_a, f_a
      integer, intent (in) :: no
      integer :: i, no_f, no_m

      m_a = 0.0
      f_a = 0.0
      no_f = 0
      no_m = 0
      do i = 1, no
        if (data(i)%sex=='M' .or. data(i)%sex=='m' &
            ) then
          m_a = m_a + data(i)%weight
          no_m = no_m + 1
        else if (data(i)%sex=='F' .or. &
                  data(i)%sex=='f') then
          f_a = f_a + data(i)%weight
          no_f = no_f + 1
        end if
      end do
      if (no_m>0) then
        m_a = m_a/no_m
      end if
      if (no_f>0) then
        f_a = f_a/no_f
      end if
    end subroutine stats
  end module subs_module
program ch2103
  use personal_module
  use subs_module
  implicit none
  type (person), dimension (:), allocatable :: &
    patient
  integer :: no_of_patients
  real :: male_average, female_average

  call read_data(patient, no_of_patients)
  call stats(patient, no_of_patients, &
            male_average, female_average)
  print *, 'average male weight is ', &
            male_average
  print *, 'average female weight is ', &
            female_average
end program ch2103
```

21.8 Example 4: A Module for Simple Timing of a Program

It is a common requirement to need timing details on how long parts of a program take. In this module we have a `start_timing` and `end_timing` subroutines and a `time_difference` real function. We will be using this module in several examples in subsequent chapters.

```
module timing_module

    implicit none
    integer, dimension (8), private :: dt
    real, private :: h, m, s, ms, tt
    real, private :: last_tt

contains

    subroutine start_timing()
        implicit none

        call date_and_time(values=dt)
        print 100, dt(1:3), dt(5:8)
        h = real(dt(5))
        m = real(dt(6))
        s = real(dt(7))
        ms = real(dt(8))
        last_tt = 60*(60*h+m) + s + ms/1000.0
100     format (1x, i4, '/', i2, '/', i2, 1x, i2, &
               ':', i2,(':', i2, 1x, i3)
        end subroutine start_timing

    subroutine end_timing()
        implicit none

        call date_and_time(values=dt)
        print 100, dt(1:3), dt(5:8)
100     format (1x, i4, '/', i2, '/', i2, 1x, i2, &
               ':', i2,(':', i2, 1x, i3)
        end subroutine end_timing

    real function time_difference()
        implicit none

        tt = 0.0
        call date_and_time(values=dt)
```

```

h = real(dt(5))
m = real(dt(6))
s = real(dt(7))
ms = real(dt(8))
tt = 60*(60*h+m) + s + ms/1000.0
time_difference = tt - last_tt
last_tt = tt
end function time_difference

end module timing_module

```

21.9 **private, public and protected** attributes

With the examples of modules so far every entity in a module has been accessible to each program unit that 'uses' the module. By default all entities in a module have the public attribute, but sometimes it is desirable to limit the access. If entities have the private attribute this limits the possibility of inadvertent changes to a variable by another program unit.

Example of using public and private attributes:

```

real, public      :: a, b, c
integer, private :: i, j, k

```

If a variable in a module is declared to be public, its access can be partially restricted by also giving it the protected attribute. This means that the variable can still be seen by program units that use the module but its value cannot be changed e.g.,

```
integer, public, protected:: i
```

21.10 The **use** statement

In its simplest form the use statement is

```
use module_name
```

which then makes all the module's public entities available to the program unit. There may be times when only certain entities should be available to a particular program unit. In Example 1 subroutine sub1 'uses' maths_module but only needs pi and not c, e and g. The use statement could therefore be

```
use maths_module, only: pi
```

There are also times when an entity in a module needs to have its name changed when used in a program unit. For example variable `g` in `maths_module` needs to be called `gravity` in subroutine `sub1` so the `use` statement becomes

```
use maths_module, gravity=> g
```

We have also used this facility in example 1 where we renamed `dp` to `wp`.

21.11 Notes on Module Usage and Compilation

If we only have one file comprising all of the program units (main program, modules, functions and subroutines) then there is little to worry about. However, it is recommended that larger-scale programs be developed as a collection of files with related program units in each file, or even one program unit per file. This is more productive in the longer term, but it will lead to problems with modules unless we compile each module before we use it in other program units.

21.12 Formal Syntax

The following is taken from the standard and describes more fully requirements in the interface area.

21.12.1 Interface

The interface of a procedure determines the forms of reference through which it may be invoked. The procedure's interface consists of its name, binding label, generic identifiers, characteristics, and the names of its dummy arguments. The characteristics and binding label of a procedure are fixed, but the remainder of the interface may differ in differing contexts

21.12.2 Implicit and Explicit Interfaces

Within the scope of a procedure identifier, the interface of the procedure is either explicit or implicit. The interface of an internal procedure, module procedure, or intrinsic procedure is always explicit in such a scope.

The interface of a subroutine or a function with a separate result name is explicit within the subprogram where the name is accessible.

21.12.3 Explicit Interface

A procedure other than a statement function shall have an explicit interface if it is referenced and

- a reference to the procedure appears
 - with an argument keyword, or
 - in a context that requires it to be pure,
- the procedure has a dummy argument that
 - has the `allocatable`, `optional`, `pointer`, `target`, or `value` attribute,
 - is an assumed-shape array,
 - is a coarray,
 - is polymorphic,
- the procedure has a result that
 - is an array,
 - is a pointer or is allocatable, or
 - has a nonassumed type parameter value that is not a constant expression,
- the procedure is elemental

21.13 Summary

We have now introduced the concept of a module, another type of program unit, probably one of the most important features of modern Fortran. We have seen in this chapter how they can be used:

- Define global data.
- Define derived data types.
- Contain explicit procedure interfaces.
- Package together procedures.

This is a very powerful addition to the language, especially when constructing large programs and procedure libraries.

21.14 Problems

21.1 Write two functions, one to calculate the volume of a cylinder $\pi r^2 l$ where the radius is r and the length is l , and the other to calculate the area of the base of the cylinder πr^2

Define π as a parameter in a module which is used by the two functions. Now write a main program which prompts the user for the values of r and l , calls the two functions and prints out the results.

21.2 Make all the real variables in the above problem have 15 significant digits and a range of 10^{-307} to 10^{+307} . Use a module.

Chapter 22

Data Structuring in Fortran

The good teacher is a guide who helps others to dispense with his services.

R.S. Peters, Ethics and Education

Aims

The aims of this chapter are to look at several complete examples illustrating data structuring in Fortran using the following

- Singly linked list
- Ragged arrays
- A perfectly balanced tree
- A date data type

22.1 Introduction

This chapter looks at simple data structuring in Fortran using a range of examples. We use modules throughout to define the data structures that we will be working with. The chapter starts with a number of pointer examples.

22.2 Example 1: Singly Linked List: Reading an Unknown Amount of Text

Conceptually a singly linked list consists of a sequence of boxes with compartments. In the simplest case the first compartment holds a data item and the second contains directions to the next box.

In the diagram below we have a singly linked list that holds characters Jane. We assume that the address of the start of the list is 100. We assume 4 bytes per character (a 32 bit word) and 4 bytes per pointer.

- Element 1 is at address 100 and holds the character J and a pointer to the next element at address 108.
- Element 2 holds the character a and a pointer to the next element at address 116.
- Element 3 holds the character n and a pointer to the next element at address 124.
- Element 4 holds the character e and does not point to anything—we use the null pointer.

```
[J : 108] -> [a : 116] -> [n : 124] -> [e : null]
```

We can construct a data structure in Fortran to work with a singly linked list by defining a link data type with two components, a character variable and a pointer variable to a link data type. A complete program to do this is given below:

```
module link_module

type link
    character (len=1) :: c
    type (link), pointer :: next => null()
end type link

end module link_module

program ch2201

use link_module
implicit none
type (link), pointer :: root, current
character (len=:), allocatable :: word
character (len=80) :: fname
integer :: io_stat_number = 0
integer :: n, i = 0
! reads an arbitrary amount of text from a file
! - eof terminates it
print *, 'Type in the file name'
read '(a)', fname
open (unit=1, file=fname, status='old')
! reads in a character at a time until eof
allocate (root)

read (unit=1, fmt='(a)', advance='no', &
iostat=io_stat_number) root%c

if (io_stat_number/=-1) then
    allocate (root%next)
    i = i + 1
end if
```

```

end if
current => root

do while (associated(current%next))
    current => current%next
    read (unit=1, fmt='(a)', advance='no', &
          iostat=io_stat_number) current%c
    if (io_stat_number/=-1) then
        allocate (current%next)
        i = i + 1
    end if
end do

print *, i, ' characters read'
! Allocate the deferred length character variable
! to the correct size and copy from the linked list.
n = i
allocate (character(len=n) :: word)
i = 0
current => root

do while (associated(current%next))
    i = i + 1
    word(i:i) = current%c
    current => current%next
end do

print *, 'text read in was:'
print *, word

end program ch2201

```

The first thing of interest is the type definition for the singly linked list. We have

```

module link_module
    type link
        character :: c
        type (link), pointer :: next => null()
    end type link
end module link_module

```

and we call the new type `link`. It comprises two component parts: the first holds a character `c`, and the second holds a pointer called `next` to allow us to refer to another instance of type `link`.

We use the intrinsic `null()` to provide an initial value for the `next` pointer.

The next item of interest is the variable definition. Here we define two variables `root` and `current` to be pointers that point to items of type `link`. In Fortran when we define a variable to be a pointer we also have to define what it is allowed to point to. This is a very useful restriction on pointers, and helps make using them more secure. The first executable statement

```
allocate(root)
```

requests that the variable `root` be allocated memory. The next statement reads a character from the file. We are using a number of additional features of the read statement, including

```
iostat=io_stat_number
advance='no'
```

and the two options combine to provide the ability to read an arbitrary number of text from a file a character at a time. If there is data in the file we allocate `root%next` and increment the character count `i`. We then loop until we reach end of file. When end of file is reached the while loop will terminate as `next` is `null()`. The statement

```
current => root
```

means that both `current` and `root` point to the same physical memory location, and this holds a character data item and a pointer. We must do this as we have to know where the start of the list is. This is now our responsibility, not the compilers. Without this statement we are not able to do anything with the list except fill it up—hardly very useful.

When end of file is reached the while loop will terminate as `next` is `null()`. We then print out the number of characters read. We then allocate a character variable of the correct size. The next statement

```
current => root
```

means that we are back at the start of the list, and in a position to traverse the list and copy each character from the linked list to the word character variable.

There is thus the concept with the pointer variable `current` of it providing us with a window into memory where the complete linked list is held, and we look at one part of the list at a time. Both while loops use the intrinsic function associated to check the association status of a pointer.

It is recommended that this program be typed in, compiled and executed. It is surprisingly difficult to believe that it will actually read in a completely arbitrary amount of text from a file. Seeing is believing.

22.3 Example 2: Reading in an Arbitrary Number of Reals Using a Linked List and Copying to an Array

In this example we will look at using a singly linked list to read in an arbitrary amount of data and then allocating an array to copy it to for normal numeric calculations at run time. Here is the program.

```
module link_module
  type link
    real :: n
    type (link), pointer :: next => null()
  end type link
end module link_module

program ch2202
  use link_module
  implicit none
  type (link), pointer :: root, current
  integer :: i = 0, m
  integer :: io_stat_number = 0
  real, allocatable, dimension (:) :: x
  character (len=80) :: fname

  print *, 'file containing real numbers?'
  read '(a)', fname
  open (unit=1, file=fname, status='old')
  allocate (root)

! read in 1st number from file
  read (unit=1, fmt=*, iostat=io_stat_number) &
    root%n
  if (io_stat_number==0) then ! not end of file
    i = i + 1
    allocate (root%next)
  end if
  current => root

! read in remaining numbers (1 per line)
  do while (associated(current%next))
    current => current%next
    read (unit=1, fmt=*, iostat=io_stat_number) &
      current%n
    if (io_stat_number==0) then
      i = i + 1
      allocate (current%next)
    end if
  end do
```

```

m = i
allocate (x(1:m))
i = 1
current => root
do while (associated(current%next))
  x(i) = current%n
  i = i + 1
  current => current%next
end do
print *, m, ' numbers read from file'
print *, m, ' elements of array x are:'
do i = 1, m
  print *, x(i)
end do
end program ch2202

```

The program is very similar to the first one. Once you have programmed a linked list for one data type it is very easy to modify it to work with another data type.

22.4 Example 3: Ragged Arrays

Arrays in Fortran are rectangular, even when allocatable. However if you wish to set up a lower triangular matrix that uses minimal memory Fortran provides a number of ways of doing this. The following example achieves it using allocatable components.

```

module ragged_module
  implicit none
  type ragged
    real, dimension (:), allocatable :: &
      ragged_row
  end type ragged
end module ragged_module

program ch2203
  use ragged_module
  implicit none
  integer :: i
  integer, parameter :: n = 3
  type (ragged), dimension (1:n) :: lower_diag
  do i = 1, n
    allocate (lower_diag(i)%ragged_row(1:i))
    print *, ' type in the values for row ', i
  end do
end program ch2203

```

```
read *, lower_diag(i)%ragged_row(1:i)
end do
do i = 1, n
    print *, lower_diag(i)%ragged_row(1:i)
end do
end program ch2203
```

Within the first do loop we allocate a row at a time and each time we go around the loop the array allocated increases in size.

22.5 Example 4: Ragged Arrays and Variable Sized Data Sets

The previous example showed how to use allocatable components in a derived type to achieve ragged arrays. We extend this simple idea in the example below. In this example both the number of stations and the number of data items for each station is read in at run time and allocated accordingly. Notice that 0 is valid as the number of data items for a station.

```
module ragged_module
type ragged
    real, allocatable, dimension(:) :: rainfall
end type ragged
end module ragged_module

program ch2204
use ragged_module
implicit none
integer :: i
integer :: nr
integer, allocatable, dimension(:) :: nc
type (ragged), allocatable, dimension(:) :: station
print *, ' enter number of stations'
read *, nr
allocate (station(1:nr))
allocate (nc(1:nr))
do i = 1, nr
    print *, ' enter the number of data values ' &
        , 'for station ', i
    read *, nc(i)
    allocate (station(i)%rainfall(1:nc(i)))
    if (nc(i)==0) then
```

```

        cycle
end if
print *, ' Type in the values for station ', &
         i
read *, station(i)%rainfall(1:nc(i))
end do
do i = 1, nr
print *, ' Row ', i, ' Data = ', &
         station(i)%rainfall(1:nc(i))
end do
end program ch2204

```

22.6 Example 5: Perfectly Balanced Tree

Let us now look at a more complex example that builds a perfectly balanced tree and prints it out. A loose definition of a perfectly balanced tree is one that has minimum depth for n nodes. More accurately a tree is perfectly balanced if for each node the number of nodes in its left and right subtrees differ by at most 1:

```

module tree_node_module
implicit none

type tree_node
    integer :: number
    type (tree_node), pointer :: &
        left => null() , right => null()
end type tree_node

end module tree_node_module

module tree_module
implicit none

contains

recursive function tree(n) result (answer)
use tree_node_module
implicit none
integer, intent (in) :: n
type (tree_node), pointer :: answer
type (tree_node), pointer :: new_node
integer :: l, r, x

```

```
if (n==0) then
    print *, ' terminate tree'
    nullify (answer)
else
    l = n/2
    r = n - l - 1
    print *, l, r, n
    print *, ' next item'
    read *, x
    allocate (new_node)
    new_node%number = x
    print *, ' left branch'
    new_node%left => tree(l)
    print *, ' right branch'
    new_node%right => tree(r)
    answer => new_node
end if
print *, ' function tree ends'
end function tree

end module tree_module

module print_tree_module
    implicit none

contains

recursive subroutine print_tree(t, h)
    use tree_node_module
    implicit none
    type (tree_node), pointer :: t
    integer :: i
    integer :: h

    if (associated(t)) then
        call print_tree(t%left, h+1)
        do i = 1, h
            write (unit=*, fmt=100, advance='no')
        end do
        print *, t%number
        call print_tree(t%right, h+1)
    end if
    100 format (' ')
end subroutine print_tree

end module print_tree_module
```

```

program ch2205
! construction of a perfectly balanced tree
use tree_node_module
use tree_module
use print_tree_module
implicit none
type (tree_node), pointer :: root
integer :: n_of_items

print *, 'enter number of items'
read *, n_of_items
root => tree(n_of_items)
call print_tree(root, 0)
end program ch2205

```

There are a number of very important concepts contained in this example and they include:

- The use of a module to define a type. For user defined data types we must create a module to define the data type if we want it to be available in more than one program unit.
- The use of a function that returns a pointer as a result.
- As the function returns a pointer we must determine the allocation status before the function terminates. This means that in the above case we use the nullify (result) statement. The other option is to target the pointer.
- The use of associated to determine if the node of the tree is terminated or points to another node.

Type the program in and compile, link and run it. Note that the tree only has the minimal depth necessary to store all of the items. Experiment with the number of items and watch the tree change its depth to match the number of items.

22.7 Example 6: Date class

The following is a complete manual rewrite of Skip Noble and Alan Millers date module. Here are two urls for this code.

<http://jblevins.org/mirror/amiller/>
<http://jblevins.org/mirror/amiller/datesub.f90>

The original worked with the built-in Fortran intrinsic data types, i.e year, month and day were plain integer data types. It has been rewritten to work with a derived date data type.

We have also added a function to print dates out in a variety of formats. This is based on a subroutine called `date_stamp` from the original code. The first key code segment is

```
type, public :: date
  private
  integer :: day
  integer :: month
  integer :: year
end type date
```

where the `date` data type is public but its components are private. This means that access to the components must be done via subroutines and functions within the `date_module` module. The next key segment is

```
character (9) :: day(0:6) = &
  ('Sunday ', 'Monday ', 'Tuesday ', &
   'Wednesday', 'Thursday ', 'Friday ', &
   'Saturday ')
character (9) :: month(1:12) = &
  ('January ', 'February ', 'March ', &
   'April ', 'May ', 'June ', &
   'July ', 'August ', 'September ', &
   'October ', 'November ', 'December ')
```

which declares the variable `day` to be an array of characters of length 9. They are initialised with the names of the days. The variable `day` is declared in the module and is available to all contained functions and subroutines.

The variable `month` is an array of characters of length 9 and is initialised to the names of the months. The variable `month` is declared in the module and is available to all contained functions and subroutines. The next key code segment is

```
public :: &
  calendar_to_julian, &
  date_, &
  date_to_day_in_year, &
  date_to_weekday_number, &
  get_day, &
  get_month, &
  get_year, &
  julian_to_date, &
  julian_to_date_and_week_and_day, &
  ndays,
```

```
print_date, &
year_and_day_to_date
```

where we explicitly make the listed subroutines and functions public, as the code segment from the top of the module,

```
private
```

defines everything to be private.

We have to provide a user defined constructor when the components of the derived type are private. This is given below:

```
function date_(dd,mm,yyyy) result (x)
implicit none
type (date) :: x
integer, intent (in) :: dd, mm, yyyy
x = date(dd,mm,yyyy)
end function date_
```

This in turn calls the built-in constructor date. As the `date_` function is now an executable statement we cannot initialise in a declaration, i.e. the following is not allowed.

```
type (date) :: date1_(11,2,1952)
```

We also provide three additional procedures to access the components of the date class:

```
get_day
get_month
get_year
```

This is common programming practice in object oriented and object based programming.

The `print_date` function also has examples of internal write statements. These are

```
write(print_date(1:2),'(i2)')x%day
write(print_date(4:5),'(i2)')x%month
write(print_date(7:10), '(i4)') x%year
write(print_date(pos:pos+1), '(i2)') x%day
write(print_date(pos:pos+3), '(i4)') x%year
```

where we construct the elements of the character variable from the integer values of the `x%day`, `x%month` and `x%year` data.

```
module date_module
implicit none

private
```

```

type, public :: date
  private
    integer :: day
    integer :: month
    integer :: year
end type date

character (9) :: day(0:6) = (/ 'Sunday   ', &
  'Monday   ', 'Tuesday  ', 'Wednesday', &
  'Thursday ', 'Friday   ', 'Saturday ' /)
character (9) :: month(1:12) = (/ 'January  ', &
  'February ', 'March    ', 'April    ', &
  'May      ', 'June     ', 'July    ', &
  'August   ', 'September', 'October  ', &
  'November ', 'December ' /)

public :: calendar_to_julian, date_, &
  date_to_day_in_year, date_to_weekday_number, &
  get_day, get_month, get_year, &
  julian_to_date, &
  julian_to_date_and_week_and_day, ndays, &
  print_date, year_and_day_to_date

```

contains

```

function calendar_to_julian(x) result (ival)
  implicit none
  integer :: ival
  type (date), intent (in) :: x

  ival = x%day - 32075 + 1461*(x%year+4800+(x%&
    month-14)/12)/4 + 367*(x%month-2-((x%month &
    -14)/12)*12)/12 - 3*((x%year+4900+(x%month &
    -14)/12)/100)/4
end function calendar_to_julian

function date_(dd, mm, yyyy) result (x)
  implicit none
  type (date) :: x
  integer, intent (in) :: dd, mm, yyyy

  x = date(dd, mm, yyyy)
end function date_

```

```
function date_to_day_in_year(x)
    implicit none
    integer :: date_to_day_in_year
    type (date), intent (in) :: x
    intrinsic modulo

    date_to_day_in_year = 3055*(x%month+2)/100 - &
        (x%month+10)/13*2 - 91 + (1-(modulo(x%year &
        ,4)+3)/4+(modulo(x%year,100)+99)/100-( &
        modulo(x%year,400)+399)/400)*(x%month+10)/ &
        13 + x%day
end function date_to_day_in_year

function date_to_weekday_number(x)
    implicit none
    integer :: date_to_weekday_number
    type (date), intent (in) :: x
    intrinsic modulo

    date_to_weekday_number = modulo((13*( &
        x%month+10-(x%month+10)/13*12)-1)/5+x%day+ &
        77+5*(x%year+(x%month-14)/12-(x%year+ &
        (x%month-14)/12)/100*100)/4+(x%year+(x% &
        month-14)/12)/400-(x%year+(x%month- &
        14)/12)/100*2, 7)
end function date_to_weekday_number

function get_day(x)
    implicit none
    integer :: get_day
    type (date), intent (in) :: x

    get_day = x%day
end function get_day

function get_month(x)
    implicit none
    integer :: get_month
    type (date), intent (in) :: x

    get_month = x%month
end function get_month
```

```
function get_year(x)
    implicit none
    integer :: get_year
    type (date), intent (in) :: x

    get_year = x%year
end function get_year

function julian_to_date(julian) result (x)
    implicit none
    integer, intent (in) :: julian
    integer :: l, n
    type (date) :: x

    l = julian + 68569
    n = 4*l/146097
    l = l - (146097*n+3)/4
    x%year = 4000*(l+1)/1461001
    l = l - 1461*x%year/4 + 31
    x%month = 80*l/2447
    x%day = l - 2447*x%month/80
    l = x%month/11
    x%month = x%month + 2 - 12*l
    x%year = 100*(n-49) + x%year + 1
end function julian_to_date

subroutine julian_to_date_and_week_and_day(jd, &
    x, wd, ddd)
    implicit none
    integer, intent (out) :: ddd, wd
    integer, intent (in) :: jd
    type (date), intent (out) :: x

    x = julian_to_date(jd)
    wd = date_to_weekday_number(x)
    ddd = date_to_day_in_year(x)
end subroutine julian_to_date_and_week_and_day

function ndays(date1, date2)
    implicit none
    integer :: ndays
    type (date), intent (in) :: date1, date2

    ndays = calendar_to_julian(date1) - &
        calendar_to_julian(date2)
end function ndays
```

```
function print_date(x, day_names, &
    short_month_name, digits)
implicit none
type (date), intent (in) :: x
logical, optional, intent (in) :: day_names, &
    short_month_name, digits
character (40) :: print_date
integer :: pos
logical :: want_day, want_short_month_name, &
    want_digits
intrinsic len_trim, present, trim

want_day = .false.
want_short_month_name = .false.
want_digits = .false.
print_date = ' '
if (present(day_names)) then
    want_day = day_names
end if
if (present(short_month_name)) then
    want_short_month_name = short_month_name
end if
if (present(digits)) then
    want_digits = digits
end if
if (want_digits) then
    write (print_date(1:2), '(i2)') x%day
    print_date(3:3) = '/'
    write (print_date(4:5), '(i2)') x%month
    print_date(6:6) = '/'
    write (print_date(7:10), '(i4)') x%year
else
    if (want_day) then
        pos = date_to_weekday_number(x)
        print_date = trim(day(pos)) // ' '
        pos = len_trim(print_date) + 2
    else
        pos = 1
        print_date = ' '
    end if
    write (print_date(pos:pos+1), '(i2)') &
        x%day
    if (want_short_month_name) then
        print_date(pos+3:pos+5) = month(x%month) &
            (1:3)
```

```
    pos = pos + 7
else
    print_date(pos+3:) = month(x%month)
    pos = len_trim(print_date) + 2
end if
write (print_date(pos:pos+3), '(i4)' ) &
      x%year
end if

return
end function print_date

function year_and_day_to_date(year, day) &
result (x)
implicit none
type (date) :: x
integer, intent (in) :: day, year
integer :: t
intrinsic modulo

x%year = year
t = 0
if (modulo(year,4)==0) then
    t = 1
end if
if (modulo(year,400)/=0 .and. &
    modulo(year,100)==0) then
    t = 0
end if
x%day = day
if (day>59+t) then
    x%day = x%day + 2 - t
end if
x%month = ((x%day+91)*100)/3055
x%day = (x%day+91) - (x%month*3055)/100
x%month = x%month - 2
if (x%month>=1 .and. x%month<=12) then
    return
end if
write (unit=*, fmt='(a,i11,a)' ) '$$year_and_d&
&ay_to_date: day of the year input &
&=', day, ' is out of range.'
end function year_and_day_to_date

end module date_module
```

```
program ch2206
  use date_module, only: calendar_to_julian, &
    date, date_, date_to_day_in_year, &
    date_to_weekday_number, get_day, get_month, &
    get_year, julian_to_date_and_week_and_day, &
    ndays, print_date, year_and_day_to_date

  implicit none
  integer :: dd, ddd, i, mm, ndiff, wd, yyyy
  integer :: val(8)
  intrinsic date_and_time
  type (date) :: date1, date2, x

  call date_and_time(values=val)
  yyyy = val(1)
  mm = 10
  do i = 31, 26, -1
    x = date_(i, mm, yyyy)
    if (date_to_weekday_number(x)==0) then
      print *, 'Turn clocks back to EST on: ', &
        i, ' October ', get_year(x)
      exit
    end if
  end do
  call date_and_time(values=val)
  yyyy = val(1)
  mm = 4
  do i = 1, 8
    x = date_(i, mm, yyyy)
    if (date_to_weekday_number(x)==0) then
      print *, 'Turn clocks ahead to DST on: ', &
        i, ' April ', get_year(x)
      exit
    end if
  end do
  call date_and_time(values=val)
  yyyy = val(1)
  mm = 12
  dd = 31
  x = date_(dd, mm, yyyy)
  if (date_to_day_in_year(x)==366) then
    print *, get_year(x), ' is a leap year'
  else
    print *, get_year(x), ' is not a leap year'
  end if
```

```
x = date_(1, 1, 1970)
call julian_to_date_and_week_and_day &
(calendar_to_julian(x), x, wd, ddd)
if (get_year(x)/=1970 .or. get_month(x)/=1 &
.or. get_day(x)/=1 .or. wd/=4 .or. ddd/=1) &
then
print *, &
'julian_to_date_and_week_and_day failed'
print *, ' date, wd, ddd = ', get_year(x), &
get_month(x), get_day(x), wd, ddd
stop
end if
date1 = date_(22, 5, 1984)
date2 = date_(22, 5, 1983)
ndiff = ndays(date1, date2)
yyyy = 1970

x = year_and_day_to_date(yyyy, ddd)

if (ndiff/=366) then
print *, 'ndays failed; ndiff = ', ndiff
else
if (get_month(x)/=1 .and. get_day(x)/=1) &
then
print *, 'year_and_day_to_date failed'
print *, ' mma, dda = ', get_month(x), &
get_day(x)
else
print *, ' calendar_to_julian OK'
print *, ' date_ OK'
print *, ' date_to_day_in_year OK'
print *, ' date_to_weekday_number OK'
print *, ' get_day OK'
print *, ' get_month OK'
print *, ' get_year OK'
print *, &
' julian_to_date_and_week_and_day OK'
print *, ' ndays OK'
print *, ' year_and_day_to_date OK'
end if
end if
```

```

x = date_(11, 2, 1952)

print *, ' print_date test'
print *, ' Single parameter      ', &
print_date(x)
print *, &
' day_names=false short_month_name=false ', &
print_date(x, day_names=.false., &
short_month_name=.false.)
print *, &
' day_names=true  short_month_name=false ', &
print_date(x, day_names=.true., &
short_month_name=.false.)
print *, &
' day_names=false short_month_name=true   ', &
print_date(x, day_names=.false., &
short_month_name=.true.)
print *, ' digits=true           ', &
print_date(x, digits=.true.)

print *, ' Test out a month'

yyyy = 1970
do dd = 1, 31
  x = year_and_day_to_date(yyyy, dd)
  print *, print_date(x, day_names=.false., &
short_month_name=.true.)
end do

end program ch2206

```

There are wrap problems with some of the lengthier arithmetic expressions. The version on the web site is obviously correct.

We also have an alternate form of array declaration in this program, which is given below. It is common in Fortran 77 style code:

```
integer :: val(8)
```

One improvement would be additional code to test the validity of dates. This would be called from within our constructor `date_`. This would mean that we could never have an invalid date when using the `date_module`. This is left as a programming exercise.

22.7.1 Notes: DST in the USA

The above program is no longer correct. Beginning in 2007, Daylight Saving Time was brought forward by 3 or 4 weeks in Spring and extended by one week in the Fall. Daylight Saving Time begins for most of the United States at 2 a.m. on the second Sunday of March. Time reverts to standard time at 2 a.m. on the first Sunday in November.

Bibliography

Chapter 2 provided details of some books that address data structuring, but mainly from an historical viewpoint.

We provide a small number of references to books that look at data structuring more generally.

Schneider, G.M., Bruell, S.C.: Advanced Programming and Problem Solving with Pascal. Wiley, New York (1981)

- The book is aimed at computer science students and follows the curriculum guidelines laid down in Communications of the ACM, August 1985, Course CS2. The book is very good for the complete beginner as the examples are very clearly laid out and well explained. There is a coverage of data structures, abstract data types and their implementation, algorithms for sorting and searching, the principles of software development as they relate to the specification, design, implementation and verification of programs in an orderly and disciplined fashion—their words.

Sedgewick, R.: Algorithms in Modula 3. Addison-Wesley, Reading (1993). ISBN 0-201-53351-0

- The Modula 3 algorithms are relatively easy to translate into Fortran.

22.8 Problems

22.1 Compile and run the examples in this chapter with your compiler.

22.2 Modify the ragged array example that processes a lower triangular matrix to work with an upper triangular matrix.

22.3 Using the balanced tree example as a basis and modify it to work with a character array rather than an integer. The routine that prints the tree will also have to be modified to reflect this.

22.4 Modify the Date program to account for the current DST in the USA.

22.5 Modify ch2204 to calculate and print the average rainfall for each station.

Chapter 23

An Introduction to Algorithms and the Big O Notation

Errors using inadequate data are much less than those using no data at all.

Charles Babbage

Aims

The aims of this chapter are to provide an introduction to algorithms and their behaviour. In Computer Science this is normally done using the so called big O notation.

We will cover briefly a small set of behaviour types including

- Order $O(1)$
- Order $O(n)$
- Order $O(\log n)$
- Order $O(n \log n)$

23.1 Introduction

A method for dealing with approximations was introduced by Bachman in 1892 in his work Analytische Zahlen Theorie. This is the big O notation.

The big O notation is used to classify algorithms by how they perform depending on the size of the input data set they are working on. This typically means looking at both their space and time behaviour.

A more detailed and mathematical coverage can be found in Knuth's Fundamental Algorithms.

Chapter one of this book looks at the basic concepts and mathematical preliminaries required for analysing algorithms, and is around 120 pages. Well worth a read.

Table 23.1 Big O notation and complexity

Notation	Name
$O(1)$	Constant
$O(n)$	Linear
$O(\log n)$	Logarithmic
$O(n \log n) = O(\log n!)$	Linearithmic, loglinear, quasilinear
$O(\log \log n)$	Double logarithmic
$O(n \log^* n)$	$n \log\star n$
$O(n^2)$	Quadratic
$O(n^c) 0 < c < 1$	Fractional power
$O(n^c) c > 1$	Polynomial or algebraic
$O(c^n) c > 1$	Exponential
$O(n!)$	Factorial

23.2 Basic Background

Table 23.1 summarises some of the details regarding commonly occurring types of problem.

23.3 Brief Explanation

- $O(1)$ Determining if a number is even or odd; using a constant-size lookup table
- $O(\log \log n)$ Finding an item using interpolation search in a sorted array of uniformly distributed values.
- $O(\log n)$ Finding an item in a sorted array with a binary search or a balanced search tree as well as all operations in a Binomial heap.
- $O(n^c) 0 < c < 1$ Searching in a kd-tree
- $O(n)$ Finding an item in an unsorted list or a malformed tree (worst case) or in an unsorted array; Adding two n-bit integers by ripple carry.
- $O(n \log^* n)$ Performing triangulation of a simple polygon using Seidel's algorithm.
- $O(n \log n)$ Performing a Fast Fourier transform; heapsort, quicksort (best and average case), or merge sort.
- $O(n^2)$ Multiplying two n-digit numbers by a simple algorithm; bubble sort (worst case or naive implementation), Shell sort, quicksort (worst case), selection sort or insertion sort.
- $O(n^c) c > 1$ Tree-adjoining grammar parsing; maximum matching for bipartite graphs.
- $O(c^n) c > 1$ Finding the (exact) solution to the traveling salesman problem using dynamic programming; determining if two logical statements are equivalent using brute-force search.

- $O(n!)$ Solving the traveling salesman problem via brute-force search; generating all unrestricted permutations of a poset; finding the determinant with expansion by minors.

23.4 Example 1

This program calculates values for 4 of the above functions, for n from 1 to 10^9 .

```

program ch2301
    implicit none

    integer, parameter :: nn = 10
    integer :: n
    integer, dimension (nn) :: nvalues = [ 1, 10, &
        100, 1000, 10000, 100000, 1000000, 10000000, &
        100000000, 1000000000 ]
    integer :: i
    character *80 heading

    heading = ' i           n   O(1)      O(n)'
    heading = trim(heading) // &
        '          O(n*n)  O(log n)  O(n log n)'
    print *, heading
    print *, ''
    do i = 1, nn
        n = nvalues(i)
        print 100, i, n, order_1(), order_n(n), &
            order_n_squared(n), order_log_n(n), &
            order_n_log_n(n)
100 format (1x, i2, 2x, i10, 2x, i4, 2x, i10, &
            2x, e10.4, 2x, f7.2, 2x, e10.4)
    end do

contains

    integer function order_1()
        order_1 = 1
    end function order_1

    integer function order_n(n)
        integer, intent (in) :: n

        order_n = n
    end function order_n

    double precision function order_n_squared(n)
        integer, intent (in) :: n

        order_n_squared = dble(n)*dble(n)
    end function order_n_squared

```

```

real function order_log_n(n)
    integer, intent (in) :: n

    order_log_n = log(real(n))
end function order_log_n

real function order_n_log_n(n)
    integer, intent (in) :: n

    order_n_log_n = n*log(real(n))
end function order_n_log_n

end program ch2301

```

Here is the output from running the program.

i	n	$O(1)$	$O(n)$	$O(n*n)$	$O(\log n)$	$O(n \log n)$
1	1	1	1	0.1000E+01	0.00	0.0000E+00
2	10	1	10	0.1000E+03	2.30	0.2303E+02
3	100	1	100	0.1000E+05	4.61	0.4605E+03
4	1000	1	1000	0.1000E+07	6.91	0.6908E+04
5	10000	1	10000	0.1000E+09	9.21	0.9210E+05
6	100000	1	100000	0.1000E+11	11.51	0.1151E+07
7	1000000	1	1000000	0.1000E+13	13.82	0.1382E+08
8	10000000	1	10000000	0.1000E+15	16.12	0.1612E+09
9	100000000	1	100000000	0.1000E+17	18.42	0.1842E+10
10	1000000000	1	1000000000	0.1000E+19	20.72	0.2072E+11

23.5 Sorting

In the book we use two sorting algorithms

- Quicksort
- Insertion sort

Table 23.2 looks at their behaviour.

Table 23.2 Quicksort and insertion sort comparison

Algorithm	Data structure	Time complexity Best			Worst case auxiliary space complexity Worst
		Best	Average	Worst	
Quicksort	Array	$O(n \log(n))$	$O(n \log(n))$	$O(n^2)$	$O(n)$
Insertion sort	Array	$O(n)$	$O(n^2)$	$O(n^2)$	$O(1)$

Table 23.3 Array and linked list performance

Data structure	Time complexity								Space complexity Worst	
	Average				Worst					
	Index	Search	Insert	Delete	Index	Search	Insert	Delete		
Basic array	$O(1)$	$O(n)$	—	—	$O(1)$	$O(n)$	—	—	$O(n)$	
Dynamic array	$O(1)$	$O(n)$	$O(n)$	$O(n)$	$O(1)$	$O(n)$	$O(n)$	$O(n)$	$O(n)$	
Singly-linked list	$O(n)$	$O(n)$	$O(1)$	$O(1)$	$O(n)$	$O(n)$	$O(1)$	$O(1)$	$O(n)$	

23.6 Basic Array and Linked List Performance

Table 23.3 that summarises the array and linked list performance.

Bibliography

The earliest books that we have used in this area are those by Donald Knuth, and details are given below in chronological order.

Volume 1, Fundamental Algorithms, first edition, 1968, xxi+634pp, ISBN 0-201-03801-3.

Volume 2, Seminumerical Algorithms, first edition, 1969, xi+624pp, ISBN 0-201-03802-1.

Volume 3, Sorting and Searching, first edition, 1973, xi+723pp+centerfold, ISBN 0-201-03803-X

Volume 1, second edition, 1973, xxi+634pp, ISBN 0-201-03809-9.

Volume 2, second edition, 1981, xiii+688pp, ISBN 0-201-03822-6.

- Knuth uses the Mix assembly language (an artificial language) and this limits the accessibility of the books.
- However within the Computer Science community they are generally regarded as the first and most comprehensive treatment of its subject.

For something more accessible, Sedgewick has written several programming language versions of a book on algorithms. He was a student of Knuth's.

The earliest used Pascal, and later editions have used C, C++ and Modula 2 and Modula 3.

Sedgewick, Robert (1992). Algorithms in C++, Addison-Wesley. ISBN 0-201-51059-6.

Sedgewick, Robert (1993). Algorithms in Modula 3, Addison-Wesley. ISBN 0-201-53351-0.

- The Modula 3 algorithms are relatively easy to translate into Fortran.

Chapter 24

Operator Overloading

All the persons in this book are real and none is fictitious even in part.

Flann O'Brien, *The Hard Life*

Aims

The aims of this chapter are to look at operator overloading in Fortran.

24.1 Introduction

In programming operator overloading can be regarded as a way of achieving polymorphism in that operators (e.g. +, -, *, / or =) can have different implementations depending on the types of their arguments.

In some programming languages overloading is defined by the language. In Fortran for example, the addition + operator invokes quite different code when used with integer, real or complex types.

Some languages allow the programmer to implement support for user defined types. Fortran introduced support for operator and assignment overloading in the 1990 standard.

24.2 Other Languages

Operator overloading is not new and several languages offer support for the feature including:

- Algol 68—1968
- Ada—Ada 83

- C++—First standard, 1998
- Eiffel—1986
- C#—2001

Java, however does not.

24.3 Example 1: Overloading the Addition (+) Operator

The following example overloads the addition operator.

```

module t_position
  implicit none
  type position
    integer :: x
    integer :: y
    integer :: z
  end type position
  interface operator (+)
    module procedure new_position
  end interface operator (+)

contains
  function new_position(a, b)
    type (position), intent (in) :: a, b
    type (position) :: new_position

    new_position%x = a%x + b%x
    new_position%y = a%y + b%y
    new_position%z = a%z + b%z
  end function new_position
end module t_position

program ch2401
  use t_position
  implicit none
  type (position) :: a, b, c

  a%x = 10
  a%y = 10
  a%z = 10
  b%x = 20
  b%y = 20
  b%z = 20

```

```
c = a + b
print *, a
print *, b
print *, c
end program ch2401
```

We have extended the meaning of the addition operator so that we can write simple expressions in Fortran based on it and have our new position calculated using a user supplied function that actually implements the calculation of the new position.

24.4 Problems

24.1 Compile and run this example. Overload the subtraction operator as well.

Chapter 25

Generic Programming

General notions are generally wrong.

Letter to Mr. Wortley Montagu, 28th March 1710.

Aims

This chapter looks at some examples that implement generic programming in Fortran.

25.1 Introduction

Fortran 77 had several generic functions, e.g. the sine function could be called with arguments of type real, double precision or complex. Fortran 90 extended the idea so that a programmer could write their own generic functions or subroutines. For example we can now write a sort routine which works with arguments of a variety of types, e.g. integer, real etc.

25.2 Generic Programming and Other Languages

Generic programming has a wider meaning in computer science and effectively is a style of computer programming in which an algorithm is written once, but can be made to work with a variety of types.

This style of programming is provided in several programming languages and in a variety of ways.

Languages that support generics include

- Ada
- C#

- Eiffel
- Java
- C++

To quote the generic programming pioneer Alexander Stepanov;

... Generic programming is about abstracting and classifying algorithms and data structures. It gets its inspiration from Knuth and not from type theory. Its goal is the incremental construction of systematic catalogs of useful, efficient and abstract algorithms and data structures. Such an undertaking is still a dream.

and quoting Bjarne Stroustrup:

... lift algorithms and data structures from concrete examples to their most general and abstract form.

We'll look at a concrete example in Fortran next.

25.3 Example 1: Sorting Reals and Integers

In Chap. 20 Example 5 had a module called `sort_data_module` that contained a `sort_data` subroutine. The `sort_data` subroutine in turn contained an internal `quicksort` subroutine that did the actual sorting.

Here is the start of the `sort_data` subroutine.

```
subroutine sort_data(raw_data, how_many)
  implicit none
  integer, intent (in) :: how_many
  real, intent (inout), dimension (...) :: raw_data
```

and we called this subroutine as shown below from the main program.

```
call sort_data(x,n)
```

The subroutine worked with an array of default real type. We will use the module `sort_data_module` and subroutine `sort_data` as the basis of a module that will work with arrays of four integer types and three real types.

The first thing we need are modules that defines kind type parameters for the three real types and four integer types.

These two modules are shown below.

```
module precision_module
  implicit none
  integer, parameter :: sp &
    = selected_real_kind( 6, 37)
  integer, parameter :: dp &
    = selected_real_kind(15, 307)
  integer, parameter :: qp &
    = selected_real_kind(30, 291)
end module precision_module
```

```
module integer_kind_module
    implicit none
    integer, parameter :: i8 &
        = selected_int_kind( 2 )
    integer, parameter :: i16 &
        = selected_int_kind( 4 )
    integer, parameter :: i32 &
        = selected_int_kind( 9 )
    integer, parameter :: i64 &
        = selected_int_kind(15)
end module integer_kind_module
```

We can now use these modules in the new module `sort_data_module` and main program.

We must use an interface to link the common calling name (`sort_data`) to the specific subroutines that handle each specific type.

Here is the interface block from the module `sort_data_module`.

```
interface sort_data
    module procedure sort_real_sp
    module procedure sort_real_dp
    module procedure sort_real_qp
    module procedure sort_integer_8
    module procedure sort_integer_16
    module procedure sort_integer_32
    module procedure sort_integer_64
end interface sort_data
```

In the original subroutine in Chap. 20 we had a call

```
call sort_date(raw_data,how_many)
```

and the subroutine `sort_data` had two arguments or parameters, a real array, and an integer for the size.

So the call is still the same, but now we can call the `sort_data` subroutine with an array of any of the four integer types or three real types.

The compiler will then look at the type, kind and ranks of the parameters in the call to the `sort_data` subroutine and call the appropriate module procedure.

Here is the new module `sort_data_module`.

```
module sort_data_module
    use precision_module
    use integer_kind_module

    interface sort_data
        module procedure sort_real_sp
        module procedure sort_real_dp
```

```
module procedure sort_real_qp
module procedure sort_integer_8
module procedure sort_integer_16
module procedure sort_integer_32
module procedure sort_integer_64
end interface sort_data

contains

subroutine sort_real_sp(raw_data, how_many)
use precision_module
implicit none
integer, intent (in) :: how_many
real (sp), intent (inout), dimension (: ) :: &
raw_data

call quicksort(1, how_many)

contains

recursive subroutine quicksort(l, r)
implicit none
integer, intent (in) :: l, r
integer :: i, j
real (sp) :: v, t

include 'quicksort_include.f90'

end subroutine quicksort

end subroutine sort_real_sp

subroutine sort_real_dp(raw_data, how_many)
use precision_module
implicit none
integer, intent (in) :: how_many
real (dp), intent (inout), dimension (: ) :: &
raw_data

call quicksort(1, how_many)

contains
recursive subroutine quicksort(l, r)
implicit none
integer, intent (in) :: l, r
```

```
integer :: i, j
real (dp) :: v, t

include 'quicksort_include.f90'

end subroutine quicksort
end subroutine sort_real_dp

subroutine sort_real_qp(raw_data, how_many)
use precision_module
implicit none
integer, intent (in) :: how_many
real (qp), intent (inout), dimension () :: &
raw_data

call quicksort(1, how_many)

contains
recursive subroutine quicksort(l, r)
implicit none
integer, intent (in) :: l, r
integer :: i, j
real (qp) :: v, t

include 'quicksort_include.f90'

end subroutine quicksort
end subroutine sort_real_qp

subroutine sort_integer_8(raw_data, how_many)
use integer_kind_module
implicit none
integer, intent (in) :: how_many
integer (i8), intent (inout), &
dimension () :: raw_data

call quicksort(1, how_many)

contains
recursive subroutine quicksort(l, r)
implicit none
integer, intent (in) :: l, r
integer :: i, j
integer (i8) :: v, t

include 'quicksort_include.f90'
```

```
    end subroutine quicksort
end subroutine sort_integer_8

subroutine sort_integer_16(raw_data, how_many)
use integer_kind_module
implicit none
integer, intent (in) :: how_many
integer (i16), intent (inout), &
dimension (:) :: raw_data

call quicksort(1, how_many)

contains
recursive subroutine quicksort(l, r)
implicit none
integer, intent (in) :: l, r
integer :: i, j
integer (i16) :: v, t

include 'quicksort_include.f90'

end subroutine quicksort
end subroutine sort_integer_16

subroutine sort_integer_32(raw_data, how_many)
use integer_kind_module
implicit none
integer, intent (in) :: how_many
integer (i32), intent (inout), &
dimension (:) :: raw_data

call quicksort(1, how_many)

contains
recursive subroutine quicksort(l, r)
implicit none
integer, intent (in) :: l, r
integer :: i, j
integer (i32) :: v, t

include 'quicksort_include.f90'

end subroutine quicksort
end subroutine sort_integer_32
```

```

subroutine sort_integer_64(raw_data, how_many)
  use integer_kind_module
  implicit none
  integer, intent (in) :: how_many
  integer (i64), intent (inout), &
    dimension (:):: raw_data

  call quicksort(1, how_many)

contains
  recursive subroutine quicksort(l, r)
    implicit none
    integer, intent (in) :: l, r
    integer :: i, j
    integer (i64) :: v, t

    include 'quicksort_include.f90'

  end subroutine quicksort

end subroutine sort_integer_64

end module sort_data_module

```

In this module we have implementations for each of the module procedures listed in the interface block.

Here is the include file, which is used in each of the seven subroutines and is effectively a common algorithm between all seven subroutines.

```

i = 1
j = r
v = raw_data(int((l+r)/2))
do
  do while (raw_data(i)<v)
    i = i + 1
  end do
  do while (v<raw_data(j))
    j = j - 1
  end do
  if (i<=j) then
    t = raw_data(i)
    raw_data(i) = raw_data(j)
    raw_data(j) = t
  end if
end do

```

```

raw_data(j) = t
i = i + 1
j = j - 1
end if
if (i>j) exit
end do
if (l<j) then
  call quicksort(l, j)
end if
if (i<r) then
  call quicksort(i, r)
end if

```

Here is the main program to test the generic sort module.

```

include 'integer_kind_module.f90'
include 'precision_module.f90'
include 'sort_data_module.f90'

program ch2501

use precision_module
use integer_kind_module
use sort_data_module

implicit none
integer, parameter :: n = 1000000
real      (sp), allocatable, dimension(:) :: x
integer (i32), allocatable, dimension(:) :: y
integer :: allocate_status
allocate_status = 0

print *, ' Program starts'
allocate (x(1:n), stat=allocate_status)

if (allocate_status/=0) then
  print *, ' Allocate failed.'
  print *, ' Program terminates'
  stop 10
end if

print *, ' Real allocate complete'
call random_number(x)
print *, ' Real array initialised'

```

```

call sort_data(x, n)
print *, ' Real sort ended'
print *, ' First 10 reals'
write (unit=*, fmt=100) x(1:10)
  100 format (5(2x,e12.6))
allocate (y(1:n), stat=allocate_status)
if (allocate_status/=0) then
  print *, ' Allocate failed.'
  print *, ' Program terminates'
  stop 10
end if
y = int(x*1000000)
deallocate (x)
print *, ' Integer array initialised'
call sort_data(y, n)
print *, ' Sort ended'
print *, ' First 10 integers'
write (unit=*, fmt=110) y(1:10)
  110 format (5(2x,i10))
deallocate (y)
print *, ' Deallocate'
print *, ' Program terminates'

end program ch2501

```

This is obviously a very significant facility to have in a programming language. Have a look at the following two examples which show the code for a generic quicksort in C++ and C#.

25.3.1 Generic Quicksort in C++

Here is the C++ program.

```

template <class Type>
void swap(Type array[],int i, int j)
{
    Type tmp=array[i];
    array[i]=array[j];
    array[j]=tmp;
}

template <class Type>
void quicksort( Type array[], int l, int r)

```

```

{
    int i=l;
    int j=r;
    Type v=array[int((l+r)/2)];
    for (;;) {
    {
        while (array[i] < v) i=i+1;
        while (v < array[j]) j=j-1;
        if (i<=j)
            { swap(array,i,j); i=i+1 ; j=j-1; }
        if (i>j) goto ended ;
    }
    ended: ;
    if (l<j) quicksort(array,l,j);
    if (i<r) quicksort(array,i,r);
}

template <class Type>
void print(Type array[],int size)
{
    cout << " [ ";
    for (int ix=0;ix<size; ++ix)
        cout << array[ix] << " ";
    cout << "] \n";
}

#include <iostream>
using namespace std;
int main()
{
    double da[] =
{1.9,8.2,3.7,6.4,5.5,1.8,9.2,3.6,7.4,5.5};
    int ia[] = {1,10,2,9,3,8,4,7,6,5};
    int size=sizeof(da)/sizeof(double);
    cout << " Quicksort of double array is \n";
    quicksort(da,0,size-1);
    print(da,size);
    size=sizeof(ia)/sizeof(int);
    cout << " Quicksort of integer array is \n";
    quicksort(ia,0,size-1);
    print(ia,size);
    return(0);
}

```

25.3.2 Generic Quicksort in C#

Here is the C# version.

```
using System;
public static class generic
{
    public static void swap< Type > (Type[] array, int i, int j)
    {
        Type tmp=array[i];
        array[i]=array[j];
        array[j]=tmp;
    }

    public static void quicksort< Type > (Type[] array, int l, int r)
        where Type : IComparable< Type >
    {
        int i=l;
        int j=r;
        Type v=array[(int)((l+r)/2)];
        for (;;)
        {
            while (array[i].CompareTo( v ) < 0 ) i=i+1;
            while (v.CompareTo(array[j]) < 0) j=j-1;
            if (i<=j)
                { swap(array,i,j); i=i+1 ; j=j-1; }
            if (i>j) goto ended ;
        }
        ended: ;
        if (l<j) quicksort(array,l,j);
        if (i<r) quicksort(array,i,r);
    }

    public static void print< Type > (Type[] array, int size)
    {
        int i;
        int l;
        l=array.Length;
        for (i=0;i<l;i++)
            Console.WriteLine(array[i]);
    }
}
```

```

public static int Main()
{
    double[] da =
    {1.9,8.2,3.7,6.4,5.5,1.8,9.2,3.6,7.4,5.5};
    int[] ia = {1,10,2,9,3,8,4,7,6,5};
    int size;
    size=da.Length;
    Console.WriteLine("Original array");
    print(da,size);
    quicksort(da,0,size-1);
    Console.WriteLine("Sorted array");
    print(da,size);
    size=ia.Length;
    Console.WriteLine("Original array");
    print(ia,size);
    quicksort(ia,0,size-1);
    Console.WriteLine("Sorted array");
    print(ia,size);
    return(0);
}
}

```

In C++ and C# we only have one version of the sort procedure and the compiler generates the code for us for each type of array we call the procedure with, which we have to actually write in Fortran.

25.4 Example 2: Generic Statistics Module

In this example we extend the statistics module from Chap. 20 (Example 4) to work with all three real kind types.

Here is the precision module.

```

module precision_module
    implicit none
    integer, parameter :: sp &
        = selected_real_kind( 6, 37)
    integer, parameter :: dp &
        = selected_real_kind(15, 307)
    integer, parameter :: qp &
        = selected_real_kind(30, 291)
end module precision_module

```

Here is the statistics module.

