

Introduction to Fortran

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Session 1

Overview

- A brief history of Fortran
- Some programming fundamentals
- Hello World
- Types and variables
- Basic grammar and operations
- Control flow

Course content

- Some experience of programming in some language very useful
- But I don't assume much!
- Covers Fortran language
- Other people covering floating point maths, compilation, performance, parallelisation
- One/two practical sessions on the basics, but most hands-on in the target application sessions

What is Fortran?

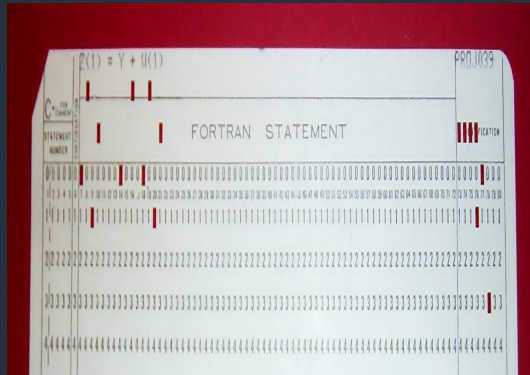
- Old language! 1956 – 62 years old
 - Oldest “high-level” language
 - Many versions over the years, latest is 2018! And next one is being worked on as we speak
- Some parts feel outdated
 - Backwards compatibility is important
 - But original reasons for some features no longer hold
- But still in use for good reason!
- Can be **very** fast
- Native multidimensional arrays
 - Very useful for scientists!

What is Fortran?

- Compiled language
 - compare with Python as interpreted language
- Statically typed:
 - types of variables must be specified at compile time and cannot be changed
 - “strong” typing, compare with C, easy to change types
- Imperative: commands executed in order
 - compare with SQL, Make, where commands are “what” vs “how”

Brief history of Fortran

- First release in 1956, FORTRAN
 - Not the first high-level language, but the first successful one
 - Let people write programs much faster, rather than in assembly
- Massively successful, ported to more than 40 different systems
- Early computers had no disks, text editors or even keyboards!
- Programs were made on punchcards



Brief history of Fortran

- FORTRAN II added functions (!)
- FORTRAN IV eventually got standardised and became FORTRAN 66
 - Starting to look like a “modern” programming language
- Next standard, FORTRAN 77, added lots of modern features
 - But still tied to format of punchcards!
- Fortran 90 finally brought language up to modern era
 - “Free” form source code
 - Made lots of “spaghetti” code features obsolescent
 - Added whole array operations, modules, derived data types
- Further revisions:
 - Fortran 95 - minor revision to F90
 - Fortran 2003 - major revision, support for object-oriented programming
 - Fortran 2008 - native support for parallelisation via coarrays
 - Fortran 2018 - minor revision to F2008, more support for parallelisation and interoperability with C

Why Fortran?

- Built for efficient mathematical calculations
- Makes it easy to write simple code that optimises well
 - For “reasonable” use cases!
- Multidimensional arrays are first-class objects
- Support for basic input files built in
- Easily fits into various parallel programming paradigms
 - Some even built right into language
- Majority of codes on UK supercomputers use Fortran
 - fluid dynamics, materials, plasmas, climate, etc.
- Portable code, several compilers available
- Interoperability features (can work with C easily)

Why not Fortran?

- Not great at problems outside of “usual” domain
 - Text processing, graphical interfaces, system programming
 - Still possible, just harder than in specialist languages!
- Historical baggage has left a very verbose language
 - Lots of typing!
- Lack of proper generics make some useful data structures tricky to implement
- Slow support from compiler vendors

Alternatives

- C++
 - Templates make it possible to express generic operations
 - Can get “close to the metal”, can get very good performance
 - Multidimensional array support poor (no native support, libraries exist)
- Python
 - Easier to use!
 - Possible cost of performance (but e.g. `numpy` uses C or Fortran under the hood!)
- Matlab
 - Expensive!

Fundamentals of Programming

- Computers understand machine code – 1s and 0s
- e.g. a `square` function might look like:

```
111100110000111100010000000001111111001100001111010110011100000011000011
```

- Exact number depends on exactly what physical processor you want to run on!
- We would much prefer to write in a human language
- “Lowest” level language is *assembly*, which just gives names to the *op codes*:

```
movss  xmm0,DWORD PTR [rdi]  ;; f3 0f 10 07
mulss  xmm0,xmm0              ;; f3 0f 59 c0
ret                                ;; c3
```

- Source code is human-readable set of instructions for computer:

```
square = x * x
```

Fundamentals of Programming

- Higher level language can abstract over assembly complications
- Need a program to convert source to machine code
- Either:
 - interpreted, like Python, convert on the fly
 - compiled, like Fortran, convert then run
- Compilation step offers opportunity to spend time *optimising* the code
 - unoptimised version of `square` above is 9 times longer!

Fundamentals of Programming

- Source code is written in plain text files (i.e. not Word!)
- Run compiler on source file to produce *executable*
- Programming languages have a strict *syntax* or grammar
- Compiler will tell you if you get this wrong
 - Read the error message, then read it again!
- Compiler can also *warn* you about suspicious code
- Compilers have many options or *flags* to control warnings, errors, optimisations, etc.

Fundamentals of Programming

- Source code is read more times than it is written, by factor 5 or more
- We use high-level languages in order to be understandable to humans
- Therefore, more important to write **readable** code than **efficient** code
- Even more important that it is correct
- Make it work -> make it readable -> make it fast
 - In that order!