```
module statistics_module

use precision_module

interface calculate_statistics
    module procedure calculate_sp
    module procedure calculate_dp
    module procedure calculate_qp
end interface calculate_statistics

contains

subroutine calculate_sp(x, n, mean, std_dev, &
    median)
    implicit none
    integer, intent (in) :: n
    real (sp), intent (in), dimension (...) :: x
    real (sp), intent (out) :: mean
    real (sp), intent (out) :: std_dev
    real (sp), intent (out) :: median
    real (sp), dimension (1:n) :: y
    real (sp) :: variance
    real (sp) :: sumxi, sumxi2

    sumxi = 0.0
    sumxi2 = 0.0
    variance = 0.0
    sumxi = sum(x)
    sumxi2 = sum(x*x)
    mean = sumxi/n
    variance = (sumxi2-sumxi*sumxi/n) / (n-1)
    std_dev = sqrt(variance)
    y = x
    if (mod(n,2)==0) then
        median = (find(n/2)+find((n/2)+1))/2
    else
        median = find((n/2)+1)
    end if

contains

function find(k)
    implicit none
```

```

real (sp) :: find
integer, intent (in) :: k
integer :: l, r, i, j
real (sp) :: t1, t2
include 'statistics_module_include_file.f90'
end function find
end subroutine calculate_sp

subroutine calculate_dp(x, n, mean, std_dev, &
median)
implicit none
integer, intent (in) :: n
real (dp), intent (in), dimension () :: x
real (dp), intent (out) :: mean
real (dp), intent (out) :: std_dev
real (dp), intent (out) :: median
real (dp), dimension (1:n) :: y
real (dp) :: variance
real (dp) :: sumxi, sumxi2

sumxi = 0.0
sumxi2 = 0.0
variance = 0.0
sumxi = sum(x)
sumxi2 = sum(x*x)
mean = sumxi/n
variance = (sumxi2-sumxi*sumxi/n)/(n-1)
std_dev = sqrt(variance)
y = x
if (mod(n,2)==0) then
    median = (find(n/2)+find((n/2)+1))/2
else
    median = find((n/2)+1)
end if
contains
function find(k)
implicit none
real (dp) :: find
integer, intent (in) :: k
integer :: l, r, i, j
real (dp) :: t1, t2
include 'statistics_module_include_file.f90'
end function find
end subroutine calculate_dp

```

```
subroutine calculate_qp(x, n, mean, &
    std_dev, median)
    implicit none
    integer, intent (in) :: n
    real (qp), intent (in), dimension () :: &
        x
    real (qp), intent (out) :: mean
    real (qp), intent (out) :: std_dev
    real (qp), intent (out) :: median
    real (qp), dimension (1:n) :: y
    real (qp) :: variance
    real (qp) :: sumxi, sumxi2

    sumxi = 0.0
    sumxi2 = 0.0
    variance = 0.0
    sumxi = sum(x)
    sumxi2 = sum(x*x)
    mean = sumxi/n
    variance = (sumxi2-sumxi*sumxi/n)/(n-1)
    std_dev = sqrt(variance)
    y = x
    if (mod(n,2)==0) then
        median = (find(n/2)+find((n/2)+1))/2
    else
        median = find((n/2)+1)
    end if
contains
    function find(k)
        implicit none
        real (qp) :: find
        integer, intent (in) :: k
        integer :: l, r, i, j
        real (qp) :: t1, t2
    include 'statistics_module_include_file.f90'
        end function find
    end subroutine calculate_qp

end module
```

Here is the common include file.

```

l = 1
r = n
do while (l<r)
    t1 = y(k)
    i = l
    j = r
    do
        do while (y(i)<t1)
            i = i + 1
        end do
        do while (t1<y(j))
            j = j - 1
        end do
        if (i<=j) then
            t2 = y(i)
            y(i) = y(j)
            y(j) = t2
            i = i + 1
            j = j - 1
        end if
        if (i>j) exit
    end do
    if (j<k) then
        l = i
    end if
    if (k<i) then
        r = j
    end if
end do
find = y(k)

```

Here is the main program to test the statistics module.

```

include 'precision_module.f90'
include 'statistics_module.f90'
include 'timing_module.f90'

program ch2502

use precision_module
use statistics_module
use timing_module

implicit none
integer :: n
real (sp) , allocatable, dimension (:) :: x
real (sp) :: x_m, x_sd, x_median

```

```
real  (dp) , allocatable, dimension () :: y
real  (dp)  :: y_m, y_sd, y_median
real  (qp) , allocatable, dimension () :: z
real  (qp)  :: z_m, z_sd, z_median
character*20 , dimension(3) :: heading &
= [ ' Allocate      ', &
  ' Random       ', &
  ' Statistics   ' ]
call start_timing()
n = 50000000
print *, ' n = ', n

print *, ' Single precision'

allocate (x(1:n))
print 100,heading(1),time_difference()
100 format(a20,2x,f8.3)
call random_number(x)
print 100,heading(2),time_difference()
call calculate_statistics &
(x, n, x_m, x_sd, x_median)
print 100,heading(3),time_difference()
write(unit=*,fmt=10) x_m
10 format(' Mean           = ',f10.6)
write(unit=*,fmt=20) x_sd
20 format(' Standard deviation = ',f10.6)
write(unit=*,fmt=30) x_median
30 format(' Median          = ',f10.6)
deallocate(x)

print *, ' Double precision'

allocate (y(1:n))
print 100,heading(1),time_difference()
call random_number(y)
print 100,heading(2),time_difference()
call calculate_statistics &
(y, n, y_m, y_sd, y_median)
print 100,heading(3),time_difference()
write(unit=*,fmt=10) y_m
write(unit=*,fmt=20) y_sd
write(unit=*,fmt=30) y_median
deallocate(y)
```

```

print *, ' Quad precision'

allocate (z(1:n))
print 100,heading(1),time_difference()
call random_number(z)
print 100,heading(2),time_difference()
call calculate_statistics &
  (z, n, z_m, z_sd, z_median)
print 100,heading(3),time_difference()
write(unit=*,fmt=10) z_m
write(unit=*,fmt=20) z_sd
write(unit=*,fmt=30) z_median
deallocate(z)

end program ch2502

```

25.5 Problems

25.1 Write a generic swap routine, that swaps two rank 1 integer arrays and two rank 1 real arrays.

25.2 Using Example 2 from Chap. 22 as a starting point convert it to a generic variant which handles files of integer data type and real data type.

Bibliography

General

This site is a collection of Alex Stepanov's papers, class notes, and source code, covering generic programming and other topics.

<http://www.stepanovpapers.com/>

C++

C++ Templates: The Complete Guide, David Vandevoorde, Nicolai M Josuttis, 2003 Addison-Wesley. ISBN 0-201-73484-2

C#

Visit the following site

[http://msdn.microsoft.com/en-us/library/512aeb7t\(v=vs.80\).aspx](http://msdn.microsoft.com/en-us/library/512aeb7t(v=vs.80).aspx)

for a very good coverage of generics and C#.

Chapter 26

Mathematical Examples

You look at science (or at least talk of it) as some sort of demoralising invention of man, something apart from real life, and which must be cautiously guarded and kept separate from everyday existence. But science and everyday life cannot and should not be separated. Science, for me, gives a partial explanation for life. In so far as it goes, it is based on fact, experience and experiment.

Rosalind Franklin

Aims

The aims of this chapter are to look at several mathematical examples in Fortran.

- Using linked lists for sparse matrix problems.
- The solution of a set of ordinary differential equations using the Runge–Kutta–Merson method, with the use of a procedure as a parameter, and the use of work arrays.
- Diagonal extraction of a matrix.
- The solution of a system of linear simultaneous equations using Gaussian Elimination
- An elemental $e^{**}x$ function

26.1 Introduction

This chapter looks at a small number of mathematical examples in Fortran.

26.2 Example 1: Using Linked Lists for Sparse Matrix Problems

A matrix is said to be sparse if many of its elements are zero. Mathematical models in areas such as management science, power systems analysis, circuit theory and structural analysis consist of very large sparse systems of linear equations. It is not possible to solve these systems with classical methods because the sparsity would be

lost and the eventual system would become too large to solve. Many of these systems consist of tens of thousands, hundreds of thousands and millions of equations. As computer systems become ever more powerful with massive amounts of memory the solution of even larger problems becomes feasible.

Direct Methods for Sparse Matrices, by Duff I.S., Erisman A.M. and Reid J.K., looks at direct methods for solving sparse systems of linear equations.

Sparse matrix techniques lend themselves to the use of dynamic data structures in Fortran. Only the nonzero elements of a sparse matrix need be stored, together with their positions in the matrix. Other information also needs to be stored so that row or column manipulation can be performed without repeated scanning of a potentially very large data structure. Sparse methods may involve introducing some new nonzero elements, and a way is needed of inserting them into the data structure. This is where the Fortran pointer construct can be used. The sparse matrix can be implemented using a linked list to which entries can be easily added and from which they can be easily deleted.

As a simple introduction, consider the storage of sparse vectors. What we learn here can easily be applied to sparse matrices, which can be thought of as sets of sparse vectors.

26.2.1 Inner Product of Two Sparse Vectors

Assume that we have two sparse vectors x and y for example

$$\underline{x} = \begin{bmatrix} 3 \\ 0 \\ 5 \\ 0 \\ 0 \\ 4 \end{bmatrix} \quad \underline{y} = \begin{bmatrix} 0 \\ 1 \\ 3 \\ 0 \\ 2 \\ 1 \end{bmatrix}$$

and we wish to calculate the inner product

$$x^T y \equiv \sum_{i=1}^n x_i y_i$$

There are a number of approaches to doing this and the one we use in the program below stores them as two linked lists. Only the nonzero elements are stored (together with their indices):

x data file	y data file
3 1	1 2
5 3	3 3
4 6	2 5
	1 6

Here is the program.

```
module sparse_vector_module
    implicit none
    type sparse_vector
        integer :: index
        real :: value
        type (sparse_vector), pointer :: next => &
            null()
    end type sparse_vector
end module sparse_vector_module

program ch2601
! this program reads the non-zero elements of
! two sparse vectors x and y together with
! their indices, and stores them in two
! linked lists. using these linked lists it
! then calculates and prints out the inner
! product. it also prints the values.
use sparse_vector_module
implicit none
character (len=30) :: filename

type (sparse_vector), pointer :: root_x, &
    current_x, root_y, current_y
real :: inner_prod = 0.0
integer :: io_status

! read non-zero elements of vector x together
! with indices into a linked list

print *, 'input file name for vector x'
read '(a)', filename
open (unit=1, file=filename, status='old', &
    iostat=io_status)
if (io_status/=0) then
    print *, 'error opening file ', filename
    stop
end if
allocate (root_x)
read (unit=1, fmt=*, iostat=io_status) &
    root_x%value, root_x%index
if (io_status/=0) then
    print *, ' error when reading from file ', &
        filename, ' or file empty'
```

```
      stop 10
      end if

! read data for vector x from file until eof

current_x => root_x
allocate (current_x%next)
do while (associated(current_x%next))
  current_x => current_x%next
  read (unit=1, fmt=*, iostat=io_status) &
    current_x%value, current_x%index
  if (io_status==0) then
    allocate (current_x%next)
    cycle
  else if (io_status>0) then

!       error on reading

  print *, &
    'error occurred when reading from ', &
    filename
  end if
end do
close (unit=1)

! read non-zero elements of vector y together
! with indices into a linked list

print *, 'input file name for vector y'
read '(a)', filename
open (unit=1, file=filename, status='old', &
  iostat=io_status)
if (io_status/=0) then
  print *, 'error opening file ', filename
  stop
end if
allocate (root_y)
read (unit=1, fmt=*, iostat=io_status) &
  root_y%value, root_y%index
if (io_status/=0) then
  print *, ' error when reading from ', &
    filename, 'or file empty'
  stop
end if
```

```
! read data for vector y from file until eof

current_y => root_y
allocate (current_y%next)
do while (associated(current_y%next))
    current_y => current_y%next
    read (unit=1, fmt=*, iostat=io_status) &
        current_y%value, current_y%index
    if (io_status==0) then
        allocate (current_y%next)
        cycle
    else if (io_status>0) then

!       error on reading

        print *, &
            'error occurred when reading from', &
            filename
        stop
    end if
end do

! data has now been read and stored in 2 linked
! lists. start at the beginning of x linked list
! and y linked list and compare indices
! in order to perform inner product

current_x => root_x
current_y => root_y
do while (associated(current_x%next))
    do while (associated(current_y%next) .and. &
        current_y%index<current_x%index)

!       move through y list

        current_y => current_y%next
    end do

!       at this point
!       current_y%index >= current_x%index
!       or 2nd list is exhausted

    if (current_y%index==current_x%index) then
        inner_prod = inner_prod + current_x%value* &
            current_y%value
```

```

    end if
    current_x => current_x%next
end do

! print out inner product

print *, &
'inner product of two sparse vectors is :', &
inner_prod

! print non-zero values of vector x and indices

print *, &
'non-zero values of vector x and indices:'
current_x => root_x
do while (associated(current_x%next))
    print *, current_x%value, current_x%index
    current_x => current_x%next
end do

! print non-zero values of vector y and indices

print *, &
'non-zero values of vector y and indices:'
current_y => root_y
do while (associated(current_y%next))
    print *, current_y%value, current_y%index
    current_y => current_y%next
end do
end program ch2601

```

26.3 Example 2: Solving a System of First-Order Ordinary Differential Equations Using Runge–Kutta–Merson

Simulation and mathematical modelling of a wide range of physical processes often leads to a system of ordinary differential equations to be solved. Such equations also occur when approximate techniques are applied to more complex problems. We will restrict ourselves to a class of ordinary differential equations called initial value problems. These are systems for which all conditions are given at the same value of

the independent variable. We will further restrict ourselves to first-order initial value problems of the form:

$$\frac{dy_1}{dt} = f_1(\underline{y}, t)$$

$$\frac{dy_2}{dt} = f_2(\underline{y}, t)$$

...

$$\frac{dy_n}{dt} = f_n(\underline{y}, t)$$

or

$$\dot{\underline{y}} = \underline{f}(\underline{y}, t) \quad (26.1)$$

with initial conditions

$$\underline{y}(t_0) = \underline{y}_0$$

where

$$\underline{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \underline{f} = \begin{pmatrix} f_1 \\ \vdots \\ f_n \end{pmatrix}, \underline{y}_0 = \begin{pmatrix} y_1(t_0) \\ \vdots \\ y_n(t_0) \end{pmatrix}$$

If we have a system of ordinary differential equations of higher order then they can be reformulated to a system of order one. See the NAG library documentation for solving ordinary differential equations.

One well-known class of methods for solving initial value ordinary differential equations is Runge-Kutta. In this example we have coded the Runge-Kutta-Merson algorithm, which is a fourth-order method and solves (26.1) from a point $t = a$ to a point $t = b$.

It starts with a step length $h = (b - a)/100$ and includes a local error control strategy such that the solution at $t + h$ is accepted if:

$$|error\ estimate| < user\ defined\ tolerance$$

If this isn't satisfied the step length h is halved and the solution attempt is repeated until the above is satisfied or the step length is too small and the problem is left unsolved. If the error criterion is satisfied the algorithm progresses with a suitable step length solving the equations at intermediate points until the end point b is reached. For a full discussion of the algorithm and the error control mechanism used see Numerical Methods in Practice by Tim Hopkins and Chris Phillips.

Here is a module containing the subroutine `runge_kutta_merson`.

```
module rkm_module
  use precision_module, wp => dp
  implicit none

contains
  subroutine runge_kutta_merson &
    (y, fun, ifail, n, a, b, tol)
!
!   runge-kutta-merson method for the solution
!   of a system of n 1st order initial value
!   ordinary differential equations.
!   the routine tries to integrate from
!   t=a to t=b with initial conditions in y,
!   subject to the condition that the
!   absolute error estimate <= tol. the step
!   length is adjusted automatically to meet
!   this condition.
!   if the routine is successful it returns with
!   ifail = 0, t=b and the solution in y.
!
!   implicit none

! define arguments

  real (wp), intent (inout), dimension (: ) :: &
    y
  real (wp), intent (in) :: a, b, tol
  integer, intent (in) :: n
  integer, intent (out) :: ifail

interface
  subroutine fun(t, y, f, n)
    use precision_module, wp => dp
    implicit none
    real (wp), intent (in), dimension (: ) :: &
      y
    real (wp), intent (out), &
      dimension (: ) :: f
    real (wp), intent (in) :: t
    integer, intent (in) :: n
  end subroutine fun
end interface

! local variables
```

```
real (wp), dimension (1:size(y)) :: s1, s2, &
    s3, s4, s5, new_y_1, new_y_2, error
real (wp) :: t, h, h2, h3, h6, h8, &
    factor = 1.e-2_wp
real (wp) :: smallest_step = 1.e-6_wp, &
    max_error
integer :: no_of_steps = 0

ifail = 0

! check input parameters

if (n<=0 .or. a==b .or. tol<=0.0) then
    ifail = 1
    return
end if

! initialize t to be start of interval and
! h to be 1/100 of interval

t = a
h = (b-a)/100.0_wp
do

! ##### beginning of
! ##### repeat loop

    h2 = h/2.0_wp
    h3 = h/3.0_wp
    h6 = h/6.0_wp
    h8 = h/8.0_wp

! calculate s1,s2,s3,s4,s5
! s1=f(t,y)

    call fun(t, y, s1, n)
    new_y_1 = y + h3*s1

!     s2 = f(t+h/3,y+h/3*s1)

    call fun(t+h3, new_y_1, s2, n)
    new_y_1 = y + h6*s1 + h6*s2

!     s3=f(t+h/3,y+h/6*s1+h/6*s2)
```

```

call fun(t+h3, new_y_1, s3, n)
new_y_1 = y + h8*(s2+3.0_wp*s3)

!      s4=f(t+h/2,y+h/8*(s2+3*s3))

call fun(t+h2, new_y_1, s4, n)
new_y_1 = y + h2*(s1-3.0_wp*s3+4.0_wp*s4)

!      s5=f(t+h,y+h/2*(s1-3*s3+4*s4))

call fun(t+h, new_y_1, s5, n)

!      calculate values at t+h

new_y_1 = y + h6*(s1+4.0_wp*s4+s5)
new_y_2 = y + h2*(s1-3.0_wp*s3+4.0_wp*s4)

!      calculate error estimate

error = abs(0.2_wp*(new_y_1-new_y_2))
max_error = maxval(error)
if (max_error>tol) then

!      halve step length and try again

if (abs(h2)<smallest_step) then
    ifail = 2
    return
end if
h = h2
else

!      accepted approximation so overwrite
!      y with y_new_1, and t with t+h

y = new_y_1
t = t + h

!      can next step be doubled?

if (max_error*factor<tol) then
    h = h*2.0_wp
end if

!      does next step go beyond interval end b,

```

```

!      if so set h = b-t

      if (t+h>b) then
          h = b - t
      end if
      no_of_steps = no_of_steps + 1
  end if
  if (t>=b) exit

! ##### end of
! ##### repeat loop

end do
end subroutine runge_kutta_merson
end module rkm_module

```

Consider trying to solve the following system of first-order ordinary differential equations:

$$\dot{y}_1 = \tan y_3$$

$$\dot{y}_2 = \frac{-0.032 \tan y_3}{y_2} - \frac{0.02 y_2}{\cos y_3}$$

$$\dot{y}_3 = -\frac{0.032}{y_2^2}$$

over an interval $t = 0.0$ to $t = 8.0$ with initial conditions

$$y_1 = 0 \quad y_2 = 0.5 \quad y_3 = \pi/5$$

The user supplied subroutine, packaged as a module procedure, is:

```

module fun1_module
    implicit none
contains
    subroutine fun1(t, y, f, n)
        use precision_module, wp => dp
        implicit none
        real (wp), intent (in), dimension (:) :: y
        real (wp), intent (out), dimension (:) :: f
        real (wp), intent (in) :: t
        integer, intent (in) :: n
        f(1) = tan(y(3))
        f(2) = -0.032_wp*f(1)/y(2) - &

```

```

0.02_wp*y(2)/cos(y(3))
f(3) = -0.032_wp/(y(2)*y(2))
end subroutine fun1
end module fun1_module

```

and the main program to solve this system of ordinary differential equations is

```

program ch2602
use precision_module, wp => dp
use rkm_module
use fun1_module
implicit none
real (wp), dimension (:), allocatable :: y
real (wp) :: a, b, tol
integer :: n, ifail, all_stat

print *, 'input no of equations'
read *, n

! allocate space for y - checking to see that it
! allocates properly

allocate (y(1:n), stat=all_stat)
if (all_stat/=0) then
    print *, ' not enough memory'
    print *, ' array y is not allocated'
    stop
end if
print *, &
    ' input start and end of interval over'
print *, ' which equations to be solved'
read *, a, b
print *, 'input initial conditions'
read *, y(1:n)
print *, 'input tolerance'
read *, tol
print 100, a
100 format ('at t= ', f5.2, &
    ' initial conditions are :')
print 110, y(1:n)
110 format (4(f5.2,2x))
call runge_kutta_merson(y, fun1, ifail, n, a, &
    b, tol)
if (ifail/=0) then
    print *, 'integration stopped with ifail = ' &
        , ifail

```

```

else
    print 120, b
    120 format ('at t= ', f5.2, ' solution is:')
    print 110, y(1:n)
end if
end program ch2602

```

The user is prompted for the number of equations—3, the start and end of the interval over which the equations are to be solved—0.0, 8.0, the initial conditions—0.0, 0.5, $\pi/5$, tolerance—1.0E-6.

26.3.1 Note: Alternative Form of the Allocate Statement

In the main program ch2602 we have defined *y* to be a deferred-shape array, allocating it space after the variable *n* is read in. In order to make sure that enough memory is available to allocate space to array *y* the allocate statement is used as follows:

```
allocate(y(1:n),stat=all_stat)
```

If the allocation is successful variable *all_stat* returns zero; otherwise it is given a processor dependent positive value. We have included code to check for this and the program stops if *all_stat* is not zero.

26.3.2 Note: Automatic Arrays

The subroutine *runge_kutta_merson* needs a number of local rank 1 arrays *s1*, *s2*, *s3*, *s4* and *s5* for workspace, their shape and size being the same as the dummy argument *y*. Fortran supplies automatic arrays for this purpose and can be declared as

```
real(wp), dimension (1:size(y)) :: &
    s1, s2, s3, s4, s5
```

The size of automatic arrays can depend on the size of actual arrays: in our example they are the same shape and size as the dummy array *y*. Automatic arrays are created when the procedure is called and destroyed when control passes back to the calling program unit. They may have different shapes and sizes with different calls to the procedure, and because of this automatic arrays cannot be saved or initialised.

A word of warning should be given at this point. If there isn't enough memory available when an automatic array needs to be created problems will occur. Unlike allocatable arrays there is no way of testing to see if an automatic array has been

created successfully. The general feeling is that even though they are nice, automatic arrays should be used with care and perhaps shouldn't be used in production code!

26.3.3 Note: Subroutine as a Dummy Procedure Argument

In order to make the use of subroutine `runge_kutta_merson` as general as possible the user can choose the name of the subroutine in which the actual system of equations to be solved is defined. In this case we have chosen `fun1` as the name of the subroutine, which is then used as an actual argument when calling `runge_kutta_merson` from the main program e.g.

```
call runge_kutta_merson(y,fun1,ifail,n,a,b,tol)
```

An explicit interface for subroutine `fun1` is provided by it being contained in a module.

The equivalent dummy subroutine argument is `fun` and this needs an explicit interface in the subroutine `runge_kutta_merson`.

26.3.4 Note: Compilation When Using Modules

When compiling this program and the modules they must be done in the correct order:

- `precision_module`
 - `rkm_module`
 - `fun1_module`
- and then
- the main program.

26.3.5 Keyword and Optional Argument Variation

In modern Fortran arguments to procedures can be optional, and can be supplied by keyword. To illustrate this we will use the previous example. The definition of subroutine `runge_kutta_merson` and its dummy arguments is:

```
subroutine runge_kutta_merson(y,fun,ifail,n,a,b,tol)
```

where `a` is the initial point, `b` is the end point at which the solution is required, `tol` is the accuracy to which the solution is required and `n` is the number of equations.

The subroutine can be called as follows:

```
call runge_kutta_merson( y , fun1 , ifail , a=0.0 , &
    b=8.0 , tol=1.0E-6 , n=3)
```

where the dummy arguments `a`, `b`, `tol` and `n` are now being used as keywords. The use of keyword arguments makes the code easier to read and decreases the need to remember their precise position in the argument list.

Also with Fortran comes the ability to specify that an argument is optional. This is very useful when designing procedures for use by a range of programmers. Inside a procedure defaults can be set for the optional arguments providing an easy-to-use interface, while at the same time allowing sophisticated users a more comprehensive one.

The `optional` attribute is needed to declare a dummy argument to be optional. In the subroutine `runge_kutta_merson` the dummy argument `tol` could be declared to be optional (although internally in the subroutine the code would have to be changed to allow for this), e.g.,

```
subroutine runge_kutta_merson(y,fun,ifail,n,a,b,tol)
use precision_module , wp => dp
real (wp) , intent(inout), optional :: tol
```

and because it is at the end of the dummy argument list, calling the subroutine with a positional argument list, `tol` can be omitted, e.g.,

```
call runge_kutta_merson(y,fun1,ifail,n,a,b)
```

The code of the subroutine will need to be changed to check to see if the argument `tol` is supplied, the intrinsic function `present` being available for this purpose. Sample code is given below:

```
subroutine runge_kutta_merson(y,fun,ifail,n,a,b,tol)
use precision_module , wp => dp
! code left out
real (wp) , intent(in) , optional :: tol
real (wp) :: internal_tol = 1.0e-3_wp
if(present(tol)) then
    internal_tol=tol
    print*, 'tol = ', internal_tol,' is supplied'
else
    print*, "tol isn't supplied, default tolerance = "
    print *,internal_tol,' is used'
endif
! code left out but all references to tol
! would have to be changed to internal_tol
end subroutine runge_kutta_merson
```

26.4 Example 3: A Subroutine to Extract the Diagonal Elements of a Matrix

A common task mathematically is to extract the diagonal elements of a matrix. For example if

$$A = \begin{pmatrix} 2 & 1 & 6 & 7 \\ 9 & 3 & 2 \\ 4 & 1 & 8 \end{pmatrix}$$

the diagonal elements are (21, 3, 8).

This can be thought of as extracting an array section, but the intrinsic function `pack` is needed. In its simplest form `pack(array, vector)` packs an array, `array`, into a rank 1 array, `vector`, according to `array`'s array element order.

Below is a complete program to demonstrate this:

```
module md_module
    implicit none

contains
    subroutine matrix_diagonal(a, diag, n)
        implicit none
        real, intent (in), dimension (:, :) :: a
        real, intent (out), dimension () :: diag
        integer, intent (in) :: n
        real, dimension (1:size(a,1)*size(a,1)) :: temp

!      subroutine to extract the diagonal
!      elements of an n * n matrix A

        temp = pack(a, .true.)
        diag = temp(1:n*n:n+1)
    end subroutine matrix_diagonal
end module md_module

program ch2603
! program reads the n * n matrix from a file
use md_module
implicit none
integer :: i, n
real, allocatable, dimension (:, :) :: a
real, allocatable, dimension () :: adiag
character (len=20) :: filename

print *, 'input name of data file'
```

```

read '(a)', filename
open (unit=1, file=filename)
read (1, *) n
allocate (a(1:n,1:n), adiag(1:n))
do i = 1, n
  read (1, *) a(i, 1:n)
end do
call matrix_diagonal(a, adiag, n)
print *, ' diagonal elements of a are:'
print *, adiag
end program ch2603

```

26.5 Example 4: The Solution of Linear Equations Using Gaussian Elimination

At this stage we have introduced many of the concepts needed to write numerical code, and have included a popular algorithm, Gaussian Elimination, together with a main program which uses it and a module to bring together many of the features covered so far.

Finding the solution of a system of linear equations is very common in scientific and engineering problems, either as a direct physical problem or indirectly, for example, as the result of using finite difference methods to solve a partial differential equation. We will restrict ourselves to the case where the number of equations and the number of unknowns are the same. The problem can be defined as:

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1$$

$$a_{22}x_2 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2$$

...

$$a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_1$$

or

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} \quad (26.2)$$

which can be written as:

$$Ax = b$$

where A is the $n \times n$ coefficient matrix, b is the right-hand-side vector and x is the vector of unknowns. We will also restrict ourselves to the case where A is a general real matrix.

Note that there is a unique solution to (26.2) if the inverse, A^{-1} , of the coefficient matrix A , exists. However, the system should never be solved by finding A^{-1} and then solving $A^{-1}b = x$ because of the problems of rounding error and the computational costs.

A well-known method for solving (26.2) is Gaussian Elimination, where multiples of equations are subtracted from others so that the coefficients below the diagonal become zero, producing a system of the form:

$$\begin{pmatrix} a_{11}^* & a_{12}^* & \cdots & a_{1n}^* \\ 0 & a_{22}^* & \cdots & a_{2n}^* \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & a_{nn}^* \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1^* \\ b_2^* \\ \vdots \\ b_n^* \end{pmatrix}$$

where A has been transformed into an upper triangular matrix. By a process of backward substitution the values of x drop out.

The subroutine `gaussian_elimination` implements the Gaussian Elimination algorithm with partial pivoting, which ensure that the multipliers are less than 1 in magnitude, by interchanging rows if necessary. This is to try and prevent the buildup of errors.

This implementation is based on two LINPACK routines SGEFA and SGESL and a Fortran 77 subroutine written by Tim Hopkins and Chris Phillips and found in their book Numerical Methods in Practice.

When the subroutine `gaussian_elimination` is called on exit both `a` and `b` are overwritten. Mathematically Gaussian Elimination is described as working on rows, and using partial pivoting row interchanges may be necessary. Due to Fortran's row element ordering, to implement this algorithm efficiently it works on columns rather than rows by interchanging elements within a column if necessary.

```
include 'precision_module.f90'

module ge_module
  use precision_module, wp => dp
  implicit none

contains
  subroutine gaussian_elimination(a, n, b, x, &
    singular)
    ! routine to solve a system ax=b
    ! using gaussian elimination
    ! with partial pivoting
  end subroutine gaussian_elimination
end module
```

```
!      the code is based on the linpack routines
!      sgefa and sgesl
!      and operates on columns rather than rows !

      implicit none

!      matrix a and vector b are over-written
!      arguments

      integer, intent (in) :: n
      real (wp), intent (inout) :: a(:, :), b(:)
      real (wp), intent (out) :: x(:)
      logical, intent (out) :: singular

!      local variables

      integer :: i, j, k, pivot_row
      real (wp) :: pivot, sum, element
      real (wp), parameter :: eps = 1.e-13_wp

!      work through the matrix column by column

      do k = 1, n - 1

!      find largest element in column k for pivot
!

      pivot_row = maxval(maxloc(abs(a(k:n,k)))) &
                  + k - 1

!      test to see if a is singular
!      if so return to main program

      if (abs(a(pivot_row,k))<=eps) then
          singular = .true.
          return
      else
          singular = .false.
      end if

!      exchange elements in column k if largest
!      is
!      not on the diagonal

      if (pivot_row/=k) then
```

```

        element = a(pivot_row, k)
        a(pivot_row, k) = a(k, k)
        a(k, k) = element
        element = b(pivot_row)
        b(pivot_row) = b(k)
        b(k) = element
        end if

!      compute multipliers
!      elements of column k below diagonal
!      are set to these multipliers for use
!      in elimination later on

        a(k+1:n, k) = a(k+1:n, k)/a(k, k)

!      row elimination performed by columns for
!      efficiency

        do j = k + 1, n
          pivot = a(pivot_row, j)
          if (pivot_row/=k) then

            !      swap if pivot row is not k

              a(pivot_row, j) = a(k, j)
              a(k, j) = pivot
              end if
              a(k+1:n, j) = a(k+1:n, j) - &
                pivot*a(k+1:n, k)
            end do

!      apply same operations to b

          b(k+1:n) = b(k+1:n) - a(k+1:n, k)*b(k)
        end do

!      backward substitution

        do i = n, 1, -1
          sum = 0.0
          do j = i + 1, n
            sum = sum + a(i, j)*x(j)
          end do
          x(i) = (b(i)-sum)/a(i, i)
        end do
    
```

```
end subroutine gaussian_elimination
end module ge_module

program ch2604
use ge_module
implicit none
integer :: i, n
real (wp), allocatable :: a(:, :), b(:, ), x(:)
logical :: singular

print *, 'number of equations?'
read *, n
allocate (a(1:n,1:n), b(1:n), x(1:n))
do i = 1, n
    print *, 'input elements of row ', i, &
        ' of a'
    read *, a(i, 1:n)
    print *, 'input element ', i, ' of b'
    read *, b(i)
end do
call gaussian_elimination(a, n, b, x, &
    singular)
if (singular) then
    print *, 'matrix is singular'
else
    print *, 'solution x:'
    print *, x(1:n)
end if
end program ch2604
```

26.5.1 Notes

26.5.1.1 Module for Kind Type

We use the module `precision_module` from Chap. 21 and choose a working precision `wp` which maps to `dp` or double precision, to specify the floating point precision to which we wish to work. This module is then used by the main program and the subroutine, and `wp` is used with all the real type definitions and any constants, e.g.

```
real(wp), parameter :: eps=1.E-13_wp
```

26.5.1.2 Deferred-Shape Arrays

In the main program matrix a and vectors b and x are declared as deferred-shape arrays, by specifying their rank only and using the allocatable attribute. Their shape is determined at run time when the variable n is read in and then the statement

```
allocate(a(1:n,1:n), b(1:n), x(1:n))
```

is used.

26.5.1.3 Intrinsic Functions `maxval` and `maxloc`

In the context of subroutine `gaussian_elimination` we have used:

```
maxval ( maxloc (abs ( a ( k:n,k ) ) ) ) + k - 1
```

Breaking this down,

```
maxloc ( abs ( a (k:n,k) ) )
```

takes the rank 1 array

$$(|a(k, k)|, |a(k + 1, k)|, \dots, |a(n, k)|) \quad (26.3)$$

where $|a(k, k)| = \text{abs}(a(k, k))$ and of length $n - k + 1$. It returns the position of the largest element as a rank 1 array of size one, e.g. 1.

Applying `maxval` to this rank 1 array 1 returns 1 as a scalar, 1 being the position of the largest element of the above array.

What we actually want is the position of the largest element of (26.3), but in the k th column of matrix a . We therefore have to add $k - 1$ to 1 to give the actual position in column k of a .

26.6 Example 5: Allocatable Function Results

A function may return an array, and in this example the array allocation takes place in the function.

```
module running_average_module
    implicit none

    contains

    function running_average(r, how_many) &
        result (rarray)
        integer, intent (in) :: how_many
```

```
real, intent (in), allocatable, &
    dimension (: ) :: r
real, allocatable, dimension (: ) :: rarray
integer :: i
real :: sum = 0.0

allocate (rarray(1:how_many))
do i = 1, how_many
    sum = sum + r(i)
    rarray(i) = sum/i
end do
end function running_average
end module running_average_module
module read_data_module
    implicit none

contains

subroutine read_data(file_name, raw_data, &
    how_many)
    implicit none
    character (len=*) , intent (in) :: file_name
    integer, intent (in) :: how_many
    real, intent (out), allocatable, &
        dimension (: ) :: raw_data
    integer :: i

allocate (raw_data(1:how_many))
open (file=file_name, unit=1)
do i = 1, how_many
    read (unit=1, fmt=*) raw_data(i)
end do

end subroutine read_data

end module read_data_module

program ch2605
    use running_average_module
    use read_data_module
    implicit none
    integer :: how_many
    character (len=20) :: file_name
    real, allocatable, dimension (: ) :: raw_data
    real, allocatable, dimension (: ) :: ra
    integer :: i
```

```

print *, ' how many data items are there?'
read *, how_many
print *, ' what is the file name?'
read '(a)', file_name
call read_data(file_name, raw_data, how_many)
allocate (ra(1:how_many))
ra = running_average(raw_data, how_many)
do i = 1, how_many
    print *, raw_data(i), ' ', ra(i)
end do
end program ch2605

```

This facility was introduced in Fortran 95.

26.7 Example 6: Elemental e**x Function

The following is an elemental version of the `etox` function covered in an earlier chapter.

```

module etox_module
    implicit none

contains
    elemental real function etox(x)
        implicit none
        real, intent (in) :: x
        real :: term
        integer :: nterm
        real, parameter :: tol = 1.0e-6

        etox = 1.0
        term = 1.0
        nterm = 0
        do
            nterm = nterm + 1
            term = (x/nterm)*term
            etox = etox + term
            if (term<=tol) exit
        end do
    end function etox
end module etox_module
program ch2606
    use etox_module

```

```

implicit none
integer :: i
real :: x
real, dimension (10) :: y

x = 1.0
do i = 1, 10
    y(i) = i
end do
print *, y
x = etox(x)
print *, x
y = etox(y)
print *, y
end program ch2606

```

Elemental functions require the use of explicit interfaces, and we have therefore used modules to achieve this.

26.8 Problems

26.1 Compile and run the sparse matrix example with the data provided.

26.2 Compile and run the Runge Kutta Merson example with the data provided.

26.3 Compile and run the Gaussian Elimination example with the following data.

$$A = \begin{pmatrix} 33 & 16 & 72 \\ -24 & -10 & -57 \\ -8 & -4 & -17 \end{pmatrix}$$

$$b = \begin{pmatrix} -359 \\ 281 \\ 85 \end{pmatrix}$$

and the solution is

$$x = \begin{pmatrix} 1 \\ -2 \\ -5 \end{pmatrix}$$

26.4 Edit the Runge Kutta Merson subroutine so that `tol` is an optional argument. Compile and run the new code for the same set of ODE's but don't provide `tol` in the main program's call to the subroutine. Next provide `tol` with a value `1.0e-4`. What results do you get?

Bibliography

Duff, I.S., Erismon, A.M., Reid J.K.: Direct Methods for Sparse Matrices, Oxford Science Publications (1986).

- Authoritative coverage of this area. Relatively old, but well regarded. Code segments and examples are a mixture of Fortran 77 and Algol 60 (which of course do not support pointers) and therefore the implementation of linked lists is done using the existing features of these languages. The onus is on the programmer to correctly implement linked lists using fixed size arrays rather than using the features provided by pointers in a language. It is remarkable how elegant these solutions are, given the lack of dynamic data structures in these two languages.

Hopkins, T., Phillips, C.: Numerical Methods in Practice, Using the NAG Library. Addison-Wesley (1988).

- Good adjunct to the NAG library documentation for the less numerate user.

Chapter 27

Parameterised Derived Types (PDTs) in Fortran

Aims

The aims of this chapter are to look at some additional data structuring examples in Fortran that use parameterised derived types—PDTs.

27.1 Introduction

Parameterized derived types were introduced in the Fortran 2003 standard. They allow the kind, length, or shape of a derived types components to be chosen when the derived type is used.

This feature was only available in two compilers (Cray and IBM) at the time of the second edition. Support for this feature is now available in three additional compilers. At the time of writing they were available in the following compilers:

- Cray
- IBM
- Intel
- Nag (partial)
- PGI

Consult our *Compiler Support for the Fortran 2003 and 2008 Standards* document

http://www.fortranplus.co.uk/resources/fortran_2003_2008_compiler_support.pdf

for up to date information.

A parameterised derived type can have the kind, length and shape of a derived type chosen at run time. All type parameters are of type `integer` and have a `kind`, `len` or `dim` attribute. A kind type parameter may be used in constant and specification expressions. A length type parameter may only be used in a specification expression, e.g. array declarations.

We have a small number of examples to illustrate their use.

27.2 Example 1: Linked List Parameterised by Real Kind

Here is the program.

```

module precision_module
    implicit none
    integer, parameter :: sp &
        = selected_real_kind( 6, 37)
    integer, parameter :: dp &
        = selected_real_kind(15, 307)
    integer, parameter :: qp &
        = selected_real_kind(30, 291)
end module precision_module

module link_module
    use precision_module
    type link(real_kind)
        integer, kind :: real_kind
        real (kind=real_kind) :: n
        type (link(real_kind)), pointer :: next
    end type link
end module link_module

program ch2701
    use precision_module
    use link_module
    implicit none
    integer, parameter :: wp = dp
    type (link(real_kind=wp)), pointer :: root, &
        current
    integer :: i = 0
    integer :: error = 0
    integer :: io_stat_number = 0
    real (wp), allocatable, dimension (:) :: x

    allocate (root)
    print *, ' type in some numbers'
    read (unit=*, fmt=*, iostat=io_stat_number) &
        root%n
    if (io_stat_number>0) then
        error = error + 1
    end if
end program ch2701

```

```

else if (io_stat_number<0) then
    nullify (root%next)
else
    i = i + 1
    allocate (root%next)
end if
current => root
do while (associated(current%next))
    current => current%next
    read (unit=*, fmt=*, iostat=io_stat_number) &
        current%n
    if (io_stat_number>0) then
        error = error + 1
    else if (io_stat_number<0) then
        nullify (current%next)
    else
        i = i + 1
        allocate (current%next)
    end if
end do
print *, i, ' items read'
print *, error, ' items in error'
allocate (x(1:i))
i = 1
current => root
do while (associated(current%next))
    x(i) = current%n
    i = i + 1
    print *, current%n
    current => current%next
end do
print *, x
end program ch2701

```

Let us look at the `link_module` in more depth.

```

type link(real_kind)
    integer, kind :: real_kind
    real (kind=real_kind) :: n
    type (link(real_kind)), pointer :: next
end type link

```

The key is in the type declaration for `link` where the `link` type takes a parameter `real_kind`.

We then can reference this parameter within the `link` kind type definition. Thus the declarations for `n` and `next` are parameterised by `real_kind`.

In the main program we have

```
integer, parameter :: wp = dp
type (link(real_kind=wp)), pointer :: root, &
    current
```

and the type declarations for `root` and `current` are parameterised by `wp`, where `wp = dp`.

This means that we write one type definition for the `link` type that will work with any supported real kind type.

Without parameterised derived type support we would have to write separate kind type definitions for each supported real kind.

27.3 Example 2: Ragged Array Parameterised by Real Kind Type

Here is the program.

```
module precision_module
    implicit none
    integer, parameter :: sp &
        = selected_real_kind( 6, 37)
    integer, parameter :: dp &
        = selected_real_kind(15, 307)
    integer, parameter :: qp &
        = selected_real_kind(30, 291)
end module precision_module

module ragged_module
    use precision_module
    implicit none
    type ragged(real_kind)
        integer, kind :: real_kind
        real (real_kind), dimension (:), &
            allocatable :: ragged_row
    end type ragged
end module ragged_module
```

```

program ch2702

use precision_module
use ragged_module
implicit none
integer, parameter :: wp = sp
integer :: i
integer, parameter :: n = 3

type (ragged(wp)), dimension (1:n) :: &
lower_diag

do i = 1, n
allocate (lower_diag(i)%ragged_row(1:i))
print *, ' type in the values for row ', i
read *, lower_diag(i)%ragged_row(1:i)
end do
do i = 1, n
print *, lower_diag(i)%ragged_row(1:i)
end do

end program ch2702

```

Let us look at the `ragged_module` in more depth.

```

module ragged_module
use precision_module
implicit none
type ragged(real_kind)
    integer, kind :: real_kind
    real (real_kind), dimension (:), &
    allocatable :: ragged_row
end type ragged
end module ragged_module

```

The key is in the type declaration for the `ragged` type.
We have

```
type ragged(real_kind)
```

so the kind definition is parameterised by `real_kind`.

The `ragged_row` array declaration is parameterised by `real_kind`.

In the main program we have

```
type (ragged(wp)), dimension (1:n) :: &
    lower_diag
```

so that the `lower_diag` declaration is parameterised by `wp`, where `wp = sp`.

So we have one declaration for the `ragged` type and can use this type with any supported real kind type.

27.4 Example 3: Specifying `len` in a PDT

In this example we use both the `kind` attribute and the `len` attribute in the type specification.

```
module precision_module
    implicit none
    integer, parameter :: sp &
        = selected_real_kind( 6, 37)
    integer, parameter :: dp &
        = selected_real_kind(15, 307)
    integer, parameter :: qp &
        = selected_real_kind(30, 291)
end module precision_module

module pdt_matrix_module

use precision_module
implicit none

type pdt_matrix(k,row,col)
    integer, kind :: k
    integer, len  :: row, col
    real(kind=k), dimension(row,col) :: m
end type pdt_matrix

interface scale_matrix
    module procedure scale_matrix_sp
    module procedure scale_matrix_dp
end interface scale_matrix

contains

subroutine scale_matrix_sp(a,scale)
    type(pdt_matrix(sp,*,*)),intent(inout):: a
```

```
real(sp):: scale
    a%m = a%m + scale
end subroutine scale_matrix_sp

subroutine scale_matrix_dp(a,scale)
type(pdt_matrix(dp,*,*)) , intent(inout):: a
real(dp):: scale
    a%m = a%m + scale
end subroutine scale_matrix_dp

end module pdt_matrix_module

program ch2703
use precision_module
use pdt_module

real(sp) :: scs
real(dp) :: scd
integer, parameter:: nr = 2,nc = 3
type(pdt_matrix(sp,nr,nc)) :: as
type(pdt_matrix(dp,nr,nc)) :: ad
!
! single precision
!
do i=1,nr
    print*, 'input row ',i,' of sp matrix'
    read *,as%m(i,1:nc)
end do
print *, 'input sp scaling factor'
read*,scs
call scale_matrix(as,scs)
print*, 'updated matrix:'
do i=1,nr
    print 100,as%m(i,1:nc)
    100 format(10(f6.2,2x))
end do
!
! double precision
!
do i=1,nr
    print*, 'input row ',i,' of dp matrix'
    read *,ad%m(i,1:nc)
end do
print *, 'input dp scaling factor'
read*,scd
```

```
call scale_matrix(ad,scd)
print*, 'updated matrix:'
do i=1,nr
    print 200,ad%m(i,1:nc)
  200 format(10(e12.5,2x))
end do

end program ch2703
```

27.5 Problems

27.1 Modify example 1 to read the data from a file.

27.2 Rewrite the tree derived type in Chap. 22 as a parameterised derived type to work with an integer of any type. Test it out.

Chapter 28

Object Oriented Programming

For Madmen only

Hermann Hesse, Steppenwolf

Aims

The aims of this chapter are to look at object oriented programming in Fortran.

28.1 Introduction

This chapter looks at object oriented programming in Fortran. The chapter on programming languages covers the topic in a broader context.

28.2 Brief Review of the History of Object Oriented Programming

Object oriented programming is not new. One of the first languages to offer support was Simula 67, a language designed for discrete event simulation by Ole Johan Dahl, Bjorn Myhrhaug and Kristen Nygaard whilst working at the Norwegian Computing Centre in Oslo in the 1960s.

One of the next major developments was in the 1970s at the Xerox Palo Alto Research Centre Learning Research Group who began working on a vision of the ways different people might effectively use computing power. One of the outcomes of their work was the Smalltalk 80 system. Objects are at the core of the Smalltalk 80 system.

The 1980s and 1990s saw a number of object oriented programming languages emerge. They include

- Eiffel. Bertrand Meyer, Eiffel Software.
- C++ from C with classes. Bjarne Stroustrup at Bell Labs.
- Oberon 2. Niklaus Wirth at ETH in Zurich.
- Java. James Gosling, originally Sun, now Oracle.
- C# is a recent Microsoft addition to the list.

Object-oriented programming is effectively a programming methodology or paradigm using objects (data structures made up of data and methods). We will use the concept of a shape class in our explanation and examples. The Simula Begin book starts with shapes, and it is often used in introductions to object oriented programming in other languages.

Some of the key concepts are

- Encapsulation or information hiding—the implementation of the data is hidden inside an object and clients or users of the data only have access to an abstract view of it. Methods are used to access and manipulate the data. For example a shape class may have an x and y position, and methods exist to get and set the positions and draw and move the shape.
- Data abstraction—if we have an abstract shape data type we can create multiple variables of that type.
- Inheritance—an existing abstract data type can be extended. It will inherit the data and methods from the base type and add additional data and methods. A key to inheritance is that the extended type is compatible with the base type. Anything that works with objects or variables of the base type also work with objects of the extended type. A circle would have a radius in addition to an x and y position, a rectangle would have a width and height.
- Dynamic binding—if we have a base shape class and derive circles and rectangles from it dynamic binding ensures that the correct method to calculate the area is called at run time.
- Polymorphism—variables can therefore be polymorphic. Using the shape example we can therefore create an array of shapes, one may be a shape, one may be a circle and another may be a rectangle.

Extensible abstract data types with dynamically bound methods are often called classes. This is the terminology we will use in what follows.

28.3 Background Technical Material

We need to look more formally at a number of concepts so that we can actually do object oriented programming in Fortran. The following sections cover some of the introductory material we need, and are taken from the standard.

28.4 Type Declaration Statements

Every data object has a type and rank and may have type parameters and other attributes that determine the uses of the object. Collectively, these properties are the attributes of the object. The type of a named data object is normally specified explicitly in a type declaration statement. All of its attributes may be included in a type declaration statement or may be specified individually in separate specification statements.

28.4.1 *Type*

A `type` type specifier is used to declare entities of a derived type. Section 1.3.147 of the standard defines it as follows:

- `type`: data type—named category of data characterized by a set of values, a syntax for denoting these values, and a set of operations that interpret and manipulate the values (4.1)

A scalar entity of derived type is a structure.

28.4.2 *Class*

A polymorphic entity is a data entity that is able to be of differing types during program execution. The type of a data entity at a particular point during execution of a program is its dynamic type. The declared type of a data entity is the type that it is declared to have, either explicitly or implicitly.

A `class` type specifier is used to declare polymorphic objects. The declared type of a polymorphic object is the specified type if the `class` type specifier contains a type name.

28.4.3 *Attributes*

The additional attributes that may appear in the attribute specification of a type declaration statement further specify the nature of the entities being declared or specify restrictions on their use in the program.

28.4.3.1 Accessibility Attribute

The accessibility attribute specifies the accessibility of an entity via a particular identifier. The following is taken from section 5.3.2 of the Fortran 2008 standard.

- access-spec is `public` or `private`
- An access-spec shall appear only in the specification-part of a module.

Identifiers that are specified in a module or accessible in that module by use association have either the `public` or `private` attribute. Identifiers for which an access-spec is not explicitly specified in that module have the default accessibility attribute for that module. The default accessibility attribute for a module is `public` unless it has been changed by a `private` statement. Only identifiers that have the `public` attribute in that module are available to be accessed from that module by use association.

28.4.4 Passed Object Dummy Arguments

Section 4.5.4.5 of the Fortran 2008 standard introduces the concept of passed object dummy argument. Here is an extract from the standard:

- A passed-object dummy argument is a distinguished dummy argument of a procedure pointer component or type-bound procedure. It affects procedure overriding (4.5.7.3) and argument association (12.5.2.2).
- If `nopass` is specified, the procedure pointer component or type-bound procedure has no passed-object dummy argument.
- If neither `pass` nor `nopass` is specified or `pass` is specified without arg-name, the first dummy argument of a procedure pointer component or type-bound procedure is its passed-object dummy argument.
- If `pass (arg-name)` is specified, the dummy argument named arg-name is the passed-object dummy argument of the procedure pointer component or named type-bound procedure.
- C456 The passed-object dummy argument shall be a scalar, nonpointer, nonallocatable dummy data object with the same declared type as the type being defined; all of its length type parameters shall be assumed; it shall be polymorphic (4.3.1.3) if and only if the type being defined is extensible (4.5.7). It shall not have the `VALUE` attribute.
- Note 4.32: If a procedure is bound to several types as a type-bound procedure, different dummy arguments might be the passed-object dummy argument in different contexts.

The key here is that we are going to use the `pass` and `nopass` attributes with type bound procedures—a component of object oriented programming in Fortran.

28.4.5 Derived Types and Structure Constructors

A derived type is a type that is not defined by the language but requires a type definition to declare its components. A scalar object of such a derived type is called a structure. Assignment of structures is defined intrinsically, but there are no intrinsic operations for structures. For each derived type, a structure constructor is available to provide values.

A derived-type definition implicitly defines a corresponding structure constructor that allows construction of values of that derived type.

28.4.6 Structure Constructors and Generic Names

A generic name may be the same as a type name. This can be used to emulate user-defined structure constructors for that type, even if the type has private components. The following example is taken from the standard to illustrate this.

```
module mytype_module
type mytype
    private
        complex value
        logical exact
end type
interface mytype
    module procedure int_to_mytype
end interface
! Operator definitions etc.
...
contains
    type(mytype) function int_to_mytype(i)
        integer,intent(in) :: i
        int_to_mytype%value = i
        int_to_mytype%exact = .true.
    end function
    ! Procedures to support operators etc.
...
end
```

28.4.7 Assignment

Execution of an assignment statement causes a variable to become defined or redefined. Simplistically

```
variable = expression
```

28.4.8 Intrinsic Assignment Statement

An intrinsic assignment statement is an assignment statement that is not a defined assignment statement. In an intrinsic assignment statement, variable shall not be polymorphic.

28.4.9 Defined Assignment Statement

A defined assignment statement is an assignment statement that is defined by a subroutine and a generic interface that specifies ASSIGNMENT (=).

28.4.10 Polymorphic Variables

Here is the definition of polymorphic taken from the standard.

- Polymorphic—Able to be of differing types during program execution. An object declared with the `class` keyword is polymorphic.

A polymorphic variable must be a pointer or allocatable variable. We will use allocatable variables to achieve polymorphism in our examples.

28.4.11 Executable Constructs Containing Blocks

The following are executable constructs that contain blocks:

- `associate` construct
- `case` construct
- `do` construct
- `if` construct
- `select type` construct

We will look at the `associate` construct and `select type` construct next.

28.4.12 The `associate` Construct

The `associate` construct associates named entities with expressions or variables during the execution of its block. These named construct entities are associating entities. The names are associate names.

The following example illustrates an association with a derived-type variable.

```
associate ( xc => ax%b(i,i)%c )
xc%dv = xc%dv + product(Xxc%ev(1:n))
end associate
```

28.4.13 The **select** Type Construct

The **select** type construct selects for execution at most one of its constituent blocks. The selection is based on the dynamic type of an expression. A name is associated with the expression, in the same way as for the **associate** construct.

Quite a lot to take in! Let's illustrate the use of the above in some actual examples.

28.5 Example 1: The Basic Shape Class

The code for the base shape class is given below.

- Shape class data: integer variables **x** and **y** for the position.
- Shape class methods: **get** and **set** for the **x** and **y** values, and **moveto** and **draw**.

We have used an **include** statement in the examples that follow to reduce code duplication. In this example we have used the default accessibility for the data and methods in the **shape_module**.

```
module shape_module

type shape_type

    integer :: x_ = 0
    integer :: y_ = 0

contains

    procedure, pass (this) :: getx
    procedure, pass (this) :: gety
    procedure, pass (this) :: setx
    procedure, pass (this) :: sety
    procedure, pass (this) :: moveto
    procedure, pass (this) :: draw

end type shape_type
```

```
contains
```

```
    include 'shape_module_common_code.f90'
```

```
end module shape_module
```

Here is the code in the include file.

```
! start shape_module_common_code
integer function getx(this)
    implicit none
    class (shape_type), intent (in) :: this

    getx = this%x_
end function getx

integer function gety(this)
    implicit none
    class (shape_type), intent (in) :: this

    gety = this%y_
end function gety

subroutine setx(this, x)
    implicit none
    class (shape_type), intent (inout) :: this
    integer, intent (in) :: x

    this%x_ = x
end subroutine setx

subroutine sety(this, y)
    implicit none
    class (shape_type), intent (inout) :: this
    integer, intent (in) :: y

    this%y_ = y
end subroutine sety

subroutine moveto(this, newx, newy)
    implicit none
    class (shape_type), intent (inout) :: this
    integer, intent (in) :: newx
    integer, intent (in) :: newy

    this%x_ = newx
```

```

    this%y_ = newy
end subroutine moveto

subroutine draw(this)
implicit none
class (shape_type), intent (in) :: this

print *, ' x = ', this%x_
print *, ' y = ', this%y_
end subroutine draw
! end shape_module_common_code

```

28.5.1 Key Points

Some of the key concepts are:

- We use a module as the organisational unit for the class.
- We use `type` and `end type` to contain the data and the procedures—called type bound procedures in Fortran terminology.
- The data in the base class is an x and y position.
- The type bound methods within the class are
 - `getx` and `setx`
 - `gety` and `sety`
 - `draw`
 - `moveto`
- We have used the default accessibility for the data and methods in the type.

Let us look at the code in stages.

```
module shape_module
```

The module is called `shape_module`

```
type shape_type
```

The type is called `shape_type`

```

integer :: x_ = 0
integer :: y_ = 0

```

The data associated with the shape type are integer variables that are the x and y coordinates of the shape. We initialise to zero.

```
contains
```

The type also contains procedures or methods.

```

procedure, pass(this) :: getx
procedure, pass(this) :: gety
procedure, pass(this) :: setx
procedure, pass(this) :: sety
procedure, pass(this) :: moveto
procedure, pass(this) :: draw

```

These are called type bound procedures in Fortran terminology. It is common in object oriented programming to have get and set methods for each of the data components of the type or object. We also have a `moveto` and `draw` method.

Each of these methods has the `pass` attribute. When a type bound procedure is called or invoked the object through which it is invoked is normally passed as a hidden parameter. We have used the `pass` attribute to explicitly confirm the default behaviour of passing the invoking object as the first parameter. We have also followed the convention in object oriented programming of using the word `this` to refer to the current object.

```
end type shape_type
```

This is the end of the type definition.

`contains`

The module then contains the actual implementation of the type bound procedures. We will look at a couple of these.

```

integer function getx(this)
implicit none
class (shape_type), intent (in) :: this
getx = this%x_
end function getx

```

As we stated earlier it is common in object oriented programming to have get and set methods for each data item in an object. This function implements the `getx` method. The first argument is the current object, referred to as `this`. We then have the type declaration for this parameter. We declare the variable using `class` rather than `type` as we want the variable to be polymorphic. The rest of the function is self explanatory.

```

subroutine setx(this,x)
implicit none
class (shape_type), intent (inout) :: this
integer, intent (in) :: x
this%x_ = x
end subroutine setx

```

The `setx` procedure is a subroutine. It takes two parameters, the current object and the new `x` value. Again we use the `class` declaration mechanism as we want the variable to be polymorphic.

Here is a program to test the above class out.

```
program ch2801
  use shape_module
  implicit none
  type (shape_type) :: s1 = shape_type(10, 20)
  integer :: x1 = 100
  integer :: y1 = 200

  print *, ' get '
  print *, s1%getx(), ' ', s1%gety()
  print *, ' draw '
  call s1%draw()
  print *, ' moveto '
  call s1%moveto(x1, y1)
  print *, ' draw '
  call s1%draw()
  print *, ' set '
  call s1%setx(99)
  call s1%sety(99)
  print *, ' draw'
  call s1%draw()
end program ch2801
```

The first statement of interest is the `use` statement, where we make available the `shape_module` to the test program. The next statement of interest is

```
type (shape_type) :: s1 = shape_type(10, 20)
```

We then have a type declaration for the variable `s1`. We also have the use of what Fortran calls a structure constructor `shape_type` to provide initial values to the `x` and `y` positions. The term constructor is used in other object oriented programming languages, e.g C++, Java, C#. It has the same name as the type or class and is created automatically for us by the compiler in this example.

The

```
print *, s1%getx(), ' ', s1%gety()
```

statement prints out the `x` and `y` values for the object `s1`. We use the standard `%` notation that we used in derived types, to separate the components of the derived types. If one looks at the implementation of the `getx` function and examines the first line, repeated below

```
integer function getx(this)
```

how we refer to the current object, `s1`, through the syntax `s1%getx()`. The following call:

```
call s1%draw()
```

shows how to invoke the draw method for the s1 object, using the s1 %draw() syntax. The first line of the draw subroutine

```
subroutine draw(this)
```

shows how the current object is passed as the first argument.

28.5.2 Notes

In this example we have accepted the default Fortran accessibility behaviour. This means that we can use the compiler provided structure constructor shape_type()

```
type (shape_type) :: s1 = shape_type(10,20)
```

in the type declaration to provide initial values, as they are public by default. Direct access to the data is often not a good idea, as it is possible to make changes to the data anywhere in the program. The next example makes the data private.

28.5.3 Example 2: Base Class with Private Data

Here is the modified base class. This example will now not compile as the default compiler provided structure constructor does not have access to the private data.

```
module shape_module

type shape_type

    integer, private :: x_ = 0
    integer, private :: y_ = 0

contains

    procedure, pass (this) :: getx
    procedure, pass (this) :: gety
    procedure, pass (this) :: setx
    procedure, pass (this) :: sety
    procedure, pass (this) :: moveto
    procedure, pass (this) :: draw

end type shape_type

contains

    include 'shape_module_common_code.f90'
end module shape_module
```

The test program is the same as in the first example.
Here is the output from trying to compile this example.

```
Error: ch2802.f90, line 4:  
Constructor for type SHAPE_TYPE has value  
for PRIVATE component X_  
Errors in declarations,  
no further processing for CH2802  
[NAG Fortran Compiler error termination, 1 error]
```

Not all compilers diagnose this problem. Test yours to see if you get an error message!

An earlier solution to this type of problem can be found in the date class in Chap. 22, where we provide our own structure constructor `date_()`. Most object oriented programming languages provide the ability to use the same name as a class as a constructor name even if the data is private. Modern Fortran provides another solution to this problem. In the example below we will provide our own structure constructor inside an interface.

28.5.4 Example 3: Using an Interface to Use the Class Name for the Structure Constructor

Here is the modified base class.

```
module shape_module

type shape_type

    integer, private :: x_ = 0
    integer, private :: y_ = 0

contains

    procedure, pass (this) :: getx
    procedure, pass (this) :: gety
    procedure, pass (this) :: setx
    procedure, pass (this) :: sety
    procedure, pass (this) :: moveto
    procedure, pass (this) :: draw

end type shape_type

interface shape_type
```

```

module procedure shape_type_constructor
end interface shape_type

contains

type (shape_type) function &
    shape_type_constructor(x, y)
    implicit none
    integer, intent (in) :: x
    integer, intent (in) :: y

    shape_type_constructor%x_ = x
    shape_type_constructor%y_ = y
end function shape_type_constructor

include 'shape_module_common_code.f90'

end module shape_module

```

The key statements are

```

interface shape_type
    module procedure shape_type_constructor
end interface

```

which enables us to map a call or reference to `shape_type` (our structure constructor name) to our implementation of `shape_type_constructor`. Here is the implementation of this structure constructor.

```

type (shape_type) function &
    shape_type_constructor(x,y)
    implicit none
    integer, intent (in) :: x
    integer, intent (in) :: y
    shape_type_constructor%x_ = x
    shape_type_constructor%y_ = y
end function shape_type_constructor

```

The function is called `shape_type_constructor` hence we use this name to initialise the components of the type, and the function returns a value of type `shape_type`.

Here is the program to test the above out.

```

program ch2803
use shape_module
implicit none
type (shape_type) :: s1

```

```
integer :: x1 = 100
integer :: y1 = 200

s1 = shape_type(10, 20)
print *, ' get '
print *, s1%getx(), ' ', s1%gety()
print *, ' draw '
call s1%draw()
print *, ' moveto '
call s1%moveto(x1, y1)
print *, ' draw '
call s1%draw()
print *, ' set '
call s1%setx(99)
call s1%sety(99)
print *, ' draw'
call s1%draw()
end program ch2803
```

Note that in this example we cannot initialise `s1` at definition time using our own (user defined) structure constructor. This must now be done within the execution part of the program. This is a Fortran restriction, and makes it consistent with the rest of the language.

These examples illustrate some of the basics of object oriented programming in Fortran. To summarise

- the data in our class is private;
- access to the data is via get and set methods;
- the data and methods are within the derived type definition—the methods are called type bound procedures in Fortran terminology;
- we can use interfaces to provide user defined structure constructors, which have the same name as the class—this is a common practice in object oriented programming;
- we have used `class` to declare the variables within the type bound methods. We need to use `class` when we want to use polymorphic variables in Fortran.

28.5.5 Public and Private Accessibility

We have only made the internal data in the class private in the above example. There will be cases where some of the methods are only used within the class, in which case they can be made private.

28.6 Example 4: Simple Inheritance

In this example we look at inheritance. We use the same base shape class and derive two classes from it—circle and rectangle.

A circle has a radius. This is the additional data component of the derived class. We also have get and set methods.

A rectangle has a width and height. These are the additional data components of the derived rectangle class. We also have get and set methods.

28.6.1 Base Shape Class

The base shape class is as in the previous example.

28.6.2 Circle—Derived Type 1

Here is the code.

```
module circle_module

use shape_module

type, extends (shape_type) :: circle_type

    integer, private :: radius_

contains

    procedure, pass (this) :: getradius
    procedure, pass (this) :: setradius
    procedure, pass (this) :: draw => &
        draw_circle

end type circle_type

interface circle_type
    module procedure circle_type_constructor
end interface circle_type

contains

    type (circle_type) function &
```

```

circle_type_constructor(x, y, radius)
implicit none
integer, intent (in) :: x
integer, intent (in) :: y
integer, intent (in) :: radius

call circle_type_constructor%setx(x)
call circle_type_constructor%sety(y)
circle_type_constructor%radius_ = radius
end function circle_type_constructor

integer function getradius(this)
implicit none
class (circle_type), intent (in) :: this

getradius = this%radius_
end function getradius

subroutine setradius(this, radius)
implicit none
class (circle_type), intent (inout) :: this
integer, intent (in) :: radius

this%radius_ = radius
end subroutine setradius

subroutine draw_circle(this)
implicit none
class (circle_type), intent (in) :: this

print *, ' x = ', this%getx()
print *, ' y = ', this%gety()
print *, ' radius = ', this%radius_
end subroutine draw_circle

end module circle_module

```

Let us look more closely at the statements within this class. Firstly we have

```
module circle_module
```

which introduces our circle module. We then

```
use shape_module
```

within this module to make available the shape class. The next statement

```
type , extends(shape_type) :: circle_type
```

is the key statement in inheritance. What this statement says is base our new `circle_type` on the base `shape_type`. It is an extension of the `shape_type`. We then have the additional data in our `circle_type`

```
integer , private :: radius_
```

and the following additional type bound procedures.

```
procedure , pass(this) :: getradius
procedure , pass(this) :: setradius
procedure , pass(this) :: draw => draw_circle
```

and we have the simple get and set methods for the radius, and a type specific draw method for our `circle_type`. It is this method that will be called when drawing with a circle, rather than the draw method in the base `shape_type`.

We then have an interface to provide us with our own user defined structure constructor for our `circle_type`.

```
interface circle_type
    module procedure circle_type_constructor
end interface
```

As has been stated earlier it is common practice in object oriented programming to use the same name as the type for constructors.

We then have the implementation of the constructor.

```
type (circle_type) function &
    circle_type_constructor(x,y,radius)
    implicit none
    integer, intent (in) :: x
    integer, intent (in) :: y
    integer, intent (in) :: radius
    call circle_type_constructor%setx(x)
    call circle_type_constructor%sety(y)
    circle_type_constructor%radius_=radius
end function circle_type_constructor
```

Note that we use the `setx` and `sety` methods to provide initial values to the `x` and `y` values. They are private in the base class so we need to use these methods.

We can directly initialise the radius as this is a data component of this class, and we have access to it.

We next have the `get` and `set` methods for the radius.

Finally we have the implementation for the draw circle method.

```
subroutine draw_circle(this)
    implicit none
    class (circle_type), intent(in) :: this
    print *, ' x = ' , this%getx()
```

```

print *, ' y = ' , this%gety()
print *, ' radius = ' , this%radius_
end subroutine draw_circle

```

Notice again that we use the `getx` and `gety` methods to access the `x` and `y` private data from the base shape class.

28.6.3 Rectangle—Derived Type 2

Here is the code for the second derived type.

```

module rectangle_module

use shape_module

type, extends (shape_type) :: rectangle_type

    integer, private :: width_
    integer, private :: height_

contains

    procedure, pass (this) :: getwidth
    procedure, pass (this) :: setwidth
    procedure, pass (this) :: getheight
    procedure, pass (this) :: setheight
    procedure, pass (this) :: draw => &
        draw_rectangle

end type rectangle_type

interface rectangle_type
    module procedure rectangle_type_constructor
end interface rectangle_type

contains

type (rectangle_type) function &
    rectangle_type_constructor(x, y, width, &
    height)
    implicit none
    integer, intent (in) :: x
    integer, intent (in) :: y
    integer, intent (in) :: width
    integer, intent (in) :: height

```

```
call rectangle_type_constructor%setx(x)
call rectangle_type_constructor%sety(y)
rectangle_type_constructor%width_ = width
rectangle_type_constructor%height_ = height
end function rectangle_type_constructor

integer function getwidth(this)
implicit none
class (rectangle_type), intent (in) :: this

getwidth = this%width_
end function getwidth

subroutine setwidth(this, width)
implicit none
class (rectangle_type), intent (inout) :: &
this
integer, intent (in) :: width

this%width_ = width
end subroutine setwidth

integer function getheight(this)
implicit none
class (rectangle_type), intent (in) :: this

getheight = this%height_
end function getheight

subroutine setheight(this, height)
implicit none
class (rectangle_type), intent (inout) :: &
this
integer, intent (in) :: height

this%height_ = height
end subroutine setheight

subroutine draw_rectangle(this)
implicit none
class (rectangle_type), intent (in) :: this

print *, ' x = ', this%getx()
print *, ' y = ', this%gety()
print *, ' width = ', this%width_
```

```
    print *, ' height = ', this%height_
end subroutine draw_rectangle

end module rectangle_module
```

The code is obviously very similar to that of the first derived type.

28.6.4 Simple Inheritance Test Program

Here is a test program that illustrates the use of the shape type, circle type and rectangle type.

```
program ch2804

use shape_module
use circle_module
use rectangle_module

implicit none

type (shape_type) :: vs
type (circle_type) :: vc
type (rectangle_type) :: vr

vs = shape_type(10, 20)
vc = circle_type(100, 200, 300)
vr = rectangle_type(1000, 2000, 3000, 4000)
print *, ' get '
print *, ' shape      ', vs%getx(), ' ', &
         vs%gety()
print *, ' circle     ', vc%getx(), ' ', &
         vc%gety(), ' radius = ', vc%getradius()
print *, ' rectangle  ', vr%getx(), ' ', &
         vr%gety(), ' width = ', vr%getwidth(), '&
         'height ', vr%getheight()
print *, ' draw '
call vs%draw()
call vc%draw()
call vr%draw()
print *, ' set '
call vs%setx(19)
call vs%sety(19)
call vc%setx(199)
call vc%sety(199)
```

```

call vc%setradius(199)
call vr%setx(1999)
call vr%sety(1999)
call vr%setwidth(1999)
call vr%setheight(1999)
print *, ' draw '
call vs%draw()
call vc%draw()
call vr%draw()
end program ch2804

```

The first statements of note are

```

use shape_module
use circle_module
use rectangle_module

```

which make available the shape, circle and rectangle types within the program.

The following statements

```

type (shape_type)      :: vs
type (circle_type)    :: vc
type (rectangle_type) :: vr

```

declare `vs`, `vc` and `vr` to be of type shape, circle and rectangle respectively. The following three statements

```

vs = shape_type(10,20)
vc = circle_type(100,200,300)
vr = rectangle_type(1000,2000,3000,4000)

```

call the three user defined structure constructor functions.

We then use the get functions to print out the values of the private data in each object.

```

print *, ' shape      ', vs%getx(), &
' ', vs%gety()
print *, ' circle     ', vc%getx(), &
' ', vc%gety(), ' radius = ', vc%getradius()
print *, ' rectangle  ', vr%getx(), &
' ', vr%gety(), ' width  = ', vr%getwidth(), '
height ', vr%getheight()

```

We then call the draw method for each type.

```

call vs%draw()
call vc%draw()
call vr%draw()

```

and the appropriate draw method is called for each type. We finally call the set functions for each variable and repeat the calls to the draw methods.

The draw methods in the derived types override the draw method in the base shape class.

28.7 Example 5: Polymorphism and Dynamic Binding

An inheritance hierarchy can provide considerable flexibility in our ability to manipulate objects, whilst still taking advantage of static or compile time type checking. If we combine inheritance with polymorphism and dynamic binding we have a very powerful programming tool. We will illustrate this with a concrete example.

28.7.1 Base Shape Class

This is our base class. A polymorphic variable is a variable whose data type may vary at run time. It must be a pointer or allocatable variable, and it must be declared using the `class` keyword. Our original base class declared variables using the `class` keyword from the beginning as we always intended to design a class that could be polymorphic.

We have had to make one change to the previous one. To make the polymorphism work we have had to provide our own assignment operator. So we have

```
interface assignment (=)
  module procedure generic_shape_assign
end interface
```

which means that our implementation of `generic_shape_assign` will replace the intrinsic assignment. Here is the actual implementation.

```
subroutine generic_shape_assign(lhs,rhs)
  implicit none
  class (shape_type), intent (out), &
    allocatable :: lhs
  class (shape_type), intent (in) :: rhs
  allocate (lhs,source=rhs)
end subroutine generic_shape_assign
```

In an assignment we obviously have

```
left_hand_side = right_hand_side
```

and in our code we have variables `lhs` and `rhs` to clarify what is happening. We also have an enhanced form of allocation statement:

```
allocate (lhs,source=rhs)
```

and the key is that the left hand side variable is allocated with the values and type of the right hand side variable. Here is the complete code.

```
module shape_module

type shape_type

    integer, private :: x_ = 0
    integer, private :: y_ = 0

contains

    procedure, pass (this) :: getx
    procedure, pass (this) :: gety
    procedure, pass (this) :: setx
    procedure, pass (this) :: sety
    procedure, pass (this) :: moveto
    procedure, pass (this) :: draw

end type shape_type

interface shape_type
    module procedure shape_type_constructor
end interface shape_type

interface assignment (=)
    module procedure generic_shape_assign
end interface assignment (=)

contains

type (shape_type) function &
    shape_type_constructor(x, y)
    implicit none
    integer, intent (in) :: x
    integer, intent (in) :: y

    shape_type_constructor%x_ = x
    shape_type_constructor%y_ = y
end function shape_type_constructor

include 'shape_module_common_code.f90'

subroutine generic_shape_assign(lhs, rhs)
    implicit none
```

```

    class (shape_type), intent (out), &
        allocatable :: lhs
    class (shape_type), intent (in) :: rhs

    allocate (lhs, source=rhs)
end subroutine generic_shape_assign

end module shape_module

```

28.7.2 Circle—Derived Type 1

The circle code is the same as before.

28.7.3 Rectangle—Derived Type 2

The rectangle code is as before.

28.7.4 Shape Wrapper Module

As was stated earlier a polymorphic variable must be a pointer or allocatable variable. We have chosen to go the allocatable route. The following is a wrapper routine to allow us to have a derived type whose types can be polymorphic.

```

module shape_wrapper_module
    use shape_module
    use circle_module
    use rectangle_module
    type shape_wrapper

        class (shape_type), allocatable :: x
    end type shape_wrapper
end module shape_wrapper_module

```

So now `x` can be of `shape_type` or of any type derived from `shape_type`. Don't panic if this isn't clear at the moment, the complete program should help out!

28.7.5 Display Subroutine

This is the key subroutine in this example. We can pass into this routine an array of type `shape_wrapper`. In the code so far we have variables of type

- `shape_type`
- `circle_type`
- `rectangle_type`

and we are passing in an array of elements and each element can be of any of these types, i.e. the `shape_array` is polymorphic.

The next statement of interest is

```
call shape_array(i)%x%draw()
```

and at run time the correct `draw` method will be called. This is called dynamic binding. Here is the complete code.

```
module display_module

contains

subroutine display(n_shapes, shape_array)
use shape_wrapper_module
implicit none
integer, intent (in) :: n_shapes
type (shape_wrapper), dimension (n_shapes) &
:: shape_array
integer :: i

do i = 1, n_shapes
    call shape_array(i)%x%draw()
end do
end subroutine display

end module display_module
```

28.7.6 Test Program for Polymorphism and Dynamic Binding

We now have the complete program that illustrates polymorphism and dynamic binding in action.

```
program ch2805
use shape_module
use circle_module
use rectangle_module
use shape_wrapper_module
use display_module
implicit none
integer, parameter :: n = 6
integer :: i
type (shape_wrapper), dimension (n) :: s
s(1)%x = shape_type(10, 20)
```

```
s(2)%x = circle_type(100, 200, 300)
s(3)%x = rectangle_type(1000, 2000, 3000, &
    4000)
s(4)%x = s(1)%x
s(5)%x = s(2)%x
s(6)%x = s(3)%x
print *, ' calling display subroutine'
call display(n, s)
print *, ' select type with get methods'
do i = 1, n
    select type (t=>s(i)%x)
        class is (shape_type)
            print *, ' x = ', t%getx(), ' y = ', &
                t%gety()
        class is (circle_type)
            print *, ' x = ', t%getx(), ' y = ', &
                t%gety()
            print *, ' radius = ', t%getradius()
        class is (rectangle_type)
            print *, ' x = ', t%getx(), ' y = ', &
                t%gety()
            print *, ' height = ', t%getheight()
            print *, ' width = ', t%getwidth()
        class default
            print *, ' do nothing'
        end select
    end do
print *, ' select type with set methods'
do i = 1, n
    select type (t=>s(i)%x)
        class is (shape_type)
            call t%setx(19)
            call t%sety(19)
        class is (circle_type)
            call t%setx(199)
            call t%sety(199)
            call t%setradius(199)
        class is (rectangle_type)
            call t%setx(1999)
            call t%sety(1999)
            call t%setheight(1999)
            call t%setwidth(1999)
        class default
            print *, ' do nothing'
    end select
```

```

end do
print *, ' calling display subroutine'
call display(n, s)
end program ch2805

```

Let us look at the key statements in more detail.

```
type (shape_wrapper), dimension (n) :: s
```

This is the key declaration statement. *s* will be our polymorphic array. The following six assignment statements

```

s(1) %x = shape_type(10,20)
s(2) %x = circle_type(100,200,300)
s(3) %x = rectangle_type(1000,2000,3000,4000)
s(4) %x = s(1)%x
s(5) %x = s(2)%x
s(6) %x = s(3)%x

```

will call our own assignment subroutine to do the assignment. The allocation is hidden in the implementation. We then have

```
call display(n,s)
```

which calls the display subroutine. The compiler at run time works out which draw method to call depending of the type of the elements in the *shape_wrapper* array.

Imagine now adding another shape type, let us say a triangle. We need to do the following

- inherit from the base shape type
- add the additional data to define a triangle
- add the appropriate get and set methods
- add a draw triangle method
- add a use statement to the *shape_wrapper*_module
- add a use statement to the main program

and we now can work with the new triangle shape type. The display subroutine is unchanged! We can repeat the above steps for any additional shape type we want. Polymorphism and dynamic binding thus shorten our development and maintenance time, as it reduces the amount of code we need to write and test.

We then have an example of the use of the *select type* statement. The compiler determines the type of the elements in the array and then executes the matching block.

```

do i=1,n
  select type ( t=>s(i) %x )
    class is (shape_type)
      print *, ' x = ', t%getx(), ' y = ', t%gety()

```

```

class is (circle_type)
    print *, ' x =      ', t%getx(), ' y = ', t%gety()
    print *, ' radius = ', t%getradius()
class is (rectangle_type)
    print *, ' x =      ', t%getx(), ' y = ', t%gety()
    print *, ' height = ', t%getheight()
    print *, ' width =   ', t%getwidth()
class default
    print *, ' do nothing'
end select
end do

```

Now imagine adding support for the new triangle type. Anywhere we have `select type` constructs we have to add support for our new triangle shape. There is obviously more work involved when we use the `select type` construct in our polymorphic code. However some problems will be amenable to polymorphism and dynamic binding, others will require the explicit use of `select type` statements. This example illustrates the use of both.

28.8 Summary

This chapter has introduced some of the essentials of object oriented programming. The first example looked at object oriented programming as an extension of basic data structuring. We used type bound procedures to implement our shape class. We used methods to access the internal data of the shape object.

The second example looked at simple inheritance. We saw in this example how we could reuse the methods from the base class and also add new data and methods specific to the new shapes—circles and rectangles.

The third example then looked at how to achieve polymorphism in Fortran. We could then create arrays of our base type and dynamically bind the appropriate methods at run time. Dynamic binding is needed when multiple classes contain different implementations of the same method, i.e. to ensure in the following code

```
call shape_array(i) %x%draw()
```

that the correct draw method is invoked on the shape object.

28.9 Problems

28.1 Compile and run all of the examples in this chapter with your compiler.

28.2 Add a triangle type to the simple inheritance example.

28.3 Add a triangle type to the polymorphic example.

Further Reading

The following book

- Rouson, D., Xia, J., Xu, X.: Scientific Software Design: The Object Oriented Way. Cambridge University Press, Cambridge (2011)

uses Fortran throughout and is a very good coverage of what is possible in modern Fortran. Well worth a read.

The second edition of the following book

- Meyer, B.: Object Oriented Software Construction. Prentice Hall, Upper Saddle River (1997)

provides a very good coverage and uses Eiffel throughout—he did design the language!

Chapter 29

Introduction to Parallel Programming

'I don't know' said Alice. *'I lost count.'*

'She can't do addition,' the Red Queen interrupted.

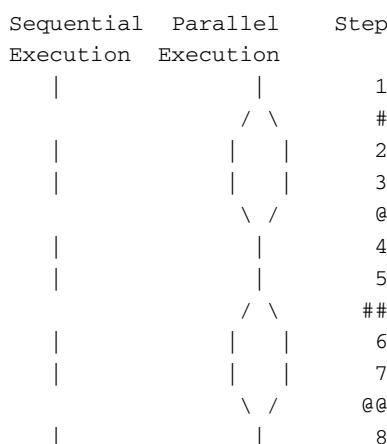
Lewis Carroll, Through the Looking Glass and What Alice Found There.

Aims

The aims of this chapter is to provide a short introduction to parallel programming.

29.1 Introduction

Parallel programming involves breaking a program down into parts that can be executed concurrently. Here is a simple diagram to illustrate the idea.



On the left hand side we have a sequential program and this steps through linearly from beginning to end. The right hand side has the same program that has been partially parallelised. There are two parallel regions and the work here is now shared between two processes or threads. At each parallel part of the program we have the following

	Parallel Region 1	Parallel Region 2
Set up cost	Step #	Step ##
Parallel section	Steps 2,3	Steps 6,7
Synchronisation cost	Step @	Step @@

The theory is that the overall run time of the program will have been reduced or we will have been able to solve a larger problem by parallelising our code. In the above example we have divided the work between two processes or threads. Here are some details of a range of processors which support multiple cores. Visit the AMD and Intel sites for up to date information.

Processor	Cores	Hyper Threading
AMD Phenom II X6	6	
Intel Core i7 920	4	* 2
Intel Core i7 2600K	4	* 2
AMD Opteron Shanghai	4	
Istanbul	6	
Magny Cours	8	
Magny Cours	12	
Intel E5-2697	12	* 2

Intel introduced hyperthreading technology in 2002. For each physical processor core the Intel chip has the operating system can see or address two virtual or logical cores, and can share the workload between them when possible. See the Wikipedia entry for more information.

<http://en.wikipedia.org/wiki/Hyper-threading>

There are several ways of doing parallel programming, and this chapter will look at three ways of doing this in Fortran. There are a common set of concepts and terminology that are useful to know about, whichever method we use, and we will cover these first.

29.2 Parallel Computing Classification

Parallel computing is often classified by the way the hardware supports parallelism. Two of the most common are:

- multi-processor and multi-core computers having multiple processing elements within a single system
- clusters or grids with multiple computers connected to work together.

Modern large systems are increasingly hybrids of the two above.

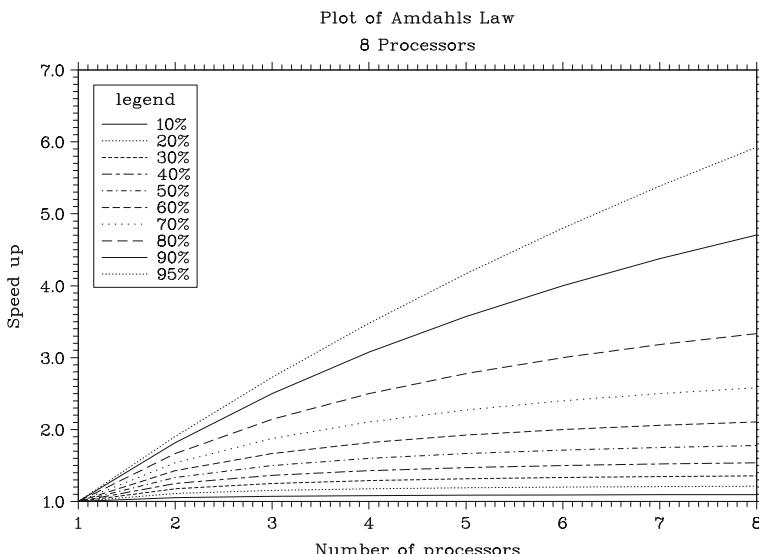
29.3 Amdahl's Law

Amdahl's law is a simple equation for the speedup of a program when parallelised. It assumes that the problem size remains the same when parallelised. In the equation below

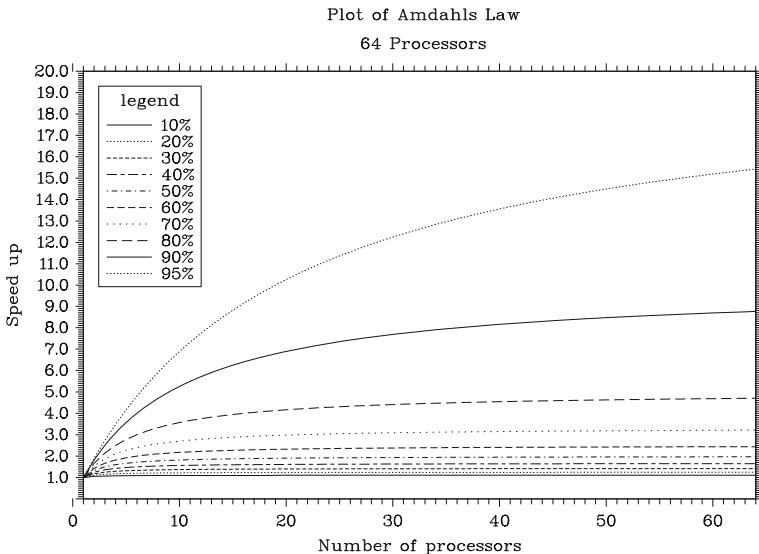
- P is the proportion of the program that can be parallelised
- $(1-P)$ is the serial proportion
- N is the number of processors
- speedup = $1/((1-P)+P/N)$

We have included a couple of graphs to illustrate the above. We have written programs that use the dislin graphics library to do the plots. More information on these programs can be found in Chap. 35, where we have a look at third party numeric and graphics libraries.

29.3.1 Amdahl's Law Graph 1–8 Processors or Cores



29.3.2 Amdahl's Law Graph 2–64 Processors or Cores



29.4 Gustafson's Law

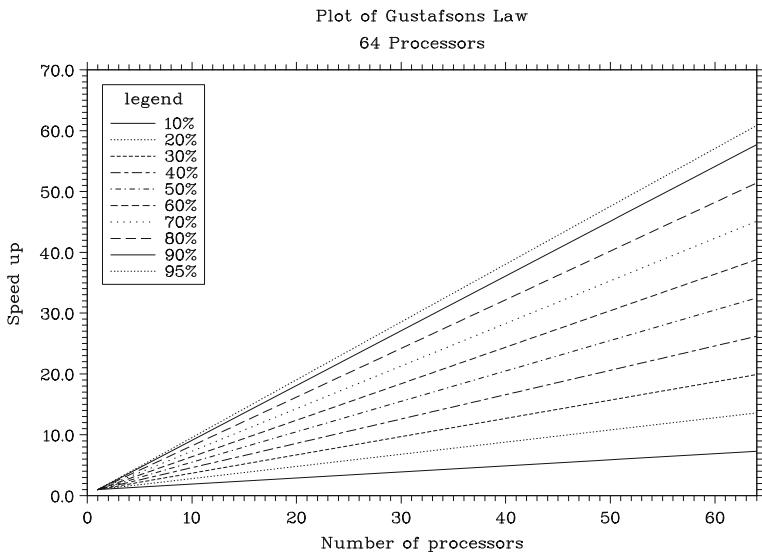
Gustafson's Law is often seen as a contradiction of Amdahl's Law. Simplistically it states that programmers solve larger problems when parallelising programs.

The equation for Gustafson's Law is given below.

- N is the number of processors
- Serial is the proportion that remains serial
- Speedup(N) = $N - \text{Serial} * (N - 1)$

We have again included a graph to illustrate the above.

29.4.1 Gustafson's Law Graph 1–64 Processors or Cores



29.5 Memory Access

Memory access times fall into two main categories that are of interest in parallel computing

- uma—uniform memory access. Each element of main memory can be accessed with the same latency and bandwidth. Multi-processor and multi-core computers typically have this behaviour.
- numa—non uniform memory access. Distributed memory systems have non-uniform memory access. Clusters or grids with multiple computers connected to work together have this behaviour.

29.6 Cache

Modern processors have a memory hierarchy. They typically have two or more levels:

- main memory
- CPU memory

and there is a speed and cost link. Main memory is cheap and relatively slow in comparison to the cpu memory.

The CPU memory or cache is used to reduce the effective access time to memory. If the information that the program requires is in the CPU cache then the average latency of memory accesses will be closer to the cache latency than to the latency of main memory. Getting high performance from a computer normally means writing cache friendly programs. This means that the data and instructions that the program needs are already in the cache and don't need to be accessed from the much slower main memory.

In a multi-core and multi-CPU system each core and CPU will have their own memory or cache. This introduces the problem of cache coherency—i.e. the consistency of data stored in local caches compared to the data in the common shared memory. This problem must obviously be addressed when doing parallel programming.

29.7 Bandwidth and Latency

Bandwidth is the rate at which data can be transferred. Latency is the start up time for a data transfer. We normally want a high bandwidth and low latency. Table 29.1 looks at some figures for several interconnects.

29.8 Flynn's Taxonomy

Flynn's taxonomy is an old, but still widely used, classification scheme for computer architecture.

- Single Instruction, Single Data stream (SISD) A sequential computer which exploits no parallelism in either the instruction or data streams. Term rarely used.
- Single Instruction, Multiple Data streams (SIMD) A computer which exploits multiple data streams against a single instruction stream to perform operations which may be naturally parallelised. For example, an array processor or GPU.
- Multiple Instruction, Single Data stream (MISD) Multiple instructions operate on a single data stream. Term rarely used.

Table 29.1 Bandwidth and latency

	MPI bandwidth or theoretical maximum (GB/s)	Latency (μs)
Gigabit ethernet	0.125	≈ 100
Infiniband	1.3	4.0
Myrinet 10-G	1.2	2.1
Quadrics QsNet II	0.9	2.7
Cray SeStar2	2.1	4.5

- Multiple Instruction, Multiple Data streams (MIMD) Multiple autonomous processors simultaneously executing different instructions on different data. Distributed systems are generally recognized to be MIMD architectures; either exploiting a single shared memory space or a distributed memory space. Essentially separate computers working together to solve a problem.

We also have the term

- Single Program Multiple Data—An identical program executes on a MIMD computer system. Conditional statements in the code mean that different parts of the program execute on each system.

29.9 Consistency Models

Parallel programming languages and parallel computers must have a consistency model (also known as a memory model). The consistency model defines rules for how operations on computer memory occur and how results are produced.

29.10 Threads and Threading

In computing a thread of execution is often regarded as the smallest unit of processing that can be scheduled by an operating system. The implementation of threads and processes generally varies with operating system.

29.11 Threads and Processes

From a strict computer science point of view threads and processes are different. However when looking simply at parallel programming the term can often be used interchangeably. In the following we use the term thread.

29.12 Data Dependencies

A data dependency is when one statement in a program depends on a calculation from a previous statement. This will obviously hinder parallelism.

29.13 Race Conditions

Race conditions can occur in programs when separate threads depend on a shared state or variable.

29.14 Mutual Exclusion-Mutex

A mutex is a programming construct that is used to allow multiple threads to share a resource. The sharing is not simultaneous. One thread will acquire the mutex and then lock the other threads from accessing it until it has completed.

29.15 Monitors

In concurrent programming, a monitor is an object or module intended to be used safely by more than one thread. The defining characteristic of a monitor is that its methods are executed with mutual exclusion. That is, at each point in time, at most one thread may be executing any of its methods. This mutual exclusion greatly simplifies reasoning about the implementation of monitors compared with code that may be executed in parallel.

29.16 Locks

In computing a lock is a synchronization mechanism for enforcing limits on access to a resource in an environment where there are many threads of execution. Locks are one way of enforcing concurrency control policies.

29.17 Synchronization

The concept of synchronisation is often split into process and data synchronisation.

In process synchronisation several processes or threads come together at a certain part of a program.

Data synchronisation is concerned with keeping data consistent.

29.18 Granularity and Types of Parallelism

Granularity is a useful concept in parallel programming. A common classification is

- Fine-grained—a lot of small components, larger amounts of communication and synchronisation
- Coarse-grained—a small number of larger components, hence smaller amounts of communication and less synchronisation

The terms are of course relative.

We also have the concept of

- Embarrassingly parallel—very little effort is required to partition the task and there is little or no communication and synchronisation.

A simple example of this would be a graphics processor processing individual pixels.

29.19 Partitioned Global Address Space—PGAS

PGAS is a parallel programming model. It assumes a global memory address space that is logically partitioned and a portion of it is local to each processor. The PGAS model is the basis of Unified Parallel C, Coarray Fortran, Titanium, Fortress, Chapel and X10.

29.20 Fortran and Parallel Programming

Most Fortran compilers now offer support for parallel programming. We next provide a brief coverage of three methods

- MPI—Message Passing Interface
- OpenMP—Open Multi-Processing
- CoArray Fortran

Subsequent chapters look at simple examples using each method.

29.21 MPI

MPI started with a meeting that was held at the Supercomputing 92 conference. The attendants agreed to develop and implement a common standard for message passing.

The first MPI standard, called MPI-1 was completed in May 1994. The second MPI standard, MPI-2, was completed in 1998.

MPI is effectively a library of C and Fortran callable routines. It has become widely used and is available on a number of platforms. Some useful web addresses are given below. The first is hosted at Argonne National Laboratory.

<http://www.mcs.anl.gov/research/projects/mpi/>

MPI was designed by a broad group of parallel computer users, vendors, and software writers. These included

- Vendors—IBM, Intel, TMC, Meiko, Cray, Convex, Ncube
- Library writers—PVM, p4, Zipcode, TCGMSG, Chameleon, Express, Linda
- Companies—ARCO, Convex, Cray Research, IBM, Intel, KAI, Meiko, NAG, nCUBE, Parasoft, Shell, TMC
- Laboratories—ANL, GMD, LANL, LLNL, NOAA, NSF, ORNL, PNL, Sandia, SDSC, SRC
- Universities—UC Santa Barbara, Syracuse University, Michigan State University, Oregon Grad Inst, University of New Mexico, Mississippi State University, University of Southampton, University of Colorado, Yale University, University of Tennessee, University of Maryland, Western Michigan University, University of Edinburgh, Cornell University, Rice University, University of San Francisco

So whilst MPI is not a formal standard like Fortran, C or C++, its development has involved quite a wide range of people. The following site has details of MPI meetings.

<http://meetings mpi-forum.org/>

The steering committee (March 2015) and affiliations are given below

- Jack Dongarra—Computer Science Department, University of Tennessee
- Al Geist—Group Leader, Computer Science Research Group, Oak Ridge National Laboratory
- Richard Graham
- Bill Gropp—Computer Science Department, University of Illinois Urbana-Champaign
- Andrew Lumsdaine—Computer Science Department, Indiana University
- Ewing Lusk—Mathematics and Computer Science Division, Argonne National Laboratory
- Rolf Rabenseifner—High Performance Computing Center, Germany

Another useful site is the Open MPI site.

<http://www.open-mpi.org/>

The following is taken from their site.

The Open MPI Project is an open source MPI implementation that is developed and maintained by a consortium of academic, research, and industry partners. Open MPI is therefore able to combine the expertise, technologies, and resources from all across the High Performance Computing community in order to build the best MPI library available. Open MPI offers advantages for system and software vendors, application developers and computer science researchers.

Both sites provide free downloadable implementations. Commercial implementations are available from

- Cray
- IBM
- Intel
- Microsoft

amongst others.

MPI is, at the time of writing, the dominant parallel programming method used in Fortran. MPI and Fortran currently account for over 80 % of the code running on the Archer Service in Edinburgh. Archer is the UK's national supercomputing resource, funded by the UK Research Councils. Visit

<http://www.archer.ac.uk>

for more information.

29.22 OpenMP

OpenMP (Open Multi-Processing) is an application programming interface that supports shared memory multiprocessing programming in three main languages (C, C++, and Fortran) on a range of hardware platforms and operating systems. It consists of a set of compiler directives, library routines, and environment variables that determine the run time behaviour of a program.

The OpenMP Architecture Review Board (ARB) has published several versions

- October 1997—OpenMP for Fortran 1.0. October the following year they released the C/C++ standard.
- 2000—Fortran version
- 2005—Fortran 2.5
- 2008—OpenMP 3.0. Included in the new features in 3.0 is the concept of tasks and the task construct.
- 2011—OpenMP 3.1
- 2013—OpenMP 4.0 was released in July 2013

A number of compilers from various vendors or open source communities implement the OpenMP API, including

- Absoft
- Cray
- gnu
- Hewlett Packard
- IBM
- Intel
- Lahey/Fujitsu
- Nag
- Oracle/Sun
- PGI

The main OpenMP web site is:

<http://www.openmp.org/>

29.23 Coarray Fortran

Coarrays became part of Fortran in the 2008 standard. The original ideas came from work by Robert Numrich and John Reid in the 1990s. They are based on a single program multiple data model. A coarray Fortran program is interpreted as if it were duplicated several times and all copies execute asynchronously. Each copy has its own set of data objects and is termed an image. The array syntax of Fortran is extended with additional trailing subscripts in square brackets to provide a concise representation of references to data that is spread across images.

The syntax is architecture independent and may be implemented on:

- Distributed memory machines.
- Shared memory machines.
- Clustered machines.

Work is underway for additional Coarray functionality for the next standard.

29.24 Other Parallel Options

There are a number of additional parallel methods. They are covered for completeness.

29.24.1 PVM

Parallel Virtual Machine consists of a library and a run-time environment which allow the distribution of a program over a network of (even heterogeneous) computers. Visit

- <http://www.epm.ornl.gov/pvm/>
- <http://www.netlib.org/pvm3/>

for more details.

29.24.2 HPF

To quote their home page

<http://hpff.rice.edu/index.htm>

'The High Performance Fortran Forum (HPFF), a coalition of industry, academic and laboratory representatives, works to define a set of extensions to Fortran 90 known collectively as High Performance Fortran (HPF). HPF extensions provide access to high-performance architecture features while maintaining portability across platforms.'

They also provide details of:

- Surveys of HPF compilers and tools.
- Currently available commercial HPF compilers.
- public domain HPF compilation systems.
- Research prototypes of HPF and HPF-related compilation systems.
- Mailing list.

29.25 Top 500 Supercomputers

Have a look at

<http://www.top500.org/>

for a lot of links to supercomputing centres and information on parallel computing in general. To see what can be done with all this processing power visit:

<http://www.met-office.gov.uk/>

29.26 Summary

Fortran has long been one of the main languages used in parallel programming. This chapter has provided a brief coverage of some of the background to parallel programming in general, and Fortran in particular.

In the next three chapters we will look at a small number of programs that introduce some of the basic syntax of parallel programming with MPI, OpenMP and Coarray Fortran. We will also look at solving one problem serially and then solve it using the parallel features provided by MPI, OpenMP and Coarray Fortran. We provide timing details so that we can see the benefits that parallel solutions offer.

Bibliography

The ideas involved in parallel computing are not new and we've included a couple of references about computer hardware and operating systems, which provide information for the more inquisitive reader. Wikipedia is an on-line source of information in this area.

Up to date hardware information can be found at most hardware vendor sites. Here are the web sites for AMD, IBM and Intel.

AMD
<http://developer.amd.com/pages/default.aspx>
IBM
<http://www.ibm.com/products/us/en/>
Intel
[http://www.intel.com/en_UK/
products/processor/index.htm](http://www.intel.com/en_UK/products/processor/index.htm)

Baer JL, Computer Systems Architecture, Computer Science Press (1980)

The chapters on the memory hierarchy and memory management are old, but well written.

Deitel HM, Operating Systems, Addison Wesley (1990).

Part two of the book (process management) has chapters on process concepts, asynchronous concurrent processes, concurrent programming and deadlock and indefinite postponement. The bibliographies at the end of each chapter are quite extensive.

The following four books provide a good coverage of the essentials of MPI and OpenMP.

Chandra R, Dagum L, Kohr D, Maydan D, McDonald J, Menon R, Parallel Programming in OpenMP, Morgan Kaufmann.

Chapman B, Jost G, Van Der Pas R, Using OpenMP, MIT Press.

Gropp W, Lusk E, Skjellum A, Using MPI: Portable Parallel Programming with the Message Passing Interface, MIT Press.

Pacheco P, Parallel Programming with MPI, Morgan Kaufmann.

Chapter 30

MPI—Message Passing Interface

In almost every computation a great variety of arrangements for the succession of the processes is possible, and various considerations must influence the selections amongst them for the purposes of a calculating engine. One essential object is to choose that arrangement which shall tend to reduce to a minimum the time necessary for completing the calculation.

Ada Lovelace

Aim

The aims of this chapter is to provide a short introduction to MPI programming in Fortran.

30.1 Introduction

Documents for the MPI standard are available from the MPI Forum. Their web address is

<http://www.mpi-forum.org>

If you are going to do MPI programming we recommend getting hold of the document that refers to your implementation.

30.2 MPI Programming

MPI programming typically requires two components, a compiler and an MPI implementation. Two common ways of doing MPI programming are

- a cluster or multiple systems running MPI
- a single system running MPI

In both cases an MPI installation will normally provide an MPI daemon or service that can then be called from an MPI program.

30.3 Compiler and Implementation Combination

A number of commercial companies provide a combined bundle including

- Cray
- IBM
- Intel
- PGI

The Cray and IBM offerings will most likely be for a cluster. Intel and PGI provide products for both clusters and single systems. You should check their sites for up to date information.

30.4 Individual Implementation

A low cost option is to get hold of an MPI implementation that works with your existing compiler, and install it yourself on your own system.

The Intel MPI product is available as a free download for evaluation purposes.

There are a number of free MPI implementations, and details are given below for two of them.

30.4.1 MPICH2

They are based at Argonne National Laboratory

<http://www.mcs.anl.gov/research/projects/mpich2/>

MPICH2 is distributed as source (with an open-source, freely available license). It has been tested on several platforms, including Linux (on IA32 and x86-64), Mac OS/X (PowerPC and Intel), Solaris (32- and 64-bit), and Windows.

30.4.2 Open MPI

They can be found at

<http://www.open-mpi.org/>

They develop Open MPI on Linux, OS X, Solaris (both 32 and 64 on all platforms) and Windows (Windows XP, Windows HPC Server 2003/2008 and also Windows 7 RC).

30.5 Compiler and MPI Combinations Used in the Book

We have used a variety of compilers and MPI combinations, including

- Intel compiler + mpich2, Windows
- Intel compiler + Intel MPI, Windows
- gfortran + openmpi, openSuSe Linux
- Cray compiler, Hector Service
- Cray compiler, Archer Service
- PGI compiler, Hector Service
- IBM compiler, Met Office Slovakia

We haven't tried out all of the examples with all of the compiler and MPI implementations.

30.5.1 Cray Archer System

The Archer hardware consists of the Cray XC30 MPP supercomputer, external login nodes and postprocessing nodes, and the associated filesystems. There are 4920 compute nodes in Archer phase 2 and each compute node has two 12-core Intel Ivy Bridge Xeon series processors (2.7 GHz Intel E5-2697) giving a total of 118,080 processing cores. Each node has a total of 64 GB of memory with a subset of large memory nodes having 128 GB. A high-performance Lustre storage system is available to all compute nodes. There is no local disk on the compute nodes as they are housed in 4-node blades (the image below shows an XC30 blade with 4 compute nodes).

30.6 The MPI Memory Model

MPI is characterised generally by distributed memory and

- All threads/processes have access to their own private memory only
- Data transfer and most synchronization has to be programmed explicitly
- All data is private
- Data is shared explicitly by exchanging buffers in MPI terminology

but in this chapter we will also show the use of MPI on one system.

30.7 Example: 1—Hello World

The first example is the classic hello world program.

```
program ch3001
use mpi
implicit none
integer :: error_number
integer :: this_process_number
integer :: number_of_processes

call mpi_init(error_number)
call mpi_comm_size(MPI_COMM_WORLD, &
    number_of_processes, error_number)
call mpi_comm_rank(MPI_COMM_WORLD, &
    this_process_number, error_number)
print *, 'Hello from process ', &
    this_process_number, ' of ', &
    number_of_processes, 'processes!'
call mpi_finalize(error_number)
end program ch3001
```

Let us look at each statement in turn.

```
use mpi
```

With most modern MPI implementations we can make available the MPI setup with a `use` statement. Older implementations required an include file option.

```
call mpi_init( error_number )
```

This must be the first MPI routine called. The Fortran binding only takes one argument, an integer variable that is used to return an `error_number`. It sets up the MPI environment.

```
call mpi_comm_size( MPI_COMM_WORLD, &
    number_of_processes , error_number )
```

is typically the second MPI routine called. All MPI communication is associated with a so called communicator that describes the communication context and an associated set of processes. In this simple example we use the default communicator, called `mpi_comm_world`. The number of processes available is returned via the second argument. This means that the above program is duplicated on each process, i.e. `number_of_processes` determines how many copies are running.

```
call mpi_comm_rank( mpi_comm_world, &
    this_process_number , error_number )
```

The call above returns the process number for this process or copy of the program.

```
print *, " Hello from process " , &
    this_process_number , " of " , &
    number_of_processes , " processes!"
```

Each copy of the program will print out this message.

```
call mpi_finalize(error_number)
```

The call to `mpi_finalize` is the last call to the MPI system we need to make. Here is the output from the Intel compiler and Intel MPI option under a Windows system.

```
mpiexec -n 8 ch3001
Hello from process      0  of      8  processes!
Hello from process      4  of      8  processes!
Hello from process      1  of      8  processes!
Hello from process      5  of      8  processes!
Hello from process      7  of      8  processes!
Hello from process      6  of      8  processes!
Hello from process      3  of      8  processes!
Hello from process      2  of      8  processes!
```

Notice that process numbering starts at 0. Note also that there is no particular order to the process numbers.

Here is the output from gfortran and openmpi on a openSuSe system. This is the same system as the above, as it is dual boot.

```
mpiexec -n 8 ch3001.out
Hello from process      0  of      8  processes!
Hello from process      1  of      8  processes!
Hello from process      2  of      8  processes!
Hello from process      3  of      8  processes!
Hello from process      4  of      8  processes!
Hello from process      5  of      8  processes!
Hello from process      6  of      8  processes!
Hello from process      7  of      8  processes!
```

Now the ordering is sequential.

Here is the output from the Cray Archer service. This uses 48 processes. The job is submitted as a batch job, via a queueing mechanism. This is a common mechanism on larger multi user systems.

```
Hello from process  1  of  48 processes!
Hello from process 11  of  48 processes!
Hello from process  6  of  48 processes!
Hello from process  7  of  48 processes!
...
Lines deleted
Hello from process 41  of  48 processes!
Hello from process 43  of  48 processes!
Hello from process 40  of  48 processes!
Hello from process 47  of  48 processes!
```

The order appears to be pretty random!

30.8 Example: 2—Hello World Using Send and Receive

The following is a variation of the above. In the first example we had no communication between processes. Sending and receiving of messages by processes is the basic MPI communication mechanism. The basic point-to-point communication operations are send and receive. Their use is shown in the example below. These are blocking send and receive operations. A blocking send does not return until the message data and envelope have been safely stored away so that the sender is free to modify the send buffer. The message might be copied directly into the matching receive buffer, or it might be copied into a temporary system buffer.

In this example process 0 is the master process and this communicates with every other process or program.

```
program ch3002
use mpi
implicit none
integer :: error_number
integer :: this_process_number
integer :: number_of_processes
integer :: i
integer, dimension (mpi_status_size) :: status

call mpi_init(error_number)
call mpi_comm_size(mpi_comm_world, &
    number_of_processes, error_number)
call mpi_comm_rank(mpi_comm_world, &
```

```

    this_process_number, error_number)
if (this_process_number==0) then
  print *, ' Hello from process ', &
    this_process_number, ' of ', &
    number_of_processes, 'processes.'
  do i = 1, number_of_processes - 1
    call mpi_recv(this_process_number, 1, &
      mpi_integer, i, 1, mpi_comm_world, &
      status, error_number)
    print *, ' Hello from process ', &
      this_process_number, ' of ', &
      number_of_processes, 'processes.'
  end do
else
  call mpi_send(this_process_number, 1, &
    mpi_integer, 0, 1, mpi_comm_world, &
    error_number)
end if
call mpi_finalize(error_number)
end program ch3002

```

The calls to

- mpi_init
- mpi_comm_size
- mpi_comm_rank
- mpi_finalize

are the same as in the first example. We have the additional code.

- A test to see if we are process 0. If we are we then print out a message saying that we are process 0. We next loop from 1 to number_of_processes -1 and call mpi_recv.
- If we are not process 0 we make a call to mpi_send—remember that the program executes on all processes.

Let us look at the calls to mpi_recv and mpi_send in more depth. Here is an extract from the MPI 2.2 specification describing mpi_recv

```

<> buf(*)
    initial address of receive buffer
integer count
    number of elements in the receive buffer
datatype
    data type of each receive buffer element
source - rank of source

```

```

tag - message tag
comm - communicator
status(MPI_STATUS_SIZE),
ierror

```

The following shows the mapping between MPI data types and Fortran data types.

mpi datatype	fortran datatype
mpi_integer	integer
mpi_real	real
mpi_double_precision	double precision
mpi_complex	complex
mpi_logical	logical
mpi_character	character(1)

our arguments to mpi_recv are

- this_process_number—process 0 is doing the receiving
- 1 item
- mpi_integer—an mpi_integer variable
- i—receive from this process
- 1—tag
- mpi_comm_world—the communicator
- status—an integer array of size mpi_status_size
- error_number

Here is an extract from the 2.2 specification regarding mpi_send

```

<> buf(*) - initial address of send buffer
integer count - number of elements in send buffer
datatype - data type of each send buffer element
dest - rank of destination
tag - message tag
comm - communicator
ierror - error number

```

the arguments to our mpi_send are

- this_process_number—send from this process
- 1
- mpi_integer
- 0—send to this process number
- 1
- mpi_comm_world—the communicator
- error_number

and as you can see the sends and receives are in matching pairs.
Here is an Intel sample run.

```
Hello from process 0 of 8 processes.
Hello from process 1 of 8 processes.
Hello from process 2 of 8 processes.
Hello from process 3 of 8 processes.
Hello from process 4 of 8 processes.
Hello from process 5 of 8 processes.
Hello from process 6 of 8 processes.
Hello from process 7 of 8 processes.
```

Here is a Cray Archer sample run.

```
Hello from process 0 of 48 processes.
Hello from process 1 of 48 processes.
Hello from process 2 of 48 processes.
Hello from process 3 of 48 processes.
Hello from process 4 of 48 processes.
```

lines deleted

```
Hello from process 43 of 48 processes.
Hello from process 44 of 48 processes.
Hello from process 45 of 48 processes.
Hello from process 46 of 48 processes.
Hello from process 47 of 48 processes.
```

30.9 Example: 3—Serial Solution for Pi Calculation

We choose numerical integration in this example. The following integral

$$\int_0^1 \frac{4}{1+x^2} dx$$

is one way of calculating an approximation to π , and is a problem that is easy to parallelise. The integral can be approximated by

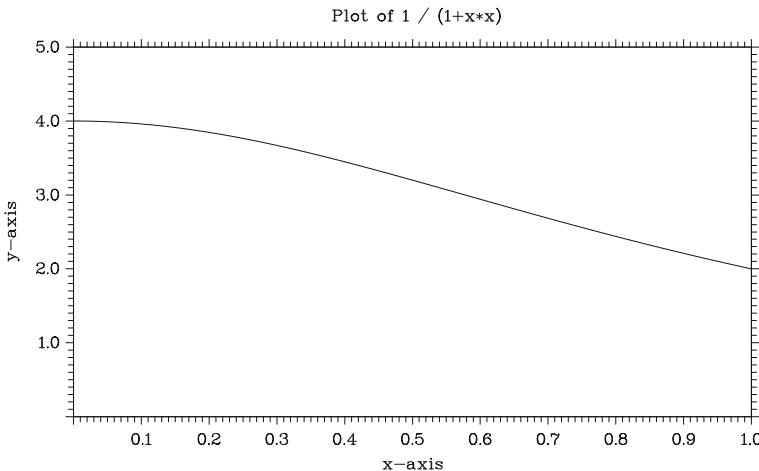
$$1/n \sum_1^n \frac{4}{1 + \left(\frac{i-0.5}{n}\right)^2}$$

According to Wikipedia π to 50 digits is

3.14159265358979323846264338327950288419716939937510

Another way of calculating π is using the formula $4 \tan^{-1}(1)$ and in Fortran this is $4.0 * \text{atan}(1.0)$.

Consider the following plot of the above equation.



To do the evaluation numerically we divide the interval between 0 and 1 into n sub intervals. The higher the value of n the more accurate our value of π will be, or should be.

Here is a serial program to do this calculation. The program is in three main parts. These are

- The module `precision_module`—to set the precision throughout the whole code.
- The module `timing_module`—a timing module to enable us to time parts of the program. We will be using this module throughout the parallel examples to provide information about the performance of the algorithms.
- the program—that actually does the integration.

The first two modules are straightforward and we will only cover the integration solution in depth. We will be using this integration example in this chapter on MPI and the subsequent two on OpenMP and coarray Fortran.

```

include 'precision_module.f90'

include 'timing_module.f90'

program ch3003
use precision_module
use timing_module

```

```
implicit none
integer :: i, j
integer :: n_intervals
real (dp) :: interval_width, x, total, pi
real (dp) :: fortran_internal_pi

call start_timing()
n_intervals = 1000000
fortran_internal_pi = 4.0_dp*atan(1.0_dp)
print *, ' fortran_internal_pi = ', &
fortran_internal_pi
print *, ''
do j = 1, 4
interval_width = 1.0_dp/n_intervals
total = 0.0_dp
do i = 1, n_intervals
x = interval_width*(real(i,dp)-0.5_dp)
total = total + f(x)
end do
pi = interval_width*total
print 100, n_intervals, time_difference()
print 110, pi, abs(pi-fortran_internal_pi)
n_intervals = n_intervals*10
end do
100 format (' N intervals = ', i12, ' time = ', &
f8.3)
110 format (' pi = ', f20.16, /, &
' difference = ', f20.16)
call end_timing()
stop

contains

real (dp) function f(x)
implicit none
real (dp), intent (in) :: x

f = 4.0_dp/(1.0_dp+x*x)
end function f

end program ch3003
```

The first part of the code has the declarations for the variables we will be using. These are

```
integer :: n_intervals
real (dp) :: interval_width, x, total, pi
real (dp) :: fortran_internal_pi
```

We have an integer variable for the number of intervals we will be using. We have made this of default integer type, which will be 32 bit on most platforms, and will be up to 2,147,483,647.

We then have the following variables

- `interval_width`
- `z`—the variable we will be calculating numerically
- `total`—our total for the integration
- `pi`—our calculated value of π
- `fortran_internal_pi`—we use a common way of defining this using the internal `atan` function.

We then call the `start_timing` routine to print out details of the start time.

We next set the number of intervals. We choose 10 as an initial value. We will be doing the calculation for a number of interval sizes.

We calculate π using the `atan` intrinsic and print out its value. We will be using this value to determine the accuracy of our calculations.

We then have the loop that does the calculations for 9 values of the interval size from 10 to 1,000,000,000.

We calculate the interval width at the start of each loop and reset the total to zero at the start of each loop.

The following

```
do i = 1, n_intervals
    x = interval_width*(real(i, dp)-0.5_dp)
    total = total + f(x)
end do
```

is the code that actually does the integration. We calculate `x` each time round the loop and then use this calculated value in our call to our function, summing up as we go along. We need to subtract `a` as we need the mid point of the interval for our value of `x`.

The loop finishes and we then calculate the value of π and print out details of the number of intervals, the calculated value of `pi` and the difference between the internal value of π and the calculated value.

We also print out timing information about this calculation. We then increment the number of intervals and repeat the above.

We need to know how long the serial version takes and how accurate our calculated value for π is.

Here is output from this program on a couple of systems and compilers.

Compiler 1—Intel compiler, Windows

```
2015/ 3/12 13:16:55 739
fortran_internal_pi = 3.14159265358979

N intervals = 1000000 time = 0.000
pi = 3.1415926535899033
difference = 0.0000000000001101
N intervals = 10000000 time = 0.031
pi = 3.1415926535896861
difference = 0.0000000000001070
N intervals = 100000000 time = 0.281
pi = 3.1415926535902168
difference = 0.0000000000004237
N intervals = 1000000000 time = 2.871
pi = 3.1415926535897682
difference = 0.000000000000249
2015/ 3/12 13:16:58 922
```

Compiler 2—gfortran, Windows

```
2015/ 3/12 15:14:42 110
fortran_internal_pi = 3.1415926535897931

N intervals = 1000000 time = 0.016
pi = 3.1415926535899601
difference = 0.0000000000001670
N intervals = 10000000 time = 0.016
pi = 3.1415926535897216
difference = 0.000000000000715
N intervals = 100000000 time = 0.281
pi = 3.1415926535900236
difference = 0.0000000000002305
N intervals = 1000000000 time = 2.793
pi = 3.1415926535896523
difference = 0.0000000000001408
2015/ 3/12 15:14:45 214
```

Compiler 3—Cray, Archer Service. Hardware details of this system are given earlier.

```
sntp1553@eslogin008:~> ./ch3003.x
2015/ 3/22 11:42: 5 50
fortran_internal_pi = 3.1415926535897931
```

```

N intervals =      1000000 time =      0.000
pi =    3.1415926535899033
difference =  0.0000000000001101
N intervals =      10000000 time =      0.023
pi =    3.1415926535896861
difference =  0.0000000000001070
N intervals =     100000000 time =      0.207
pi =    3.1415926535902168
difference =  0.0000000000004237
N intervals =    1000000000 time =      2.074
pi =    3.1415926535897682
difference =  0.000000000000249
2015/ 3/22 11:42: 7 356
STOP

```

The three sample serial runs provide us with information that we can use as a basis for an analysis of our parallel solution. We have information about the accuracy of the solution and timing details.

30.10 Example: 4—Parallel Solution for Pi Calculation

This example is a parallel solution to the above problem using MPI. We only show the parallel program. The precision and timing modules are the same as in the previous example.

```

include 'precision_module.f90'

include 'timing_module.f90'

program ch3004
use precision_module
use timing_module
use mpi
implicit none
real (dp) :: fortran_internal_pi
real (dp) :: partial_pi
real (dp) :: total_pi
real (dp) :: width
real (dp) :: partial_sum
real (dp) :: x
integer :: n
integer :: this_process
integer :: n_processes

```

```
integer :: i
integer :: j
integer :: error_number

call mpi_init(error_number)
call mpi_comm_size(MPI_COMM_WORLD, &
    n_processes, error_number)
call mpi_comm_rank(MPI_COMM_WORLD, &
    this_process, error_number)
n = 100000
fortran_internal_pi = 4.0_dp*atan(1.0_dp)
if (this_process==0) then
    call start_timing()
    print *, ' fortran_internal_pi = ', &
        fortran_internal_pi
end if
do j = 1, 5
    width = 1.0_dp/n
    partial_sum = 0.0_dp
    do i = this_process + 1, n, n_processes
        x = width*(real(i,dp)-0.5_dp)
        partial_sum = partial_sum + f(x)
    end do
    partial_pi = width*partial_sum
    call mpi_reduce(partial_pi, total_pi, 1, &
        MPI_DOUBLE_PRECISION, MPI_SUM, 0, &
        MPI_COMM_WORLD, error_number)
    if (this_process==0) then
        print 100, n, time_difference()
        print 110, total_pi, abs(total_pi- &
            fortran_internal_pi)
    end if
    n = n*10
end do
call mpi_finalize(error_number)
100 format (' N intervals = ', i12, ' time = ', &
    f8.3)
110 format (' pi = ', f20.16, ', &
    ' difference = ', f20.16)
```

contains

```
real (dp) function f(x)
implicit none
real (dp), intent (in) :: x
```

```

f = 4.0_dp/(1.0_dp+x*x)
end function f

end program ch3004

```

The first difference is the

```
use mpi
```

statement. This makes available the MPI functionality. We next have several variable declarations.

```

real (dp) :: fortran_internal_pi
real (dp) :: partial_pi
real (dp) :: total_pi
real (dp) :: width
real (dp) :: partial_sum
real (dp) :: x
integer :: n
integer :: this_process
integer :: n_processes
integer :: i
integer :: j
integer :: error_number

```

The variables `partial_pi`, `total_pi` and `partial_sum` are required by our parallel algorithm. The variable `n` is the number of intervals and we start this at 100,000 rather than 10 as we have seen from the serial solution that there are quite large differences between the internal value of pi and the calculated value below 100,000.

The variables `this_process`, `n_processes` and `error_number` are required for the MPI solution.

The real work is done in the following do loop.

```

do i = this_process + 1, n, n_processes
  x = width*(real(i,dp)-0.5_dp)
  partial_sum = partial_sum + f(x)
end do

```

The key is to split up the work of the calculation between the processes we have available. The following shows how the work will be split up for `n = 10` and with the number of processes ranging from 1 to 8.

```

n_processes=1 do i=1,n,1  1,2,3,4,5,6,7,8,9,10
n_processes=2 do i=1,n,2  1,3,5,7,9
    do i=2,n,2  2,4,6,8,10
n_processes=4 do i=1,n,4  1,5,9
    do i=2,n,4  2,6,10
    do i=3,n,5  3,7
    do i=4,n,4  4,8
n_processes=8 do i=1,n,8  1,9
    do i=2,n,8  2,10
    do i=3,n,8  3
    do i=4,n,8  4
    do i=5,n,8  5
    do i=6,n,8  6
    do i=7,n,8  7
    do i=8,n,8  8

```

The above also shows how the algorithm balances the load of the computation across the processes.

Each process has its own `partial_sum` and `partial_pi`. We then use the call to the MPI subroutine `mpi_reduce` to calculate the total value of pi from the partial values of pi. Here is the MPI description of the `mpi_reduce` routine

```

MPI_REDUCE( sendbuf, recvbuf, count,
            datatype, op, root, comm)
IN  sendbuf address of send buffer (choice)
OUT recvbuf address of receive buffer
    (choice, significant only at root)
IN  count number of elements in send buffer
    (non-negative integer)
IN  datatype data type of elements of send buffer
    (handle)
IN  op reduce operation (handle)
IN  root rank of root process (integer)
IN  comm communicator (handle)

```

and

```

partial_pi is our send buffer
total_pi is our receive buffer
1 - the number of elements
mpi_double_precision - the type of the elements
mpi_sum - the reduction operation
0 - the root process
mpi_comm_world - the communicator
error_number - the error number

```

We then control the printing from process 0.

Here is sample output from the Intel compiler on a 6 core AMD system.

```
mpiexec -n 6 ch3004.exe
2015/ 3/12 13:16:39 671
fortran_internal_pi = 3.14159265358979
N intervals = 100000 time = 0.000
pi = 3.1415926535981256
difference = 0.00000000000083324
N intervals = 1000000 time = 0.000
pi = 3.1415926535898762
difference = 0.0000000000000830
N intervals = 10000000 time = 0.000
pi = 3.1415926535897674
difference = 0.0000000000000258
N intervals = 100000000 time = 0.062
pi = 3.1415926535897389
difference = 0.0000000000000542
N intervals = 1000000000 time = 0.637
pi = 3.1415926535898402
difference = 0.0000000000000471
```

We get a nearly linear speed up over the serial version, which shows how good the parallel solution is. Note that the time value is not the total time taken by all processes, but rather the effective running time of the program. If we are sat in front of the pc the program would complete in about a quarter of the time of the serial version. The numerical results are similar to the serial solution.

Table 30.1 summarises the output from the Intel compiler on an Intel I7 system. The table has the execution time details when running the program on 1–8 cores. The timing for cores 1–4 are for the program runs on real physical cores. The timing for cores 5–8 are when running on hyperthreaded cores. The execution time is worse when running on 5–7 cores. You should time your programs on hyperthreaded systems to see if running on the extra cores brings any benefit.

Table 30.1 Intel I7 with hyperthreading

Intervals	Cores							
	1	2	3	4	5	6	7	8
100,000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1,000,000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
10,000,000	0.016	0.016	0.012	0.000	0.016	0.000	0.000	0.016
100,000,000	0.234	0.109	0.078	0.062	0.094	0.094	0.078	0.062
1,000,000,000	2.203	1.141	0.816	0.609	0.984	0.812	0.703	0.594

As can be seen the performance for 5–8 cores is similar to that for 4 cores. Cores 5–8 represent the hyperthreaded cores.

Here is the output from the Cray at the Archer service. This is for 48 processes running on 2 nodes.

```
2015/ 3/21 1:11:47 841
  fortran_internal_pi = 3.1415926535897931
N intervals =      1000000 time =      0.004
pi = 3.141592653589757
difference = 0.0000000000000826
N intervals =      10000000 time =      0.000
pi = 3.1415926535897958
difference = 0.0000000000000027
N intervals =      100000000 time =      0.006
pi = 3.1415926535897909
difference = 0.0000000000000022
N intervals =      1000000000 time =      0.054
pi = 3.1415926535897949
difference = 0.0000000000000018
```

30.11 Example: 5—Work Sharing Between Processes

This example looks at one way of splitting work up between processes. We use the process number of determine which process does which work.

```
program ch3005
  use mpi
  implicit none
  integer :: error_number
  integer :: this_process_number
  integer :: number_of_processes
  integer, dimension (mpi_status_size) :: status
  integer, allocatable, dimension(:) :: x
  integer :: n
  integer, parameter :: factor = 5
  integer :: i, j, k
  integer :: start
  integer :: end
  integer :: recv_start

  call mpi_init(error_number)
  call mpi_comm_size(mpi_comm_world, &
```

```

        number_of_processes, error_number)
call mpi_comm_rank(mpi_comm_world, &
    this_process_number, error_number)
n = number_of_processes*factor
allocate (x(1:n))
x = 0
start = (factor*this_process_number) + 1
end = factor*(this_process_number+1)
print 100, this_process_number, start, end
do i = start, end
    x(i) = i*factor
end do
do i = 1, n
    print 110, this_process_number, i, x(i)
end do
if (this_process_number==0) then
    do i = 1, number_of_processes - 1
        recv_start = (factor*i) + 1
        call mpi_recv(x(recv_start), factor, &
            mpi_integer, i, 1, mpi_comm_world, &
            status, error_number)
    end do
else
    call mpi_send(x(start), factor, mpi_integer, &
        0, 1, mpi_comm_world, error_number)
end if
if (this_process_number==0) then
    do i = 1, n
        print 120, i, factor, x(i)
    end do
end if
call mpi_finalize(error_number)
100 format (' Process number = ', i3, ' start ', &
    i3, ' end ', i3)
110 format (1x, i4, ' i ', i4, ' x(i) ', i4)
120 format (1x, i4, ' * ', i2, ' = ', i5)
end program ch3005

```

What we are going to do is allocate an array based on the number of processes and then split the (simple) work on the array up between the processes. We will calculate array indices from the process numbers.

```
n = number_of_processes*factor
```

This statement calculates the array size based on the number of processes and a constant factor.

```
allocate (x(1:n))
```

This statement allocates the array.

```
x = 0
```

This statement initialises the whole array to zero. The following statements define the start and end points for the array processing for each process.

```
start = (factor*this_process_number) + 1
end = factor*(this_process_number+1)
```

and partition the work up between the processes. Each process will have its own start and end values. The following do loop does the work:

```
do i = start, end
    x(i) = i*factor
end do
```

and all we are doing as this is filling sections of the array up with data based in process numbers.

The following

```
if (this_process_number==0) then
    do i = 1, number_of_processes - 1
        recv_start = (factor*I) + 1
        call mpi_recv(x(recv_start), &
                      factor,mpi_integer,i,1,mpi_comm_world,&
                      status ,error_number)
    end do
else
    call mpi_send(x(start),factor, &
                  mpi_integer,0,1,mpi_comm_world,error_number)
end if
```

uses sends and receives to transfer the updated array sections back to process zero. We are using `recv_start` to specify the starting point for the array transfer, and `x(start)` is the starting point for the transfer from the `x` array to process zero.

Here is sample output from the program when the number of processes is three.

```
mpiexec -n 3 ch3005
Process number =    2 start   11 end   15
Process number =    1 start     6 end   10
 1 I      1 x(i)      0
 1 I      2 x(i)      0
 1 I      3 x(i)      0
 1 I      4 x(i)      0
 1 I      5 x(i)      0
 1 I      6 x(i)     30
 1 I      7 x(i)     35
 1 I      8 x(i)     40
 1 I      9 x(i)     45
 1 I     10 x(i)     50
 1 I     11 x(i)      0
 1 I     12 x(i)      0
Process number =    0 start     1 end     5
 0 I      1 x(i)      5
 0 I      2 x(i)     10
 0 I      3 x(i)     15
 0 I      4 x(i)     20
 0 I      5 x(i)     25
 0 I      6 x(i)      0
 0 I      7 x(i)      0
 0 I      8 x(i)      0
 0 I      9 x(i)      0
 0 I     10 x(i)      0
 0 I     11 x(i)      0
 0 I     12 x(i)      0
 0 I     13 x(i)      0
 0 I     14 x(i)      0
 0 I     15 x(i)      0
 1 * 5 =      5
 2 * 5 =     10
 3 * 5 =     15
 4 * 5 =     20
 5 * 5 =     25
 6 * 5 =     30
 7 * 5 =     35
 2 I      1 x(i)      0
 2 I      2 x(i)      0
 2 I      3 x(i)      0
 2 I      4 x(i)      0
 2 I      5 x(i)      0
 2 I      6 x(i)      0
 2 I      7 x(i)      0
```

```
2 I    8 x(i)    0
2 I    9 x(i)    0
2 I   10 x(i)    0
2 I   11 x(i)   55
2 I   12 x(i)   60
2 I   13 x(i)   65
2 I   14 x(i)   70
2 I   15 x(i)   75
1 I   13 x(i)    0
1 I   14 x(i)    0
1 I   15 x(i)    0
8 * 5 =    40
9 * 5 =    45
10 * 5 =   50
11 * 5 =   55
12 * 5 =   60
13 * 5 =   65
14 * 5 =   70
15 * 5 =   75
```

So with three processes we have an array of size 15, and the work that each process does is

```
Process number = 0 start 1 end 5
Process number = 1 start 6 end 10
Process number = 2 start 11 end 15
```

and each process works on its own section of the array. At the end we use the sends and receives to make sure that the x array on process zero now has all of the updated values.

This code achieves load balancing across the processes.

30.12 Summary

The programs in this chapter provide an introduction to the use of MPI to achieve parallel programs in Fortran. We have also seen some of the timing benefits of parallel programming with MPI.

30.13 Problems

30.1 Compile and run the programs with your compiler and implementation of MPI. You should get similar results.

Chapter 31

OpenMP

The best way to have a good idea is to have a lot of ideas.
Linus Pauling

Aim

The aims of this chapter is to provide a short introduction to OpenMP programming in Fortran.

31.1 Introduction

The main OpenMP site is

<http://openmp.org/wp/>

and this has details about the various specifications

<http://openmp.org/wp/openmp-specifications/>

We recommend downloading the documentation if you are going to do OpenMP programming. You should visit

<http://openmp.org/wp/openmp-compilers/>

to see an up to date list of what compilers support the OpenMP specification, and at what level.

The OpenMP site has a range of resources available, check out

<http://openmp.org/wp/resources>

for more information.

We've run the examples in this chapter with one or more of the following compilers

- Cray
- gfortran
- Intel
- Nag

31.2 OpenMP Memory Model

OpenMP is a shared memory programming model. It has several features including

- All threads have access to the same shared memory
- Data can be shared or private
- Data transfer is transparent to the programmer
- Synchronization takes place and is generally implicit

We will look at a small number of examples to highlight some of the key features. We provide a brief coverage of some of the OpenMP glossary to provide a basic background to OpenMP.

- Threading Concepts
 - Thread—An execution entity with a stack and associated static memory, called threadprivate memory.
 - OpenMP thread—A thread that is managed by the OpenMP runtime system.
 - Thread-safe routine—A routine that performs the intended function even when executed concurrently (by more than one thread).
- OpenMP language terminology
 - Structured block—for Fortran, a block of executable statements with a single entry at the top and a single exit at the bottom.
 - Loop directive—an OpenMP executable directive whose associated user code must be a loop that is a structured block. For Fortran, only the do directive and the optional end do directive are loop directives.
 - Master thread—the thread that encounters a parallel construct, creates a team, generates a set of tasks, then executes one of those tasks as thread number 0.
 - Worksharing construct—a construct that defines units of work, each of which is executed exactly once by one of the threads in the team executing the construct. For Fortran, worksharing constructs are do, sections, single and workshare.
 - Barrier—a point in the execution of a program encountered by a team of threads, beyond which no thread in the team may execute until all threads in the team have reached the barrier and all explicit tasks generated by the team have executed to completion.
- Data Terminology
 - Variable—a named data object, whose value can be defined and redefined during the execution of a program. Only an object that is not part of another object is

considered a variable. For example, array elements, structure components, array sections and substrings are not considered variables.

- Private variable—With respect to a given set of task regions that bind to the same parallel region, a variable whose name provides access to a different block of storage for each task region.
- Shared variable—With respect to a given set of task regions that bind to the same parallel region, a variable whose name provides access to the same block of storage for each task region.

- Execution Model

- The OpenMP API uses the fork-join model of parallel execution. Multiple threads of execution perform tasks defined implicitly or explicitly by OpenMP directives. OpenMP is intended to support programs that will execute correctly both as parallel programs (multiple threads of execution and a full OpenMP support library) and as sequential programs (directives ignored and a simple OpenMP stubs library).

The above coverage should be enough to get started with OpenMP and understand the examples that follow.

31.3 Example 1: Hello World

This is the classic hello world program.

```
program ch3101
  use omp_lib
  implicit none
  integer :: nthreads
  integer :: thread_number
  integer :: i

  nthreads = omp_get_max_threads()
  print *, ' Number of threads = ', nthreads
!$omp parallel do
  do i = 1, nthreads
    print *, ' Hello from thread ', &
              omp_get_thread_num()
  end do
!$omp end parallel do
end program ch3101
```

Let us go through the program one statement at a time.

```
use omp_lib
```

This use statement makes available the OpenMP environment. OpenMP statements are treated as comments without this statement.

```
nthreads = omp_get_max_threads()
print *, ' Number of threads = ', nthreads
```

The first statement sets the variable nthread to the value returned by the OpenMP function `omp_get_max_threads()`. We then print out this value.

```
!$omp parallel do
```

OpenMP directives in Fortran start with the comment character (!), followed by a \$ symbol and the characters omp. We use this form as it works with both free format and fixed format Fortran source code.

The parallel do words indicate that the code that follows is a parallel region construct. In this case a do loop. Here is a small table listing some of the OpenMP directives.

Parallel region construct

```
!$omp parallel [clause]
structured block
!$omp end parallel
```

Work sharing constructs

```
!$omp do [clause] ...
do loop
!$omp end parallel
!$omp sections [clause] ...
[ !$omp section
structured block ] ...
!$omp end sections [nowait]
!$omp single [clause]
structured block
!$omp end single [nowait]
```

Combined parallel work sharing constructs

```
!$omp parallel do [clause]
structured block
!$omp end parallel do
!$omp parallel sections [clause] ...
[ !$omp section
```

```

structured block ] ...
!$omp end parallel sections

Synchronisation constructs

!$omp master
structured block
!$omp end master
!$omp critical [(name)]
structured block
!$omp end critical [(name)]
!$omp barrier
$omp atomic
expression list
!$omp flush
!$omp ordered
structured block
!$omp end ordered

Data environment

!$omp threadprivate (/c1/,/c2/)
```

We next have the parallel do.

```

do i = 1, nthreads
    print *, 'Hello from thread ', &
        omp_get_thread_num()
end do
```

This loop prints out a message from each thread showing the thread number.

```
!$omp end parallel do
```

This marks the end of the OpenMP parallel loop.

So at the start of the loop the OpenMP run time system does a fork and creates multiple threads. At the end of the loop we have a join operation and we are back to one thread of execution.

Here is the output from the Intel compiler on an Intel i7 system.

Number of threads =	8
Hello from thread	0
Hello from thread	4
Hello from thread	2
Hello from thread	3
Hello from thread	1
Hello from thread	7

Hello from thread	6
Hello from thread	5

These Intel systems have four real cores and each core supports hyper threading in Intel terminology. So the OpenMP system sees eight threads.

Here is the output from the gfortran compiler on the same system.

Number of threads =	8
Hello from thread	1
Hello from thread	3
Hello from thread	2
Hello from thread	4
Hello from thread	5
Hello from thread	6
Hello from thread	0
Hello from thread	7

The output is very similar, as one would expect.

31.4 Example 2: Hello World Using Default Variable Data Scoping

This is a simple variation on the first example. At first sight it appears to be identical in effect to example one.

```
program ch3102
  use omp_lib
  implicit none
  integer :: nthreads
  integer :: thread_number
  integer :: i

  nthreads = omp_get_max_threads()
  print *, ' Number of threads = ', nthreads
  !$omp parallel do
  do i = 1, nthreads
    thread_number = omp_get_thread_num()
    print *, ' Hello from thread ', &
              thread_number
  end do
  !$omp end parallel do
end program ch3102
```

However we have introduced a variable `thread_number` and are using the OpenMP default data scoping rules, i.e. we have said nothing. Here is the output from the Intel compiler.

Number of threads =	8
Hello from thread	4
Hello from thread	5
Hello from thread	0
Hello from thread	1
Hello from thread	2
Hello from thread	3
Hello from thread	7
Hello from thread	6

We appear to have a working program. Here is the output from the gfortran compiler.

```
$ ./a.exe
Number of threads = 8
Hello from thread 6
Hello from thread 7
```

Now something appears to be not quite right! The default variable scoping rules mean that the variable `thread_number` is available to all threads—in OpenMP terminology it is shared. The opposite of shared is private and each thread has their own copy. Example 3 corrects this problem.

31.5 Example 3: Hello World with Private `thread_number` variable

```
program ch3103
use omp_lib
implicit none
integer :: nthreads
integer :: thread_number
integer :: i

nthreads = omp_get_max_threads()
print *, ' Number of threads = ', nthreads
! $omp parallel do private(thread_number)
do i = 1, nthreads
    thread_number = omp_get_thread_num()
```

```

print *, ' Hello from thread ', &
    thread_number
end do
! $omp end parallel do
end program ch3103

```

Here is the output from the gfortran compiler.

```

$ ./a.exe
Number of threads =          8
Hello from thread      2
Hello from thread      1
Hello from thread      4
Hello from thread      3
Hello from thread      0
Hello from thread      6
Hello from thread      5
Hello from thread      7

```

Care must be taken with variables in OpenMP to ensure they have the correct data scoping state.

31.6 Example 4: Parallel Solution for Pi Calculation

This is an OpenMP parallel implementation of the integration problem (Example 3) from the previous chapter. You should compare it with the MPI solution—example 4 in the last chapter.

```

include 'precision_module.f90'

include 'timing_module.f90'

program ch3104
use precision_module
use timing_module
use omp_lib
implicit none
real (dp) :: fortran_internal_pi
real (dp) :: partial_pi
real (dp) :: openmp_pi
real (dp) :: width
real (dp) :: x
integer :: nthreads
integer :: i
integer :: j

```

```

integer :: k
integer :: n

nthreads = omp_get_max_threads()
fortran_internal_pi = 4.0_dp*atan(1.0_dp)
print *, ' Maximum number of threads is ', &
nthreads
do k=1,nthreads
    call start_timing()
    n = 100000
    call omp_set_num_threads(k)
    print *, ' Number of threads = ', k
    do j = 1, 5
        width = 1.0_dp/n
        partial_pi = 0.0_dp
    !$omp parallel do private(x) &
    !$omp shared(width) reduction(+:partial_pi)
        do i = 1, n
            x = width*(real(i,dp)-0.5_dp)
            partial_pi = partial_pi + f(x)
        end do
    !$omp end parallel do
        openmp_pi = width*partial_pi
        print 100, n, time_difference()
        print 110, openmp_pi, abs(openmp_pi- &
            fortran_internal_pi)
        n = n*10
    end do
end do
100 format (' N intervals = ', i12, ' time =', &
f8.3)
110 format (' openmp_pi = ', f20.16, /, &
'difference = ', f20.16)
call end_timing()
stop

```

contains

```

real (dp) function f(x)
implicit none
real (dp), intent (in) :: x

f = 4.0_dp/(1.0_dp+x*x)
end function f

```

```
end program ch3104
```

Here is the output from the Intel compiler.

```
Maximum number of threads is          8
..
Number of threads =                  1
N intervals =      100000  time =  0.004
openmp_pi =      3.1415926535981167
difference =    0.0000000000083236
N intervals =      1000000  time =  0.012
openmp_pi =      3.1415926535899033
difference =    0.000000000001101
N intervals =     10000000  time =  0.051
openmp_pi =      3.1415926535896861
difference =    0.000000000001070
N intervals =    100000000  time =  0.449
openmp_pi =      3.1415926535902168
difference =    0.000000000004237
N intervals =   1000000000  time =  4.398
openmp_pi =      3.1415926535897682
difference =    0.000000000000249
..
Number of threads =                  2
N intervals =      100000  time =  0.000
openmp_pi =      3.1415926535981260
difference =    0.0000000000083329
N intervals =     1000000  time =  0.000
openmp_pi =      3.1415926535898624
difference =    0.000000000000693
N intervals =    10000000  time =  0.020
openmp_pi =      3.1415926535897829
difference =    0.00000000000102
N intervals =   100000000  time =  0.219
openmp_pi =      3.1415926535898926
difference =    0.000000000000995
N intervals =   1000000000  time =  2.195
openmp_pi =      3.1415926535897380
difference =    0.000000000000551
..
Number of threads =                  4
N intervals =      100000  time =  0.004
openmp_pi =      3.1415926535981287
difference =    0.0000000000083356
N intervals =     1000000  time =  0.004
openmp_pi =      3.1415926535898726
difference =    0.000000000000795
```

```
N intervals =      10000000 time =   0.027
openmp_pi =    3.1415926535898153
difference =  0.0000000000000222
N intervals =      100000000 time =   0.137
openmp_pi =    3.1415926535898038
difference =  0.0000000000000107
N intervals =     1000000000 time =   1.781
openmp_pi =    3.1415926535898544
difference =  0.0000000000000613
..
Number of threads =          8
N intervals =     100000 time =   0.000
openmp_pi =    3.1415926535981278
difference =  0.0000000000083347
N intervals =     1000000 time =   0.004
openmp_pi =    3.1415926535898784
difference =  0.000000000000853
N intervals =     10000000 time =   0.016
openmp_pi =    3.1415926535897962
difference =  0.000000000000031
N intervals =     100000000 time =   0.113
openmp_pi =    3.1415926535898162
difference =  0.000000000000231
N intervals =     1000000000 time =   1.137
openmp_pi =    3.1415926535898824
difference =  0.000000000000893
```

We have similar timing improvements to the MPI solutions.

31.7 Summary

This chapter briefly introduced the essentials of OpenMP programming. We have also seen the timing benefits that OpenMP programming can offer in the solution of the same problem.

31.8 Problems

- 31.1** Compile and run the examples in this chapter with your compiler and compare the results.

Chapter 32

Coarray Fortran

Science is a wonderful thing if one does not have to earn one's living at it.

Einstein

Aim

The aims of this chapter is to provide a short introduction to coarray programming in Fortran.

32.1 Introduction

Coarrays were the major component of the Fortran 2008 standard. As stated earlier they are based on a single program multiple data model. Coarrays are a simple parallel programming extension to Fortran. They are effectively variables that can be shared across multiple instances of the same program or images in Fortran terminology.

Coarray variables look like conventional Fortran arrays, except that they use [] brackets instead of () brackets. In the simple declaration below

```
character(len=20) :: name[*]='*****'
```

We declare name to be a coarray and the * in the [] brackets means that the bounds of the coarray are calculated at run time, rather than compile time.

```
read *, name
```

is a reference to the coarray on the current image.

We can then use the following statement

```
name[i] = name
```

to broadcast the value read in to each of the other images.

Note the Fortran coarray syntax here. We use the [] brackets to reference the coarray variable on other images and the omission of the [] brackets is a reference to the coarray variable on the current image.

32.2 Coarray Terminology

The following is taken from the standard and covers some of the basic coarray terminology.

- codimension attribute—The codimension attribute specifies that an entity is a coarray. The coarray-spec specifies its corank or corank and cobounds.
- Allocatable coarray—A coarray with the allocatable attribute has a specified corank, but its cobounds are determined by allocation or argument association.
- Explicit-coshape coarray—An explicit-coshape coarray is a named coarray that has its corank and cobounds declared by an explicit-coshape-spec.
- Coindexed named objects—A coindexed-named-object is a named scalar coarray variable followed by an image selector.
- Image selectors—An image selector determines the image index for a coindexed object.
- Image execution control and image control statements—The execution sequence on each image is specified in 2.3.5 of the standard.
- Execution of an image control statement divides the execution sequence on an image into segments. Each of the following is an image control statement:
 - sync all statement;
 - sync images statement;
 - sync memory statement;
 - allocate or deallocate statement that has a coarray allocate-object;
 - critical or end critical;
 - lock or unlock statement;
 - Any statement that completes execution of a block or procedure and which results in the implicit deallocation of a coarray;
 - stop statement;
 - end statement of a main program.
- Coarray—A coarray is a data entity that has nonzero corank; it can be directly referenced or defined by any image. It may be a scalar or an array.
- Coarray dummy variables—if the dummy argument is a coarray, the corresponding actual argument shall be a coarray and shall have the volatile attribute if and only if the dummy argument has the volatile attribute.
- Coarray intrinsics
 - image_index—convert a cosubscript to an image index
 - lcobound—cobounds of a coarray
 - num_images—the number of images

- `this_image`—image index or cosubscripts
- `ucobound`—cobounds of a coarray

Let us look now at some simple examples.

32.3 Example 1: Hello World

The first is the classic Hello world.

```
program ch3201

implicit none

print *, 'Hello world from image ', &
this_image()

end program ch3201
```

Here is the output from the Intel compiler.

Hello world from image	5
Hello world from image	3
Hello world from image	4
Hello world from image	8
Hello world from image	1
Hello world from image	6
Hello world from image	2
Hello world from image	7

Here is sample output from the Cray Archer service.

Hello world from image	16
Hello world from image	6
Hello world from image	13
Hello world from image	25
Hello world from image	34

lines deleted

Hello world from image	38
Hello world from image	44
Hello world from image	35
Hello world from image	28
Hello world from image	33
Hello world from image	32
Hello world from image	30
Hello world from image	29

The output is obviously very similar to the corresponding MPI and OpenMP versions.

32.4 Example 2: Broadcasting Data

Here is a simple program that broadcasts data from one image to the rest. This is a common requirement in parallel programming.

```
program ch3202

implicit none

integer :: i
character (len=20) :: name [ * ] = '*****'

print 100, name, this_image()

if (this_image()==1) then
    print *, ' Type in your name'
    read *, name
    do i = 2, num_images()
        name [ i ] = name
    end do
end if

sync all

print 100, name, this_image()
100 format (1x, ' Hello ', a20, &
' from image ', i3)

end program ch3202
```

Here is the output from the Intel compiler.

Hello *****	from image	1
Hello *****	from image	3
Hello *****	from image	5
Hello *****	from image	7
Hello *****	from image	2
Hello *****	from image	4
Hello *****	from image	8

```
Type in your name
Hello *****          from image  6
Jane
Hello Jane           from image  4
Hello Jane           from image  8
Hello Jane           from image  2
Hello Jane           from image  6
Hello Jane           from image  7
Hello Jane           from image  3
Hello Jane           from image  5
Hello Jane           from image  1
```

Again no particular ordering of the image numbers.

32.5 Example 3: Parallel Solution for Pi Calculation

```
include 'precision_module.f90'

include 'timing_module.f90'

program ch3203

use precision_module
use timing_module

implicit none

real (dp) :: fortran_internal_pi
real (dp) :: partial_pi
real (dp) :: coarray_pi
real (dp) :: width
real (dp) :: total_sum
real (dp) :: x
real (dp), codimension [ * ] :: partial_sum

integer :: n_intervals
integer :: i
integer :: j
integer :: current_image
integer :: n_images

fortran_internal_pi = 4.0_dp*atan(1.0_dp)
n_images = num_images()
```

```

current_image = this_image()

if (current_image==1) then
  print *, ' Number of images = ', n_images
end if

n_intervals = 100000

do j = 1, 5
  if (current_image==1) then
    call start_timing()
  end if
  width = 1.0_dp/real(n_intervals, dp)
  total_sum = 0.0_dp
  partial_sum = 0.0_dp
  do i = current_image, n_intervals, n_images
    x = (real(i,dp)-0.5_dp)*width
    partial_sum = partial_sum + f(x)
  end do
  partial_sum = partial_sum*width
  sync all
  if (current_image==1) then
    do i = 1, n_images
      total_sum = total_sum + partial_sum [ i &
        ]
    end do
    coarray_pi = total_sum
    print 100, n_intervals, time_difference()
    print 110, coarray_pi, abs(coarray_pi- &
      fortran_internal_pi)
  end if
  n_intervals = n_intervals*10
  sync all
end do

100 format (' n intervals = ', i12, &
  ' time =', f8.3)
110 format (' pi = ', f20.16, /, &
  ' difference = ', f20.16)
```

contains

```

real (dp) function f(x)
implicit none
real (dp), intent (in) :: x
```

```
f = 4.0_dp/(1.0_dp+x*x)

end function f

end program ch3203
```

Here is the output from the Intel compiler.

```
Number of images =          8
2011/ 6/10 13:40:48 479
n intervals =      100000  time =   0.004
pi =    3.1415926535981260
difference =  0.00000000000083329
2011/ 6/10 13:40:48 486
n intervals =      1000000  time =   0.004
pi =    3.1415926535898802
difference =  0.0000000000000870
2011/ 6/10 13:40:48 490
n intervals =      10000000  time =   0.012
pi =    3.1415926535897936
difference =  0.0000000000000004
2011/ 6/10 13:40:48 500
n intervals =      100000000  time =   0.105
pi =    3.1415926535897749
difference =  0.0000000000000182
2011/ 6/10 13:40:48 605
n intervals =      1000000000  time =   0.992
pi =    3.1415926535898455
difference =  0.0000000000000524
```

Here is the output from the Cray compiler.

```
Number of images =  48
2015/ 3/21 1:11:50 130
n intervals =      100000  time =   0.005
pi =    3.1415926535981265
difference =  0.00000000000083333
2015/ 3/21 1:11:50 135
n intervals =      1000000  time =   0.000
pi =    3.1415926535898762
difference =  0.0000000000000830
2015/ 3/21 1:11:50 135
n intervals =      10000000  time =   0.001
pi =    3.1415926535897953
difference =  0.0000000000000022
2015/ 3/21 1:11:50 136
```

```

n intervals =    100000000 time =    0.006
pi =    3.1415926535897905
difference =    0.0000000000000027
2015/ 3/21  1:11:50 142
n intervals =    1000000000 time =    0.054
pi =    3.1415926535897949
difference =    0.0000000000000018

```

We get the time improvement we have seen with both the MPI and OpenMP solutions.

32.6 Example 4: Work Sharing

This example looks at one way of splitting work up between images. We use the image number to determine which image does which work. It is a coarray version of the MPI work sharing example.

```

program ch3204
  implicit none
  integer :: n, i, j
  integer :: me, nim, start, end
  integer, parameter :: factor = 5
  integer, dimension (1:factor), &
    codimension [ * ] :: x

  nim = num_images()
  me = this_image()
  n = nim*factor
  x = 0
  start = factor*(me-1) + 1
  end = factor*me
  j = 1
  do i = start, end
    x(j) = i*factor
    print *, 'on image ', me, 'j = ', j, &
      ' x(j) = ', x(j)
    j = j + 1
  end do
! sync all
  if (me==1) then
    print *, 'coarray x on image ', me, ' is: ', &
      x
    do i = 2, nim

```

```

!      print*, 'coarray x on image ', I, ' is:
!      ', x(:)[I]
      end do
      end if
end program ch3204

```

The following statements define the start and end points for the array processing for each image:

```

start = factor*(me-1) + 1
end   = factor*me

```

and partitions the work between the images. Each image will have its own start and end values. The following do loop does the work:

```

do i=start,end
  x(j) = i*factor
  print*, 'on image ', me, ' j = ', j, ' x(j) = ', x(j)
  j    = j + 1
end do

```

We need the

```
sync all
```

to ensure that each image has completed before further processing, and we then print out the data from each image on image 1.

Here is a subset of the output from the Intel compiler. This example runs on 8 images.

```

on image      2 j =      1 x(j) =      30
on image      7 j =      1 x(j) =     155
on image      8 j =      1 x(j) =     180
on image      8 j =      2 x(j) =     185
on image      8 j =      3 x(j) =     190
on image      8 j =      4 x(j) =     195
on image      8 j =      5 x(j) =     200
on image      6 j =      1 x(j) =     130
on image      6 j =      2 x(j) =     135
on image      6 j =      3 x(j) =     140
...
...
...
coarray x on image           1 is:

```

```

      5          10
15
20          25
on image    4 j =      1 x(j) =     80
on image    4 j =      2 x(j) =     85
on image    4 j =      3 x(j) =     90
on image    4 j =      4 x(j) =     95
on image    4 j =      5 x(j) =    100
coarray x on image           2 is:
      30          35
40
45          50
coarray x on image           3 is:
      55          60
65
70          75
coarray x on image           4 is:
      80          85
90
95          100
coarray x on image           5 is:
      105         110
      120         125
coarray x on image           6 is:
      130         135
140
145         150
coarray x on image           7 is:
      155         160
165
170         175
coarray x on image           8 is:
      180         185
190
195         200

```

Here is a sample of the output from the Cray compiler on the Archer service. This example runs on 48 images.

```

on image  1 j =  1 x(j) =  5
on image  1 j =  2 x(j) = 10
on image  3 j =  1 x(j) = 55
on image  3 j =  2 x(j) = 60

```

```
stuff deleted
```

```
on image 22 j = 5 x(j) = 550
coarray x on image 1 is: 5, 10, 15, 20, 25
on image 21 j = 1 x(j) = 505

stuff deleted

on image 20 j = 3 x(j) = 490
on image 6 j = 3 x(j) = 140
on image 13 j = 2 x(j) = 310
on image 6 j = 4 x(j) = 145

stuff deleted

on image 7 j = 1 x(j) = 155
on image 10 j = 2 x(j) = 235

stuff deleted

on image 27 j = 2 x(j) = 660
on image 41 j = 4 x(j) = 1020
on image 28 j = 2 x(j) = 685

stuff deleted

on image 33 j = 5 x(j) = 825
on image 36 j = 5 x(j) = 900
on image 40 j = 1 x(j) = 980

stuff deleted

on image 40 j = 2 x(j) = 985
on image 40 j = 3 x(j) = 990
on image 40 j = 4 x(j) = 995
on image 40 j = 5 x(j) = 1000
on image 45 j = 4 x(j) = 1120
on image 46 j = 5 x(j) = 1150
on image 45 j = 5 x(j) = 1125

Application 13271719 resources: utime ~7s,
stime ~52s, Rss ~4288,
inblocks ~22292, outblocks ~39436
```

32.7 Summary

This chapter has looked briefly at some of the simple syntax of coarrays using a small set of examples. We have also seen the timing benefits that coarray programming can offer in the solution of the same problem.

32.8 Problems

- 32.1** Compile and run the examples in this chapter with your compiler.

Chapter 33

C Interop

We can't solve problems by using the same kind of thinking we used when we created them.

Einstein

Aim

This chapter looks briefly at C interoperability.

33.1 Introduction

C is a widely used programming language and there is a considerable amount of software written in C or with a C calling interface. Fortran 2003 introduced a standardised mechanism for interoperating with C.

There were limitations to this interoperability and ISO TS 29113 significantly extended the scope of the interoperation facilities. The TS was published in 2012.

In this chapter we provide a brief coverage of some of the technical details required for interoperability and then have a look at a couple of examples.

33.2 The `iso_c_binding` Module

There is an intrinsic module called `iso_c_binding` that contains named constants, derived types and module procedures to support interoperability.

33.3 Named Constants and Derived Types in the Module

In Table 33.1 the entities listed in the second column are named constants of type default integer.

Table 33.1 iso_c_binding module—named constants

Fortran type	Named constant from the iso_c_binding module (kind type parameter is positive if supported)	C type
Integer	c_int	int
	c_short	short int
	c_long	long int
	c_long_long	long long int
	c_signed_char	signed char
		unsigned char
	c_size_t	size_t
	c_int8_t	int8_t
	c_int16_t	int16_t
	c_int32_t	int32_t
	c_int64_t	int64_t
	c_int_least8_t	int_least8_t
	c_int_least16_t	int_least16_t
	c_int_least32_t	int_least32_t
	c_int_least64_t	int_least64_t
	c_int_fast8_t	int_fast8_t
	c_int_fast16_t	int_fast16_t
	c_int_fast32_t	int_fast32_t
	c_int_fast64_t	int_fast64_t
	c_intmax_t	intmax_t
	c_intptr_t	intptr_t
Real	c_float	float
	c_double	double
	c_long_double	long double
Complex	c_float_complex	float complex
	c_double_complex	double complex
	c_long_double_complex	long double complex
Logical	c_bool	bool
Character	c_char	char

33.4 Character Interoperability

Table 33.2 shows the mapping between Fortran and C character types. The semantics of these values are explained in 5.2.1 and 5.2.2 of the C International Standard.

Table 33.2 C Interop character interoperability

Name	C definition	<code>c_char = -1</code>	<code>c_char/ = -1</code>
<code>c_null_char</code>	null character	<code>char(0)</code>	<code>'\0'</code>
<code>c_alert</code>	alert	<code>achar(7)</code>	<code>'\a'</code>
<code>c_backspace</code>	backspace	<code>achar(8)</code>	<code>'\b'</code>
<code>c_form_feed</code>	form feed	<code>achar(12)</code>	<code>'\f'</code>
<code>c_new_line</code>	new line	<code>achar(10)</code>	<code>'\n'</code>
<code>c_carriage_return</code>	carriage return	<code>achar(13)</code>	<code>'\r'</code>
<code>c_horizontal_tab</code>	horizontal tab	<code>achar(9)</code>	<code>'\t'</code>
<code>c_vertical_tab</code>	vertical tab	<code>achar(11)</code>	<code>'\v'</code>

33.5 Procedures in the Module

There are several procedures in this module. In the descriptions below, procedure names are generic and not specific.

A C procedure argument is often defined in terms of a C address. The `c_loc` and `c_funloc` functions are provided so that Fortran applications can determine the appropriate value to use with C facilities.

The `c_associated` function is provided so that Fortran programs can compare C addresses.

The `c_f_pointer` and `c_f_procpointer` subroutines provide a means of associating a Fortran pointer with the target of a C pointer.

More information can be found in Chap. 15 of the Fortran 2008 standard.

33.6 Interoperability of Intrinsic Types

Table 33.1 shows the interoperability between Fortran intrinsic types and C types. A Fortran intrinsic type with particular type parameter values is interoperable with a C type if the type and kind type parameter value are listed in the table on the same row as that C type; if the type is character, interoperability also requires that the length type parameter be omitted or be specified by an initialization expression whose value is one. A combination of Fortran type and type parameters that is interoperable with a C type listed in the table is also interoperable with any unqualified C type that is compatible with the listed C type.

The second column of the table refers to the named constants made accessible by the `iso_c_binding` intrinsic module.

A combination of intrinsic type and type parameters is interoperable if it is interoperable with a C type.

The above mentioned C types are defined in the C International Standard, clauses 6.2.5, 7.17, and 7.18.1.

33.7 Other Aspects of Interoperability

There are considerable restrictions on other aspects of interoperability. The following provides some brief details of other areas:

33.7.1 Interoperability with C Pointer Types

`c_ptr` and `c_funptr` shall be derived types with private components. `c_ptr` is interoperable with any C object pointer type. `c_funptr` is interoperable with any C function pointer type.

33.7.2 Interoperability of Scalar Variables

A scalar Fortran variable is interoperable if its type and type parameters are interoperable and it has neither the pointer nor the allocatable attribute.

An interoperable scalar Fortran variable is interoperable with a scalar C entity if their types and type parameters are interoperable.

33.7.3 Interoperability of Array Variables

An array Fortran variable is interoperable if its type and type parameters are interoperable and it is of explicit shape or assumed size.

33.7.4 Interoperability of Procedures and Procedure Interfaces

A Fortran procedure is interoperable if it has the `bind` attribute, that is, if its interface is specified with a proc-language-binding-spec.

33.7.5 Interoperation with C Global Variables

A C variable with external linkage may interoperate with a common block or with a variable declared in the scope of a module. The common block or variable shall be specified to have the `bind` attribute.

33.7.6 Binding Labels for Common Blocks and Variables

The binding label of a variable or common block is a value of type default character that specifies the name by which the variable or common block is known to the companion processor.

33.7.7 Interoperation with C Functions

A procedure that is interoperable may be defined either by means other than Fortran or by means of a Fortran subprogram, but not both.

Another useful source can be found in the December 2009 edition of Fortran Forum. Details are given at the end of the chapter.

33.8 Compilers Used in the Examples

Not all Fortran compilers work with all C and C++ compilers and vice versa.

Table 33.3 has some details of the compilers we have used in the examples that follow.

Table 33.3 Compilers used

Main program	Subprogram	Operating system
gfortran	gcc	cygwin, Windows
gfortran	gcc	MinGW-W64, Windows
gfortran	gcc	openSuSe 13.1
Intel Fortran	Microsoft Visual C++	Windows
Nag Fortran	gcc	openSuSe 13.1
Nag Fortran	Nag integrated gcc	Windows
Nag Fortran	gcc	MinGW-W64, Windows
Oracle Fortran	Oracle cc	openSuSe 13.1
gcc	gfortran	cygwin, Windows
gcc	gfortran	openSuSe 13.1
Intel C	Intel Fortran	openSuSe 13.1
Oracle C	Oracle Fortran	openSuSe 13.1
g++	gfortran	cygwin, Windows
g++	gfortran	openSuSe 13.1
Intel C++	Intel Fortran	openSuSe 13.1
Microsoft Visual C++	Intel Fortran	Windows
Oracle C++	Oracle Fortran	openSuSe 13.1

33.9 Example 1: Kind Type Support

This example uses Table 33.1 as its basis. It prints out the kind types for each of the kind types in the table. If the value of one of the named constants is positive it will be a valid kind value for the intrinsic type, i.e. the corresponding C type is interoperable with the Fortran intrinsic type of that kind. If the value of one of the named constants is negative then there is no interoperable Fortran kind for that C type.

```
program ch3301
use iso_c_binding
implicit none

print *, 'integer support'
print *, 'c_int = ', c_int
print *, 'c_short = ', c_short
print *, 'c_long = ', c_long
print *, 'c_long_long = ', c_long_long
print *, 'c_signed_char = ', c_signed_char
print *, 'c_size_t = ', c_size_t
print *, 'c_int8_t = ', c_int8_t
print *, 'c_int16_t = ', c_int16_t
print *, 'c_int32_t = ', c_int32_t
print *, 'c_int64_t = ', c_int64_t
print *, 'c_int_least8_t = ', c_int_least8_t
print *, 'c_int_least16_t = ', &
         c_int_least16_t
print *, 'c_int_least32_t = ', &
         c_int_least32_t
print *, 'c_int_least64_t = ', &
         c_int_least64_t
print *, 'c_int_fast8_t = ', c_int_fast8_t
print *, 'c_int_fast16_t = ', c_int_fast16_t
print *, 'c_int_fast32_t = ', c_int_fast32_t
print *, 'c_int_fast64_t = ', c_int_fast64_t
print *, 'c_intmax_t = ', c_intmax_t
print *, 'c_intptr_t = ', c_intptr_t
print *, 'real support'
print *, 'c_float = ', c_float
print *, 'c_double = ', c_double
print *, 'c_long_double = ', c_long_double
print *, 'complex support'
print *, 'c_float_complex = ', &
         c_float_complex
print *, 'c_double_complex = ', &
         c_double_complex
```

```

print *, ' c_long_double_complex = ', &
         c_long_double_complex
print *, 'logical support'
print *, ' c_bool = ', c_bool
print *, 'character support'
print *, ' c_char = ', c_char
end program ch3301

```

Table 33.4 summarises support for several compilers.

Table 33.4 Basic C Interop table

Compiler vendors	gfortran	Intel	Nag	Sun
C Interop type				
C_INT	4	4	4	4
C_SHORT	2	2	2	2
C_LONG	8	4	4	8
C_LONG_LONG	8	8	8	8
C_SIGNED_CHAR	1	1	1	1
C_SIZE_T	8	8	8	8
C_INT8_T	1	1	1	1
C_INT16_T	2	2	2	2
C_INT32_T	4	4	4	4
C_INT64_T	8	8	8	8
C_INT_LEAST8_T	1	1	1	1
C_INT_LEAST16_T	2	2	2	2
C_INT_LEAST32_T	4	4	4	4
C_INT_LEAST64_T	8	8	8	8
C_INT_FAST8_T	1	1	1	1
C_INT_FAST16_T	8	2	2	2
C_INT_FAST32_T	8	4	4	4
C_INT_FAST64_T	8	8	8	8
C_INTMAX_T	8	8	8	8
C_INTPTR_T	8	8	8	8
C_FLOAT	4	4	4	4
C_DOUBLE	8	8	8	8
C_LONG_DOUBLE	10	8	-4	-3
C_FLOAT_COMPLEX	4	4	4	4
C_DOUBLE_COMPLEX	8	8	8	8
C_LONG_DOUBLE_COMPLEX	10	8	-4	-3
C_BOOL	1	1	1	1
C_CHAR	1	1	1	1

A negative number means not supported

33.10 Example 2: Fortran Calling a C Function

Here is the Fortran source.

```
program ch3302
  use iso_c_binding
  interface
    real (c_float) function reciprocal(x) &
      bind (c, name='reciprocal')
    use iso_c_binding
    real (c_float), value :: x
  end function reciprocal
end interface
real :: x

x = 10.0
print *, 'Fortran calling C function'
print *, x, 'reciprocal = ', reciprocal(x)
end program ch3302
```

Here is the C source.

```
float reciprocal(float x)
{
    return(1.0f/x);
}
```

The first key statement is

```
use iso_c_binding
```

which makes available named constants, derived types and module procedures to support interoperability.

The next part of the program

```
interface
  real (c_float) function reciprocal(x) &
    bind(c,name='reciprocal')
  use iso_c_binding
  real (c_float) , value :: x
end function reciprocal
end interface
```

provides the compiler with details of the C function that is being called. It is called `reciprocal`, takes an argument of type `real` in Fortran or `float` in C terminology, and returns a value of type `real` in Fortran or `float` in C terminology.

33.11 Example 3: C Calling a Fortran Function

Here is the Fortran source.

```
function reciprocal(x) bind (c, name= &
    'reciprocal')
use iso_c_binding
implicit none
real (c_float), intent (in) :: x
real (c_float) :: reciprocal

    reciprocal = 1.0/x
end function reciprocal
```

Here is the C source.

```
#include <stdio.h>
float reciprocal(float *x);

int main()
{
    float x;
    x=10.0f;
    printf(" C calling a Fortran function\n");
    printf(" (1 / %f ) = %f \n" ,x,reciprocal(&x));
    return(0);
}
```

Let us look at the Fortran code first.

```
function reciprocal(x) bind(c,name=reciprocal)
```

This line tells the compiler that the `reciprocal` function has to have a name and calling convention that is interoperable with C.

```
real (c_float), intent(in) :: x
```

says that the argument `x` is `intent(in)` and is of type `real` in Fortran and type `float` in C.

```
real (c_float) :: reciprocal
```

says that the function will return a value of type `real` in Fortran or `float` in C terminology.

The function prototype

```
float reciprocal(float *x);
```

is required in the C source code to tell the compiler about the `reciprocal` function.

33.12 Example 4: C++ Calling a Fortran Function

Here is the Fortran source.

```
function reciprocal(x) bind (c, name= &
    'reciprocal')
use iso_c_binding
implicit none
real (c_float), intent (in) :: x
real (c_float) :: reciprocal

reciprocal = 1.0/x
end function reciprocal
```

Here is the C++ source.

```
#include <iostream>
using namespace std;
extern "C" { float reciprocal(float *); }
int main()
{
    float x;
    x=10.0f;
    cout << " C++ calling a Fortan function" << endl;
    cout << " x = " << x << " reciprocal = ";
    cout << reciprocal(&x) << endl;
    return(0);
}
```

The Fortran code and explanation is as for the previous example.

The

```
extern "C" { float reciprocal(float *); }
```

code is required in the C++ code to tell the compiler about the Fortran function reciprocal.

In C++ we have to tell the compiler that the function has C calling semantics.

33.13 Example 5: Passing an Array from Fortran to C

Here is the Fortran source.

```
program ch3305
use iso_c_binding
interface
```

```

function summation(x, n) bind (c, &
    name='summation')
use iso_c_binding
integer (c_int), value :: n
real (c_float), dimension (1:n), &
    intent (in) :: x
real (c_float) :: summation
end function summation
end interface
integer, parameter :: n = 10
real, dimension (1:n) :: x = 1.0

print *, ' Fortran calling c function'
print *, ' 1 d array as parameter'
print *, summation(x, n)
end program ch3305

```

Here is the C source.

```

float summation(float *x,int n)
{
    int i;
    float t;
    t=0.0f;
    for (i=0;i<n;i++)
    {
        t+=x[i];
    }
    return(t);
}

```

The following code

```

interface
    function summation(x,n) bind(c,name=summation)
        use iso_c_binding
        integer (c_int) , value :: n
        real (c_float), dimension(1:n) , intent(in) :: x
        real (c_float) :: summation
    end function summation
end interface

```

is required to tell the Fortran compiler the details of the C function.

Arrays in C are passed as pointers or by address so we have the following signature

```
float summation(float *x,int n)
```

in the C code.

33.14 Example 6: Passing an Array from C to Fortran

Here is the Fortran source.

```
function summation(x, n) bind (c, &
    name='summation')
use iso_c_binding
implicit none
integer (c_int), value :: n
real (c_float), dimension (1:n), &
    intent (in) :: x
real (c_float) :: summation

summation = sum(x(1:n))
end function summation
```

Here is the C source.

```
#include <stdio.h>
float summation(float *x,int n);

int main()
{
    const int n=10;
    float x[n];
    int i;
    for (i=0;i<n;i++)
        x[i]=1.0;
    printf(" C calling Fortran\n");
    printf(" 1 d array as parameter\n");
    printf(" Sum is = %f \n" ,summation(x,n));
    return(0);
}
```

The `bind(c)` attribute is required to tell the Fortran compiler that the function will be called from C.

The other declarations provide details of the parameters passed into the function from the C calling routine.

The following function prototype

```
float summation(float *x,int n);
```

is required to tell the C compiler the details of the Fortran function.

33.15 Example 7: Passing an Array from C++ to Fortran

Here is the Fortran source.

```
function summation(x, n) bind (c, &
    name='summation')
use iso_c_binding
implicit none
integer (c_int), value :: n
real (c_float), dimension (1:n), &
    intent (in) :: x
real (c_float) :: summation
integer :: i

summation = sum(x(1:n))
end function summation
```

Here is the C++ source.

```
#include <iostream>
using namespace std;
extern "C" float summation(float *,int );
int main()
{
    const int n=10;
    float *x;
    int i;
    x = new float[n];
    for (i=0;i<n;i++)
        x[i]=1.0f;
    cout << " C++ calling Fortran" << endl;
    cout << " 1 d array as parameter" << endl;
    cout << " Sum is " << summation(x,n) << endl;
    return(0);
}
```

The explanation of the Fortran source is the same as for the previous example.
The following function prototype

```
float summation(float *x,int n);
```

is required to tell the C++ compiler about the Fortran function.

33.16 Example 8: Passing a Rank 2 Array from Fortran to C

Here is the Fortran source.

```

program ch3308
use iso_c_binding
interface
    subroutine reciprocal(nr, nc, x, y) bind (c, &
        name='reciprocal')
        use iso_c_binding
        integer (c_int), value :: nr
        integer (c_int), value :: nc
        real (c_float), dimension (nr, nc) :: x
        real (c_float), dimension (nr, nc) :: y
    end subroutine reciprocal
end interface
integer, parameter :: nr = 2
integer, parameter :: nc = 6
integer :: i
real, dimension (nr, nc) :: x
real, dimension (nr, nc) :: y
real, dimension (nr*nc) :: t = [ (i,i=1,nr*nc) &
    ]
integer :: r
integer :: c

x = reshape(t, (/nr,nc/), order=(/2,1/) )
print *, ' Fortran calling C'
print *, ' two d array as parameter'
print *, ' using C 99 VLA'
do r = 1, nr
    print 100, x(r, 1:nc)
100 format (10(f5.1))
end do
call reciprocal(nr, nc, x, y)
do r = 1, nr
    print 110, y(r, 1:nc)
110 format (10(f6.3))
end do
end program ch3308

```

Here is the C source.

```

void reciprocal(int nrow,int ncol,
    float matrix1[nrow][ncol],
    float matrix2[nrow][ncol])

```

```
{
    int i;
    int j;
    for (i=0;i<nrow;i++)
        for (j=0;j<ncol;j++)
            matrix2[i][j]=1.0f/matrix1[i][j];
}
```

In this example we are using the variable length array syntax that was introduced in the C 99 standard.

This feature is not supported in all C compilers.

This enables us to use the following syntax in C.

```
void reciprocal(int nrow,int ncol,
float matrix1[nrow][ncol],
float matrix2[nrow][ncol])
```

33.17 Example 9: Passing a Rank 2 Array from C to Fortran

Here is the Fortran source.

```
subroutine reciprocal(nr, nc, x, y) bind (c, &
    name='reciprocal')
use iso_c_binding
implicit none
integer (c_int), value :: nr
integer (c_int), value :: nc
real (c_float), dimension (1:nr, 1:nc), &
    intent (in) :: x
real (c_float), dimension (1:nr, 1:nc), &
    intent (out) :: y

y = 1.0/x
end subroutine reciprocal
```

Here is the C source.

```
#include <stdio.h>
void reciprocal(int nr,int nc,
                float x[nr][nc],
                float y[nr][nc]);
int main()
{
    const int nr=2;
    const int nc=5;
```

```

float x[nr][nc];
float y[nr][nc];
int r;
int c;
int i=1;
for (r=0;r<nr;r++)
    for (c=0;c<nc;c++)
    {
        x[r][c]=(float)(i);
        i++;
    }
printf(" C calling Fortran\n");
printf(" 2 d array as parameter\n");
printf(" C99 vla\n");
for (r=0;r<nr;r++)
{
    for (c=0;c<nc;c++)
    {
        printf(" %5.2f " , x[r][c]);
    }
    printf("\n");
}
reciprocal(nr,nc,x,y);
for (r=0;r<nr;r++)
{
    for (c=0;c<nc;c++)
    {
        printf(" 1 / %5.2f = %6.3f \n"
, x[r][c],y[r][c]);
    }
    printf("\n");
}
return(0);
}

```

We use C99 VLAs in this example too.

33.18 Example 10: Passing a Rank 2 Array from C++ to Fortran

Here is the Fortran source.

```

subroutine reciprocal(nr, nc, x, y) bind (c, &
name='reciprocal')

```

```

use iso_c_binding
implicit none
integer (c_int), value :: nr
integer (c_int), value :: nc
real (c_float), dimension (1:nr, 1:nc), &
    intent (in) :: x
real (c_float), dimension (1:nr, 1:nc), &
    intent (out) :: y

y = 1.0/x
end subroutine reciprocal

```

Here is the C++ source.

```

#include <iostream>
using namespace std;
extern "C" void reciprocal(int nr,int nc,
                           float *x,float *y);
int main()
{
    const int nr=2;
    const int nc=5;
    float x[nr][nc];
    float y[nr][nc];
    int r;
    int c;
    int i=1;
    for (r=0;r<nr;r++)
        for (c=0;c<nc;c++)
        {
            x[r][c]=(float)(i);
            i++;
        }
    cout << " C++ calling Fortran" << endl;
    cout << " 2 d array as parameter\n";
    for (r=0;r<nr;r++)
    {
        for (c=0;c<nc;c++)
        {
            cout << " " << x[r][c] << " ";
        }
        cout << endl;
    }
    reciprocal(nr,nc,(float*)x,(float*)y);
    for (r=0;r<nr;r++)
    {

```

```

    for (c=0;c<nc;c++)
        cout << " 1 / " << x[r][c] << " = "
                << y[r][c] << endl;
}
return(0);
}

```

The key syntax in this example is

```
extern "C" void reciprocal(int nr,int nc,
float *x,float *y);
```

where we have to pass pointers to the two d arrays.

33.19 Example 11: Passing a Rank 2 Array from C++ to Fortran and Taking Care of Array Storage

Two dimensional arrays are stored by column in Fortran and by row in C++. In this example we take care of the array element ordering changes between C++ and Fortran. We handle the change in the Fortran subroutine.

Here is the C++ calling program.

```
#include <iostream>
#include <iomanip>
using namespace std;
extern "C" void sums(int nr,int nc,
    int *x,int *rsum, int *csum);
int main()
{
    const int nr=2;
    const int nc=6;
    int x[nr][nc];
    int rsum[nr];
    int csum[nc];
    int r;
    int c;
    int i=1;
    for (r=0;r<nr;r++)
        for (c=0;c<nc;c++)
    {
        x[r][c]=i;
        i++;
    }
    for (r=0;r<nr;r++)
```

```

rsum[r]=0;
for (c=0;c<nc;c++)
    csum[c]=0;
cout << " C++ calling Fortran" << endl;
cout << " 2 d array as parameter\n";
cout << " Original 2 d array" << endl;
cout << endl;
for (r=0;r<nr;r++)
{
    for (c=0;c<nc;c++)
    {
        cout << setw(3) << x[r][c] << " ";
    }
    cout << endl;
}
cout << endl;
sums(nr,nc,(int*)x,rsum,csum);
for (r=0;r<nr;r++)
{
    for (c=0;c<nc;c++)
    {
        cout << setw(3) << x[r][c] << " ";
    }
    cout << " = " << rsum[r] << endl;
}
cout << endl;
for (c=0;c<nc;c++)
    cout << setw(3) << csum[c] << " ";
cout << endl;
return(0);
}

```

Here is the Fortran subroutine.

```

subroutine sums(nr, nc, x, rsum, csum) bind (c, &
name='sums')
! g++ needs -lgfortran to link
use iso_c_binding
implicit none
integer (c_int), value :: nr
integer (c_int), value :: nc
integer (c_int), dimension (1:nr, 1:nc), &
intent (in) :: x
integer (c_int), dimension (1:nr), &
intent (out) :: rsum
integer (c_int), dimension (1:nc), &

```

```

intent (out) :: csum
integer (c_int), dimension (1:nc, 1:nr) :: t

t = reshape(x, (/nc,nr/) )
rsum = sum(t, dim=1)
csum = sum(t, dim=2)
end subroutine sums

```

The key syntax in the C++ code is shown below.

```
extern "C" void sums(int nr,int nc,
int *x,int *rsum, int *csum);
```

where all arrays are passed by address.

The key statements in the Fortran are

```
t=reshape(x, (/nc,nr/))
```

where we use the `reshape` intrinsic to transform from row storage to column storage.

The `reshape` intrinsic and the following statements

```
rsum=sum(t,dim=1)
csum=sum(t,dim=2)
```

show the power and expressiveness of array handling in Fortran compared to the C family of languages (C, C++, C# and Java).

33.19.1 Compiler Switches

We now have to ensure that we include the necessary components of the Fortran run time system.

Here are details of how to make this work with the following compiler combinations.

```
gfortran and g++, openSuSe 13.1 and Windows
```

```
gfortran -c ch3311.f90 -o ch3111_f.o
g++          ch3311.c      ch3111_f.o -lgfortran
```

```
ifort and icc, openSuSe 13.1
```

```
ifort -c ch3311.f90 -o ch3111_f.o
icc       ch3311.cxx     ch3111_f.o
```

```
sunf90 and sunCC, openSuSe 13.1

sunf90 -c ch3311.f90 -o ch3111_f.o
sunCC      ch3312.cxx      ch3111_c.o -xlang=f90
```

33.20 Example 12: Passing a Rank 2 Array from C to Fortran and Taking Care of Array Storage

Two dimensional arrays are stored by column in Fortran and by row in C. In this example we take care of the array element ordering changes between C and Fortran. We handle the change in the Fortran subroutine.

Here is the C calling program.

```
#include <stdio.h>
void sums(int nr,int nc,int x[nr][nc],
           int * rsum, int * csum);
int main()
{
    const int nr=2;
    const int nc=6;
    int x[nr][nc];
    int rsum[nr];
    int csum[nc];
    int r;
    int c;
    int i=1;
    for (r=0;r<nr;r++)
        rsum[r]=0;
    for (c=0;c<nc;c++)
        csum[c]=0;
    for (r=0;r<nr;r++)
        for (c=0;c<nc;c++)
    {
        x[r][c]=i;
        i++;
    }
    printf(" C calling Fortran\n");
    printf(" 2 d array as parameter\n");
    printf(" c99 vla\n");
    for (r=0;r<nr;r++)
    {
        for (c=0;c<nc;c++)
    {
```

```

        printf(" %3d " , x[r][c]);
    }
    printf("\n");
}
printf("\n");
sums(nr,nc,x,rsum,csum);
for (r=0;r<nr;r++)
{
    for (c=0;c<nc;c++)
    {
        printf(" %3d " , x[r][c]);
    }
    printf(" %3d ",rsum[r]);
    printf("\n");
}
printf("\n");
for (c=0;c<nc;c++)
    printf(" %3d ",csum[c]);
printf("\n");
return(0);
}

```

Here is the Fortran subroutine.

```

subroutine sums(nr, nc, x, rsum, csum) bind (c, &
name='sums')
! gcc requires -lgfortran
use iso_c_binding
implicit none
integer (c_int), value :: nr
integer (c_int), value :: nc
integer (c_int), dimension (1:nr, 1:nc), &
intent (in) :: x
integer (c_int), dimension (1:nr), &
intent (out) :: rsum
integer (c_int), dimension (1:nc), &
intent (out) :: csum
integer (c_int), dimension (1:nc, 1:nr) :: t

t = reshape(x, (/nc,nr/))
rsum = sum(t, dim=1)
csum = sum(t, dim=2)
end subroutine sums

```

33.20.1 Compiler Switches

In this example we are calling a Fortran subroutine from C and the subroutine calls the `reshape` intrinsic function.

We now have to ensure that we include the necessary components of the Fortran run time system.

Here are details of how to make this work with the following compiler combinations.

gfortran and gcc, openSuSe 13.1 and Windows

```
gfortran -c ch3312.f90 -o ch3112_f.o
gcc         ch3312.c       ch3112_f.o -lgfortran
```

ifort andicc, openSuSe 13.1

```
ifort -c ch3312.f90 -o ch3112_f.o
icc      ch3312.c       ch3112_f.o
```

sunf90 and sunc99, openSuSe 13.1

```
sunf90 -c ch3312.f90 -o ch3112_f.o
sunc99 -c ch3312.c   -o ch3112_c.o
sunf90   ch3312_f.o   ch3112_c.o
```

33.21 Acknowledgements

Thanks to Steve Clamage of Oracle and Themis Tsikas of Nag for technical advice with some of C interop examples.

33.22 c_loc Examples on our Web Site

We have examples of using the `c_loc` function on our web site for both 32 bit and 64 bit operating systems.

<http://www.fortranplus.co.uk/>

Here is some background technical information on `c_loc` from the Fortran 2008 standard.

33.22.1 c_loc(x) Description

Description: Returns the C address of the argument.

Class: Inquiry function.

Argument: *x* shall either

- (1) have interoperable type and type parameters and be
 - (a) a variable that has the `target` attribute and is interoperable,
 - (b) an allocated allocatable variable that has the `target` attribute and is not an array of zero size, or
 - (c) an associated scalar pointer, or
- (2) be a nonpolymorphic scalar, have no length type parameters, and be
 - (a) a nonallocatable, nonpointer variable that has the `target` attribute,
 - (b) an allocated allocatable variable that has the `target` attribute, or
 - (c) an associated pointer.

Result Characteristics: Scalar of type `c_ptr`.

Result Value: The result value will be described using the result name `cptr`.

- (1) If *x* is a scalar data entity, the result is determined as if `c_ptr` were a derived type containing a scalar pointer component `px` of the type and type parameters of *x* and the pointer assignment

```
cptr%px => x
```

were executed.

- (2) If *x* is an array data entity, the result is determined as if `c_ptr` were a derived type containing a scalar pointer component `px` of the type and type parameters of *x* and the pointer assignment of `cptr%px` to the first element of *x* were executed.

If *x* is a data entity that is interoperable or has interoperable type and type parameters, the result is the value that the C processor returns as the result of applying the unary `&` operator (as defined in the C International Standard, 6.5.3.2) to the target of `cptr`.

The result is a value that can be used as an actual `cptr` argument in a call to `c_f_pointer` where `fptr` has attributes that would allow the pointer assignment

```
fptr => x
```

Such a call to `c_f_pointer` shall have the effect of the pointer assignment

```
fptr => x
```

NOTE 15.6—Where the actual argument is of noninteroperable type or type parameters, the result of `c_loc` provides an opaque “handle” for it. In an actual implementation, this handle may be the C address of the argument; however, portable C

functions should treat it as a `void` (generic) C pointer that cannot be dereferenced (6.5.3.2 in the C International Standard).

The key issues are that we must take care with the argument to the function, the return value is of type `c_ptr`, and that this is an opaque type. Let us now look at some examples using this function.

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33.23 Problems

33.1 Compile and run the example programs in this chapter with your compiler and examine the output.

Chapter 34

IEEE Arithmetic

Any effectively generated theory capable of expressing elementary arithmetic cannot be both consistent and complete. In particular, for any consistent, effectively generated formal theory that proves certain basic arithmetic truths, there is an arithmetical statement that is true, but not provable in the theory.

Godel, First incompleteness theorem

Aims

The aims of this chapter are to look in more depth at arithmetic and in particular at the support that Fortran provides for the IEEE 754 and later standards. There is a coverage of:

- hardware support for arithmetic.
- integer formats.
- floating point formats: single and double.
- special values: denormal, infinity and not a number—nan.
- exceptions and flags: divide by zero, inexact, invalid, overflow, underflow.

34.1 Introduction

The literature contains details of the IEEE arithmetic standards. The bibliography contains details of a number of printed and on-line sources.

34.2 History

When we use programming languages to do arithmetic two major concerns are the ability to develop reliable and portable numerical software. Arithmetic is done in hardware and there are a number of things to consider:

- the range of hardware available both now and in the past.
- the evolution of hardware.

Table 34.1 Computer hardware and manufacturers

CDC	Cray	IBM	ICL
Fujitsu	DEC	Compaq	Gateway
Sun	Silicon Graphics	Hewlett Packard	Data General
Harris	Honeywell	Elliot	Mostek
National Semiconductors	Intel	Zilog	Motorola
Signetics	Amdahl	Texas Instruments	Cyrix
AMD	NEC		

Table 34.2 Operating systems

NOS	NOS/BE	Kronos	UNIX
VMS	Dos	Windows 3.x	Windows 95
Windows 98	Windows NT	Windows 2000	Windows XP
Windows Vista	Windows 7.x	Windows 8.x	MVS
VM	VM/CMS	CP/M	Macintosh
OS/2	Linux (too many)		

There has been a very considerable change in arithmetic units since the first computers. Table 34.1 is a list of hardware and computing systems that the authors have used or have heard of. It is not exhaustive or definitive, but rather reflects the authors' age and experience.

Table 34.2 lists some of the operating systems.

Again the list is not exhaustive or definitive. The intention is simply to provide some idea of the wide range of hardware, computer manufacturers and operating systems that have been around in the past 50 years.

To cope with the anarchy in this area Doctor Robert Stewart (acting on behalf of the IEEE) convened a meeting which led to the birth of IEEE 754.

The first draft, which was prepared by William Kahan, Jerome Coonen and Harold Stone, was called the KCS draft and eventually adopted as IEEE 754. A fascinating account of the development of this standard can be found in An Interview with the Old Man of Floating Point, and the bibliography provides a web address for this interview. Kahan went on to get the ACM Turing Award in 1989 for his work in this area.

This has become a de facto standard amongst arithmetic units in modern hardware. Note that it is not possible to describe precisely the answers a program will give, and the authors of the standard knew this. This goal is virtually impossible to achieve when one considers floating point arithmetic. Reasons for this include:

- the conversions of numbers between decimal and binary formats.
- the use of elementary library functions.
- results of calculations may be in hardware inaccessible to the programmer.
- intermediate results in subexpressions or arguments to procedures.

The bibliography contains details of a paper that addresses this issue in much greater depth—Differences Among IEEE 754 Implementations.

Fortran is one of a small number of languages that provides access to IEEE arithmetic, and it achieves this via TR1880 which is an integral part of Fortran 2003. The C standard (C9X) addresses this issue and Java offers limited IEEE arithmetic support. More information can be found in the references at the end of the chapter.

34.3 IEEE 754 Specifications

The standard specifies a number of things including:

- single precision floating point format.
- double precision floating point format.
- two classes of extended floating point formats.
- accuracy requirements on the following floating point operations:
 - add.
 - subtract.
 - multiply.
 - divide.
 - square root.
 - remainder.
 - round numbers in floating point format to integer values.
 - convert between different floating point formats.
 - convert between floating point and integer format.
 - compare.
- base conversion, i.e., when converting between decimal and binary floating point formats and vice versa.
- exception handling for:
 - divide by zero.
 - overflow.
 - underflow.
 - invalid operation.
 - inexact.
- rounding directions.
- rounding precisions.

We will look briefly at each of these requirements.

34.3.1 Single Precision Floating Point Format

This is a 32-bit quantity made up of a sign bit, 8-bit biased exponent and 23-bit mantissa. The standard also specifies that certain of the bit patterns are set aside and do not represent normal numbers. This means that valid numbers are in the range 3.40282347E+38–1.17549435E-38 and the precision is between 6 and 9 digits depending on the numbers.

The special bit patterns provide the following:

- +0
- -0
- subnormal numbers in the range 1.17549421E-38–1.40129846E-45
- $+\infty$
- $-\infty$
- quiet NaN (Not a Number)
- signalling NaN

One of the first systems that the authors worked with that had special bit patterns set aside was the CDC 6000 range of computers that had negative indefinite and infinity. Thus the ideas are not new, as this was in the late 1970s.

The support of positive and negative zero means that certain problems can be handled correctly including:

- The evaluation of the log function which has a discontinuity at zero.
- The equation $\sqrt{1/z} = 1/z$ can be solved when $z = -1$

See also the Kahan paper *Branch Cuts for complex Elementary functions, or Much Ado About Nothing's Sign Bit* for more details.

Subnormals, which permit gradual underflow, fill the gap between 0 and the smallest normal number.

Simply stated underflow occurs when the result of an arithmetic operation is so small that it is subject to a larger than normal rounding error when stored. The existence of subnormals means that greater precision is available with these small numbers than with normal numbers. The key features of gradual underflow are:

- When underflow does occur there should never be a loss of accuracy any greater than that from ordinary roundoff.
- The operations of addition, subtraction, comparison and remainder are always exact.
- Algorithms written to take advantage of subnormal numbers have smaller error bounds than other systems.
- if x and y are within a factor of 2 then $x-y$ is error free, which is used in a number of algorithms that increase the precision at critical regions.

The combination of positive and negative zero and subnormal numbers means that when x and y are small and $x-y$ has been flushed to zero the evaluation of $1/(x-y)$ can be flagged and located.

Certain arithmetic operations cause problems including:

- $0 * \infty$
- $0/0$
- \sqrt{x} when $x < 0$

and the support for NaN handles these cases.

The support for positive and negative infinity allows the handling of $x/0$ when x is nonzero and of either sign, and the outcome of this means that we write our programs to take the appropriate action. In some cases this would mean recalculating using another approach.

For more information see the references in the bibliography.

34.3.2 Double Precision Floating Point Format

This is a 64-bit quantity made up of a sign bit, 11-bit biased exponent and 52-bit mantissa. As with single precision the standard specifies that certain of the bit patterns are set aside and do not represent normal numbers. This means we have valid numbers in the range $1.7976931348623157E308$ – $2.2250738585072014E-308$ and precision between 15 and 17 digits depending on the numbers.

As with single precision there are bit patterns set aside for the same special conditions.

Note that this does not mean that the hardware has to handle the manipulation of this 64-bit quantity in an identical fashion. The Sparc and Intel family handle the above as two 32-bit quantities but the order of the two component parts is reversed—so-called big endian and little endian.

34.3.3 Two Classes of Extended Floating Point Formats

These formats are not mandatory. A number of variants of double extended exist including:

- Sun—four 32-bit words, one sign bit, 15-bit biased exponent and 112-bit mantissa, numbers in the range $3.362E-4932$ – $1.189E4932$, 33–36 digits of significance.
- Intel—10 bytes—one sign bit, 15-bit biased exponent, 63-bit mantissa, numbers in the range $3.362E-4932$ to $1.189E4932$, 18–21 digits of significance.
- PowerPC—as Sun.

34.3.4 Accuracy Requirements

Remainder and compare must be exact. The rest should return the exact result if possible. If not, there are well-defined rounding rules to apply.

34.3.5 Base Conversion—Converting Between Decimal and Binary Floating Point Formats and Vice Versa

These results should be exact if possible; if not the results must differ by tolerances that depend on the rounding mode.

34.3.6 Exception Handling

It must be possible to signal to the user the occurrence of the following conditions or exceptions:

- divide by zero.
- overflow.
- underflow.
- invalid operation.
- inexact.

The ability to detect the above is a big step forward in our ability to write robust and portable code. These operations do occur in calculations and it is essential for the programmer to have control over what action to take.

34.3.7 Rounding Directions

Four rounding directions are available:

- nearest—the default.
- down.
- up.
- chop.

Access to directed rounding can be used to implement interval arithmetic, for example.

34.3.8 Rounding Precisions

The only mandatory part here is that machines that perform computations in extended mode let the programmer control the precision via a control word. This means that if software is being developed on machines that support extended modes those machines can be switched to a mode that would enable the software to run on a system that didn't support extended modes. This area looks like a can of worms. Look at the Kahan paper for more information—*Lecture Notes on the Status of IEEE 754*.

34.4 Resume

The above has provided a quick tour of IEEE 754. We'll now look at what Fortran has to offer to support it.

34.5 Fortran Support for IEEE Arithmetic

Fortran first introduced support for IEEE arithmetic in ISO TR 15580. The Fortran 2003 standard integrated support into the main standard. It is Sect. 14 of the standard.

The intrinsic modules

- `ieee_features`
- `ieee_exceptions`
- `ieee_arithmetic`

provide support for exceptions and IEEE arithmetic. Whether the modules are provided is processor dependent. If the module `ieee_features` is provided, which of the named constants defined in this standard are included is processor dependent. The module `ieee_arithmetic` behaves as if it contained a `use` statement for `ieee_exceptions`; everything that is public in `ieee_exceptions` is public in `ieee_arithmetic`.

The first thing to consider is the degree of conformance to the IEEE standard. It is possible that not all of the features are supported. Thus the first thing to do is to run one or more test programs to determine the degree of support for a particular system.

34.6 Derived Types and Constants Defined in the Modules

The modules

- ieee_exceptions
- ieee_arithmetic
- ieee_features

define five derived types, whose components are all private.

34.6.1 *ieee_exceptions*

This module defines ieee_flag_type, for identifying a particular exception flag.

Possible values are

```
ieee_invalid
ieee_overflow
ieee_divide_by_zero
ieee_underflow
ieee_inexact
```

The module also defines the array named constants

```
ieee_usual = (/ ieee_overflow, &
              ieee_divide_by_zero, ieee_invalid /)

ieee_all = (/ ieee_usual, ieee_underflow, &
            ieee_inexact /)

ieee_status_type
```

The last is for saving the current floating point status.

34.6.2 *ieee_arithmetic*

This module defines ieee_class_type, for identifying a class of floating-point values.

Possible values are:

```
ieee_signaling_nan  
ieee_quiet_nan  
ieee_negative_inf  
ieee_negative_normal  
ieee_negative_denormal  
ieee_negative_zero  
ieee_positive_zero  
ieee_positive_denormal  
ieee_positive_normal  
ieee_positive_inf  
ieee_other_value
```

The module defines `ieee_round_type`, for identifying a particular rounding mode. Its only possible values are those of named constants defined in the module: `ieee_nearest`, `ieee_to_zero`, `ieee_up`, and `ieee_down` for the `ieee_modes`; and `ieee_other` for any other mode.

The elemental operator `==` for two values of one of these types to return true if the values are the same and false otherwise.

The elemental operator `/=` for two values of one of these types to return true if the values differ and false otherwise.

34.6.3 ieee_features

This module defines `ieee_features_type`, for expressing the need for particular `ieee_features`. Its only possible values are those of named constants defined in the module: `ieee_datatype`, `ieee_denormal`, `ieee_divide`, `ieee_halting`, `ieee_inexact_flag`, `ieee_inf`, `ieee_invalid_flag`, `ieee_nan`, `ieee_rounding`, `ieee_sqrt`, and `ieee_underflow_flag`.

34.6.4 Further Information

There are a number of additional sources of information.

- The standard.
- Documentation that comes with your compiler.

The latter has the benefit of describing what is supported in that compiler.

34.7 Example 1: Testing IEEE Support

The first examples test basic IEEE arithmetic support.

Here is a program to illustrate the above.

```
program ch3401

use precision_module
use ieee_arithmetic

implicit none

real (sp) :: x = 1.0
real (dp) :: y = 1.0_dp
real (qp) :: z = 1.0_qp

if (ieee_support_datatype(x)) then
    print *, ' 32 bit IEEE support'
end if
if (ieee_support_datatype(y)) then
    print *, ' 64 bit IEEE support'
end if
if (ieee_support_datatype(z)) then
    print *, ' 128 bit IEEE support'
end if

end program ch3401
```

Table 34.3 summarises the support for a number of compilers.

Table 34.3 Compiler IEEE support for various precisions

Precision	gfortran	intel	nag	sun
32 bit IEEE support	Yes	Yes	Yes	Yes
64 bit IEEE support	Yes	Yes	Yes	Yes
128 bit IEEE support	No	Yes	No	Yes

34.8 Example 2: Testing What Flags are Supported

Here is a program to illustrate the above.

```
program ch3402

use precision_module
use ieee_arithmetic

implicit none

real (sp) :: x = 1.0
real (dp) :: y = 1.0_dp
real (qp) :: z = 1.0_qp

integer :: i

character *20, dimension (5) :: flags = (/ &
'IEEE_DIVIDE_BY_ZERO ', &
'IEEE_INEXACT ', &
'IEEE_INVALID ', &
'IEEE_OVERFLOW ', &
'IEEE_UNDERFLOW ' /)

do i = 1, 5
  if (ieee_support_flag(ieee_all(i),x)) then
    write (unit=*, fmt=100) flags(i)
100   format (a20, ' 32 bit support')
  end if
  if (ieee_support_flag(ieee_all(i),y)) then
    write (unit=*, fmt=110) flags(i)
110   format (a20, ' 64 bit support')

  end if
  if (ieee_support_flag(ieee_all(i),z)) then
    write (unit=*, fmt=120) flags(i)
120   format (a20, '128 bit support')
  end if
end do

end program ch3402
```

Here is the output from the Intel compiler.

IEEE_DIVIDE_BY_ZERO	32 bit support
IEEE_DIVIDE_BY_ZERO	64 bit support
IEEE_DIVIDE_BY_ZERO	128 bit support
IEEE_INEXACT	32 bit support
IEEE_INEXACT	64 bit support
IEEE_INEXACT	128 bit support
IEEE_INVALID	32 bit support
IEEE_INVALID	64 bit support
IEEE_INVALID	128 bit support
IEEE_OVERFLOW	32 bit support
IEEE_OVERFLOW	64 bit support
IEEE_OVERFLOW	128 bit support
IEEE_UNDERFLOW	32 bit support
IEEE_UNDERFLOW	64 bit support
IEEE_UNDERFLOW	128 bit support

34.9 Example 3: Overflow

Here is a program to illustrate the above.

```

program ch3403

use ieee_arithmetic

implicit none
integer :: i
real :: x = 1.0
logical :: overflow_happened = .false.

if (ieee_support_datatype(x)) then
print *, &
      ' IEEE support for default precision'
end if

do i = 1, 50
  if (overflow_happened) then
    print *, ' overflow occurred '
    print *, ' program terminates'
    stop 20
  else
    print 100, i, x
  100 format (' ', i3, ' ', e12.4)
end if

```

```
    end if
    x = x*10.0
    call ieee_get_flag(ieee_overflow, &
        overflow_happened)
end do
end program ch3403
```

34.10 Example 4: Underflow

Here is a program to illustrate the above.

```
program ch3404

use ieee_arithmetic

implicit none
integer :: i
real :: x = 1.0
logical :: underflow_happened = .false.

if (ieee_support_datatype(x)) then
    print *, ' IEEE arithmetic '
    print *, &
        ' is supported for default precision'
end if

do i = 1, 50
    if (underflow_happened) then
        print *, ' underflow occurred '
        print *, ' program terminates'
        stop 20
    else
        print 100, i, x
    end if
    x = x/10.0
    call ieee_get_flag(ieee_underflow, &
        underflow_happened)
end do
end program ch3404
```

34.11 Example 5: Inexact Summation

Here is a program to illustrate the above.

```

program ch3405

use ieee_arithmetic
implicit none

integer :: i
real :: computed_sum
real :: real_sum
integer :: array_size

logical :: inexact_happened = .false.
integer :: allocate_status

character *13, dimension (3) :: heading = (/ &
    ' 10,000,000', ' 100,000,000', &
    '1,000,000,000' /)

real, allocatable, dimension(:) :: x

if (ieee_support_datatype(x)) then
    print *, &
        ' IEEE support for default precision'
end if

! 1234567

array_size = 10000000

do i = 1, 3
    write (unit=*, fmt=100) array_size, &
        heading(i)
100 format (' Array size = ', i15, 2x, a13)
    allocate (x(1:array_size), stat= &
        allocate_status)
    if (allocate_status/=0) then
        print *, ' Allocate fails, program ends'
        stop
    end if
    x = 1.0
    computed_sum = sum(x)

```

```
call ieee_get_flag(ieee_inexact, &
    inexact_happened)
real_sum = array_size*1.0
write (unit=*, fmt=110) computed_sum
110 format (' Computed sum = ', e12.4)
write (unit=*, fmt=120) real_sum
120 format (' Real sum      = ', e12.4)
if (inexact_happened) then
    print *, ' inexact arithmetic'
    print *, ' in the summation'
    print *, ' program terminates'
    stop 20
end if
deallocate (x)
array_size = array_size*10
end do

end program ch3405
```

Here is the output from several compilers.

gfortran

```
IEEE support for default precision
Array size =          10000000      10,000,000
Computed sum =     0.1000E+08
Real sum      =     0.1000E+08
Array size =          100000000      100,000,000
Computed sum =     0.1000E+09
Real sum      =     0.1000E+09
inexact arithmetic
in the summation
program terminates
```

Intel

```
IEEE support for default precision
Array size =          10000000      10,000,000
Computed sum =     0.1000E+08
Real sum      =     0.1000E+08
Array size =          100000000      100,000,000
```

```
Computed sum = 0.1000E+09
Real sum      = 0.1000E+09
inexact arithmetic
in the summation
program terminates
```

nag

```
IEEE support for default precision
Array size = 10000000 10,000,000
Computed sum = 0.1000E+08
Real sum      = 0.1000E+08
Array size = 100000000 100,000,000
Computed sum = 0.1678E+08
Real sum      = 0.1000E+09
inexact arithmetic
in the summation
program terminates
```

sun/oracle

```
IEEE support for default precision
Array size = 10000000 10,000,000
Computed sum = 0.1000E+08
Real sum      = 0.1000E+08
Array size = 100000000 100,000,000
Computed sum = 0.1678E+08
Real sum      = 0.1000E+09
inexact arithmetic
in the summation
program terminates
```

What do you notice about the value of the computed sum?

34.12 Example 6: NAN and Other Specials

Here is a program to illustrate some additional IEEE functionality.

```
program ch3406
```

```
use precision_module
use ieee_arithmetic
implicit none

real (sp) :: x0 = 0.0
real (dp) :: y0 = 0.0_dp
real (qp) :: z0 = 0.0_qp

real (sp) :: x1 = 1.0
real (dp) :: y1 = 1.0_dp
real (qp) :: z1 = 1.0_qp

real (sp) :: xnan = 1.0
real (dp) :: ynan = 1.0_dp
real (qp) :: znan = 1.0_qp

real (sp) :: xinfinite = 1.0
real (dp) :: yinfinite = 1.0_dp
real (qp) :: zinfinite = 1.0_qp

xinfinite = x1/x0
yinfinite = y1/y0
zinfinite = z1/z0
xnan = x0/x0
ynan = y0/y0
znan = z0/z0

if (ieee_support_datatype(x1)) then
    print *, ' 32 bit IEEE support'
    print *, '      inf ', ieee_support_inf(x1)
    print *, '      nan ', ieee_support_nan(x1)
    print *, ' 1/0 finite', ieee_is_finite( &
        xinfinite)
    print *, ' 0/0 nan', ieee_is_nan(xnan)
end if

if (ieee_support_datatype(y1)) then
    print *, ' 64 bit IEEE support'
    print *, '      inf ', ieee_support_inf(y1)
    print *, '      nan ', ieee_support_nan(y1)
    print *, ' 1/0 finite', ieee_is_finite( &
        yinfinite)
    print *, ' 0/0 nan', ieee_is_nan(ynan)
end if
```

```

if (ieee_support_datatype(z1)) then
    print *, ' 128 bit IEEE support'
    print *, '      inf ', ieee_support_inf(z1)
    print *, '      nan ', ieee_support_nan(z1)
    print *, ' 1/0 finite', ieee_is_finite( &
        zinfinite)
    print *, ' 0/0 nan', ieee_is_nan(znan)
end if

end program ch3406

```

34.13 Summary

Compiler support in this area is now quite widespread as the above examples have shown.

Bibliography

Hauser, J.R.: Handling floating point exceptions in numeric programs. ACM Trans. Program. Lang. Syst. **18**(2), 139–174 (1996)

- The paper looks at a number of techniques for handling floating point exceptions in numeric code. One of the conclusions is for better structured support for floating point exception handling in new programming languages, or of course better standards for existing languages.

IEEE: IEEE Standard for Binary Floating-Point Arithmetic, ANSI/IEEE Std 754-2008, Institute of Electrical and Electronic Engineers Inc.

- The formal definition of IEEE 754. This is available for purchase as both a pdf and printed version—see the address below.

[http://www.techstreet.com/standards/
IEEE/754_2008?product_id=1745167](http://www.techstreet.com/standards/IEEE/754_2008?product_id=1745167)

This standard specifies formats and methods for floating-point arithmetic in computer systems: standard and extended functions with single, double, extended, and extendable precision, and recommends formats for data interchange. Exception conditions are defined and standard handling of these conditions is specified. Keywords: 754-2008, arithmetic, binary, computer, decimal, exponent, floating-point, format, interchange, NaN, number, rounding, significand, subnormal. Product Code(s): STDPD95802, STD95802

Knuth, D.: Seminumerical Algorithms. Addison-Wesley (1969)

- There is a coverage of floating point arithmetic, multiple precision arithmetic, radix conversion and rational arithmetic.

Sun: Numerical Computation Guide. SunPro.

- Very good coverage of the numeric formats for IEEE Standard 754 for Binary Floating-Point Arithmetic. All SunPro compiler products support the features of the IEEE 754 standard.

Web-Based Sources

<http://validgh.com/goldberg/addendum.html>

- Differences Among IEEE 754 Implementations. The material in this paper will eventually be included in the Sun Numerical Computation Guide as an addendum to Appendix C, David Goldberg's What Every Computer Scientist Should Know about Floating Point Arithmetic.

<http://docs.oracle.com/cd/E19422-01/819-3693/819-3693.pdf>
<http://docs.sun.com/>

- The Numerical Computation Guide can be browsed on-line or downloaded as a pdf file. The last time we checked it was 294 pages. Good source of information if you have Sun equipment.

<http://babbage.cs.qc.edu/courses/cs341/IEEE-754references.html>

- Brief coverage of IEEE arithmetic with pointers to further sources. There is also a coverage of the storage layout and ranges of floating point numbers. Computer Science 341 is an introduction to the design of a computer's hardware, particularly the CPU and memory systems.

<http://www.math.psu.edu/dna/disasters/ariadne.html>

- The Explosion of the Ariane 5: A 64-bit floating point number relating to the horizontal velocity of the rocket with respect to the platform was converted to a 16-bit signed integer. The number was larger than 32,768, the largest integer storeable in a 16-bit signed integer, and thus the conversion failed.

Hardware Sources

Amd—Visit

<http://developer.amd.com/documentation/guides/pages/default.aspx>

for details of the AMD manuals. The following five manuals are available for download as pdf's from the above site.

- AMD64 Architecture Programmer's Manual Volume 1: Application Programming
- AMD64 Architecture Programmer's Manual Volume 2: System Programming
- AMD64 Architecture Programmer's Manual Volume 3: General Purpose and System Instructions
- AMD64 Architecture Programmer's Manual Volume 4: 128-bit and 256 bit media instructions
- AMD64 Architecture Programmer's Manual Volume 5: 64-Bit Media and x87 Floating-Point Instructions

Intel—Visit

<http://www.intel.com/products/processor/manuals/index.htm>

for a list of manuals. The following three manuals are available for download as pdf's from the above site.

- Intel 64 and IA-32 Architectures Software Developer's Manual. Volume 1: Basic Architecture
- Intel 64 and IA-32 Architectures Software Developer's Manual. Combined Volumes 2A and 2B: Instruction Set Reference, A-Z.
- Intel 64 and IA-32 Architectures Software Developer's Manual. Combined Volumes 3A and 3B: System Programming Guide, Parts 1 and 2

Osbourne, A., Kane, G.: 4-bit and 8-bit Microprocessor Handbook. Osbourne and McGraw Hill (1981)

- Good source of information on 4-bit and 8-bit microprocessors.

Osbourne, A., Kane, G.: 16-Bit Microprocessor Handbook. Osbourne and McGraw Hill (1981)

- Ditto 16-bit microprocessors.

Bhandarkar, D.P.: Alpha Implementations and Architecture: Complete Reference and Guide. Digital Press (1996)

- Looks at some of the trade-offs and design philosophy behind the alpha chip. The author worked with VAX, MicroVAX and VAX vectors as well as the Prism. Also looks at the GEM compiler technology that DEC/Compaq use.

Various companies home pages.

<http://www.ibm.com/>
IBM home page.
<http://www.sgi.com/>
Silicon Graphics home page.

Operating Systems

Deitel, H.M.: An Introduction to Operating Systems. Addison-Wesley (1990)

- The revised first edition includes case studies of UNIX, VMS, CP/M, MVS and VM. The second edition adds OS/2 and the Macintosh operating systems. There is a coverage of hardware, software, firmware, process management, process concepts, asynchronous concurrent processes, concurrent programming, deadlock and indefinite postponement, storage management, real storage, virtual storage, processor management, distributed computing, disk performance optimisation, file and database systems, performance, coprocessors, risc, data flow, analytic modelling, networks, security and it concludes with case studies of the these operating systems. The book is well written and an easy read.

34.14 Problems

34.1 Compile and run each of the examples in this chapter with your compiler(s). If you have access to more than one compiler do the compilers behave in the same way?

Chapter 35

Miscellaneous Examples

*The Analytical Engine weaves algebraic patterns, just as the
Jacquard loom weaves flowers and leaves.*

Ada Lovelace

Aims

We look at a number of additional examples including

- the earlier date derived type extended with US and ISO date formats
- a binary search example
- three sorting examples, including a recursive algorithm, a non recursive algorithm and a parallelised subroutine from the Nag library
 - timing details for our generic serial Quicksort algorithm for five of the numeric kind types
 - timing details of the Netlib serial non recursive Quicksort for 32 bit integers, 32 bit reals and 64 bit reals
 - a comparison of the timing of the above two sorting algorithms
 - the Nag SMP sorting routine m01caf for 64 bit reals
 - timing details of the parallel Nag sorting subroutine
- graphics libraries
- the dislin graphics library
- examples calling the dislin library.

35.1 Example 1: Date Data Type with USA and ISO Support

In Chap. 22 Example 6, we introduced a derived date type. To handle the other two date formats we have added an extra component to this derived type. Here is the updated type.

```
type, public :: date
private
integer :: day
```

```
integer :: month
integer :: year
integer :: date_type = 1
end type date
```

When we use the default constructor we set the `date_type` to 1. An integer variable is often used in a problem like this. In the `date_iso` constructor we set `date_type` to 3 and in the `date_us` constructor set `date_type` to 2.

The only other method we have to alter is the `print_date` method. In this method we have an `if` then `else` construct to choose how to print the date, based on the date type.

We have solved the problem of how to handle a variety of date formats in a simple, non object oriented fashion. Here is the complete program and module from Chap. 22.

```
module date_module
  implicit none

  private

  type, public :: date
    private
    integer :: day
    integer :: month
    integer :: year
    integer :: date_type = 1
  end type date

  character (9) :: day(0:6) = (/ 'Sunday  ', &
    'Monday  ', 'Tuesday  ', 'Wednesday', &
    'Thursday ', 'Friday   ', 'Saturday  ' /)
  character (9) :: month(1:12) = (/ 'January  ', &
    'February ', 'March    ', 'April    ', &
    'May      ', 'June     ', 'July     ', &
    'August   ', 'September', 'October  ', &
    'November ', 'December ' /)

  public :: calendar_to_julian, date_, date_iso, &
    date_us, date_to_day_in_year, &
    date_to_weekday_number, get_day, get_month, &
    get_year, julian_to_date, &
    julian_to_date_and_week_and_day, ndays, &
    print_date, year_and_day_to_date

contains

  function date_(dd, mm, yyyy) result (x)
    implicit none
    type (date) :: x
    integer, intent (in) :: dd, mm, yyyy
    integer :: dt = 1

    x = date(dd, mm, yyyy, dt)
  end function date_
```

```
function date_iso(yyyy, mm, dd) result (x)
    implicit none
    type (date) :: x
    integer, intent (in) :: dd, mm, yyyy
    integer :: dt = 3

    x = date(dd, mm, yyyy, dt)
end function date_iso

function date_us(mm, dd, yyyy) result (x)
    implicit none
    type (date) :: x
    integer, intent (in) :: dd, mm, yyyy
    integer :: dt = 2

    x = date(dd, mm, yyyy, dt)
end function date_us

include 'date_module_common_code.f90'

function print_date(x, day_names, &
    short_month_name, digits)
    implicit none
    type (date), intent (in) :: x
    logical, optional, intent (in) :: day_names, &
        short_month_name, digits
    character (30) :: print_date
    integer :: pos
    logical :: want_day, want_short_month_name, &
        want_digits
    integer :: l, t
    intrinsic len_trim, present, trim

    want_day = .false.
    want_short_month_name = .false.
    want_digits = .false.
    print_date = ' '
    if (present(day_names)) then
        want_day = day_names
    end if
    if (present(short_month_name)) then
        want_short_month_name = short_month_name
    end if
    if (present(digits)) then
        want_digits = digits
    end if
! Start of code dependent on date_type
! day month year
    if (x%date_type==1) then
        if (want_digits) then
            write (print_date(1:2), '(i2)') x%day
            print_date(3:3) = '/'
            write (print_date(4:5), '(i2)') x%month
            print_date(6:6) = '/'
            write (print_date(7:10), '(i4)') x%year
        else
```

```

if (want_day) then
    pos = date_to_weekday_number(x)
    print_date = trim(day(pos)) // ''
    pos = len_trim(print_date) + 2
else
    pos = 1
    print_date = ''
end if
write (print_date(pos:pos+1), '(i2)') &
    x%day
if (want_short_month_name) then
    print_date(pos+3:pos+5) =
        = month(x%month)(1:3)
    pos = pos + 7
else
    print_date(pos+3:) = month(x%month)
    pos = len_trim(print_date) + 2
end if
write (print_date(pos:pos+3), '(i4)') &
    x%year
end if
else if (x%date_type==2) then
! month day year
    if (want_digits) then
        write (print_date(1:2), '(i2)') x%month
        print_date(3:3) = '/'
        write (print_date(4:5), '(i2)') x%day
        print_date(6:6) = '/'
        write (print_date(7:10), '(i4)') x%year
    else
        pos = 1
        if (want_short_month_name) then
            print_date(pos:pos+2) = month(x%month) &
                (1:3)
            pos = pos + 4
        else
            print_date(pos:) = month(x%month)
            pos = len_trim(print_date) + 2
        end if
        if (want_day) then
            t = date_to_weekday_number(x)
            l = len Trim(day(t))
            print_date(pos:pos+1) = trim(day(t)) &
                // ''
            pos = len Trim(print_date) + 2
        end if
        write (print_date(pos:pos+1), '(i2)') &
            x%day
        pos = pos + 3
        write (print_date(pos:pos+3), '(i4)') &
            x%year
    end if
else if (x%date_type==3) then
! year month day
    if (want_digits) then
        write (print_date(1:4), '(i4)') x%year

```

```

print_date(5:5) = '/'
write (print_date(6:7), '(i2)') x%month
print_date(8:8) = '/'
write (print_date(9:10), '(i2)') x%day
else
  pos = 1
  write (print_date(pos:pos+3), '(i4)') &
    x%year
  pos = pos + 5
  if (want_short_month_name) then
    print_date(pos:pos+2) = month(x%month) &
      (1:3)
    pos = pos + 4
  else
    print_date(pos:) = month(x%month)
    pos = len_trim(print_date) + 2
  end if
  if (want_day) then
    t = date_to_weekday_number(x)
    l = len_trim(day(t))
    print_date(pos:pos+l) = trim(day(t))
    pos = pos + l + 1
  end if
  write (print_date(pos:pos+1), '(i2)') &
    x%day
  end if
end if
return
end function print_date

end module date_module

include 'date_module.f90'

program ch3501
use date_module, only: calendar_to_julian, &
  date, date_, date_iso, date_us, &
  date_to_day_in_year, date_to_weekday_number, &
  get_day, get_month, get_year, &
  julian_to_date_and_week_and_day, ndays, &
  print_date, year_and_day_to_date

implicit none
integer :: i
integer, parameter :: n = 3
type (date), dimension (1:n) :: x

x(1) = date_(11, 2, 1952)
x(2) = date_us(2, 11, 1952)
x(3) = date_iso(1952, 2, 11)

do i = 1, 3
  print *, print_date(x(i))
end do

end program ch3501

```

35.2 Example 2: Binary Search Example

Searching is a common problem in programming. Wirth's book has a short chapter on searching, with coverage of

- linear search
- binary search
- table search
- straight string search
- the Knuth-Morris-Pratt string search
- the Boyer-Moore string search

A linear search of a collection can obviously be quite an expensive operation. The worst case is that the object of interest is the last member of the collection.

In this example we make the assumption that the data is sorted and can then use a very efficient algorithm—a binary search. Here is the program.

```
include 'timing_module.f90'

module character_binary_search_module

contains

function binary_search(x,n,key) result (position)
implicit none

! Algorithm taken from Algorithms +
! Data Structures - N. Wirth
! ISBN 0-13-021999-1
! Pages 57:59
integer , intent(in) :: n
character*32 , dimension(1:n) , intent(in) :: x
character*32 , intent(in) :: key

integer :: position
integer :: l,r,m

l=1
r=n

do while(l<r)
  m=(l+r)/2
  if ( x(m) < key ) then
    l=m+1
  else
    r=m
  end if
end do

if ( x(r) == key ) then
  position = r
else
  position = 0
endif
```

```
end function binary_search

end module character_binary_search_module

program ch3502
use character_binary_search_module
use timing_module
implicit none

integer , parameter :: nwords=173528
character*32 , dimension(1:nwords) :: dictionary
character*32 :: word
character*1 :: answer
integer :: position

call start_timing()

call read_words()

write (*,10) time_difference()
10 format(2x,f7.3)

do

print * , 'Type in the word you are looking for'
read * , word

write (*,10) time_difference()

position=binary_search(dictionary,nwords,word)

write (*,10) time_difference()

if (position == 0) then
print *, 'Word not found'
else
write (*,20) trim(word) , position
20 format( a , ' found at position ',i6)
end if

print *, ' Try again (y/n) ?'
read *,answer

if ( (answer == 'y') .or. (answer=='Y') ) then
cycle
else
exit
endif

end do

call end_timing()

contains

subroutine read_words()
```

```

implicit none
integer :: i
character*80 :: file_name = "words.txt"

open(unit=10,file=file_name)
do i=1,nwords
    read (10,10) dictionary(i)
    10 format(a)
end do
close(10)

end subroutine read_words

end program ch3502

```

The program reads in a dictionary. Historically on Unix systems there was a spelling checker, and there would be a *words* file, often in

/etc

This is an example of one of these files. Many language versions were available. We then search the dictionary to see if the word entered is in the dictionary. The program provides timing information.

Here is the output from a sample run. The data was read from a file.

```

2015/ 3/10 14:56: 8 430
 0.070
Type in the word you are looking for
 0.000
 0.000
qwerty found at position 122712
Try again (y/n) ?
Type in the word you are looking for
 0.000
 0.000
Word not found
Try again (y/n) ?
Type in the word you are looking for
 0.000
 0.000
albumin found at position   3309
Try again (y/n) ?
Type in the word you are looking for
 0.000
 0.000
transubstantiation found at position 158170
Try again (y/n) ?
2015/ 3/10 14:56: 8 500

```

As can be seen the timing reading in the file takes less than one tenth of a second, and the search takes less than a microsecond—the resolution made available via the `date_time` subroutine.

The dictionary has over 170,000 words. Handy for Scrabble!

35.3 Comparison of Three Sorting Methods

We next look at a comparison of the timing details of three sorting methods. We use a serial recursive Quicksort, a serial non-recursive Quicksort and the Nag library parallel sorting routine m01caf. The Nag library works with 64 bit reals.

35.4 Example 3: Generic Recursive Quicksort Example with Timing Details

This example has several components

- a module called `precision_module` from Chap. 21
- a module called `integer_kind_module` from Chap. 25
- a timing module
- the generic Quicksort module from Chap. 25
- a main program to provide the timing information

Here is the source code for the main program. The source code for the other modules is the same as in earlier chapters.

```
include 'integer_kind_module.f90'
include 'precision_module.f90'
include 'sort_data_module.f90'
include 'timing_module.f90'

program ch3503

use sort_data_module
use timing_module

implicit none
integer , parameter :: n =      100000000
character*12          :: nn = "100,000,000"
character*80          :: report_file_name = &
                        "ch3503.report"

real     (sp)  , allocatable, dimension(:) :: x_sp
real     (dp)  , allocatable, dimension(:) :: x_dp
real     (qp)  , allocatable, dimension(:) :: x_qp
integer (i32) , allocatable, dimension(:) :: y_i32
integer (i64) , allocatable, dimension(:) :: y_i64

integer :: allocate_status=0

character*20 , dimension(5) :: heading1 &
= [ ' 32 bit real' , &
  ' 32 bit int' , &
  ' 64 bit real' , &
  ' 64 bit int' , &
  ' 128 bit real' ]
```

```

character*20 , dimension(3) :: heading2 &
= [ '      Allocate ', &
  '      Random   ', &
  '      Sort     ' ]

print *, 'Program starts'
print * , 'N = ',nn
call start_timing()

open(unit=100,file=report_file_name)

print * , heading1(1)

allocate (x_sp(1:n),stat=allocate_status)
if (allocate_status /= 0) then
  print *, 'Allocate failed. Program terminates'
  stop 10
end if

print 100,heading2(1),time_difference()
100 format(a20,2x,f8.3)
call random_number(x_sp)
print 100,heading2(2),time_difference()
call sort_data(x_sp,n)
print 100,heading2(3),time_difference()
write(unit=100,fmt='(a)')' First 10 32 bit reals'
write(unit=100,fmt=30) x_sp(1:10)
30 format(5(2x,e14.6))

print * , heading1(2)

allocate (y_i32(1:n),stat=allocate_status)
if (allocate_status /= 0) then
  print *, 'Allocate failed. Program terminates'
  stop 20
end if
print 100,heading2(1),time_difference()
y_i32=int(x_sp*1000000000,i32)
deallocate(x_sp)
print 100,heading2(2),time_difference()
call sort_data(y_i32,n)
print 100,heading2(3),time_difference()
write(unit=100,fmt='(a)' &
  'First 10 32 bit integers'
write(unit=100,fmt=40) y_i32(1:10)
40 format(5(2x,i10))
deallocate(y_i32)

print * , heading1(3)

allocate (x_dp(1:n),stat=allocate_status)
if (allocate_status /= 0) then
  print *, 'Allocate failed. Program terminates'
  stop 30
end if

```

```
print 100,heading2(1),time_difference()
call random_number(x_dp)
print 100,heading2(2),time_difference()
call sort_data(x_dp,n)
print 100,heading2(3),time_difference()
write(unit=100,fmt='(a)' ) &
  'First 10 64 bit reals'
write(unit=100,fmt=30) x_dp(1:10)

print * , heading1(4)

allocate (y_i64(1:n),stat=allocate_status)
if (allocate_status /= 0) then
  print *, 'Allocate failed. Program terminates'
  stop 40
end if

print 100,heading2(1),time_difference()
y_i64 = int(x_dp * 1000000000000000_i64,i64)
deallocate(x_dp)
print 100,heading2(2),time_difference()
call sort_data(y_i64,n)
print 100,heading2(3),time_difference()
write( unit=100,fmt='(a)' ) &
  'First 10 64 bit integers'
write(unit=100,fmt=40) y_i64(1:10)
deallocate(y_i64)

print * , heading1(5)

allocate (x_qp(1:n),stat=allocate_status)
if (allocate_status /= 0) then
  print *, 'Allocate failed. Program terminates'
  stop 50
end if

print 100,heading2(1),time_difference()
call random_number(x_qp)
print 100,heading2(2),time_difference()
call sort_data(x_qp,n)
print 100,heading2(3),time_difference()
write( unit=100,fmt='(a)' ) &
  'First 10 128 bitreals'
write(unit=100,fmt=30) x_qp(1:10)

close(200)
print *, 'Program terminates'
call end_timing()

end program ch3503
```

Table 35.1 Generic recursive quicksort timing

		gfortran	Intel	Nag	Oracle	Mean	StdDev
Allocate	32 bit real	0.008	0.000	0.000	0.000	0.002	0.004
Allocate	32 bit int	0.000	0.000	0.000	0.008	0.002	0.004
Allocate	64 bit real	0.094	0.031	0.031	0.000	0.039	0.039
Allocate	64 bit int	0.016	0.000	0.016	0.000	0.008	0.009
Allocate	128 bit real	0.156	0.047	0.047	0.000	0.063	0.066
Allocate	Total	0.274	0.078	0.094	0.008	0.114	0.113
Random	32 bit real	0.562	0.422	0.609	2.125	0.930	0.801
Random	32 bit int	0.219	0.172	0.328	0.062	0.195	0.110
Random	64 bit real	1.492	0.594	0.531	2.219	1.209	0.804
Random	64 bit int	0.414	0.328	0.609	0.133	0.371	0.197
Random	128 bit real	11.203	3.797	1.070	3.625	4.924	4.368
Random	Total	13.890	5.313	3.147	8.164	7.629	4.653
Sort	32 bit real	13.742	12.328	15.063	11.586	13.180	1.541
Sort	32 bit int	3.492	2.891	4.781	2.203	3.342	1.095
Sort	64 bit real	14.945	13.266	16.078	12.664	14.238	1.561
Sort	64 bit int	2.742	2.312	2.906	1.633	2.398	0.568
Sort	128 bit real	45.703	33.141	18.750	36.633	33.557	11.201
Sort	Total	80.624	63.938	57.578	64.719	66.715	9.809
Overall	Total	94.788	69.329	60.819	72.891	74.457	14.469

Table 35.1 has timing information for four compilers.

Here are some simple observations about the timing information in this table:

- allocation is a negligible component of the overall time
- random number generation takes between 5 and 15 % of total timing
- integer sorting is much faster than real sorting
- sorting of 32 and 64 bit reals is similar
- overall processing of the Nag format 128 bit real is much faster than the other 128 bit formats

35.5 Example 4: Non Recursive Quicksort Example with Timing Details

The following subroutine is a serial non recursive Fortran 77 implementation of Quicksort. It is taken from the Netlib site. Their web address is

<http://www.netlib.org/>

The following is taken directly from their FAQ.

- What is Netlib? The Netlib repository contains freely available software, documents, and databases of interest to the numerical, scientific computing, and other communities. The repository is maintained by AT&T Bell Laboratories, the University of Tennessee and Oak Ridge National Laboratory, and by colleagues world-wide. The collection is replicated at several sites around the world, automatically synchronized, to provide reliable and network efficient service to the global community.

The routines we are interested in are in the following directory.

<http://www.netlib.org/slatec/src/>

Three versions are provided.

<http://www.netlib.org/slatec/src/isort.f>
<http://www.netlib.org/slatec/src/ssort.f>
<http://www.netlib.org/slatec/src/dsort.f>

The complete modified source can be found on our web site. They are fixed form Fortran 77. We will cover the changes we have made below for one of the three source files.

Here is the subroutine header for the double precision subroutine.

SUBROUTINE DSORT (DX, DY, N, KFLAG)

The routine takes 4 parameters and we look at the implementation of the `dsort` routine to find out more details about each parameter. This line

C***TYPE DOUBLE PRECISION (SSORT-S, DSORT-D, ISORT-I)

provides the first clue as to the nature of the parameters.

The following provide some more.

```
C      Description of Parameters
C      DX - array of values to be sorted    (usually abscissas)
C      DY - array to be (optionally) carried along
C      N - number of values in array DX to be sorted
C      KFLAG - control parameter
C              = 2 means sort DX in increasing order and carry DY
C              along.
C              = 1 means sort DX in increasing order (ignoring DY)
C              = -1 means sort DX in decreasing order (ignoring DY)
C              = -2 means sort DX in decreasing order and carry DY
C              along.
```

The following lines then complete the information.

```
C      .. Scalar Arguments ..
      INTEGER KFLAG, N
C      .. Array Arguments ..
      DOUBLE PRECISION DX(*), DY(*)
```

If we set the fourth parameter to 1, we can use the same array for the first and second arguments.

We have made source code changes regarding the external error handling subroutine. We can comment out the calls to this subroutine.

```

      IF (NN .LT. 1) THEN
          CALL XERMSG ('SLATEC', 'DSORT',
+             'The number of values to be sorted is not positive.',
1, 1)
          RETURN
      ENDIF
and
      IF (KK.NE.1 .AND. KK.NE.2) THEN
          CALL XERMSG ('SLATEC', 'DSORT',
+             'The sort control parameter, K, is not 2, 1, -1, or -2.',
2,
+             1)
          RETURN
      ENDIF

```

We have also commented out the EXTERNAL statement reference to this subroutine.

The following lines

```

C***REFERENCES R. C. Singleton, Algorithm 347, An efficient algorithm
C                 for sorting with minimal storage, Communications
of
C                 the ACM, 12, 3 (1969), pp. 185-187.
C***ROUTINES CALLED XERMSG
C***REVISION HISTORY (YYMMDD)
C   761101 DATE WRITTEN
C   761118 Modified to use the Singleton quicksort algorithm. (JAW)
C   890531 Changed all specific intrinsics to generic. (WRB)
C   890831 Modified array declarations. (WRB)
C   891009 Removed unreferenced statement labels. (WRB)
C   891024 Changed category. (WRB)
C   891024 REVISION DATE from Version 3.2
C   891214 Prologue converted to Version 4.0 format. (BAB)
C   900315 CALLs to XERROR changed to CALLs to XERMSG. (THJ)
C   901012 Declared all variables; changed X,Y to DX,DY; changed
C           code to parallel SSORT. (M. McClain)
C   920501 Reformatted the REFERENCES section. (DWL, WRB)
C   920519 Clarified error messages. (DWL)
C   920801 Declarations section rebuilt and code restructured to
use
C           IF-THEN-ELSE-ENDIF. (RWC, WRB)

```

provide details about the algorithm and its revision history. This information is extremely useful when working with the subroutine.

We are now going to look at one solution to the problem of how to integrate the original program and the three sorting subroutines. We can independently compile the three routines as Fortran 77 source.

Here is the main program.

```

include 'precision_module.f90'
include 'integer_kind_module.f90'
include 'timing_module.f90'

```

```
program ch3504
use precision_module
use integer_kind_module
use timing_module
implicit none
integer, parameter :: n = 100000000
character *12 :: nn = '100,000,000'
character *80 :: report_file_name = &
    'ch3502.report'
real (sp), allocatable, dimension () :: x_sp
real (dp), allocatable, dimension () :: x_dp
integer (i32), allocatable, dimension () :: &
    y_i32

integer :: allocate_status
character *20, dimension (5) :: heading1 = [ &
    ' 32 bit real ', ' 32 bit int ', &
    ' 64 bit real ', ' 64 bit int ', &
    ' 128 bit real ' ]

character *20, dimension (3) :: heading2 = [ &
    ' Allocate ', ' Random ', &
    ' Sort ' ]

allocate_status = 0

print *, 'Program starts'
print *, 'N = ', nn
call start_timing()

open (unit=100, file=report_file_name)

print *, heading1(1)

allocate (x_sp(1:n), stat=allocate_status)
if (allocate_status/=0) then
    print *, &
        ' Allocate failed. Program terminates'
    stop 10
end if
print 100, heading2(1), time_difference()
100 format (a20, 2x, f8.3)
call random_number(x_sp)
print 100, heading2(2), time_difference()
call ssort(x_sp, x_sp, n, 1)
print 100, heading2(3), time_difference()
write (unit=100, fmt='(a)') &
    ' First 10 32 bit reals'
write (unit=100, fmt=110) x_sp(1:10)
110 format (5(2x,e14.6))

print *, heading1(2)

allocate (y_i32(1:n), stat=allocate_status)
if (allocate_status/=0) then
    print *, &
```

```

        ' Allocate failed. Program terminates'
        stop 20
end if
print 100, heading2(1), time_difference()
y_i32 = int(x_sp*1000000000, i32)
deallocate (x_sp)
print 100, heading2(2), time_difference()
call isort(y_i32, y_i32, n, 1)
print 100, heading2(3), time_difference()
write (unit=100, fmt='(a)') &
        'First 10 32 bit integers'
write (unit=100, fmt=120) y_i32(1:10)
120 format (5(2x,i10))
deallocate (y_i32)

print *, heading1(3)

allocate (x_dp(1:n), stat=allocate_status)
if (allocate_status/=0) then
    print *, &
        ' Allocate failed. Program terminates'
    stop 30
end if
print 100, heading2(1), time_difference()
call random_number(x_dp)
print 100, heading2(2), time_difference()
call dsort(x_dp, x_dp, n, 1)
print 100, heading2(3), time_difference()
write (unit=100, fmt='(a)') &
        'First 10 64 bit reals'
write (unit=100, fmt=110) x_dp(1:10)

print *, ' Program terminates'
call end_timing()

end program ch3504

```

Table 35.2 summarises the timing information for the above four compilers.
Here are some simple observations about the timing information in this table:

- allocation is again a negligible component of the overall time
- random number generation takes between 5 and 15 % of total timing
- integer sorting is much faster than real sorting
- sorting of 32 and 64 bit reals is similar
- the sums for the sorting are very similar, as the standard deviation shows

Table 35.2 Non recursive quicksort timing

		gfortran	Intel	Nag	Oracle	Mean	StdDev
Allocate	32 bit real	0.000	0.016	0.008	0.000	0.006	0.008
Allocate	32 bit int	0.000	0.000	0.000	0.000	0.000	0.000
Allocate	64 bit real	0.094	0.023	0.031	0.004	0.038	0.039
Allocate	Sum	0.094	0.039	0.039	0.004	0.044	0.037
Random	32 bit real	0.562	0.609	0.625	2.062	0.965	0.732
Random	32 bit int	0.203	0.375	0.297	0.066	0.235	0.133
Random	64 bit real	1.484	0.523	0.516	2.090	1.153	0.772
Random	Sum	2.249	1.507	1.438	4.218	2.353	1.296
Sort	32 bit real	11.508	11.563	11.852	12.207	11.783	0.321
Sort	32 bit int	2.945	2.961	3.000	2.242	2.787	0.364
Sort	64 bit real	12.625	12.406	12.320	12.953	12.576	0.282
Sort	Sum	27.078	26.930	27.172	27.402	27.146	0.198
Overall	Sum	29.421	28.476	28.649	31.624	29.543	1.447

35.5.1 Notes—Version Control Systems

The original program had the following statement

```
*DECK DSORT
```

and this statement was one used in version control or revision control software of the time. Two version control programs that were available on CDC systems from the 1970s and 1980s were called `update` and `modify` that used the above. In computer programming, revision control is any practice that tracks and provides control over changes to source code. Software developers also use revision control software to maintain documentation and configuration files as well as source code.

The use of this kind of software is common for medium to large scale program development.

Wikipedia provides a comparison of what is currently available. See

[http://en.wikipedia.org/wiki/
Comparison_of_revision_control_software](http://en.wikipedia.org/wiki/Comparison_of_revision_control_software)

for more information.

35.6 Subroutine and Function Libraries

A software library is a set of precompiled program units (functions and subroutines) that has been written to solve common problems.

In a university environment many departments (e.g. Mechanical Engineering, Electrical Engineering, Mathematics, Physics etc.) have libraries that solve common problems in each discipline.

In this chapter we will look at examples of the use of a numerical library and a graphics library.

35.7 Numerical Libraries

The major commercial cross platform numerical library is the Nag library.

More information can be found at:

http://www.nag.co.uk/numeric/numerical_libraries.asp

The library is available on a range of platforms.

- Windows
- Linux (including 64-bit)
- Solaris
- Mac OS X
- AIX

A subset of the library is thread safe.

35.8 Serial and Parallel Libraries

Libraries exist in both serial and parallel versions.

35.9 The Nag Library for SMP and Multicore

Nag provide an SMP and multicore version of their library.

<http://www.nag.co.uk/numeric/FL/FSdescription.asp>

Many of the algorithms, or routines, in the library are specifically tuned to run significantly faster on multi-socket and multicore systems. We will look at timing information for one of the sorting routines and compare the times to those of our serial sorting routines.

35.10 Example 5: Calling the Nag M01caf Sorting Routine

Here is the program source.

```
include 'precision_module.f90'
include 'timing_module.f90'

program ch3505

use precision_module
use timing_module

implicit none
integer , parameter :: n = 100000000
character*12 :: nn = "100,000,000"
character*80 :: report_file_name = &
               "ch3505.report"

real (dp) , allocatable, dimension(:) :: x_dp

integer :: allocate_status=0
integer :: ifail=0

character*20 , dimension(5) :: heading1 &
= [ ' 32 bit real' , &
  ' 32 bit int' , &
  ' 64 bit real' , &
  ' 64 bit int' , &
  ' 128 bit real' ]

character*20 , dimension(3) :: heading2 &
= [ ' Allocate ' , &
  ' Random ' , &
  ' Sort ' ]

print *, 'Program starts'
print * , 'N = ',nn
call start_timing()

open(unit=100,file=report_file_name)

100 format(a20,2x,f8.3)
30 format(5(2x,e14.6))
40 format(5(2x,i10))

print * , heading1(3)

allocate (x_dp(1:n),stat=allocate_status)
if (allocate_status /= 0) then
    print *,'Allocate failed. Program terminates'
    stop 30
end if

print 100,heading2(1),time_difference()
call random_number(x_dp)
print 100,heading2(2),time_difference()
```

```

call m01caf(x_dp,1,n,'A',ifail)
if (ifail /= 0) then
    print *, 'sort failed. Program terminates'
    stop 100
end if

print 100,heading2(3),time_difference()
write(unit=100,fmt='(a)')'First 10 64 bit reals'
write(unit=100,fmt=30) x_dp(1:10)

close(200)
print *, 'Program terminates'
call end_timing()

end program ch3505

```

Table 35.3 has details of timing information for the serial sorting algorithms.

The non recursive solution is faster for three out of four compilers.

Table 35.4 has the timing information for the Nag SMP routine, for 1–8 cores.

As can be seen the Nag m01caf timing is faster for one core and shows a very impressive speed up as the number of cores goes up. The system is an Intel I7 system, which has 4 physical cores and is also hyper-threaded giving 8 cores overall.

This link

http://www.nag.co.uk/numeric/f1/performance_examples.asp

has some examples of how the NAG SMP library performance scales on multiple cores. At the time of writing they were drawn from the following library chapters

- Sorting
- Correlation and Regression Analysis
- Wavelet Transforms
- Interpolation
- Random number generators
- Special Functions

This link

http://www.nag.co.uk/numeric/f1/nagdoc_f124/html/GENINT/smptuned.html

has details of the tuned routines in the SMP library.

Here are some details that were correct at the time of writing.

Table 35.3 Sixty four bit real sort timings

		gfortran	Intel	Nag	Oracle	Mean	StdDev
Recursive sort	64 bit real	14.945	13.266	16.078	12.664	14.238	1.561
Non-recursive sort	64 bit real	12.625	12.406	12.320	12.953	12.576	0.282

Table 35.4 Nag sort m01caf timing

N threads	Time
1	11.938
2	6.773
3	5.047
4	4.211
5	4.094
6	3.703
7	3.586
8	3.391

- There are 77 tuned LAPACK routines
- There are 149 Tuned NAG-specific routines within the Library

The Nag library may well offer you a very cost effective way to improve the speed of your programs. Nag have effectively done the work of parallelising many common problems and sub problems and thus the use of their library routines may save you significant development time and help you produce programs that run faster.

As you are probably aware by now parallelising your own code can be hard work!

35.11 Graphics Libraries

Our resource file

http://www.fortranplus.co.uk/resources/fortran_resources.pdf

provides details of some of the graphics libraries available.
We will be using the Dislin library in our examples.

35.12 The Dislin Graphics Library

This is the dislin home page.

<http://www.mps.mpg.de/dislin/>

Here is a description of the software from the above page.

- The software is available for several C, Fortran 77 and Fortran 90/95 compilers on the operating systems UNIX, Linux, FreeBSD, OpenVMS, Windows, Mac OSX and MS-DOS. DISLIN programs are very system-independent, they can be ported from one operating system to another without any changes.

35.12.1 Dislin Example 1: Amdahl's Law Graph 1–8 Processors or Cores

Here is the source code for this program.

```

program ch35_dislin_01
  use dislin
  implicit none
  integer :: i, j
! Total number of processors and hence data points
  integer, parameter :: nprocs = 8
! Number of percentage values from
! 10% -> 90% 9
! 95% 1
! Total 10
  integer, parameter :: nn = 10
  real, dimension (nn) :: pp = &
(/0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 0.95/)
  real, dimension (nprocs) :: x
  real, dimension (nprocs) :: y
  real, dimension (nprocs,nn) :: ydata
  integer :: nx
  integer :: ny
  character*30 cbuf
  do i = 1, nprocs
    x(i) = real(i)
  end do
! Amdahl calculations. Store in 2 d array and then
! assign to 1 d array for plotting.
  do i = 1, nprocs
    do j = 1, nn
      ydata(i,j) = 1/((1-pp(j))+pp(j)/i)
    end do
  end do
! Write the data to a file for verification purposes
  open (unit=10,file='amdahl_table_08.txt')
  do i = 1, nprocs
    write (unit=10,fmt=100) x(i), ydata(i,1:nn)
  100 format (11(f7.2,2x))
  end do
  close (10)
  call disini
  call complx
  call axspos(450,1800)
  call axslen(2200,1400)
  call name('Number of processors','x')
  call name('Speed up','y')
  call titlin('Plot of Amdahls Law',1)
  call titlin('8 Processors',3)
  call labdig(-1,'x')
  call ticks(10,'xy')
  call graf(1.0,8.0,1.0,1.0,1.0,7.0,1.0,1.0)
  call title
  call xaxgit
  call chncrv('line')

```

```
! Plot the curves. Copy from 2 d array to 1 d array
! before the call to curve.
do i = 1, nm
  y = ydata(1:nprocs,i)
  call curve(x,y,nprocs)
end do
call legini(cbuf,10,3)
! Coordinates of the start of the legend
! for the curves.
nx = 500
ny = 450
call legpos(nx,ny)
call leglin(cbuf,'10%',1)
call leglin(cbuf,'20%',2)
call leglin(cbuf,'30%',3)
call leglin(cbuf,'40%',4)
call leglin(cbuf,'50%',5)
call leglin(cbuf,'60%',6)
call leglin(cbuf,'70%',7)
call leglin(cbuf,'80%',8)
call leglin(cbuf,'90%',9)
call leglin(cbuf,'95%',10)
call legit('legend')
call legend(cbuf,3)
call disfin
end program ch35_dislin_01
```

35.12.2 Dislin Example 2: Amdahl's Law Graph 2–64 Processors or Cores

The source code can be found on our web site. It is similar to the previous example.

35.12.3 Dislin Example 3: Gustafson's Law Graph 1–64 Processors or Cores

The source code can be found on our web site. It is similar to the first example.

35.12.4 Dislin Example 4: The Display of Tsunami Events

Here is the source code for this program.

```
program ch35_dislin_04
use dislin
logical :: trial, screen
```

```
real :: long, lat

screen = .false.
trial = .false.

! read in the tsunami data

call datain(trial)

! i now have all the tsunami data latitude and
! longitude
! values read in to the arrays in the tsunam
! common block.

iproj = 1
lat = 0.0
long = 180.0

nreg = 0

! dislin initialisation routines and setting of
! some basic components
! of the plot. these are based on two sample
! dislin programs.

! initialise dislin

call disini

! choose font

call psfont('times-roman')

! determines the position of an axis system.
! the lower left corner of the axis system

call axspos(400, 1850)

! the size of the axis system
! are the length and height of an axis system in
! plot coordinates. the default
! values are set to 2/3 of the page length and
! height.

call axslen(2400, 1400)

! define axis title

call name('longitude', 'x')

! define axis title

call name('latitude', 'y')

! this routine plots a title over an axis
! system.
```

```
call titlin('plot of 3034 tsunami events ', 3)

! determines which label types will be plotted
! on an axis.
! map defines geographical labels which are
! plotted as non negative floating-point
! numbers with the following characters 'w',
! 'e', 'n' and 's'.

call labels('map', 'xy')

! plots a geographical axis system.

call grafmp(-180., 180., -180., 90., -90., &
90., -90., 30.)

! the statement call gridmp (i, j) overlays an
! axis system with a longitude
! and latitude grid where i and j are the number
! of grid lines between labels in
! the x- and y-direction.

call gridmp(1, 1)

! the routine world plots coastlines and lakes.

call world

! the angle and height of the characters can be
! changed with the routines
! angle and height.

call height(50)

! this routine plots a title over an axis
! system.
! the title may contain up to four lines of text
! designated
! with titlin.

call title

! this is a call to the routine that actually
! plots each event.

call plotem(trial, nreg)

! disfin terminates dislin and prints a message
! on the screen.
! the level is set back to 0.

call disfin

end program ch35_dislin_04

subroutine datain(trial)
```

```

common /tsunam/reg0la(378), reg0lo(378), &
       reg1la(206), reg1lo(206), reg2la(41), &
       reg2lo(41), reg3la(54), reg3lo(54), &
       reg4la(60), reg4lo(60), reg5la(1540), &
       reg5lo(1540), reg6la(80), reg6lo(80), &
       reg7la(144), reg7lo(144), reg8la(245), &
       reg8lo(245), reg9la(285), reg9lo(285)

logical :: trial
character (80) :: filnam
if (trial) then
    print *, ' entering data input phase'
end if
filnam = 'tsunami.txt'
open (unit=50, file=filnam, err=100, &
      status='old')
go to 110
100 print *, ' error opening data file'
    print *, ' program terminates'
    stop
110 do i = 1, 378
    read (unit=50, fmt=100) reg0la(i), reg0lo(i)
end do
100 format (1x, f7.2, 2x, f7.2)
do i = 1, 206
    read (unit=50, fmt=100) reg1la(i), reg1lo(i)
end do
do i = 1, 41
    read (unit=50, fmt=100) reg2la(i), reg2lo(i)
end do
do i = 1, 54
    read (unit=50, fmt=100) reg3la(i), reg3lo(i)
end do
do i = 1, 60
    read (unit=50, fmt=100) reg4la(i), reg4lo(i)
end do
do i = 1, 1540
    read (unit=50, fmt=100) reg5la(i), reg5lo(i)
end do
do i = 1, 80
    read (unit=50, fmt=100) reg6la(i), reg6lo(i)
end do
do i = 1, 144
    read (unit=50, fmt=100) reg7la(i), reg7lo(i)
end do
do i = 1, 245
    read (unit=50, fmt=100) reg8la(i), reg8lo(i)
end do
do i = 1, 285
    read (unit=50, fmt=100) reg9la(i), reg9lo(i)
end do
if (trial) then
    do i = 1, 10
        print *, reg0la(i), ' ', reg0lo(i)
    end do
    print *, ' exiting data input phase'

```

```

    read *, dummy
    end if
end subroutine datain

subroutine plotem(trial, nreg)
use dislin
common /tsunam/reg0la(378), reg0lo(378), &
    reg1la(206), reg1lo(206), reg2la(41), &
    reg2lo(41), reg3la(54), reg3lo(54), &
    reg4la(60), reg4lo(60), reg5la(1540), &
    reg5lo(1540), reg6la(80), reg6lo(80), &
    reg7la(144), reg7lo(144), reg8la(245), &
    reg8lo(245), reg9la(285), reg9lo(285)

! this subroutine plots all of the tsunamis onto
! the map as coloured
! points, with a different colour per region. i
! have chosen
! a dot size of 1 mm, and step through the
! colour palette.
! the default may not be appropriate.

logical :: trial
integer :: nreg
integer :: kolour = 10
data dwidth/1.0/
if (trial) then
    dwidth = 5.0
    print *, ' entering plot points'
end if
call incmrk(-1)
if (nreg==0) then
    call setclr(kolour)
    call curvmp(reg0lo, reg0la, 378)
    kolour = kolour + 30
    call setclr(kolour)
    call curvmp(reg1lo, reg1la, 206)
    kolour = kolour + 30
    call setclr(kolour)
    call curvmp(reg2lo, reg2la, 41)
    kolour = kolour + 30
    call setclr(kolour)
    call curvmp(reg3lo, reg3la, 54)
    kolour = kolour + 30
    call setclr(kolour)
    call curvmp(reg4lo, reg4la, 60)
    kolour = kolour + 30
    call setclr(kolour)
    call curvmp(reg5lo, reg5la, 1540)
    kolour = kolour + 30
    call setclr(kolour)
    call curvmp(reg6lo, reg6la, 80)
    kolour = kolour + 30
    call setclr(kolour)
    call curvmp(reg7lo, reg7la, 144)
    kolour = kolour + 30

```

```

call setclr(kolour)
call curvmp(reg8lo, reg8la, 245)
kolour = kolour + 30
call setclr(kolour)
call curvmp(reg9lo, reg9la, 285)
else if (nreg==1) then
  kolour = 10
  call setclr(kolour)
  call curvmp(reg0lo, reg0la, 378)
else if (nreg==2) then
  kolour = 20
  call setclr(kolour)
  call curvmp(reg1lo, reg1la, 206)
else if (nreg==3) then
  kolour = 30
  call setclr(kolour)
  call curvmp(reg2lo, reg2la, 41)
else if (nreg==4) then
  kolour = 40
  call setclr(kolour)
  call curvmp(reg3lo, reg3la, 54)
else if (nreg==5) then
  kolour = 50
  call setclr(kolour)
  call curvmp(reg4lo, reg4la, 60)
else if (nreg==6) then
  kolour = 60
  call setclr(kolour)
  call curvmp(reg5lo, reg5la, 1540)
else if (nreg==7) then
  kolour = 70
  call setclr(kolour)
  call curvmp(reg6lo, reg6la, 80)
else if (nreg==8) then
  kolour = 80
  call setclr(kolour)
  call curvmp(reg7lo, reg7la, 144)
else if (nreg==9) then
  kolour = 90
  call setclr(kolour)
  call curvmp(reg8lo, reg8la, 245)
else if (nreg==10) then
  kolour = 100
  call setclr(kolour)
  call curvmp(reg9lo, reg9la, 285)
end if
if (trial) then
  print *, ' exiting plot points'
end if

end subroutine plotem

```

The original program on which this is based was written by Ian whilst he was on secondment to the United Nations Environment Programme. Section 35.9 of their Environmental Data Reports cover natural disasters and these include

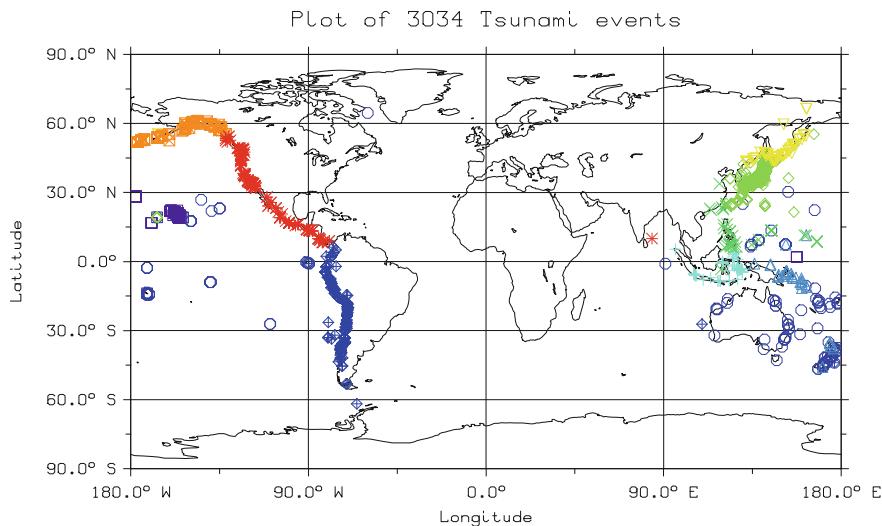
- Earthquakes
- Volcanoes
- Tsunamis
- Floods
- Landslides
- Natural dams
- Droughts
- Wildfires

See the bibliography for more details of these publications. The tsunami data sets are from this chapter.

The tsunami data file and graphics program can be found at:

<http://www.fortranplus.co.uk/>

Here is the plot produced by this program.



As you can see there are a lot of tsunami events in the Pacific area. A colour A4 pdf of the plot can be found at the Fortranplus website.

It is a common requirement in science and engineering to have to produce graphical output and we have now briefly covered some of the capability of the dislin library. Most graphics libraries will offer similar functionality.

35.13 Problems

35.1 Try out the first two examples on your system. What timing details do you get?

35.2 Using the non recursive 32 bit integer sort subroutine as a starting point produce a 64 bit integer version. How long did it take to get a working version?

35.3 If you have successfully solved the above problem now produce subroutines for 8 bit and 16 bit integers.

35.4 Using the non recursive 64 bit real subroutine as a starting point produce a 128 bit version. How long did this take?

Bibliography

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Wirth N., Algorithms & Data Structures, Prentice-Hall, 1986.

Chapter 36

Converting from Fortran 77

*Twas brillig, and the slithy toves did gyre and gimble in the
wabe; All mimsy were the borogoves, And the mome raths
outgrabe.*

Lewis Carroll

Aim

This chapter looks at some of the options available when working with older Fortran code.

36.1 Introduction

This chapter looks at converting Fortran 77 code to a modern Fortran style.

The aim is to provide the Fortran 77 programmer (and in particular the person with legacy code) with some simple guidelines for conversion.

The first thing that one must have is a thorough understanding of the newer, better language features of Fortran. It is essential that the material in the earlier chapters of this book are covered, and some of the problems attempted. This will provide a feel for modern Fortran.

The second thing one must have is a thorough understanding of the language constructs used in your legacy code. Use should be made of the compiler documentation for whatever Fortran 77 compiler you are using, as this will provide the detailed (often system specific) information required. The recommendations below are therefore brief.

It is possible to move gradually from Fortran 77 to modern Fortran. In many cases existing code can be quite simply recompiled by a suitable choice of compiler options. This enables us to mix and match old and new in one program. This process is likely to highlight nonstandard language features in your old code. There will inevitably be some problems here.

The standard identifies two kinds of decremented features; deleted and obsolescent. It is extremely unwise to consider the long-term use of these features as they are candidates for removal from future standards.

36.2 Deleted Features

The list of deleted features for Fortran 2008 is empty, i.e., there are none.

36.3 Obsolescent Features

The obsolescent features are those for which better methods are available. They are given below with alternatives.

36.3.1 Arithmetic If

Use the if statement.

36.3.2 Real and Double Precision Do Control Variables

Use integer.

36.3.3 Shared do Termination and Non-enddo Termination

Use an end do.

36.3.4 Alternate Return

Use a case statement on return. An error code has to be returned.

36.3.5 Pause Statement

System specific. Normally easily replaced with a suitable read statement.

36.3.6 Assign and Assigned Goto Statements

Fortunately rarely used.

36.3.7 Assigned Format Statements

Use character arrays, arrays and constants.

36.3.8 H Editing

Use character edit descriptor.

36.4 Better Alternatives

Below we are looking at the new features of the Fortran standard, and how we can replace our current coding practices with the better facilities that now exist.

- double precision—use the module `precision_module` which was introduced in Chap. 21 and used subsequently throughout the book.
- fixed format—use free format
- implicit typing—use `implicit none`
- block data—use modules
- common statement—use modules
- equivalence—Invariably the use of this feature requires considerable system specific knowledge. There will be cases where there have been extremely good reasons why this feature has been used, normally efficiency related. However with the rapid changes taking place in the power and speed of hardware these reasons are diminishing.
- assumed-size / explicit-shape dummy array arguments—if a dummy argument is assumed-size or explicit-shape (the only ones available in Fortran 77) then the ranks of the actual argument and the associated argument don't have to be the same. With modern Fortran arrays are now objects instead of a linear sequence of elements, as was the case with Fortran 77, and now for array arguments the fundamental rule

is that actual and dummy arguments have the same rank and same extents in each dimension, i.e., the same shape, and this is done using assumed-shape dummy array arguments. An explicit interface is mandatory for assumed-shape arrays.

- entry statement—use module plus use statement.
- statement functions—use internal function, see Chap. 12.
- computed goto—use case statement, see Chap. 13.
- alternate return—use error flags on calling routine.
- external statement for dummy procedure arguments—use modules and interface blocks. See the Runge-Kutta-Merson example in Chap. 26.

Use explicit interfaces everywhere, i.e., use module procedures. This also provides argument checking and other benefits.

36.5 Commercial Conversion Tools

At the time of writing there are several options. Have a look at our Fortran resource file:

http://www.fortranplus.co.uk/resources/fortran_resources.pdf

for up to date information.

Here are brief details of the tools currently available.

36.5.1 Convert

Fortran 77 to Fortran 90 converter by Mike Metcalf.

<http://www.nag.co.uk/nagware/Examples/convert.f90>

36.5.2 Forcheck

A Fortran analyzer and programming aid.

<http://www.forcheck.nl/>

36.5.3 Forstruct

Restructures FORTRAN into Clean, Maintainable Code.

<http://www.cobalt-blue.com/fs/fsmain.htm>

36.5.4 Forstudy

Analyzes and Documents your FORTRAN code.

<http://www.cobalt-blue.com/>

36.5.5 Plusfort

Fortran 77 to Fortran 90 converter.

<http://www.polyhedron.com/>

36.5.6 VAST/77to90

Fortran 77 to Fortran 90 translator

http://www.crescentbaysoftware.com/vast_77to90.html

36.6 Example of PlusFORT Capability from Polyhedron Software

Below is an example from their site that looks at the same subroutine in Fortran 66, 77 and 90 styles.

36.6.1 Original Fortran 66

This subroutine picks off digits from an integer and branches depending on their value.

```
SUBROUTINE OBACT(TODO)
INTEGER TODO,DONE,IP,BASE
COMMON /EG1/N,L,DONE
PARAMETER (BASE=10)
13 if(TODO.EQ.0) GO TO 12
      I=MOD(TODO,BASE)
      TODO=TODO/BASE
      GO TO(62,42,43,62,404,45,62,62,62),I
      GO TO 13
42 CALL COPY
      GO TO 127
43 CALL MOVE
      GO TO 144
404 N=-N
44 CALL DELETE
      GO TO 127
45 CALL print
      GO TO 144
62 CALL BADACT(i)
      GO TO 12
127 L=L+N
144 DONE=DONE+1
      CALL RESYNC
      GO TO 13
12 RETURN
END
```

36.6.2 Fortran 77 Version

In addition to restructuring, SPAG has renamed some variables, removed the unused variable IP, inserted declarations, and used upper and lower case to distinguish different types of variable:

```
SUBROUTINE OBACT(TODO)
IMPLICIT NONE
C*** START OF DECLARATIONS INSERTED BY SPAG
      INTEGER ACT , LENGTH , NCHAR
C*** END OF DECLARATIONS INSERTED BY SPAG
```

```

INTEGER TODO , DONE , BASE
COMMON /EG1      / NCHAR , LENGTH , DONE
PARAMETER (BASE=10)
100 IF ( TODO.NE.0 ) THEN
      ACT = MOD(TODO,BASE)
      TODO = TODO/BASE
      IF ( ACT.EQ.1 .OR. ACT.EQ.4 .OR.
&          ACT.EQ.7 .OR. ACT.EQ.8 .OR.
&          ACT.EQ.9 ) THEN
          CALL BADACT(ACT)
          GOTO 200
      ELSEIF ( ACT.EQ.2 ) THEN
          CALL COPY
          LENGTH = LENGTH + NCHAR
      ELSEIF ( ACT.EQ.3 ) THEN
          CALL MOVE
      ELSEIF ( ACT.EQ.5 ) THEN
          NCHAR = -NCHAR
          CALL DELETE
          LENGTH = LENGTH + NCHAR
      ELSEIF ( ACT.EQ.6 ) THEN
          CALL PRINT
      ELSE
          GOTO 100
      ENDIF
      DONE = DONE + 1
      CALL RESYNC
      GOTO 100
  ENDIF
200 RETURN
END

```

36.6.3 Fortran 90 Version

SPAG has used do while, select case, exit and cycle. No GOTOs or labels remain.

```

subroutine obact(todo)
implicit none
C*** start of declarations inserted by spag
integer act , length , nchar
C*** end of declarations inserted by spag
integer todo , done , base

```

```
common /eg1    / nchar , length , done
parameter (base=10)
do while ( todo.ne.0 )
    act = mod(todo,base)
    todo = todo/base
    select case (act)
    case (1,4,7,8,9)
        call badact(act)
        exit
    case (2)
        call copy
        length = length + nchar
    case (3)
        call move
    case (5)
        nchar = -nchar
        call delete
        length = length + nchar
    case (6)
        call print
    case default
        cycle
    end select
    done = done + 1
    call resync
enddo
return
end
```

This tool suite can also be used in the maintenance of code during development.

36.7 Summary

This chapter has shown some of the options open to you when working with legacy code. The emphasis has been on relatively straightforward code restructuring. The use of software tools to aid in this is highly recommended as converting manually using an editor is obviously going to involve much more work.

Appendix A

Glossary

Actual argument entity that appears in a procedure reference

Allocatable having the allocatable attribute

Array set of scalar data, all of the same type and type parameters, whose individual elements are arranged in a rectangular pattern

Array element scalar individual element of an array

Array pointer array with the pointer attribute

Array section array subobject designated by array-section, and which is itself an array

Assumed-shape array nonallocatable nonpointer dummy argument array that takes its shape from its effective argument

Assumed-size array dummy argument array whose size is assumed from that of its effective argument

Deferred-shape array allocatable array or array pointer, declared with a deferred-shape-spec-list

Explicit-shape array array declared with an explicit-shape-spec-list, which specifies explicit values for the bounds in each dimension of the array

Associate name name of construct entity associated with a selector of an associate or select type construct

Association inheritance association, name association, pointer association, or storage association. Name association is further subcategorized as argument association, construct association, host association, linkage association, or use association

Argument association association between an effective argument and a dummy argument

Host association name association, other than argument association, between entities in a submodule or contained scoping unit and entities in its host

Inheritance association association between the inherited components of an extended type and the components of its parent component

Pointer association association between a pointer and an entity with the target attribute

Storage association association between storage sequences

Use association association between entities in a module and entities in a scoping unit that references that module, as specified by a use statement

Attribute property of an entity that determines its uses

Automatic data object **Automatic object** nondummy data object with a type parameter or array bound that depends on the value of a specification-expr that is not an initialization expression

Binding label default character value specifying the name by which a global entity with the bind attribute is known to the companion processor

Block is a bounded sequence of executable constructs and statements that is treated as a unit. It may be empty.

Block data program unit program unit whose initial statement is a block data statement, used for providing initial values for data objects in named common blocks

Bound array bound limit of a dimension of an array

Character context within a character literal constant or within a character string edit descriptor

Characteristics either of a procedure, the properties listed in; of a dummy argument, being a dummy data object, dummy procedure, or an asterisk (alternate return indicator); of a dummy data object, the properties listed in; of a dummy procedure or dummy procedure pointer, the properties listed in; or of a function result, the properties listed in

Coarray data entity that has nonzero corank

Cobound bound (limit) of a codimension

Codimension dimension of the pattern formed by corresponding coarrays

Coindexed object data object whose designator includes an image-selector

Corank number of codimensions of a coarray (zero for objects that are not coarrays)

Cosubscript scalar integer expression in an image-selector

Collating sequence one-to-one mapping from a character set into the nonnegative integers

Common block block of physical storage specified by a common statement

Blank common unnamed common block

Companion processor processor-dependent mechanism by which global data and procedures may be referenced or defined

Component part of a derived type, or of an object of derived type, defined by a component-def-stmt

Direct component one of the components, or one of the direct components of a nonpointer nonallocatable component

Parent component component of an extended type whose type is that of the parent type and whose components are inheritance associated with the inherited components of the parent type

Subcomponent of a structure, direct component that is a subobject of that structure

Ultimate component a component that is of intrinsic type, a pointer, or allocatable; or an ultimate component of a nonpointer nonallocatable component of derived type

Component order ordering of the nonparent components of a derived type that is used for intrinsic formatted input/output and structure constructors (where component keywords are not used)

Conformable of two data entities, having the same shape, or one being an array and the other being scalar

Connected relationship between a unit and a file: each is connected if and only if the unit refers to the file

Constant data object that has a value and which cannot be defined, redefined, or become undefined during execution of a program

Literal constant constant that does not have a name

Named constant named data object with the parameter attribute

Construct entity entity whose identifier has the scope of a construct index variable of a `forall` construct or `do concurrent` construct, associate name of an associate construct or select type construct, or entity declared in the specification part of a block construct other than only in `asynchronous` and `volatile` statements

Data entity data object, result of the evaluation of an expression, or the result of the execution of a function reference

Data object object constant, variable, or subobject of a constant

Decimal symbol character that separates the whole and fractional parts in the decimal representation of a real number in a file

Declaration specification of attributes for various program entities. Note that often this involves specifying the type of a named data object or specifying the shape of a named array object

Default initialization mechanism for automatically initializing pointer components to have a defined pointer association status, and nonpointer components to have a particular value

Default-initialized of a subcomponent, being subject to a default initialization specified in the type definition for that component

Definable being capable of definition and permitted to become defined

Defined either

of a data object, the property of having a valid value, or
of a pointer, the property of having a pointer association status of associated or
disassociated

Defined assignment assignment defined by a procedure

Defined input/output input/output defined by a procedure

Defined operation operation defined by a procedure

Definition either

the specification of derived types, enumerations, and procedures, or
the process by which a data object becomes defined

Designator name followed by zero or more component selectors, complex part selectors, array section selectors, array element selectors, image selectors, and substring selectors

Complex part designator designator that designates the real or imaginary part of a complex data object, independently of the other part

Object designator data object designator designator for a data object. an object name is a special case of an object designator

Procedure designator designator for a procedure

Disassociated either

the pointer association status of not being associated with any target and not being undefined or
of a pointer, having that pointer association status

Dummy argument entity whose identifier appears in a dummy argument list in a function, subroutine, entry, or statement function statement, or whose name can be used as an argument keyword in a reference to an intrinsic procedure or a procedure in an intrinsic module

Dummy data object dummy argument that is a data object

Dummy function dummy procedure that is a function

Effective argument entity that is argument-associated with a dummy argument

Effective item scalar object resulting from the application of the rules in to an input/output list

Elemental independent scalar application of an action or operation to elements of an array or corresponding elements of a set of conformable arrays and scalars, or possessing the capability of elemental operation. combination of scalar and array operands or arguments combine the scalar operand(s) with each element of the array operand(s)

Elemental assignment assignment that operates elementally

Elemental operation operation that operates elementally

Elemental operator operator in an elemental operation

Elemental procedure elemental intrinsic procedure or procedure defined by an elemental subprogram

Elemental reference reference to an elemental procedure with at least one array actual argument

Elemental subprogram subprogram with the elemental prefix

End statement end-block-data-stmt, end-function-stmt, end-module-stmt, end-mp-subprogram-stmt, end-program-stmt, end-submodule-stmt, or end-subroutine-stmt

Explicit initialization initialization of a data object by a specification statement

Explicit interface interface of a procedure that includes all the characteristics of the procedure and names for its dummy arguments except for asterisk dummy arguments

Extent number of elements in a single dimension of an array

External file file that exists in a medium external to the program

External unit external input/output unit entity that can be connected to an external file

File storage unit unit of storage in a stream file or an unformatted record file

Final subroutine subroutine whose name appears in a final statement in a type definition, and which can be automatically invoked by the processor when an object of that type is finalized

Finalizable either

of a type, having a final subroutine or a nonpointer nonallocatable component of finalizable type, or of a nonpointer data entity, being of finalizable type

Finalization the process of calling final subroutines when one of the events listed in occurs

Function procedure that is invoked by an expression

Generic identifier lexical token that identifies a generic set of procedures, intrinsic operations, and/or intrinsic assignments

Generic interface set of procedure interfaces identified by a generic identifier

Host scoping unit host the scoping unit immediately surrounding another scoping unit, or the scoping unit of the parent of a submodule

Image instance of a fortran program

Image index integer value identifying an image

Implicit interface interface of a procedure that includes only the type and type parameters of a function result (,)

Inherit of an extended type, to acquire entities (components, type-bound procedures, and type parameters) through type extension from the parent type

Initialization expression expression that satisfies the rules in

Inquiry function intrinsic function, or function in an intrinsic module, whose result depends on the properties of one or more of its arguments instead of their values

Interface block abstract interface block, generic interface block, or specific interface block

Abstract interface block interface block with the abstract keyword; collection of interface bodies that specify abstract interfaces

Generic interface block interface block with a generic-spec; collection of interface bodies and procedure statements that are to be given that generic identifier

Specific interface block interface block with no generic-spec or abstract keyword; collection of interface bodies that specify the interfaces of procedures

Interface body scoping unit that specifies an abstract interface or the interface of a dummy procedure, external procedure, procedure pointer, or separate module procedure

Interoperable interoperable with a c entity

Intrinsic and accessible without further definition or specification, or a procedure or module provided by a processor but

Standard intrinsic

Nonstandard intrinsic

Internal file character variable that is connected to an internal unit

Internal unit input/output unit that is connected to an internal file

Keyword statement keyword, argument keyword, type parameter keyword, or component keyword

Argument keyword word that identifies the corresponding dummy argument in an actual argument list

Component keyword word that identifies a component in a structure constructor

Statement keyword word that is part of the syntax of a statement

Type parameter keyword word that identifies a type parameter in a type parameter list

Line sequence of zero or more characters

Main program program unit that is not a subprogram, module, submodule, or block data program unit

Module program unit containing (or accessing from other modules) definitions that are to be made accessible to other program units

Name identifier of a program constituent, formed according to the rules given in

Nan not a number, a symbolic floating-point datum (ieee international standard)

Operand data value that is the subject of an operator

Operator either a prefix syntax specifying a computation involving one (unary operator) data value, or an infix syntax specifying a computation involving two (binary operator) data values

Passed-object dummy argument dummy argument of a type-bound procedure or procedure pointer component that becomes associated with the object through which the procedure is invoked

Pointer data pointer or procedure pointer

Data pointer data entity with the pointer attribute

Procedure pointer procedure with the external and pointer attributes

Pointer assignment association of a pointer with a target, by execution of a pointer assignment statement or an intrinsic assignment statement for a derived-type object that has the pointer as a subobject

Polymorphic data entity declared with the class keyword, able to be of differing dynamic types during program execution

Preconnected of a file or unit, connected at the beginning of execution of the program

Procedure entity encapsulating an arbitrary sequence of actions that can be invoked directly during program execution

Dummy procedure procedure that is a dummy argument

External procedure procedure defined by an external subprogram or by means other than fortran

Internal procedure procedure defined by an internal subprogram

Module procedure procedure that is defined by a module subprogram

Pure procedure procedure declared or defined to be pure according to the rules in

Processor combination of a computing system and mechanism by which programs are transformed for use on that computing system

Processor dependent not completely specified in the standard, having methods and semantics determined by the processor

Program set of fortran program units and global entities defined by means other than fortran that includes exactly one main program

Program unit main program, external subprogram, module, submodule, or block data program unit

Record sequence of values or characters in a file

Reference data object reference, procedure reference, or module reference

Data object reference appearance of a data object designator in a context requiring its value at that point during execution

Function reference appearance of the procedure designator for a function, or operator symbol in a context requiring execution of the function during expression evaluation

Module reference appearance of a module name in a use statement

Procedure reference appearance of a procedure designator, operator symbol, or assignment symbol in a context requiring execution of the procedure at that point during execution; or occurrence of defined input/output or derived-type finalization

Rank number of array dimensions of a data entity (zero for a scalar entity)

Result variable variable that returns the value of a function

Saved having the save attribute

Scalar data entity that can be represented by a single value of the type and that is not an array

Scoping unit either

a program unit or subprogram, excluding any scoping units in it,
a derived-type definition, or
an interface body, excluding any scoping units in it

Sequence set of elements ordered by a one-to-one correspondence with the numbers 1, 2 to n

Empty sequence sequence containing no elements

Shape array dimensionality of a data entity, represented as a rank-one array whose size is the rank of the data entity and whose elements are the extents of the data entity. thus the shape of a scalar data entity is an array with rank one and size zero

Size of an array, the total number of elements in the array

Specification expression expression that satisfies the rules in

Standard-conforming program program that uses only those forms and relationships described in, and which has an interpretation according to,

Statement sequence of one or more complete or partial lines satisfying a syntax rule that ends in -stmt

Executable statement statement that is a member of the syntactic class executable-construct, excluding those in the specification-part of a block construct

Nonexecutable statement statement that is not an executable statement

Statement entity entity whose identifier has the scope of a statement or part of a statement

Statement label label unsigned positive number of up to five digits that refers to an individual statement

Storage sequence contiguous sequence of storage units

Storage unit unit of storage; a character storage unit, numeric storage unit, file storage unit, or unspecified storage unit

Character storage unit storage unit for holding a default character value

Numeric storage unit storage unit for holding a default real, default integer, or default logical value

Unspecified storage unit storage unit for holding a value that is not default character, default real, double precision real, default logical, or default complex

Structure scalar data object of derived type

Structure component component of a structure

Structure constructor syntax (structure-constructor), that specifies a structure value or which creates such a value

Submodule program unit that extends a module or another submodule

Subobject portion of data object that can be referenced, and if it is a variable defined, independently of any other portion

Subprogram function-subprogram or subroutine-subprogram

External subprogram subprogram that is not contained in a main program, module, submodule, or another subprogram

Internal subprogram subprogram that is contained in a main program or another subprogram

Module subprogram subprogram that is contained in a module or submodule but which is not an internal subprogram

Subroutine procedure invoked by a call statement, by defined assignment, or by some operations on derived-type entities

Target entity that is pointer-associated with a pointer, entity on the right-hand-side of a pointer assignment statement, or entity with the target attribute

Transformational function intrinsic function, or function in an intrinsic module, which is neither elemental nor an inquiry function

Type data type named category of data characterized by a set of values, a syntax for denoting these values, and a set of operations that interpret and manipulate the values

Abstract type type with the abstract attribute

Declared type type that a data entity is declared to have, either explicitly or implicitly

Derived type type defined by a type definition or by an intrinsic module

Dynamic type type of a data entity at a particular point during execution of a program

Extended type type with the extends attribute

Extensible type type that has neither the bind attribute nor the sequence attribute and which therefore may be extended using the extends clause

Extension type relationship between two types: a type is an extension type of another if the other is the same type, the parent type, or an extension of the parent type

Intrinsic type

Numeric type one of the types integer, real, and complex

Parent type of an extended type, the type named in its extends clause

Type compatible of one entity with respect to another, compatibility of the types of the entities for purposes such as argument association, pointer association, and allocation

Type parameter value used to parameterize a type, further specifying the set of data values, syntax for denoting those, and the set of operations available

Assumed type parameter length type parameter that assumes the type parameter value from another entity, which is the selector for an associate name, the initialization-expr for a named constant of type character, and the effective argument for a dummy argument

Deferred type parameter length type parameter whose value can change during execution of a program and whose type-param-value is a colon

Kind type parameter type parameter whose value is required to be defaulted or given by an initialization expression

Length type parameter type parameter whose value is permitted to be assumed, deferred, or given by a specification expression

Type parameter inquiry syntax (type-param-inquiry) that is used to inquire the value of a type parameter of a data object

Type parameter order ordering of the type parameters of a type used for derived-type specifiers (derived-type-spec,)

Type-bound procedure procedure bound to a type

Ultimate argument nondummy entity with which a dummy argument is associated via a chain of argument associations

Undefined either

of a data object, the property of not having a valid value, or
of a pointer, the property of having not having a pointer association status of associated or disassociated

Unit input/output unit means, specified by an io-unit, for referring to a file

Unsaved not having the save attribute

Variable data entity that can be defined and redefined during execution of a program

Local variable variable in a scoping unit or block construct that is not a dummy argument or part thereof, is not a global entity or part thereof, and is not accessible outside that scoping unit or construct

Vector subscript section-subscript that is an array

Whole array array designated by a name

Appendix B

Intrinsic Functions and Procedures

This appendix has a brief coverage of some of the more commonly used intrinsic functions and procedures.

Chapter 13 of the standard should be consulted for an exhaustive coverage. The following abbreviations and typographic conventions are used in this appendix.

Argument type and return type

i	integer
r	real
c	complex
n	numeric (any of integer, real, complex)
l	logical
p	pointer
p*	polymorphic
t	target
dp	double precision
char	character, length = 1.
s	character
boz	boz-literal-constant
co	coarray or coindexed object

There are several classes of function in Fortran and they are documented below.

Class

a	indicates that the procedure is an atomic subroutine
e	indicates that the procedure is an elemental function
es	indicates that the procedure is an elemental subroutine
i	indicates that the procedure is an inquiry function
ps	indicates that the procedure is a pure subroutine
s	indicates that the procedure is an impure subroutine
t	indicates that the procedure is a transformational function

Arguments in italics are optional arguments.

In the example `ALL (mask, dim) dim` may be omitted.

Common optional arguments

back	controls the direction of string scan, forward or backward
dim	a selected dimension of an array argument
kind	describes the kind type parameter of the result. If the kind argument is absent the result is the same type as the first argument.
mask	a mask may be applied to the arguments
size	of an array, the total number of elements

Double precision

Before Fortran 90 if you required real variables to have greater precision than the default real then the only option available was to declare them as double precision. With the introduction of kind types with Fortran 90 the use of double precision declarations is not recommended, and instead real entities with a kind type offering more than the default precision should be used.

Result type

When the result type is the same as the argument type then the result is not just the same type as the argument but also the same kind.

Miscellaneous rules

When the argument is `back` it is of logical type.

When the argument is `count_rate`, `count_max`, `dim`, `kind`, `len`, `order`, `n_copies`, `shape`, `shift`, `values` it is of integer type.

When the argument is `mask` it is of logical type.

When the argument is `target` it is of pointer or target type.

Fortran 2008 introduced several changes to Fortran 2003 that affects intrinsic procedures.

- The following functions can now have arguments of type complex: `acos`, `asin`, `atan`, `cosh`, `sinh`, `tan` and `tanh`.
- The intrinsic function `atan2` can be referenced by the name `atan`.
- The intrinsic functions `lge`, `lgf`, `lle` and `llt` can have arguments of ASCII kind.
- The intrinsic functions `maxloc` and `minloc` have an additional `back` argument
- The intrinsic function `selected_real_kind` has an additional `radix` argument

ABS(a): Absolute value.

argument: a	type: n
result: as argument	class: e

Note(s): If a is complex(x,y) then the functions returns $\sqrt{x^2 + y^2}$

Example(s): r1=abs (a)

ACHAR(i, kind): Returns character in the ASCII character set.

argument: i	type: i
result: char	class: e

Note(s): Inverse of the iachar function.

Example(s): c=achar (i)

ACOS(x): Arccosine, inverse cosine.

argument: x	type: r,c
result: as argument	class: e

Note(s): $|x| \leq 1$

Example(s): y=acos (x)

ACOSH(x): Inverse hyperbolic cosine function.

argument: x	type: r,c
result: as argument	class: e

Example(s): y = acosh (x)

ADJUSTL(string): Adjust string left, removing leading blanks and inserting trailing blanks.

argument: string	type: s
result: as argument	class: e

Example(s): s=adjustl (s)

ADJUSTR(string): Adjust string right, removing trailing blanks and inserting leading blanks.

argument: string	type: s
result: as argument	class: e

Example(s): s=adjustr (s)

AIMAG(z): Imaginary part of complex argument.

argument: z	type: c
result: as argument	class: e

Example(s): `y=aimag(z)`

AINT(a, kind): Truncation toward zero to a whole number.

argument: a	type: r
result: as a	class: e

Example(s): `y=aint(z)`

When $z=0.3$ $y=0$; when $z=2.73$ $y=2.0$; when $z=-2.73$ $y=-2.0$

ALL(mask, dim): Determines whether all values are true in mask along dimension dim.

argument: mask	type: l
result: l	class: t

Note(s): dim must be a scalar in the range $1 \leq dim \leq n$ where n is the rank of mask. The result is scalar if dim is absent or mask has rank 1. Otherwise it works on the dimension dim of mask and the result is an array of rank $n - 1$

Example(s): `t=all(m)`

ALLOCATED(variable): returns true if and only if the allocatable variable is allocated.

argument: variable	type: any
result: l	class: i

Note(s): variable must be declared with the allocatable attribute and can be an array or a scalar.

Example(s): `if (allocated(array)) then ...`

ANINT(a, kind): Nearest whole number.

argument: a	type: r
result: as a	class: e

Example(s): `z=anint(a)`

If $a = 5.63$ $z = 6$; if $a=-5.7$ $z = -6.0$

ANY(mask, dim): Determines whether any value is true in mask along dimension dim.

argument: mask	type: l
result: l	class: t

Note(s): mask must be an array. The result is a scalar if dim is absent or if mask is of rank 1. Otherwise it works on the dimension dim of mask and the result is an array of rank $n - 1$

Example(s): `t=any (a)`

ASIN(x): Arcsine.

argument: x	type: r,c
result: as argument	class: e

Example(s): `z=asin (x)`

ASINH(x): Inverse hyperbolic sine function.

argument: x	type: r,c
result: as argument	class: e

Example(s): `y = asinh (x)`

ASSOCIATED(pointer, target): Returns the association status of the pointer.

argument: pointer	type: p
result: l	class: i

Note(s):

1. If `target` is absent then the result is true if pointer is associated with a target, otherwise false.
2. If `target` is present and is a target, the result is true if pointer is currently associated with target and false if it is not.
3. If `target` is present and is a pointer, the result is true if both pointer and target are currently associated with the same target, and is false otherwise. If either `pointer` or `target` is disassociated the result is false.

Example(s): `t=associated (p)`

ATAN(x): Arctangent.

argument: x	type: r,c
result: as argument	class: e

Example(s): `z=atan (x)`

ATAN(y, x): Arctangent.

argument: y	type: r,c
argument: x	type: same as y
result: same as <code>atan (y, x)</code>	class: e

Note(s):

1. If `y` has the value zero, `x` shall not have the value zero.

Example(s): `z=atan(x)`

ATAN2(y, x): Arctangent of y/x .

argument: y	type: r
result: as arguments	class: e

Example(s): `z=atan2(y, x)`

ATANH(x): Inverse hyperbolic tangent function.

argument: x	type: r,c
result: as argument	class: e

Example(s): `y = atanh(x)`

BESSEL_J0(x): Bessel function of the first kind, order 0.

argument: x	type: r
result: as argument	class: e

Example(s): `y = bessel_j0(1.0)`

Has the value 0.765 (approximately)

BESSEL_J1(x): Bessel function of the first kind, order 1.

argument: x	type: r
result: as argument	class: e

Example(s): `y = bessel_j1(1.0)`

has the value 0.440 (approximately).

BESSEL_JN(n, x): Bessel functions of the first kind.

arguments: n, x	type: n is i, x is r
result: as x	class: e

Example(s): `y = bessel_jn(2, 1.0)`

has the value 0.115 (approximately).

BESSEL_JN(n1, n2, x): Bessel functions of the first kind.

arguments: n1, n2, x	type: n1, n2 are i, x is r
result: See note below.	class: t

Note(s): Result: is a real rank-one array with extent `max(n2-n1+1, 0)`. Element i of the result value is a processor-dependent approximation to the bessel function of the first kind and order $n1 + i - 1$ of x .

BESSEL_Y0(x): Bessel function of the second kind, order 0.

argument: x	type: r
result: as argument	class: e

Example(s): `y = bessel_y0(1.0)`
has the value 0.088 (approximately).

BESSEL_Y1(x): Bessel function of the second kind, order 1.

argument: x	type: r
result: as argument	class: e

Example(s): `y = bessel_y1(1.0)`
has the value -0.781 (approximately).

BESSEL_YN(n, x): Bessel functions of the second kind.

arguments: n, x	type: n is i, x is r
result: is same type and kind as x.	class: e

Example(s): `y = bessel_yn(2, 1.0)`
has the value -1.651 (approximately).

BESSEL_YN(n1, n2, x): Bessel functions of the second kind.

arguments: n1, n2, x	type: n1, n2 are i, x is r
result: See note below.	class: t

Note(s): Is a real rank-one array with extent `max(n2-n1+1, 0)`. Element i of the result value is a processor-dependent approximation to the bessel function of the second kind and order $n1 + i - 1$ of x.

BGE(i, j) : True if i is bitwise greater than or equal to j.

arguments: i,j	type: i or boz
result: l	class: e

Example(s): If `bit_size(j)` has the value 8 `bge(z'ff', j)` has the value true for any value of j. `bge(0, -1)` has the value false.

BGT(i, j): True if i is bitwise greater than j

arguments: i,j	type: i or boz
result: l	class: e

The result is true if the sequence of bits represented by i is greater than the sequence of bits represented by j, according to the method of bit sequence comparison in 13.3.2 of the standard; otherwise the result is false.

Example(s): `bgt(z'ff', z'fc')` has the value true. `bgt(0, -1)` has the value false.

BLE(i,j): True if i is bitwise less than or equal to j.

arguments: i,j	type: i or boz
result: l	class: e

The result is true if the sequence of bits represented by i is less than or equal to the sequence of bits represented by j, according to the method of bit sequence comparison in 13.3.2 of fortran 2008 standard; otherwise the result is false.

Example(s): `ble(0, j)` has the value true for any value of j. `ble(-1, 0)` has the value false.

BLT(i,j): Bitwise less than.

arguments: i,j	type: i or boz
result: l	class: e

The result is true if the sequence of bits represented by i is less than the sequence of bits represented by j, according to the method of bit sequence comparison in 13.3.2 of fortran 2008 standard; otherwise the result is false.

Example(s): `blt(0, -1)` has the value true. `blt(z'ff', z'fc')` has the value false.

BIT_SIZE(i): Returns the number of bits, as defined by the model of Sect. 13.3 of the standard.

argument: i	type: i
result: as argument	class: i

Example(s): `n_bits=bit_size(i)`

BTEST(i, pos): True if and only if a specified bit of an integer value is one.

argument: i	type: i
result: l	class: e

Example(s): `t=btest(i, pos)`

CEILING(a, kind): Least integer greater than or equal to a.

argument: a	type: r
result: i	class: e

Note(s): If kind is present the result has the kind type parameter kind. otherwise the result is of type default integer.

Example(s): `i=ceiling(a)` If `a=12.21` then `i=13`, if `a=-3.16` then `i=-3`.

CHAR(i, kind): Returns the character in a given position in the processor collating sequence associated with the specified kind type parameter. It is the inverse of the ICHAR function.

argument: i **type:** i
result: char **class:** e

Note(s): ASCII is the default character set.

Example(s): `c=char(65)` and for the ASCII character set `c='a'`.

CMPLX(x, y, kind): Converts to complex from integer, real and complex.

argument: x **type:** n
result: c **class:** e

Note(s):

1. If `x` is complex and `y` is absent it is as if `y` were present with the value `a(x)`.
2. If `x` is not complex and `y` is absent, it is as if `y` were present with the value 0.

Example(s): `z=cmplx(x,y)`

COMMAND_ARGUMENT_COUNT(): Number of command arguments.

arguments: none **result:** i
class: t

The result value is equal to the number of command arguments available. If there are no command arguments available or if the processor does not support command arguments, then the result has the value zero. If the processor has a concept of a command name, the command name does not count as one of the command arguments.

Example(s): `i = command_argument_count()`

CONJG(z): Conjugate of a complex argument.

argument: z **type:** c
result: as z **class:** e

Example(s): `z1=conjg(z)`

COS(x): Cosine.

argument: x **type:** r, c
result: as argument **class:** e

Note(s): The arguments of all trigonometric functions should be in radians, not degrees.

Example(s): `a=cos (x)`

COSH(x): Hyperbolic cosine.

argument: x	type: r,c
result: as argument	class: e

Example(s): `z=cosh (x)`

COUNT(mask, dim, kind): Returns the number of true elements in mask along dimension dim.

argument: mask	type: l
result: i	class: t

Note(s): dim must be a scalar in the range $1 \leq dim \leq n$, where n is the rank of mask. The result is scalar if dim is absent or mask has rank 1. Otherwise it works on the dimension dim of mask and the result is an array of rank $n - 1$.

Example(s): `n=count (a)`

CPU_TIME(time): returns the processor time.

argument: time	type: r
result: n/a	class: s

Example(s): `call cpu_time(time)`

CSHIFT(array, shift, dim): Circular shift on a rank 1 array or rank 1 sections of higher-rank arrays.

argument: array	type: any
result: as array	class: t

Note(s): array must be an array, shift must be a scalar if array has rank 1, otherwise it is an array of rank $n - 1$, where n is the rank of array. dim must be a scalar with a value in the range $1 \leq dim \leq n$.

Example(s): `array=cshift (array,10)`

DATE_AND_TIME(date, time, zone, values): Returns the current date and time (compatible with ISO 8601:1988).

argument: date	type: s
result: n/a	class: s

Time and zone are of type s.

Note(s):

1. Date is optional and must be scalar and 8 characters long in order to return the complete value of the form ccyyymmdd, where cc is the century, yy is the year, mm is the month and dd is the day. It is intent (out).

2. Time is optional and must be scalar and 10 characters long in order to return the complete value of the form hhmmss . sss where hh is the hour, mm is the minutes and ss . sss is the seconds and milliseconds. It is intent (out).

3. Zone is optional and must be scalar and must be 5 characters long in order to return the complete value of the form hhmm where hh and mm are the time differences with respect to coordinated universal time in hours and minutes. it is intent (out).

4. Values is optional and a rank 1 array of size 8. It is intent (out). The values returned are as follows:

values(1) = the year
 values(2) = the month
 values(3) = the day
 values(4) = the time with respect to coordinated universal time in minutes.
 values(5) = the hour (24 hour clock)
 values(6) = the minutes
 values(7) = the seconds
 values(8) = the milliseconds in the range 0 – 999.

Example(s): call date_time(d,t,z,v)

DBLE(a): converts to double precision from integer, real, and complex

argument: a	type: n
result: dp	class: e

Example(s): d=dble(a)

DIGITS(x): returns the number of significant digits of the argument as defined in the numeric models for integer and reals in Chap. 5.

argument: x	type: i,r
result: i	class: i

Example(s): i=digits(x)

DIM(x, y): difference of two values if positive or zero otherwise.

argument: x	type: i
result: as arguments	class: e

Example(s): z=dim(x,y)

DOT_PRODUCT(vector_1,vector_2): Performs the mathematical dot product of two rank 1 arrays.

argument: vector_1	type: n
result: as arguments	class: t

vector_2 is as vector_1.

Note(s):

1. For integer and real `vector_1` result has the value `sum(vector_1*vector_2)`.
2. For complex `vector_1` result has the value `sum(conjg(vector_1)*vector_2)`.
3. For logical `vector_1` result has the value `any(vector_1 .and. vector_2)`.

Example(s): `a=dot_product(x,y)`

DPROD(x, y): Double precision product of two reals.

argument: x	type: r
result: dp	class: e

Example(s): `d=dprod(x,y)`

DSHIFTL(i, j, shift): Combined left shift.

arguments: i,j	type: i or boz
argument: shift	type: i
result: See note below.	class: e

Note(s): Result type: Same as i if i is of type integer; otherwise, same as j. if either i or j is a boz-literal-constant, it is first converted as if by the intrinsic function int to type integer with the kind type parameter of the other. the rightmost shift bits of the result value are the same as the leftmost bits of j, and the remaining bits of the result value are the same as the rightmost bits of i. this is equal to `ior(shiftl(i, shift), shiftr(j, bit size(j)-shift))`. the model for the interpretation of an integer value as a sequence of bits is in Sect. 13.3 of the standard.

Example(s): `dshiftl(1, 2**30, 2)` has the value 5 if default integer has 32 bits. `dshiftl(i, i, shift)` has the same result value as `ishftc(i, shift)`.

DSHIFTR(i, j, shift): Combined right shift.

arguments: i,j	type: i or boz
argument: shift	type: i
result: See note below.	class: e

Note(s): Result: Same as i if i is of type integer; otherwise, same as j. if either i or j is a boz-literal-constant, it is first converted as if by the intrinsic function int to type integer with the kind type parameter of the other. the leftmost shift bits of the result value are the same as the rightmost bits of i, and the remaining bits of the result value are the same as the leftmost bits of j. this is equal to `ior(shiftl(i, bit size(i)-shift), shiftr(j, shift))`. the model for the interpretation of an integer value as a sequence of bits is in 13.3 of fortran 2008 standard.

Example(s): `dshiftr(1, 16, 3)` has the value 229 +2 if default integer has 32 bits. `dshiftr(i, i, shift)` has the same result value as `ishftc(i,-shift)`.

EOSHIFT(array, shift, boundary, dim): End of shift of a rank 1 array or rank 1 section of a higher-rank array.

argument: array	type: any
result: as array	class: t

Note(s):

1. boundary is as array.
2. Array must be an array, shift must be a scalar if array has rank 1, otherwise it is an array of rank $n - 1$, where n is the rank of array. boundary must be scalar if array has rank 1, otherwise it must be either scalar or of rank $n - 1$. dim must be a scalar with a value in the range $1 \leq dim \leq n$.

Example(s): `a=eoshift(a,shift)`

EPSILON(x): Smallest difference between two reals of that kind. See Chap. 5 and real numeric model.

argument: x	type: r
result: as argument	class: i

Example(s): `tiny=epsilon(x)`

ERF(x): Error function.

argument: x	type: r
result: as x	class: e

Example(s): `y = erf(1.0)` has the value 0.843 (approximately).

ERFC(x): Complementary error function.

argument: x	type: r
result: as x	class: e

Example(s): `y = erfc(1.0)` has the value 0.157 (approximately).

ERFC_SCALED(x): Scaled complementary error function.

argument: x	type: r
result: as x	class: e

Example(s): `y = erfc_scaled(20.0)` has the value 0.0282 (approximately).

EXECUTE_COMMAND_LINE(command, wait, exitstat, cmdstat, cmdmsg): Execute a command line.

Note(s):

argument: command—shall be a default character scalar. it is an intent(in) argument. its value is the command line to be executed. the interpretation is processor dependent.

argument: wait -(optional) shall be a default logical scalar. it is an intent(in) argument. if wait is present with the value false, and the processor supports asynchronous execution of the command, the command is executed asynchronously; otherwise it is executed synchronously.

argument: exitstat -(optional) shall be a default integer scalar. it is an intent(inout) argument. if the command is executed synchronously, it is assigned the value of the processor-dependent exit status. otherwise, the value of exitstat is unchanged.

argument: cmdstat -(optional) shall be a default integer scalar. it is an intent(out) argument. it is assigned the value -1 if the processor does not support command line execution, a processor-dependent positive value if an error condition occurs, or the value -2 if no error condition occurs but wait is present with the value false and the processor does not support asynchronous execution. otherwise it is assigned the value 0.

argument: cmdmsg -(optional) shall be a default character scalar. it is an intent(inout) argument. if an error condition occurs, it is assigned a processor-dependent explanatory message. otherwise, it is unchanged.

Example(s): call execute_command_line('pwd') will print the full pathname of the current directory under unix and an error message from windows.

EXP(x): Exponential. e^x

argument: x	type: r, c
result: as argument	class: e

Example(s): y=exp (x)

EXPONENT(x): Returns the exponent component of the argument. See Chap. 5 and the real numeric model.

argument: x	type: r
result: i	class: e

Example(s): i=exponent (x)

EXTENDS_TYPE_OF(a, mold): Query dynamic type for extension.

arguments: a, mold	type: p*
result: l	class: i

Note(s): If mold is unlimited polymorphic and is either a disassociated pointer or unallocated allocatable variable, the result is true; otherwise if a is unlimited polymorphic and is either a disassociated pointer or unallocated allocatable variable, the result is false; otherwise if the dynamic type of a or mold is extensible, the result is true if and only if the dynamic type of a is an extension type of the dynamic type of mold; otherwise the result is processor dependent.

Example(s):

```
if(extends_type_of(a, mold)) then
    print *, 'dynamic type of a is an '
```

```

print *, 'extension of dynamic type of mold'
end if

```

FINDLOC(array, value, dim, mask, kind, back):**FINDLOC(array, value, mask, kind, back):** Location(s) of a specified value.**Note(s):**

argument: array **type:** shall be an array of intrinsic type

argument: value **type:** shall be scalar and in type conformance with array, as specified in Table 7.2 for relational intrinsic operations 7.1.5.5.2 of the standard).

argument: dim **type:** shall be an integer scalar with a value in the range 1 dim n, where n is the rank of array. the corresponding actual argument shall not be an optional dummy argument.

argument: mask **type:**(optional) shall be of type logical and shall be conformable with array.

argument: kind **type:**(optional) shall be a scalar integer constant expression.

argument: back **type:**(optional) shall be a logical scalar.

class: t

FLOOR(a, kind): Returns the greatest integer less than or equal to the argument

argument: a	type: r
result: i	class: e

Note(s): if kind is present the result has the kind type parameter kind, otherwise the result is of type default integer.

Example(s): i=floor(a) when a=5.2 i has the value 5, when a=-9.7 i has the value -10.

FRACTION(x): Returns the fractional part of the real numeric model of the argument. See Chap. 5 and the real numeric model.

argument: x	type: r
result: as x	class: e

Example(s): f=fraction(x)

GAMMA(x): Gamma function.

argument: x	type: r
result: as x	class: e

Example: y = gamma(1.0) has the value 1.000 (approximately).

GET_COMMAND(command, length, status): Query program invocation command.**GET_COMMAND_ARGUMENT(number, value, length, status):** Query arguments from program invocation.

GET_ENVIRONMENT_VARIABLE(name, value, length, status, trim name):
Query environment variable.

HUGE(x): Returns the largest number for the kind type of the argument. See Chap.[5](#) and the real and integer numeric models.

argument: x	type: i,r
result: as argument	class: i

Example h=huge (x)

HYPOT(x, y): Euclidean distance function.

arguments: x,y	type: r
result: r	class: e

Example: h = hypot (3.0, 4.0) has the value 5.0(approximately).

IACHAR(c): Returns the position of the character argument in the ASCII collating sequence.

argument: c	type: char
result: i	class: e

Example(s): i=ichar ('a') returns the value 65.

IALL(array, dim, mask) or IALL(array, mask): Reduce array with bitwise and operation.

IAND(i, j): Performs a logical and on the arguments.

argument: i	type: i
result: as arguments	class: e

Example(s): k=iand (i, j)

IANY(array, dim, mask) or IANY(array, mask): Reduce array with bitwise or operation.

IBCLR(i, pos): Clears one bit of the argument to zero.

argument: i	type: i
result: as i	class: e

Note(s): $0 \leq pos \leq \text{bitsize}(i)$

Example(s): `i=ibclr(i, pos)`

IBITS(i, pos, len): Returns a sequence of bits.

argument: i	type: i
result: as i	class: e

Note(s):

$0 \leq pos$
 $(pos + length) \leq bit_size(i)$
 $len \geq 0$

Example(s): `slice=ibits(i, pos, len)`

IBSET(i, pos): Sets one bit of the argument to one.

argument: i	type: i
result: as i	class: e

Note(s):

$0 \leq pos \leq bitsize(i)$

Example(s): `i=ibset(i, pos)`

ICHAR(c): Returns the position of a character in the processor collating sequence associated with the kind type parameter of the argument. normally the position in the ASCII collating sequence.

argument: c	type: char
result: i	class: e

Example(s): `i=ichar('a')` would return the value 65 for the ASCII character set.

IEOR(i, j): Performs an exclusive or on the arguments.

argument: i	type: i
result: Same as i if i is of type integer; otherwise, same as j.	class: e

Example(s): `i=ieor(i, j)`

IMAGE_INDEX(coarray, sub): convert cosubscripts to image index.

argument: coarray	type: co
argument: sub	type: rank-one integer array
result: i	class: i

Example(s):

```
integer, codimension[0:*]:: x
integer, dimension(10,15), &
codimension[3,0:1,-1:*]:: z
```

```
print*, image_index(x, (/0/));
print*, image_index(z, (/2, 0, -1/))
```

would print 1 and 2 respectively.

INDEX(string, substring, back, kind): locates one substring in another, i.e., returns position of substring in character expression string.

argument: string	type: s
result: i	class: e

substring is of type s.

Note(s):

1. if back is absent or present with the value .false. then the function returns the start position of the first occurrence of the substring. if len(substring) = 0 then one is returned.
2. if back is present with the value .true. then the function returns the start position of the last occurrence of the substring. if len(substring) = 0 then the value(len(string) + 1) is returned.
3. if the substring is not found the result is zero.
4. if len(string) < len(substring) the result is zero.

Example(s):

```
where=index(' hello world hello','hello')
the result 2 is returned.
```

```
where=index(' hello world hello','hello',.true.)
the result 14 is returned.
```

INT(a, kind): converts to integer from integer, real, and complex.

argument: a	type: n
result: i	class: e

Example(s): i=int (f)

IOR(i, j): performs an inclusive or on the arguments.

argument: i	type: i
result: as i	class: e

Example(s): i=ior (i, j)

IPARITY(array, dim, mask) or IPARITY(array, mask): reduce array with bitwise exclusive or operation.

ISHFT(i, shift): performs a logical shift. The bits of i are shifted by shift positions.

argument: i **type:** i
result: as i **class:** e

Note(s):

$|shift| \leq bitsize(i)$

Example(s): `i=ishift(i, shift).`

ISHFTC(i, shift, size): performs a circular shift of the rightmost bits. The size rightmost bits of i are circularly shifted by shift positions.

argument: i **type:** i
result: i **class:** e

Note(s):

$|shift| < size$

$0 \leq size \leq bitsize(i)$

If size is absent it is as if it were present with the value of `bit_size(i)`.

If shift is positive the shift is to the left.

If shift is negative the shift is to the right.

If shift is zero no shift is performed.

`i=ishftc(i,shift,size)`

IS_CONTIGUOUS(array): test contiguity of an array.

argument: array **type:** any
result: l **class:** i

Example(s):

```
integer,target, dimension(10)::a
integer,pointer,dimension(:) :: p
p= a(1:10:2); print*,is_contiguous(p)
```

would print 'f'.

IS_IOSTAT_END(i): test iostat value for end-of-file.

argument: i **type:** i
result: l **class:** e

Example: `is_iostat_end(i)` returns value true if i is an i/o status value that corresponds to an end-of-file condition, and false otherwise.

```
read(unit=1,fmt=*, iostat=ist)y(i)
if(is_iostat_end(ist)) then
    print*, 'end of file!'
endif
```

IS_IOSTAT_EOR(i): test iostat value for end-of-record.

argument: i	type: i
result: l	class: e

Example(s): `is_iostat_eor(i)` returns the value true if i is an i/o status value that corresponds to an end-of-record condition, and false otherwise.

KIND(x): returns the kind type parameter of the argument.

argument: x	type: any
result: i	class: i

Example(s): `i=kind(x)`

LBOUND(array, dim, kind): Lower bound(s) of an array.

argument: array	type: any
result: i	class: i

Note(s):

1. `dim` optional. $1 \leq dim \leq n$ Where n is the rank of array. the result is scalar if `dim` is present otherwise the result is an array of rank 1 and size n. The result is scalar if `dim` is present, otherwise a rank 1 array and size n.
2. if `array` is a whole array and either array is an assumed-size array of rank `dim` or dimension `dim` of array has nonzero extent, `lbound (array, dim)` has a value equal to the lower bound for subscript `dim` of `array`. Otherwise the result value is 1.

Example(s): `i=lbound(array)`

LCOBOUND(coarray, dim, kind): lower cobound(s) of a coarray.

argument: coarray	type: co
argument: dim (optional)	type: i
argument: kind(optional)	type: i
result: i	class: i

Example(s):

```
integer, codimension[:, :, :], allocatable::a
allocate(a[2:3, 7:*)]
```

`lcbound(a)` is [2,7] and `lcobound(a, dim=2)` is 7

Note(s):

1. `lcobound(coarray, dim)` has a value equal to the lower cobound for cosubscript `dim` of coarray.

LEADZ(i): Number of leading zero bits.

argument: i	type: i
result: i	class: e

Example: leadz(1) has the value 31 if bit size(1) has the value 32.

LEN(string): Length of a character entity.

argument: string	type: s
result: i	class: i

Example(s): i=len(string)

LEN_TRIM(string): Length of character argument less the number of trailing blanks.

argument: string	type: s
result: i	class: e

Example(s): i=len_trim(string)

LGE(string_1, string_2):

Lexically greater than or equal to and this is default character or ASCII.

argument: string_1	type: s,ASCII
result: l	class: e

string_2 is of type s.

Example(s): l=lge(s1,s2)

LGT(string_1, string_2): Lexically greater than and this is based on the ASCII collating sequence.

argument: string_1	type: s
---------------------------	----------------

Example(s): l=lgte(s1,s2)

LLE(string_1, string_2): Lexically less than or equal to and this is based on the ASCII collating sequence.

argument: string_1	type: s
result: l	class: e

string_2 is of type s.

Example(s): l=llte(s1,s2)

LLT(string_1, string_2): Lexically less than and this is based on the ASCII collating sequence.

argument: string_1	type: s
result: l	class: e

Example(s): `l=llt(s1,s2)`

LOG(x): natural logarithm.

argument: x	type: r, c
result: as argument	class: e

Example(s): `y=log(x)`

LOG_GAMMA(x): logarithm of the absolute value of the gamma function.

argument: x	type: r
result: r	class: e

Example(s): `log_gamma(3.0)` has the value 0.693 (approximately).

LOG10(x): common logarithm, log10

argument: x	type: r
result: as argument	class: e

Example(s): `y=log10(x)`

LOGICAL(l, kind): converts between different logical kind types, i.e., performs a type cast.

argument: l	type: l
result: l	class: e

Example(s): `l=logical(k,kind)`

MASKL(i, kind): left justified mask.

argument: i	type: i
result: i	class: e

Example: `maskl(4)` has the value `shiftl(15, bit_size(0) - 4)`

MASKR(i, kind): right justified mask.

argument: i	type: i
result: i	class: e

Example(s): `maskr(4)` has the value 15.

MATMUL(matrix_1, matrix_2): performs mathematical matrix multiplication of the array arguments.

argument: matrix_1	type: n,l
result: as arguments	class: t

`matrix_2` is as `matrix_1`.

Note(s):

1. matrix_1 and matrix_2 must be arrays of rank 1 or 2. if matrix_1 is of numeric type so must matrix_2.
2. if matrix_1 has rank 1, matrix_2 must have rank 2.
3. if matrix_2 has rank 1, matrix_1 must have rank 2.
4. the size of the first dimension of matrix_2 must equal the size of the last dimension of matrix_1.
5. if matrix_1 has shape(n,m) and matrix_2 has shape(m,k) the result has shape (n,k).
6. if matrix_1 has shape(m) and matrix_2 has shape(m,k) the result has shape (k). 7. if matrix_1 has shape(n,m) and matrix_2 has shape(m) the result has shape(n).

Example(s): `r=matmul (m_1 , m_2)`

MAX(a1, a2, a3,...): returns the largest value.

argument: a1	type: i,r,s
result: as arguments	class: e

a2, a3,.. are as a1.

Example(s): `a=max (a1 , a2 , a3 , a4)`

MAXEXPONENT(x): returns the maximum exponent. See Chap. 5 and numeric models.

argument: x	type: r
result: i	class: i

Example(s): `i=maxexponent (x)`

MAXLOC(array, dim, mask, kind, back): location(s) of maximum value.

Alternate form: **MAXLOC(array, mask, kind, back)**

argument: array	type: i,r,s
result: i	class: t

Note(s):

1. dim shall be an integer scalar with a value in the range $1 \leq dim \leq n$, where n is the rank of array. The corresponding actual argument shall not be an optional dummy argument.
2. mask (optional) shall be of type logical and shall be conformable with array.
3. kind (optional) shall be a scalar integer constant expression.
4. back (optional) shall be scalar and of type logical.
5. The result of maxloc (array) is a rank-one array whose element values are the values of the subscripts of an element of array whose value equals the maximum value of all of the elements of array. The ith subscript returned lies in the range 1 to ei, where ei is the extent of the ith dimension of array. If array has size zero, all elements of the result are zero.

6. The result of `maxloc(array, mask = mask)` is a rank-one array whose element values are the values of the subscripts of an element of `array`, corresponding to a true element of `mask`, whose value equals the maximum value of all such elements of `array`. The *i*th subscript returned lies in the range 1 to `ei`, where `ei` is the extent of the *i*th dimension of `array`. If `array` has size zero or every element of `mask` has the value false, all elements of the result are zero.

Example(s):

```
a=(/5,6,7,8/)
i=maxloc(a)
```

is (4), which is the subscript of the location of the first occurrence of the maximum value in the rank 1 array.

If

$$A = \begin{pmatrix} 1 & 8 & 5 \\ 9 & 3 & 6 \\ 4 & 2 & 7 \end{pmatrix}$$

`i = maxloc(a, dim=1)`

is (2,1,3) returning the position of the largest in each column.

`i = maxloc(a, dim=2)`

is (2,1,3) returning the position of the largest in each row.

MAXVAL(array, dim, mask): maximum value(s) of `array`.

There is an alternate form: **MAXVAL(array, mask)**.

argument: array		type: i,r,s
result: as argument		class: t

Note(s):

0. Note all cases are considered below. Refer to the standard for the full capability of this intrinsic.

1. `dim` shall be an integer scalar with a value in the range $1 \leq dim \leq n$, where `n` is the rank of `array`. The corresponding actual argument shall not be an optional dummy argument.

2. `mask` (optional) shall be of type logical and shall be conformable with `array`.

3. The result of `maxval(array)` has a value equal to the maximum value of all the elements of `array` if the size of `array` is not zero. If `array` has size zero and type integer or real, the result has the value of the negative number of the largest magnitude supported by the processor for numbers of the type and kind type parameter of `array`. If `array` has size zero and type character, the result has the value of a string of characters of length `len(array)`, with each character equal to `char(0, kind(array))`.

4. The result of `maxval(array, mask=mask)` has a value equal to that of `maxval(pack(array, mask))`.

Example(s): `maxval((/1,2,3/))` returns the value 3. `maxval(c,mask=c < 0.0)` returns the maximum of the negative elements of c.

For

$$B = \begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix}$$

`maxval(b,dim=1)` returns (2,4,6)
`maxval(b,dim=2)` returns (5,6)

MERGE(true, false, mask): chooses alternative values according to the value of a mask.

argument: true **type:** any
result: as true **class:** e

Example(s): For

$$true = \begin{pmatrix} 2 & 6 & 10 \\ 4 & 8 & 12 \end{pmatrix}, false = \begin{pmatrix} 1 & 5 & 9 \\ 3 & 7 & 11 \end{pmatrix}, \text{and } mask = \begin{pmatrix} T & F & T \\ F & T & F \end{pmatrix}$$

$$result = \begin{pmatrix} 2 & 5 & 10 \\ 3 & 8 & 11 \end{pmatrix}$$

MERGE_BITS(i, j, mask): merge of bits under mask.

argument: i **type:** i or boz
argument: j i or boz
argument: mask i or boz
result: same as i if integer,
otherwise same as j.
class: e

Example(s): `merge_bits(14, 18, 22)` has the value 6.

MIN(a1, a2, a3,...): chooses the smallest value.

argument: a1 **type:** i, r, s
result: as arguments **class:** e

Example(s): `y=min(x1, x2, x3, x4, x5)`

MINEXPONENT(x): returns the minimum exponent. See Chap. 5 and numeric models.

argument: x **type:** r
result: i **class:** i

Example(s):`i=minexponent(x)`

MINLOC(array, dim, mask, kind, back): Location of minimum value. Alternate form **MINLOC(array, mask, kind, back).**

argument: array	type:	i,r
result: i	class:	t

Note(s):

0. For full coverage of the capability of this function consult the standard. Some simple cases are covered below.
1. `dim` shall be an integer scalar with a value in the range $1 \leq dim \leq n$, where `n` is the rank of `array`. The corresponding actual argument shall not be an optional dummy argument.
2. `mask` (optional) shall be of type logical and shall be conformable with `array`.
3. `kind` (optional) shall be a scalar integer constant expression.
4. `back` (optional) shall be scalar and of type logical.
5. The result of `minloc(array)` is a rank-one array whose element values are the values of the subscripts of an element of `array` whose value equals the maximum value of all of the elements of `array`. The *i*th subscript returned lies in the range 1 to `ei`, where `ei` is the extent of the *i*th dimension of `array`. If `array` has size zero, all elements of the result are zero.
6. The result of `minloc(array, mask = mask)` is a rank-one array whose element values are the values of the subscripts of an element of `array`, corresponding to a true element of `mask`, whose value equals the maximum value of all such elements of `array`. The *i*th subscript returned lies in the range 1 to `ei`, where `ei` is the extent of the *i*th dimension of `array`. If `array` has size zero or every element of `mask` has the value false, all elements of the result are zero.

Example(s):`i=minloc(array)`

In the above example if `array` is a rank 2 array of shape (5,10) and the smallest value is in position (2,1) then the result is the rank 1 array `i` with shape (2) and `i(1)=2` and `i(2)=1`.

See `maxloc` for further examples.

MINVAL(array, dim, mask): Minimum value(s) of `array`. Alternate form `appcminval(array, mask)`.

argument: array	type:	i,r
result: as array	class:	t

Note(s):

1. `dim` shall be an integer scalar with a value in the range $1 \leq dim \leq n$, where `n` is the rank of `array`. The corresponding actual argument shall not be an optional dummy argument.
2. `mask` (optional) shall be of type logical and shall be conformable with `array`.

3. The result of `minval(array)` has a value 1 equal to the minimum value of all the elements of `array` if the size of `array` is not zero. If `array` has size zero and type integer or real, the result has the value of the positive number of the largest magnitude supported by the processor for numbers of the type and kind type parameter of `array`. If `array` has size zero and type character, the result has the value of a string of characters of length `len(array)`, with each character equal to `char(n-1,kind(array))`.
4. The result of `minval(array,mask=mask)` has a value equal to that of `minval(pack(array,mask))`.

Example(s):

`minval((/1,2,3/))` returns the value 1.

`minval(c,mask=c>0.0)` returns the minimum of the positive elements of c.

For

$$B = \begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix}$$

`minval(b,dim=1)` returns (1,3,5).

`minval(b,dim=2)` returns (1,2).

MOD(a,b): returns the remainder when first argument divided by second.

argument: a	type: i, r
result: as arguments	class: e

Note(s): if b=0 the result is processor dependent. for b 0 the result is $a - \text{int}(a/b) * b$.

Example(s): `r=mod(a,b)` if a=8 and b=5 then r=3; if a=-8 and b=5 then r=-3; if a=8 and b=-5 then r=3; if a=-8 and b=-5 then r=-3.

MODULO(a,b): returns the modulo of the arguments.

argument: a	type: i,r
result: as a	class: e

Note(s):

1. if b=0 then the result is processor dependent.

2. For integer a the result is r where $a = q * b + r$ and q is integer. The inequalities $0 \leq r < b$ holds if $b > 0$, and $b < r \leq 0$ holds if $b < 0$. 3. For real a the result is $a - \text{floor}(a/b) * b$.

Example(s): `r=modulo(a,b)` if a=8 and b=5 then r=3; if a=-8 and b=5 then r=2; if a=8 and b=-5 then r=-2; if a=-8 and b=-5 then r=-3.

MOVE_ALLOC(from,to): move an allocation.**Note(s):**

argument: `from` may be any type and rank. It shall be allocatable. It is `intent(inout)`.

argument: to type compatible with from and same rank. It shall be allocatable.
class: pure subroutine

Example(s):

```
real,allocatable :: grid(:,tempgrid(:)
...
allocate(grid(-n:n))
! initial allocation of grid
...
! "reallocation" of grid to
! allow intermediate points
allocate(tempgrid(-2*n:2*n))
! allocate bigger grid
tempgrid(:2)=grid
! distribute values to new locations
call move_alloc(to=grid,from=tempgrid)
! old grid is deallocated because to is
! intent (out), and grid then "takes over"
! new grid allocation
```

MVBITS(from, frompos, len, to, topos): copies a sequence of bits from one data object to another.

argument: from	type: i
result: n/a	class: s

all arguments are of integer type.

Note(s):

from shall be of type integer. It is an intent(in) argument. frompos shall be of type integer and nonnegative. It is an intent(in) argument. $frompos + len \leq bit_size(from)$. len shall be of type integer and nonnegative. It is an intent(in) argument. to shall be a variable of the same type and kind type parameter value as from and may be associated with from. It is an intent(inout) argument. to is defined by copying the sequence of bits of length len, starting at position frompos of from to position topos of to. No other bits of to are altered. On return, the len bits of to starting at topos are equal to the value that the len bits of from starting at frompos had on entry. topos shall be of type integer and nonnegative. It is an intent(in) argument. $topos + len \leq bit_size(to)$.

Example(s):

```
If to has the initial value 6,
the value of to after the statement
call mvbits (7, 2, 2, TO, 0) is 5.
```

Example(s): call mvbits(f,fp,l,t,tp)

NEAREST(x,next): returns the nearest different number. See Chap. 5 and the real numeric model.

argument: x	type:	r
result: as x	class:	e

next is of type r.

Example(s):n=nearest (x, next)

NEW_LINE(a): returns newline character used for formatted stream output.

argument: a	type:	char
result: char	class:	i

Example(s):

```
open(2,file='nline.txt', access='stream', form='formatted')
write(2,'(a)')'hola'//new_line('a')//'mundo'
```

This will write 2 lines to the file nline.txt.

NINT(a, kind): yields nearest integer.

argument: a	type:	r
result: i	class:	e

Note(s):

1. $a > 0$, the result is $\text{int}(a+0.5)$.
2. $a \leq 0$, the result is $\text{int}(a-0.5)$.

Example(s): i=int (x)

NORM2(x, dim): l2 norm of an array.

argument: x	type:	r array
argument: dim	type:	See note below.
result: r	class:	t

Note(s):

1. type: dim (optional) shall be an integer scalar with a value in the range $1 \leq dim \leq n$, where n is the rank of x. The corresponding actual argument shall not be an optional dummy argument.
2. The result of norm2 (x) has a value equal to a processor-dependent approximation to the generalized l2 norm of x, which is the square root of the sum of the squares of the elements of x.
3. If dim is present the array is reduced as for sum (x, dim) except that norm2 is applied to the reduced vectors.

Example(s): See below.

```
norm2([3.0, 4.0]) is 5.0.
If x has the value
  1.0 2.0
  3.0 4.0
norm2(x,dim=1) is [3.162, 4.472]
norm2(x,dim=2) is [2.236,5.0]
approximately.
```

NOT(i): returns the logical complement of the argument.

argument: i	type: i
result: as i	class: e

Example(s): i=not (i)

NULL(mold): Returns a disassociated pointer.

argument: mold	type: p
result: as argument	class: t

Note(s): If the argument mold is present the result is the same as mold. Otherwise it is determined by context.

Example(s): real , pointer :: p=>null()

NUM_IMAGES(): Number of images.

argument: none	
result: i	class: t

Example(s): print*, ' number of images = ', num_images()

PACK(array, mask, vector): Packs an array into an array of rank 1, under the control of a mask.

argument: array	type: any
result: as array	class: t

Note(s):

1. array must be an array.
2. mask be conformable with array.
3. vector must have rank 1 and have at least as many elements as there are true elements in mask.
4. if mask is scalar with the value true. vector must have at least as many elements as there are in array.
5. the result is an array of rank 1.
6. if vector is present the result size is that of vector.

7. if vector is not present the result size is t, the number of true elements in mask, unless mask is scalar with a value true in which case the result size is the size of array.

Example(s): `r=pack(a, m)`

PARITY(mask, dim): Reduce array with `.neqv.` operation.

argument: mask	type: l array
argument: dim shall be an	
integer scalar in the range	
1 <= dim <= n where n is	
rank of mask.	

Example(s): If t has the value `true` and f has the value `false` `parity([t, t, t, f])` is `true`.

POPCNT(i): Number of one bits in the sequence of bits of i.

argument: i	type: i
result: i	class: e

Example: `popcnt([1, 2, 3, 4, 5, 6, 7])` has the value [1, 1, 2, 1, 2, 2, 3].

POPPAR(i): returns the parity of the bit count of an integer expressed as 0 or 1.

argument: i	type: i
result: i	type: e

Example(s): `poppar([1, 2, 3, 4, 5, 6, 7])` has the value [1, 1, 0, 1, 0, 0, 1]

PRECISION(x): Returns the decimal precision of the argument. See Chap. 5 and numeric models.

argument: x	type: r, c
result: i	class: i

Example(s): `i=precision(x)`

PRESENT(a): Returns whether an optional argument is present.

argument: a	type: any
result: l	class: i

Note(s): a must be an optional argument of the procedure in which the present function reference appears.

Example(s): `if(present(a)) then`

PRODUCT(array, dim, mask): The product of all of the elements of array along the dimension dim corresponding to the true elements of mask. There is an alternate form **PRODUCT(array, mask)**

argument: array **type:** n
result: as array **class:** t

Note(s):

1. array must be an array.
2. $1 \leq dim \leq n$ n where n is the rank of array.
3. mask must be conformable with array.
4. result is scalar if dim is absent, or array has rank 1, otherwise the result is an array of rank n-1.

Example:

```
product((/1,2,3/)) the result is 6.  

product( c , mask = c > 0.0) forms the product of the positive elements of c.
```

If

$$B = \begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix}$$

```
product(b, dim=1)  

is (2,12,30)  

product(b, dim=2)  

is (15,48)
```

RADIX(x): Returns the base of the numeric argument. See Chap. 5 and numeric models.

argument: x **type:** i,r
result: i **class:** i

Example(s): base=radix(x)

RANDOM_NUMBER(x): Returns one pseudorandom number or an array of pseudorandom numbers from the uniform distribution over the range $0 \leq x < 1$

argument: x **type:** r
result: n/a **class:** s

Note(s): x is intent(out).

Example(s): call random_number(x)

RANDOM_SEED(size, put, get): Restarts (seeds) or queries the pseudorandom generator used by random_number.

argument: size **type:** i
result: n/a **class:** s

All arguments are of integer type.

Note(s):

1. `size` is `intent(out)`. It is set to the number `n` of integers that the processor uses to hold the value of the seed.
2. `put` is `intent(in)`. It is an array of rank 1 and `size >= n`. It is used by the processor to set the seed value.
3. `get` is `intent(out)`. It is an array of rank 1 and `size >= n`. It is set by the processor to the current value of the seed.

Example(s): call `random_seed`

RANGE(x): Returns the decimal exponent range of the real argument. See Chap. 5 and the numeric model representing the argument.

<code>argument: x</code>	<code>type: n</code>
<code>result: i</code>	<code>class: i</code>

Example(s): `i=range(n)`

REAL(a, kind): Converts to real from integer, real or complex.

<code>argument: a</code>	<code>type: n</code>
<code>result: r</code>	<code>class: e</code>

Example(s): `x=real(a)`

REPEAT(string, n_copies): Concatenate several copies of a string.

<code>argument: string</code>	<code>type: s</code>
<code>result: s</code>	<code>class: t</code>

Example(s): `new_s=repeat(s, 10)`

RESHAPE(source, shape, pad, order): Constructs an array of a specified shape from the elements of a given array.

<code>argument: source</code>	<code>type: any</code>
<code>result: as source</code>	<code>class: t</code>

Note(s):

1. `source` must be an array. If `pad` is absent or of size zero the size of `source` must be `product(shape)`.
2. `shape` must be a rank 1 array and $0 \leq size < 8$
3. `pad` must be an array.
4. `order` must have the same shape as `shape` and its value must be a permutation of $(1, 2, \dots, n)$ where n is the size of `shape`. If absent it is as if it were present with the value $(1, 2, \dots, n)$.
5. the result is an array of shape `shape`

Example(s):

```
reshape((/1,2,3,4,5,6/),(/2,3/))
```

has the value

$$\begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix}$$

```
reshape((/1,2,3,4,5,6/),(/2,4/),(/0,0/),(/2,1/))
```

has the value

$$\begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 0 & 0 \end{pmatrix}$$

RRSPACING(x): returns the reciprocal of the relative spacing of model numbers near the argument value. See Chap. 5 and the real numeric model.

argument: x	type: r
result: as x	class: e

Example: z=rrspacing(x)

SAME_TYPE_AS(a, b): Query dynamic types for equality. If the dynamic type of a or b is extensible, the result is true if and only if the dynamic type of a is the same as the dynamic type of b. If neither a nor b has extensible dynamic type, the result is processor dependent.

Note(s):

argument: a an object of extensible declared type or unlimited polymorphic. If it is a pointer, it shall not have an undefined association status.

argument: b an object of extensible declared type or unlimited polymorphic. If it is a pointer, it shall not have an undefined association status.

result: l

type: i

SCALE(x, i): returns xb^i where b is the base in the model representation of x. See Chap. 5 and the real numeric model.

argument: x	type: r
result: as x	class: e

Note(s): i is of integer type.

Example: z=scale(x, i)

SCAN(string, set, back): scans a string for any one of the characters in a set of characters.

argument: string		type: s
result: i		class: e

Note(s):

1. the default is to scan from the left, and will only be from the right when back is present and has the value true.
2. zero is returned if the scan fails.

Example: w=scan(string, set)

SELECTED_CHAR_KIND(name): returns the kind value for the character set whose name is given by the character string name or -1 if not supported.

argument: name		type: char
result: i		class: t

Note(s):

if name has the value:

default:

the result is the kind of the default character type.

ASCII:

the result is the kind of the ASCII character type.

ISO_10646:

the result is the kind of the ISO (IEC) 10646 UCS-4 character type.

SELECTED_INT_KIND(r): returns a value of the kind type parameter of an integer data type that represents all integer values n with $-10^r < n < 10^r$

argument: r		type: i
result: i		class: t

Note(s): r must be scalar.

If a kind type parameter is not available then the value -1 is returned.

Example: i=selected_int_kind(2)

SELECTED_REAL_KIND(p,r,radix): returns a value of the kind type parameter of a real data type with decimal precision of at least p digits and a decimal exponent range of at least r.

argument: p and r		type: i
result: i		class: t

Note(s):

0. at least one argument must be present.
1. p, r and radix must be integer scalars.

2. The result is -1 if the processor supports a real type with radix `radix` and exponent range of at least `r` but not with precision of at least `p`; -2 if the processor supports a real type with radix `radix` and precision of at least `p` but not with exponent range of at least `r`; -3 if the processor supports a real type with radix `radix` but with neither precision of at least `p` nor exponent range of at least `r`; -4 if the processor supports a real type with radix `radix` and either precision of at least `p` or exponent range of at least `r` but not both together; -5 if the processor supports no real type with radix `radix`.

Example: `i=selected_real_kind(p,r)`

SET_EXPONENT(x,i): returns the model number whose fractional part is the fractional part of the model representation of `x` and whose exponent part is `i`.

argument: <code>x</code>	type: <code>r</code>
result: <code>as x</code>	class: <code>e</code>

Note(s): `i` is of integer type.

Example(s): `exp_part=set_exponent(x,i)`

SHAPE(source, kind): Returns the shape of the array argument or scalar.

argument: <code>source</code>	type: any
result: <code>i</code>	class: <code>i</code>

Note(s):

1. `source` may be array valued or scalar. It must not be a pointer that is disassociated or an allocatable array that is not allocated. It must not be an assumed-size array.
2. the result is an array of rank 1 whose size is equal to the rank of `source`.

Example: `s=shape(a(2:5,-1:1))` yields `s=(4,3)`

SHIFTA(i, shift): Right shift with fill.

argument: <code>i</code>	type: <code>i</code>
argument: <code>shift</code>	type: <code>i</code>
result: same as <code>i</code>	class: <code>e</code>

Note(s):

1. `shift` shall be nonnegative and less than or equal to `bit_size(i)`
2. If `shift` is zero the result is `i`. Bits shifted out from the right are lost. The model for the interpretation of an integer value as a sequence of bits is in 13.3 of the standard.

Example(s): `shifta(ibset(0, bit_size(0)), 2)`

is equal to `shiftl(7, bit_size(0) 3)`.

Example: `shifta(ibset(0, bit_size(0) -1), 2)`

is equal to `shiftl(7, bit_size(0) - 3)`.

SHIFTL(i, shift): Shift left.

argument: i	type: i
argument: shift	type: i
result: same as i	class: e

Note(s):

- shift shall be nonnegative and less than or equal to `bit_size(i)`

Example(s): `shiftl(4, 1)` is 8

SHIFTTR(i, shift): Shift right.

argument: i	type: i
type: i, non-negative and.	result: same as i
type: $i \leq bit_size(i)$.	
class: e	

Note(s):

- shift shall be nonnegative and less than or equal to `bit_size(i)`

Example(s): `shifttr(4, 1)` is 2.

SIGN(a, b): absolute value of a times the sign of b.

argument: a	type: i, r
result: as a	class: e

Note(s):

- If $b > 0$, the value of the result is $|a|$.
- If $b < 0$, the value of the result is $-|a|$.
- If b is of type integer and $b = 0$, the value of the result is $|a|$.
- If b is of type real and is zero, then:
if the processor cannot distinguish between positive and negative real zero, or if b is positive real zero, the value of the result is $|a|$;
if b is negative real zero, the value of the result is $-|a|$.

Example(s): `a=sign(a, b)`

SIN(x): sine.

argument: x	type: r, c
result: as argument	class: e

Note(s): the argument is in radians.

Example `z=sin(x)`

SINH(x): hyperbolic sine.

argument: x	type: r,c
result: as argument	class: e

Example `z=sinh(x)`

SIZE(array, dim, kind): Extent of an array along a specified dimension or the total number of elements in the array.

argument: array	type: any
result: i	class: i

Note(s):

1. `array` shall be a scalar or array of any type. It shall not be an unallocated allocatable variable or a pointer that is not associated. If `array` is an assumed-size array, `dim` shall be present with a value less than the rank of `array`.
2. `dim` (optional) shall be an integer scalar with a value in the range $1 \leq \text{dim} \leq n$, where n is the rank of `array`.
3. `kind` (optional) shall be a scalar integer constant expression.
4. `result` is equal to the extent of dimension `dim` of `array`, or if `dim` is absent, the total number of elements of `array`.

Example(s): `a=size(array)`

SPACING(x): returns the absolute spacing of model numbers near the argument value. See Chap. 5 and the real numeric model.

argument: x	type: r
result: as x	class: e

Example(s): `s=spacing(x)`

SPREAD(source, dim, n_copies): creates an array with an additional dimension, replicating the values in the original array.

argument: source	type: any
result: as source	class: t

Note(s): 1. Source may be array valued or scalar, with rank less than 15. 2. `dim` must be scalar and in the range $1 \leq \text{dim} \leq n + 1$ where n is the rank of `source`. 3. `n_copies` must be scalar. 4. the result is an array of rank $n + 1$.

Example(s):

If *a* is the array (2,3,4) then `spread(a, dim=1, ncopies=3)` then the result is the array

$$\begin{pmatrix} 2 & 3 & 4 \\ 2 & 3 & 4 \\ 2 & 3 & 4 \end{pmatrix}$$

SQRT(x): square root.

argument: <i>x</i>	type: r, c
result: as argument	class: e

Example(s): `a=sqrt(b)`

STORAGE_SIZE(*a, kind*) : Storage size in bits that an array element of the same dynamic type and type parameters of *a* would have.

argument: <i>a</i>	type: scalar or array of any type.
argument: <i>kind</i> (optional)	result: i
class: i	

Note(s):

1. An array element might take more bits to store than an isolated scalar, since any hardware-imposed alignment requirements for array elements might not apply to a simple scalar variable.
2. This is intended to be the size in memory that an object takes when it is stored; this might differ from the size it takes during expression handling (which might be the native register size) or when stored in a file. If an object is never stored in memory but only in a register, this function nonetheless returns the size it would take if it were stored in memory.

Example(s): `storage_size(1.0)` has the same value as the named constant `numeric_storage_size` in the intrinsic module `iso_fortran_env`.

SUM(array, dim, mask) or **SUM(array, mask)**: returns the sum of all elements of array along the dimension *dim* corresponding to the true elements of *mask*.

argument: <i>array</i>	type: n
result: as array	class: t

Note(s):

1. *array* must be an array.
2. $1 \leq dim \leq n$ where *n* is the rank of *array*.
3. *mask* must be conformable with *array*.

4. result is scalar if dim is absent, or array has rank 1, otherwise the result is an array of rank $n - 1$.

Example(s):

```
sum( (/1,2,3/) )
```

the result is 6.

```
sum(c, mask=c> 0.0)
```

forms the arithmetic sum of the positive elements of c.

If

$$B = \begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix}$$

```
sum(b, dim=1)
```

is (3,7,11)

```
sum(b, dim=2)
```

is (9,12)

SYSTEM_CLOCK(*count*, *count_rate*, *count_max*): returns integer data from a real time clock.

argument: <i>count</i>	type: i
result: n/a	class: s

Note(s):

1. *count* is intent (out) and is set to a processor dependent value based on the current value of the processor clock or to -huge (0) if there is no clock. It lies in the range 0 to *count_max* if there is a clock.
2. *count_rate* is intent (out) and it is set to the number of processor clock counts per second, or zero if there is no clock.
3. *count_max* is intent (out) and is set to the maximum value that *count* can have or to zero if there is no clock.

```
call system_clock(c,r,m)
```

TAN(x): tangent.

argument: x	type: r,c
result: as argument	class: e

Note(s): x must be in radians.

Example $y=\tan(x)$

TANH(x): hyperbolic tangent.

argument: x	type: r,c
result: as argument	class: e

```
y=tanh(x)
```

THIS_IMAGE(), THIS_IMAGE(coarray, dim) : Index of the invoking image, a single cosubscript, or a list of cosubscripts.

Note(s):

argument: coarray shall be a coarray of any type. If it is allocatable it shall be allocated.

argument: dim (optional) shall be a default integer scalar. Its value shall be in the range $1 \leq dim \leq n$, where n is the corank of coarray. The corresponding actual argument shall not be an optional dummy argument.

class: t

Note(s):

case(i) The result of `this_image()` is a scalar with a value equal to the index of the invoking image.

case(ii) The result of `this_image(coarray)` is the sequence of cosubscript values for `coarray` that would specify the invoking image.

case(iii) The result of `this_image(coarray, dim)` is the value of cosubscript dim in the sequence of cosubscript values for `coarray` that would specify the invoking image.

Example:

```
integer, dimension(10,20), &
    codimension[10,0:9,0:*] :: a
```

then on image 5, `this_image()` has the value 5 and `this_image(a)` has the value [3,1,2].

TINY(x): returns the smallest positive number in the model representing numbers of the same type and kind type parameter as the argument.

argument: x	type: r
result: as x	class: i

Example(s): `t=tiny(x)`

TRAILZ(i): number of trailing zero bits. If all of the bits of i are zero, the result value is `bit_size(i)`. Otherwise, the result value is the position of the rightmost 1 bit in i.

argument: i	type: i
result: i	class: e

Example(s):

```
trailz(4)
has the value 2.
```

TRANSFER(source, mold, size): returns a result with a physical representation identical to that of source, but interpreted with the type and type parameters of mold.

argument: source	type: any
result: as mold	class: t

Warning: A thorough understanding of the implementation specific internal representation of the data types involved is necessary for successful use of this function. Consult the documentation that accompanies the compiler that you work with before using this function.

TRANSPOSE(matrix): transposes an array of rank 2.

argument: matrix	type: any
result: as argument	class: t

Note(s): matrix must be of rank 2. If its shape is (n, m) then the resultant matrix has shape (m, n)

Example(s):

```
transpose(a)
```

$$a = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix} \text{ yields } \begin{pmatrix} 1 & 4 & 7 \\ 2 & 5 & 8 \\ 3 & 6 & 9 \end{pmatrix}$$

TRIM(string): returns the argument with trailing blanks removed.

argument: string	type: s
result: as string	class: t

Note(s): string must be a scalar.

Example: t_s=trim(s)

UBOUND(array, dim, kind): Upper bound(s) of an array.

argument: array	type: any
result: i	class: i

Note(s):

1. dim optional. shall be an integer scalar with a value in the range $1 \leq dim \leq n$, where n is the rank of array. The corresponding actual argument shall not be an optional dummy argument.
2. For an array section or for an array expression, other than a whole array, ubound(array, dim) has a value equal to the number of elements in the given dimension; otherwise, it has a value equal to the upper bound for subscript dim of

array if dimension `dim` of `array` does not have size zero and has the value zero if dimension `dim` has size zero.

Example: `z=ubound(a)`

UCOBOUND(coarray, dim, kind): upper cobound(s) of a coarray.

argument: coarray	type: co
argument: dim (optional)	type: i
argument: kind(optional)	type: i
result: i	class: i

UNPACK(vector,mask,field): unpacks an array of rank 1 into an array under the control of a mask.

argument: vector	type: any
result: as vector	class: t

Note(s):

1. `vector` must have rank 1. Its size must be at least `t`, where `t` is the number of true elements in `mask`.
2. `mask` must be array valued.
3. `field` must be conformable with `mask`. Result is an array with the same shape as `mask`.

Example(s):

With `vector=(1, 2, 3)`

$$\text{and } \text{mask} = \begin{pmatrix} f & t & f \\ t & f & f \\ f & f & t \end{pmatrix} \text{ and } \text{field} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ the result is } \begin{pmatrix} 1 & 2 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 3 \end{pmatrix}$$

VERIFY(string, set, back, kind): verify that a set of characters contains all the characters in a string by identifying the position of the first character in a string of characters that does not appear in a given set of characters.

argument: string	type: s
result: i	class: e

Note(s):

1. The default is to scan from the left, and will only be from the right when `back` is present and has the value true.
2. The value of the result is zero if each character in `string` is in `set`, or if `string` has zero length.

Example `i=verify(string, set)`

Appendix C

Text Extracts, English, Latin and coded

English and Latin

YET IF HE SHOULD GIVE UP WHAT
HE HAS BEGUN, AND AGREE TO MAKE US OR
OUR KINGDOM SUBJECT TO THE KING OF ENGLAND
OR THE ENGLISH, WE SHOULD
EXERT OURSELVES AT ONCE TO DRIVE HIM OUT AS
OUR ENEMY AND A SUBVERTER
OF HIS OWN RIGHTS AND OURS, AND MAKE SOME
OTHER MAN WHO WAS ABLE TO
DEFEND US OUR KING; FOR, AS LONG AS BUT A
HUNDRED OF US REMAIN ALIVE,
NEVER WILL WE ON ANY CONDITIONS BE BROUGHT
UNDER ENGLISH RULE. IT
IS IN TRUTH NOT FOR GLORY, NOR RICHES, NOR
HONOURS THAT WE ARE FIGHTING,
BUT FOR FREEDOM - FOR THAT ALONE, WHICH NO
HONEST MAN GIVES UP BUT
WITH LIFE ITSELF.

QUEM SI AB INCEPTIS
DIESISTERET, REGI ANGLORUM AUT ANGLICIS NOS
AUT
REGNUM NOSTRUM VOLENS SUBICERE, TANQUAM
INIMICUM NOSTRUM ET SUI NOSTRIQUE
JURIS SUBUERSOREM STATIM EXPELLERE NITEREMUR
ET ALIUM REGEM NOSTRUM
QUI AD DEFENSIONEM NOSTRAM SUFFICERET
FACEREMUS. QUIA QUANDIU CENTUM
EX NOBIS VIUI REMANSERINT, NUCQUAM ANGLORUM
DOMINIO ALIQUATENUS VOLUMUS

SUBIUGARI. NON ENIM PROPTER GLORIAM,
DIUICIAS AUT HONORES PUGNAMUS
SET PROPTER LIBERATEM SOLUMMODO QUAM NEMO
BONUS NISI SIMUL CUM VITA
AMITTIT.

from 'The Declaration of Arbroath'
c.1320. The English translation is by
Sir James Fergusson.

Coded

OH YABY NSFOUN, YAN DUBZY LZ DBUYLTUBFAJ
BYYBOHNX GPDA FNUZNDYOLH
YABY YAN SBF LZ B GOHTMN FULWOHDN DLWNUNX
YAN GFBDN LZ BH NHYOUN DOYJ,
BHX YAN SBF LZ YAN NSFOUN OYGNMZ BH NHYOUN
FULWOHDN. OH YAN DLPUGN
LZ YOSN, YANGN NKYNHGOWN SBFG VNUN ZLPHX
GLSNALV VBHYOHT, BHX GL YAN
DLMMNTN LZ DBUYLTUBFANUG NWLMWNX B SBF LZ
YAN NSFOUN YABY VBG YAN
GBSN GDBMN BG YAN NSFOUN BHX YABY DLOHDOXNX
VOYA OY FLOHY ZLU FLOHY.
MNGG BYYNYHOWN YL YAN GYPXJ LZ DBUYLTUBFAJ,
GPDDNNXOHT TNHNUBYOLHG
DBSN YL RPXTN B SBF LZ GPDA SBTHOYPXN
DPSENUGLSN, BHX, HLY VOYALPY
OUUNWNUNHDN, YANJ BEBXLHNX OY YL YAN
UOTLPUG LZ GPH BHX UBOH. OH
YAN VNGYNUH XNGNUYG, YBYYNUNX ZUBTSNHYG LZ
YAN SBF BUN GYOMM YL EN
ZLPHX, GANMYNUOHT BH LDDBGOLHBM ENBGY LU
ENTTBU; OH YAN VALMN HBYOLH,
HL LYANU UNMOD OG MNZY LZ YAN XOGDOFMHN LZ
TNLTUBFAJ.

Appendix D

Formal Syntax

Statement ordering

Format statements may appear anywhere between the use statement and the contains statement.

The following table summarises the usage of the various statements within individual scoping units.

Kind of scoping unit	Main program	Module	External sub program	Module sub program	Internal sub program	Interface body
use	Y	Y	Y	Y	Y	Y
format	Y	N	Y	Y	Y	N
Misc Dec.	Y	Y	Y	Y	Y	Y
Derived type definition	Y	Y	Y	Y	Y	Y
interface block	Y	Y	Y	Y	Y	Y
Executable statement	Y	N	Y	Y	Y	N
contains	Y	Y	Y	Y	N	N

Misc Dec. (Miscellaneous declaration) are parameter statements, implicit statements, type declaration statements and specification statements.

Syntax summary of some frequently used Fortran constructs

The following provides simple syntactical definitions of some of the more frequently used parts of Fortran.

Main program

```
program [ program-name ]
[ specification-construct ] ...
[ executable-construct ] ...
[ contains
  [ internal procedure ] ... ]
end [ program [ program-name ] ]
```

Subprogram

procedure heading
 [specification-construct] ...
 [executable-construct] ...
 [contains
 [internal procedure] ...]
 procedure ending

module

module name
 [specification-construct] ...
 [contains
 subprogram
 [subprogram] ...]
 end [module [module-name]]

Internal procedure

procedure heading
 [specification construct] ...
 [executable construct] ...
 procedure ending

procedure heading

[recursive] [type specification] function function-name
 ([dummy argument list]) [result (result name)]
 [recursive] subroutine subroutine name
 [([dummy argument list])]

procedure ending

end [function [function name]]
 end [subroutine [subroutine name]]

Specification construct

derived type definition
 interface block
 specification statement

Derived type definition

type [[, access specification] ::] type name
 [private]
 [sequence]
 [type specification [[, pointer] ::] component specification list]
 ...
 end type [type name]

interface block

interface [generic specification]
 [procedure heading
 [specification construct] ...
 procedure ending] ...

[module procedure module procedure name list] ...
 end interface

Specification statement

allocatable [::] allocatable array list
 dimension array dimension list
 external external name list
 format ([format specification list])
 implicit implicit specification
 intent (intent specification) :: dummy argument name list
 intrinsic intrinsic procedure name list
 optional [::] optional object list
 parameter (named constant definition list)
 pointer [::] pointer name list
 public [::] module entity name list]
 private[[::] module entity name list]
 save[[::] saved object list]
 target [::] target name list
 use module name [, rename list]
 use module name , only : [access list]
 type specification [[, attribute specification] ... :: object declaration list]

type specification

integer [([kind=] kind parameter)]
 real[([kind=] kind parameter)]
 complex[([kind=] kind parameter)]
 character[([kind=] kind parameter)]
 character[([kind=] kind parameter)]
 [len=] length parameter)
 logical[([kind=] kind parameter)]
 type (type name)

Attribute specification

allocatable
 dimension (array specification)
 external
 intent (intent specification)
 intrinsic
 optional
 parameter
 pointer
 private
 public
 save
 target

Executable construct

action statement
case construct
do construct
if construct
where construct

Action statement

allocate (allocation list) [,stat= scalar integer variable])
call subroutinename [([actual argument specification list])]
close (close specification list)
cycle [do construct name]
deallocate(name list) [, stat= scalar integer variable])
endfile external file unit
exit [do construct name]
goto label
if (scalar logical expression) action statement
inquire (inquire specification list) [output item list]
nullify (pointer object list)
open [and close] (connect specification list)
print format [, output item list]
read (i/o control specification list) [input item list]
read format [, output item list]
return [scalar integer expression]
rewind (position specification list)
stop [access code]
where (array logical expression) array assignment expression
write (i/o control specification list) [output item list]
pointer variable => target expression
variable = expression

Appendix E

Compiler Options

In this appendix we look at some of compiler options we have used during the development of the programs in the book.

Cray

Debug

-G Debug level -R run time checks

Optimise

default compiler options

gfortran

Debug

gfortran -W -Wall -fbounds-check -pedantic-errors -std=f2003 -Wunderflow

-O -fbacktrace -ffpe-trap=zero,overflow,underflow -g

Optimise

gfortran -ffast-math -funroll-loops -O3

Intel

Debug

ifort /check:all /debug:all /gen-interfaces /Qopenmp /standard-semantics
/traceback /warn:all

ifort /check:all /fpe:0 /heap-arrays /traceback /warn:all,nodec,interfaces
/Qfp-stack-check /automatic /gen_interfaces

Optimise

Intel (autoparallel)

ifort /fast /Qparallel /link /heap-arrays

Intel

ifort /fast /link /heap-arrays

Nag

Debug

nagfor -C=all -C=undefined -f2008 -info -g -gline -ieee=stop -info
-mtrace=verbose -thread_safe

Optimise

nagfor -O4 -openmp -thread_safe

Polish

The Nag compiler has a *polish* option. Here are some of the options used in the reformatting of the examples in the book. The examples in the book were set with a line length of 48 to fit the printed page. The examples on the web site were set with a line length of 132.

```
nagfor =polish -alter_comments -noblank_cmt_to_blank_line  
-blank_line_after_decls -break_long_comment_word  
-format_start=100 -format_step=10 -idcase=L -indent=2  
-indent_continuation=2 -indent_max=16 -keep_blank_lines  
-keep_comments -kwcase=L -leave_formats_in_place  
-margin=0 -noindent_comment_marker  
-noseparate_format_numbering -relational=F90+ -renumber  
-renumber_start=100 -renumber_step=10  
-separate_format_numbering -terminate_do_with_enddo -width=48
```

Sun

Debug

```
sunf95 -ansi -w4 -xcheck=all -C -ftrap=common,overflow,underflow
```

Optimise

Intel hardware

```
sunf95 -fast -xtarget=nehalem -xipo=2 -m64 -xvector=simd
```

AMD hardware

```
sunf95 -fast -xtarget=native
```

Index

A

Abs function, 211
Abstraction, stepwise refinement and modules, 24
ACM Fortran Forum, 39
Actual argument, 297, 301, 302, 304, 305, 329, 400, 502, 536, 593
Ada, 2, 26
Addition operator, 366, 367
Additional forms of the dimension attribute and do loop statement, 122
a edit descriptor, 153, 251
Algol, 2, 20
Algol 68, 2
Algorithm, 1, 5, 8, 14, 16, 359
 big O notation, 359
 complexity, 359
Allocatable arrays, 35, 115, 116, 399
Allocatable attribute, 116, 126, 301, 308, 408, 502
Allocatable dummy arrays, 302, 315
Allocatable function results, 408
Allocatable variable, 426, 445
Allocate statement, 126, 283, 399
Alpha hardware, 150
Alternate return, 592
Alternative form of the allocate statement, 399
AMD, 150
Amdahl's Law, 453
Amdahl's Law Graph 1–8 Processors or Cores, 453
Amdahl's Law graph 2–64 Processors or Cores, 454
APL, 2, 23
Argument keyword, 335
Argument list, 227, 298, 299, 302, 324, 401

Arguments, 294
Arithmetic assignment statement, 52, 53, 64, 66, 98, 218
Arithmetic expressions, 63, 64, 68, 97
Arithmetic if, 592
Arithmetic operators, 64, 133, 256, 270, 271
Arithmetic units, 540
Array
 allocatable, 115
 allocatable arrays, 116
 attribute
 dimension, 112
 control structure
 do loop, 106
 dimension, 106
 index, 106
 setting the size with a parameter, 110
 varying the size at run time, 115
Array arguments, 212, 227, 308, 593
Array constructor, 131, 133, 138, 140, 149
Array element, 131, 132, 135, 141, 148, 172, 212, 253, 402, 491
Array element order, 131, 132, 135, 141, 148, 172, 402
Array element ordering, 132, 147
Array initialisation, 134, 138, 139
Array pointer, 301
Array section, 136, 138, 143, 153, 171, 189, 402, 485, 491
Array size, 110, 115, 485
Arrays, 103
 allocatable attribute, 116
 allocate statement, 117
 array constructors, 138
 array element ordering, 132, 147
 assignment, 132
 bounds, 131

- conformable, 131
 - expressions, 133
 - higher dimension arrays, 117
 - implied do loops, 119
 - initialisation, 134
 - rank, 131
 - rank 2 array sections, 136
 - reshape, 141
 - order, 141
 - pad, 141
 - reshape example, 141
 - reshape function, 140
 - sections, 131, 136
 - shape, 131
 - size, 131
 - sum
 - two d arrays, 144
 - sum intrinsic, 144
 - two Dimensional arrays, 117
 - whole array manipulation, 131, 132
 - whole arrays, 131
 - Arrays in Fortran, 106
 - Artificial language, 7
 - Assign and assigned goto statements, 593
 - Assigned format statements, 593
 - Assignment, 425
 - Assignment statement, 52, 53, 64, 66, 97, 98, 100, 107, 218, 284, 285, 425, 426, 448
 - Associate construct, 426
 - Associated intrinsic function, 285
 - Association status, 35, 284
 - Assumed-shape array, 301, 305, 308, 335, 594
 - Assumed shape parameter passing, 303
 - Assumed-size, 593
 - Attribute
 - allocatable, 149
 - asynchronous, 149
 - bind, 149
 - dimension, 149
 - external, 149
 - intent, 149
 - intrinsic, 149
 - optional, 149
 - parameter, 149
 - pointer, 149
 - private, 149
 - protected, 149
 - public, 149
 - save, 149
 - target, 149
 - value, 149
 - volatile, 149
 - Attribute specification, 423
 - Automatic array, 302, 308, 312, 399, 400
 - Automatic arrays and median calculation, 308
- B**
- Bandwidth, 455, 456
 - Bandwidth and latency, 456
 - Base class, 429, 432, 433, 438, 443, 449
 - Base class with private data, 432
 - Base shape class, 436, 443
 - Base type, 265, 276, 422, 449
 - Basic, 2, 23
 - Basic array and linked list performance, 363
 - Basic module syntax, 324
 - The basic shape class, 427
 - Better alternatives, 593
 - Binary representation of a real number, 91
 - Binary representation of different integer kind type numbers, 89
 - Bit integers, 360, 561
 - Bit reals, 561
 - Block if construct, 233
 - Block if statement, 232
 - Block structure, 20
 - Bottom-up, 8
 - Brief review of the history of object oriented programming, 421
- C**
- C, 2, 23
 - C++, 2, 31, 386
 - C#, 2, 33, 386
 - Cache, 455
 - Call statement, 293, 296, 299
 - Calling the dislin library to display tsunami events, 583
 - Calling the Nag m01caf sorting routine, 579
 - Case statement, 231, 237, 238, 592, 594
 - Character arguments and assumed-length dummy arguments, 305
 - Character data, 249
 - Character data type, 249
 - Character functions, 254
 - Character input, 51, 250
 - Character interoperability, 514
 - Character operators, 251
 - Character output and the a edit descriptor, 163
 - Character string, 90, 163, 229, 250, 252, 255, 257, 260

- Character string arguments, 257
Character substrings, 253
Character variables, 50, 163, 250, 251, 253, 254, 257
Characters
 * edit descriptor, 251
 // character operator, 251
 a edit descriptors, 251
 ASCII character set, 249
 character functions, 254
 character input, 250
 character operators, 251
 character variables, 250
 collating sequence, 256
 delimiters, 250
 len function, 255
 len_trim function, 255
 scan function, 258
 substrings, 253
Characters and the a format or edit descriptor, 163
Chomsky and program language development, 20
Choosing the decimal symbol, 172
C Interop
 binding labels for common blocks and variables, 517
 C calling a Fortran function, 521
 C++ calling a Fortran function, 522
 c_loc description, 536
 c_loc examples, 535
 derived types, 513
 Fortran calling a C function, 520
 interoperability of intrinsic types, 515
 interoperability of procedures and procedure interfaces, 516
 interoperability of scalar variables, 516
 interoperability with C pointer types, 516
 interoperation with C functions, 517
 interoperation with C global variables, 516
 iso_c_binding module, 513
 module procedures, 513
 named constants and derived types in the module, 513
 other aspects of interoperability, 516
 passing a rank 2 array from C to Fortran, 527
 passing a rank 2 array from C to Fortran and taking care of array storage, 533
 passing a rank 2 array from C++ to Fortran, 528
passing a rank 2 array from C++ to Fortran and taking care of array storage, 533
passing a rank 2 array from Fortran to C, 526
passing an array from C to Fortran, 524
passing an array from C++ to Fortran, 525
passing an array from Fortran to C, 522
Circle-derived type 1, 436, 445
Class, 423
Class keyword, 443
Close statement, 153, 166, 194
Coarray
 broadcasting data, 504
 parallel solution for pi calculation, 505
 work sharing, 508
Coarray allocate-object, 502
Coarray Fortran, 462
Coarray programming, 512
Coarray terminology, 502
Cobol, 2, 19
Collating sequence, 256, 260
Column information, 181
Commercial Conversion tools, 594
Commercial numerical and statistical subroutine libraries, 322
Common programming error, 219
Compilation when using modules, 400
Compiler documentation, 58
Compiler options, 59, 287, 591
Complex and kind type, 268
Complex arithmetic, 265
Complex data type, 265
Complex numbers, 265
Computer programming, 369, 577
Computer systems, 79, 388
Consistency models, 457
Contains statement, 219, 224
Control statements, 24, 245
Control structure, 26, 34, 49, 103, 106, 113, 115, 124, 125, 215, 231, 232, 245
Control Structure formal Syntax, 245
Convert, 594
Counting vowels, consonants, etc., 238
Cycle and exit, 241
Cycle statement, 231, 241

D

- Data dependencies, 457
Data description statements, 49
Data entity, 423, 502, 536

- Data file, 128, 185–188, 194, 320, 589
 Data items, 343
 Data object, 423, 424, 462, 490
 Data structures, 103, 337, 357, 370, 412, 422
 Data structuring, 337
 - date data type or class, 346
 - perfectly balanced tree, 344
 - ragged arrays, 337, 342
 - singly linked list, 337
 Data structuring and procedural programming, 25
 Data transfer statements, 200
 Data type, 23–25
 Data-Processing statements, 49
 Date calculation, 236
 Date class, 346
 Date data type, 276
 Dc edit descriptor, 172
 Debugging, 271
 Decimal point, 66, 154, 156, 157, 160
 Decremented features, 592
 Default kind, 87, 97
 Deferred-shape array, 301, 308
 Defined assignment statement, 426
 Defined types, 275, 279, 280, 365
 Defined variable, 298
 Deleted features, 592
 Denormal, 539
 Derived data types, 323, 329, 335
 Derived type definition, 435
 Derived types, 37, 275, 276, 431, 443, 513
 Derived types and structure constructors, 425
 Detailed design, 11
 Dimension attribute, 106, 115, 122, 123
 Disassociated pointer, 284
 Dislin graphics library, 561, 581
 Display subroutine, 445
 Do concurrent, 37
 Do construct, 126
 Do loop, 91, 103, 108, 113–115, 119, 120, 122–127, 135, 138, 139, 170, 171, 216, 231, 239, 480, 485, 492, 509
 Do loops and straight repetition, 124
 Do statement, 103, 108, 114, 115, 123, 124, 238, 241
 Dot product, 133, 140
 Dot_product function, 213
 Double precision, 85, 86, 325, 369, 407, 592
 Dp edit descriptor, 172
 DST in the USA, 357
 DTR 19767 enhanced module facilities, 37
 Dummy argument, 219, 225, 297, 298, 301, 302, 304–306, 329, 334, 335, 399, 401, 424, 502, 594
 Dummy arguments or parameters and actual arguments, 296
 Dummy procedure argument, 400, 594
 Dynamic binding, 422, 443, 446, 448, 449
 Dynamic data structures, 412
 Dynamic type, 423, 427
- E**
 Easter calculation, 214
 Edit descriptor, 153–156, 161, 163, 171, 175, 194, 251, 272, 593
 - a, 175
 - b, 175
 - d, 175
 - dt, 175
 - e, 175
 - en, 175
 - es, 175
 - f, 175
 - g, 175
 - l, 175
 - o, 175
 - z, 175
 e edit descriptor, 153, 171
 E formats, 195, 561
 Eiffel, 31
 Elemental e**x function, 410
 Elemental function, 227, 318
 Elemental function use, 212
 Elemental functions, 209, 212, 226
 Elemental procedure, 35, 319
 Elemental subroutine, 318
 Elements of a programming language, 48
 Else block, 221
 Elsewhere block, 146
 End do statement, 238
 End type, 429
 End-of-file, 203
 End-of-file condition, 202
 end= specifier, 202
 Enhanced module facilities, 37
 Environment variables, 36, 59, 461
 eor= specifier, 202
 err= specifier, 202
 Error condition, 202, 203
 Error message, 61, 255, 272, 287, 292, 433
 Error number, 468, 472
 Error, end of record and end of file, 202
 Evaluation and testing, 12

Exception handling, 32, 34, 556
Executable constructs containing blocks, 426
Execution sequence, 502
Execution time, 148, 222
Exit statement, 231, 238, 241
Explicit interface, 219, 227, 298, 335, 400, 411, 594
Explicit type specification, 36
Explicit-shape array, 302
Expression equivalence, 68
Expressions, 133
External, 145, 168
Extracting the diagonal elements of a matrix, 402

F

Feasibility study and fact finding, 11
f edit descriptor, 153, 156
F format, 174, 347
File access, 198
File name, 205, 306
Files in Fortran, 165
Finalisers, 36
Floating point, 24, 66, 77, 88, 91, 97, 98, 170, 235, 327, 407, 556, 557
Floating point arithmetic, 97, 98, 557
Flynn's taxonomy, 456
Forall construct, 146
Forall statement, 146
Forcheck, 594
Format specification using a character variable, 174
Format specification using a string, 173
Format statement, 154, 155, 162, 164, 171, 175, 185, 189, 195, 593
Forstruct, 595
Forstudy, 595
Fortran 2003, 36
Fortran 2008, 37
Fortran 2015, 37
Fortran 77, 19
Fortran 77 Version, 596
Fortran 90, 34
Fortran 90 Version, 597
Fortran 95, 35
Fortran and parallel programming, 459
Fortran and the IEEE 754 standard, 96
Fortran character set, 54
Fortran discussion lists, 38
Fortran operator hierarchy, 271
Fortran operators and the arithmetic assignment statement, 64

Fortran representational models, 79
Fortran support for IEEE arithmetic, 545
Fortran's origins, 18
Function argument, 227
Function formal syntax, 227
Function header, 220, 221, 228
Function name, 218, 227, 228
Function result, 408
Function side effect, 218
Functions, 293

G

g edit descriptor, 153
Generic function, 209, 211, 216, 369
Generic interface, 426
Generic name, 425
Generic programming, 369, 370, 386
Generic programming and other languages, 369
Generic quicksort in C++, 377
Generic quicksort in C#, 379
Generic recursive quicksort with timing details, 569
Generic statistics module, 380
Gfortran, 58
Good Programming guidelines, 55
Goto statement, 232, 248, 593
Granularity and types of parallelism, 459
Graphics library, 453, 578, 581
Gustafson's law, 454
Gustafson's Law graph 1–64 processors or cores, 455, 583

H

Hardware sources, 557
H editing, 593
High-level languages, 18, 22, 23
Higher-dimension arrays, 117
HOPL, 40, 41
Host association, 36
HPF, 463

I

IBM, 58
ICON, 2, 29
i edit descriptor, 153
IEEE
 accuracy requirements, 544
 accuracy requirements on floating point operations, 541
denormal, 539

- derived types and constants defined in the modules, 546
- divide by zero, 539
- double precision floating point format, 543
- exception handling, 544
- floating point formats, 539
- inexact, 539
- inexact summation example, 552
- infinity, 539
- integer formats, 539
- invalid, 539
- NAN, 539
- NAN and other specials example, 554
- overflow, 539
- rounding directions, 544
- rounding mode, 544
- rounding precisions, 545
- single precision floating point format, 542
- subnormals, 542
- testing IEEE support, 548
- testing what flags are supported, 549
- two classes of extended floating point formats, 543
- underflow, 539, 542
- IEEE 754, 24
- IEEE 754 floating point support, 24
- IEEE 754 Specifications, 541
- IEEE double precision floating point format, 541
- IEEE extended floating point formats, 541
- IEEE single precision floating point format, 541
- Ieee_arithmetic, 546
- Ieee_exceptions, 546
- Ieee_features, 547
- If statement, 269, 592
- If then else if endif construct, 231
- If then endif construct, 231
- Image control statements, 502
- Image index, 502, 503
- Image numbers, 505
- Imaginary part of complex number, 265
- Implicit and explicit interfaces, 334
- Implicit none statement, 54
- Index, 106
- The index character function, 254
- Initial value problems, 393
- Initial values, 53, 138, 139, 276, 431, 432, 438
- Initialisation of physical constants, version 1, 92
- Initialisation of physical constants, version 2, 94
- Initialisation of physical constants, version 3, 94
- Initialising a rank 2 array, 140, 141
- Inner product of two sparse vectors, 388
- Input and output (I/O) statements, 49
- Input-item-list, 54
- Inquire statement, 201, 203
- Integer argument, 92, 229, 256
- Integer arrays, 386
- Integer data, 95, 347, 386
- Integer data type, 80, 347, 386
- Integer declaration, 218
- Integer division, 70, 71, 97, 236
- Integer division and real assignment, 70
- Integer expression, 147
- Integer formats, 539
- Integer kind type, 63, 83, 95
- Integer overflow and the i edit descriptor, 155
- Integer representation, 107
- Integer scalar, 86
- Integer variable, 92, 97, 174, 285, 429
- Integers and the i format or edit descriptor, 154
- Intel, 59, 151
- Intent, 297
 - in, 297
 - inout, 297
 - out, 297
- Intent attribute, 293
- Interface, 334
- Interface block, 302, 371, 375, 594
- Internal file, 190, 191, 194, 197, 202, 203
- Internal function, 223, 224, 227, 594
- Internal procedure, 323, 334
- Internal subroutines and scope, 311
- Internal user defined functions, 209
- Interoperability of array variables, 516
- Intrinsic assignment, 426, 443
- Intrinsic assignment statement, 426
- Intrinsic data type, 47, 347
- Intrinsic function, 73, 97, 140, 143, 144, 150, 209–211, 216, 226, 227, 265, 266, 302, 321, 401
- Intrinsic module, 203
- Intrinsic procedure, 59, 133, 134, 216, 334
- Intrinsic subroutine, 315
- Intrinsic types, 81, 275, 515
- I/O concepts and statements, 197
- Iomsg= specifier, 203
- Iostat= specifier, 203

ISO technical reports TR15580 and TR15581, 35
Iterative do loop, 231

J

Java, 2, 32, 33

K

Keyword and optional argument variation, 400
Keyword and optional arguments, 302
Keyword argument, 302, 401
Kind parameter, 81
Kind type parameter, 83, 86, 87, 327, 370, 515
Kind types, 63, 81, 83, 85, 87, 95, 229, 268, 325, 380, 561

L

Language strengths and weaknesses, 48
Leap year, 236
Len and len_trim functions, 255
Len and len_trim usage, 255
Linked list, 337–339, 363, 387, 388, 412
Linked list parameterised by real kind, 414
Linked lists for sparse matrix problems, 387
Lisp, 2, 21
List directed input, 179
Literal real constants in a calculation, 87
Loc function usage, 291
Local variables, 219, 225, 227, 297, 312
Local variables and the save attribute, 297
Locks, 458
Logic programming, 28, 43
Logical data type, 269
Logical expression, 147, 231, 233, 234, 240, 269, 270
Logical i/o, 272
Logical operators, 231, 269–271
Logical variable, 233, 269, 272, 298
Logo, 2, 27
Lower bound, 36, 143, 243, 305

M

Main program, 218, 219, 221, 278, 294, 298–300, 302, 303, 305, 306, 308, 315, 318, 323, 327, 329, 330, 336, 370, 371, 376, 384, 399, 400, 403, 407, 408, 448, 502, 569, 574
Maintenance, 12

Masked array assignment, 145
Masked array assignment and the where statement, 145

Matrix multiplication, 134, 308

Memory access, 455

Memory leak example, 288

Met office historic station data, 183

Modula, 2, 26

Modula 2, 2, 27

Modular programming, 10

Module

basic syntax, 324

Module for simple timing of a program, 332

Module procedures, 298, 299, 375, 594

Module usage and compilation, 334

Modules, 323

containing procedures, 323

derived types, 323

module usage and compilation, 334

precision definition, 324

the use statement, 323

Modules containing procedures, 298

Modules for derived data types, 323, 329

Modules for global data, 323, 324

Modules for globally sharing data, 327

Modules for precision specification and constant definition, 325

Monitors, 458

More memory leaks, 289

MPI, 459

compiler and implementation combination, 466

compiler and MPI combinations used in the book, 467

hello world using send and receive, 470

individual implementation, 466

MPI memory model, 467

parallel solution for pi calculation, 478

work sharing between processes, 483

MPI programming, 465

MPICH2, 466

Mutual exclusion - mutex, 458

N

Nag, 60

Nag SMP library, 578

Narrow field widths and the f edit descriptor, 158

Natural language, 6, 51, 257

Nested user defined types, 280

Netlib, 572

Non recursive Quicksort with timing details, 572

- Notations, 7
 Numeric models, 63
 Numerical libraries, 578
- O**
 Oberon, 2, 30
 Oberon 2, 2, 30
 Object file, 299
 Object oriented programming, 10, 29, 30, 32, 44, 421, 422, 424, 430, 431, 433, 435, 438, 449
 Obsolescent features, 592
 Open and close usage, 166
 Open MPI, 466
 Open statement, 165, 198
 OpenMP, 461
 - hello world using default variable data scoping, 494
 - hello world with private thread_number variable, 496
 - OpenMP memory model, 490
 - parallel solution for pi calculation, 496
 Operating systems, 42, 46, 57, 176, 461, 540, 559, 581
 Operator hierarchy, 271
 Operator overloading, 365
 Optional argument, 302, 400, 401
 Oracle/Sun, 60
 Order of evaluation, 68
 Ordinary differential equations, 387, 392, 393
 Original Fortran 66, 596
 Other parallel options, 462
 Output formats, 195
 Output formatting, 129
 Output-item-list, 54
 Overflow, 77, 550
 Overflow and the f edit descriptor, 158
 Overflow and underflow, 77
- P**
 Parallel computing, 455
 Parallel computing classification, 452
 Parallel programming, 451, 452, 456, 457, 459, 461, 464, 487, 501, 504
 Parallel solution, 464, 478, 482
 Parameter attribute, 63, 72, 73, 97
 Parameter passing, 294, 301, 305
 Parameterised derived types, 36, 413
 Parameters, 294
 Partitioned global address space (PGAS), 459
- Pascal, 2, 15, 22
 Pass control, 241
 Passed object dummy arguments, 424
 Pause statement, 593
 Perfectly balanced tree, 344
 Person data type, 329
 Physical and virtual memory, 148
 Pi calculation, 478, 496, 505
 PL/I, 2
 PL/I and Algol 68, 22
 Plusfort, 595
 PlusFORT capability, 595
 Pointer allocation and assignment, 288
 Pointer assignment, 36, 283, 285, 286, 536
 Pointer association, 284
 Pointer attribute, 283
 Pointer component, 424, 536
 Pointer initialisation, 284
 Pointer variables, 284, 286
 Polymorphic entity, 423
 Polymorphic variables, 426
 Polymorphism and dynamic binding, 443, 449
 Positional number systems, 63, 79, 98
 Positive integers, 80
 Positive values, 145
 Postscript language, 40
 Postscript TeX and L^AT_EX, 28
 Print statement, 135, 154, 155, 157, 171, 176
 Private attribute, 333
 Private, public and protected attributes, 333
 Problem definition, 10
 Problem solving, 5
 - algorithm, 5, 8
 - algorithmic problem solving, 5
 - artificial language, 7
 - bottom-up, 8
 - modular programming, 10
 - natural language, 6
 - notations, 7
 - algebra, 7
 - calculus, 7
 - logic, 7
 - object oriented programming, 10
 - software engineering, 5
 - stepwise refinement, 9
 - systems analysis and design, 5, 10
 - analysis, 10
 - detailed design, 10
 - evaluation, 10
 - evaluation and testing, 12
 - feasibility study and fact finding, 10
 - implementation, 10

- initial design, 10
 - maintenance, 10
 - problem definition, 10
 - technical terminology, 7
 - top-down, 8
 - UML, 5
 - Unified Modelling Language - UML, 13
 - Procedure pointer component, 424
 - Procedures, 293
 - Program development, 60
 - Program execution, 283, 423, 426
 - Program statement, 53, 54
 - Program unit, 112, 149, 218, 219, 278, 296–300, 302, 323, 324, 329, 330, 333, 334, 346, 399, 577
 - Programming languages, 1, 17, 18, 20, 22, 23, 33, 39, 43, 45–47, 53, 107, 365, 369, 421, 457, 539
 - abstraction, 24
 - Ada, 26
 - Algol, 20
 - Algol 68, 22
 - APL, 23
 - B, 23
 - Basic, 23
 - C, 23
 - C++, 31
 - C#, 33
 - Chomsky, 20
 - classes, 29
 - Cobol, 19
 - data structuring, 25
 - dynamically bound procedure calls, 29
 - early theoretical work, 17
 - engineering, 18
 - extensible data types, 29
 - Fortran
 - 1966 standard, 19
 - 1977 standard, 19
 - Fortran 2003, 36
 - Fortran 2008, 37
 - Fortran 2015, 37
 - Fortran 90, 34
 - Fortran 95, 35
 - Fortran discussion lists, 38
 - Fortran's origins, 18
 - ICON, 29
 - instances of a class, 29
 - Java, 32
 - L^AT_EX, 28
 - Lisp, 21
 - Logo, 27
 - messages, 29
- methods, 29
 - Modula, 26
 - Modula 2, 27
 - modules, 24
 - Oberon, 30
 - Oberon 2, 30
 - object oriented programming, 29
 - objects, 29
 - Pascal, 22
 - PL/I, 22
 - Postscript, 28
 - procedural programming, 25
 - Prolog, 28
 - second generation languages, 22
 - Simula, 22, 30
 - Smalltalk, 30
 - Snobol, 21
 - SQL, 28
 - standardisation, 25
 - stepwise refinement, 24
 - structured programming, 24
 - T_EX, 28
 - Turing, 17
 - von Neumann, 17
 - Prolog, 2, 28
 - Protected attribute, 323, 333
 - Public and private accessibility, 435
 - Public attribute, 333
 - Pure constraints, 225
 - Pure functions, 35, 209, 224, 226
 - Pure procedure, 225, 226
 - PVM, 463
- Q**
- Quadratic roots, 235
- R**
- Race conditions, 458
 - Ragged array parameterised by real kind type, 416
 - Ragged arrays, 342
 - Ragged arrays and variable sized data sets, 343
 - Random number, 320
 - Range, precision and size of numbers, 76
 - Rank 1 array and the sum intrinsic function, 143
 - Rank 1 array initialisation — explicit values, 138
 - Rank 1 array initialisation using an implied do loop, 139
 - Rank 1 array sections, 136

- Rank 1 whole array, 134
- Rank 2 array sections, 136
- Rank 2 arrays and the sum intrinsic function, 144
- Rank 2 whole array, 135
- Read statement, 203, 250, 340, 593
- Reading formatted files, 192
- Reading from files, 179
- Reading in an arbitrary number of reals using a linked list and copying to an array, 341
- Reading integer data, 179
- Reading one column of data from a file, 184
- Reading real data, 182
- Reading several files, 187
- Reading unformatted files, 193
- Reading using array sections, 189
- Reading using internal files, 190
- Real and double precision do control variables, 592
- Real function, 332
- Real kind type, 63, 95, 229, 268, 380
- Real literal constant, 87
- Real part of complex number, 265
- Real variable, 87, 123, 336
- Reals and the e edit descriptor, 159
- Reals and the g edit descriptor, 161
- Records, 198
- Rectangle-derived type 2, 439, 445
- Recursion and problem solving, 230
- Recursive factorial evaluation, 220
- Recursive functions, 209, 220, 227, 312
- Recursive gcd function, 222
- Recursive subroutines, 312
- Referencing a subroutine, 296
- Referencing pointer variables before allocation or pointer assignment, 286
- Relational operator, 233, 234
- Relative and absolute errors, 74
- Repeat until loop, 240
- Repetition and whole array output, 171
- Result clause, 228
- Result value, 536
- Return statement, 227
- Rkm, 400
- Round off errors and computer arithmetic, 73
- Rounding and truncation, 69
- Rounding problem, 89
- Rules and restrictions on functions, 228

- S**
- Save attribute, 225, 293
- Scalar variable, 128
- Scan function, 258
- Scan function usage, 259
- Scope of variables, 219, 298
- Second-generation languages, 22
- Select type, 36, 426, 449
- Select type construct, 427
- Selection among courses of action, 232
- Sentinel usage, 240
- Serial and parallel libraries, 578
- Serial non recursive Quicksort, 561
- Serial recursive Quicksort, 561
- Setting the array size with a parameter, 110
- Shape wrapper module, 445
- Shared do termination and non-endo , 592
- Side effect, 224
- Significant digits, 74, 159, 160
- Simple arithmetic expressions in Fortran, 65
- Simple function usage, 210
- Simple g edit descriptor example, 161
- Simple inheritance, 436
- Simple inheritance test program, 441
- Simple memory leak, 289
- Simple user defined function, 216
- Simula, 2, 22, 30
- Sine function, 212, 369
- Sin function, 212
- Singly linked list: reading an unknown amount of text, 337
- Skipping lines in a file, 186
- Smalltalk, 2, 30
- Snobol, 2, 21
- Software tools, 15
- Solution of linear equations using Gaussian Elimination, 403
- Sorting, 362
- Sorting reals and integers, 370
- Source code, 33, 386, 569, 574, 577, 582, 583
- Source files, 573
- Spaces, 162
- Sparse matrix problems, 283, 387
- SQL, 2, 28
- Standardisation, 25
- Stepwise refinement, 9, 11, 12, 16, 24
- Stirling's approximation, 224
- Stop statement, 226
- Storage size, 83, 86
- Stripping blanks from a string, 253
- Structure component, 491
- Structure constructor, 36, 425, 431–435, 438, 442

- Structure constructors and generic names, 425
Structured programming, 14, 24, 25, 232, 248
Subroutine
 arguments, 294
 parameter passing, 294
 intent, 297
 parameters, 294
Subroutine and function libraries, 577
Subroutine as a dummy procedure argument:, 400
Subroutine statement, 302, 324
Subroutine subprograms, 302
Subroutines, 293
 actual arguments, 302
 allocatable dummy arrays, 302
 automatic arrays, 302, 308
 character arguments, 305
 elemental subroutines, 318
 keyword and optional arguments, 302
 local variables, 297
 save attribute, 297
 parameter passing, 301
 allocatable dummy arrays, 315
 arrays, 301
 assumed shape arrays, 301
 deferred shape arrays, 301
 scalars, 301
 rank 2 arrays as parameters, 306
 recursive subroutines, 312
 scope of variables, 298
Subtraction operator, 367
Summary of how to select the appropriate kind type, 95
Summation and finite precision, 88
Supplying your own functions, 216
Sync all, 502
Sync images, 502
Sync memory, 502
Synchronization, 458
Systems analysis, 1, 5, 10, 14, 16, 387
Systems analysis and design, 1, 5, 10, 14, 16
- T**
Tabular output, 119
Target attribute, 283
Templates, 369
Threads and processes, 457
Threads and threading, 457
Three-dimensional spatial problems, 283
Three forms of the do statement, 239
- Three ways of generating spaces, 162
Time taken for light to travel from the Sun to Earth, 71
Timing of reading formatted files, 192
Timing of reading unformatted files, 193
Top 500 supercomputers, 463
Top-down, 1, 8, 9, 11, 14
Trailing blanks, 252, 255, 260
Transformational function use, 212
Transformational functions, 209, 212, 213
TS 29113 Further Interoperability of Fortran with C, 37
Two-dimensional spatial problems, 283
Type, 423
Type-bound procedure, 36, 424
Type construct, 277, 427, 449
Type conversion, 72
Type conversion across the = sign, 70
Type conversion and assignment, 69
Type declaration, 53, 72, 116, 228, 278, 423, 430–432
Type declaration statement, 423
Type definition, 277, 324, 339, 407, 425, 430, 435
Type integer, 218
Type statement, 73, 96, 297
Type transfer functions, 31
- U**
Underflow, 78, 79, 159, 165, 287, 539, 542, 551
Unformatted files, 170, 193, 194
Unified modeling language (UML), 13, 15
Unit numbering, 207
Unit numbers, 194
UNIX, 23
Upper bound, 143, 243, 305
Use association, 424
Use statement, 333
User defined elemental functions, 209
User defined functions, 209, 223, 226, 227, 294
User defined pure functions, 209
User defined types, 275, 279, 280
Using an interface to use the class name for the structure constructor, 433
Using iostat to test for errors, 204
Using modules, 324, 329, 400
Using the numeric inquiry functions with integer types, 82
Using the numeric inquiry functions with real types, 84

V

Variable declarations, 480
Variable definition, 277
Variable names, 250
Variable status, 96
Variable types, 265, 272
Variables—name, type and value, 51
Varying the array size at run time, 115
VAST/77to90, 595
Version control systems, 577
Volatile attribute, 36

W

Wave breaking on an offshore reef, 243

Where construct, 35, 146

While loop, 243, 340
Whole array, 131, 134, 135, 144, 145, 149,
153, 171, 172, 485
Whole array manipulation, 132
Work sharing, 508
Write statement, 175, 203
Writing formatted files, 167
Writing unformatted files, 169

X

x edit descriptor, 153