Some conventions

- `<something>` means “something” is mandatory, but up to you
- `{something}` means “something” is optional, but has to be exactly `something`
 - `{<something>}` means “something” is optional and up to you!
- These two are red in code blocks, as they won’t compile!
- If a code block has numbers on the left, it’s from an example file, which will be available from
<https://github.com/ZedThree/HPCAcademyFortran/tree/master/examples>
- I usually don’t show the whole file, but the whole file will compile and work
- I don’t always follow best practices to make things fit on slides!
 - Do as I say, not as I do!
- Words like `this` are either keywords or tiny code snippets
- Words like *this* are (usually) technical words, either common usage or from the Fortran standard
- Words like **this** are just emphasis
- I use Fortran 2018, but everything should compile with gfortran 7

Hello world

```
1 program hello
2   implicit none
3   ! Print to screen:
4   print*, "Hello, World!"
5 end program hello
```

- Lines 1 & 5: All programs must start with `program <label>` and end with `end program <label>`
- Line 2: `implicit none`: Historical reasons! Old Fortran had implicit typing: more on this later
- Line 3: A comment, begins with `!` (ignore everything after this)
- Line 4: Print some text to screen

Compiling code

This will be covered more in depth later on

Basic compilation is as so:

- `gfortran source.f90 -> a.out`
- `gfortran source.f90 -o executable -> executable`

And running like

- `./executable`

Compiler flags

Some basic, very helpful flags you should use:

- `-Wall`: “commonly used” warnings
- `-Wextra`: additional warnings
- `-fcheck=all`: various run-time checks
 - This isn't free!
- `-g`: debug symbols
 - Can give better error messages, required for debuggers like `gdb`
- `-O1/-O2/-O3`: optimisations
 - Can speed up code at cost of longer compile times

Full compile line might look like:

- `gfortran -Wall -Wextra -fcheck=all -g -O2 hello.f90 -o hello`

Build systems like `CMake` or `Makefile` help simplify this

Types

There are 5 fundamental types in Fortran:

- `integer`
- `real` – floating point numbers
- `logical` – booleans, two values: `.true.`/`.false.`
- `character` – text, also called strings
- `complex` – floating point complex numbers

(later, we will look at derived types)

What, exactly, is a type?

- Computers store **everything** in binary, ones and zeros, called *bits*
- Given a set of bits, what does it mean?
 - Could be a number, could be some text
 - Could be an instruction!
- Binary: 000000000000000001001011001110000
- As an *integer*: 38512
- As a *real*: 5.39668e-41
- As a *character*: p
- As an instruction: XCHG

What, exactly, is a type?

- We need to tell computer how to interpret the set of bits
 - We're free to lie to the computer and change our minds about how to interpret a given set of bits
- Would be very tedious if we had to tell the computer every time we wanted to do an operation on some bits what type they represented
 - plus potential for mistakes
- Types tell the *compiler* our intent: these bits are an integer, those are text
- Compiler then checks we're doing sensible things
 - `4 + 6` makes sense
 - `4 + "hello"` doesn't make any sense
 - `4 + 5.3` might do

Literals

- Very common to need **literally** “this value”
- `integer`:
 - `1, -2, 1e3, 42`
- `real`:
 - `2., 0.3, 4.6E4, 0.02e-3`
 - Note: `real` literals are single-precision by default (more on this later)
- `complex`:
 - `(0.0, 1.0), (3.2, 4.3e9)`
- `character`:
 - `"either double quotes", 'or single quotes are fine'`
- `logical`:
 - `.true., .false.`
 - But often printed as `T` and `F`!

Variables

- A variable is label for some value in memory used in a program
- In Fortran, we must tell the compiler up front what type a variable is, and this is fixed
 - In other languages, like Python, we can change our minds
- Variables are declared like:

```
<type> :: <name> {, <name>}
```

- Note: `::` not always needed, but never hurts!

```
integer :: grid_points
```

```
real :: energy, mass
```


Variable names

- Variable names must start with a letter, and are limited to ASCII lower/uppercase, numbers and underscore
- Valid:
 - `a`, `NUMBER5`, `nitrogen_mass`, `O2_concentration`
- Invalid:
 - `1a`: must start with a letter
 - `_b`: must start with a letter
 - `Pounds£`: contains non-valid character `£`
 - `a-b`: parsed as “subtract `b` from `a`”

Variable names

- Pick variable names wisely!
 - in F2003, you can have up to 63 characters in a name
- Good names:
 - `distance_to_next_atom`
 - `temperature`
 - `total_energy`
- Less good names:
 - `distnxtatm`
 - `temp`
 - `E`
- “Writing code is a form of communication” - Kate Gregory
- Be kind to future readers, dnt ndlssly shrtn nms
- Your code will live longer than you think!

Hello world again

```
1  program hello_input
2      implicit none
3      character(len=20) :: name
4      integer :: number
5      print*, "What is your name?"
6      read*, name
7      print*, "What is your favourite integer?"
8      read*, number
9      print*, "Hello, ", name, &
10         & ", your favourite number is ", number, "!"
11 end program hello_input
```

- Line 3: `character(len=20)`: we need to say up-front how long how strings are via the `len` type parameter (we'll cover this a bit more later on)
- Line 6: `read*,`: read a variable from stdin/command line
- Line 9: `&`: line continuation for long lines

What's this `implicit none`?

- Always, **always** use `implicit none`
- Early Fortran done on punch cards
- Assume anything starting with `i-n` is an `integer`, otherwise it's `real`
- Very easy to make a typo and use an undefined value, get the wrong answer
- One `implicit none` at the top of the program (or module, see later) is sufficient
 - You may like to keep it in every function, see later

Some points on Fortran grammar: whitespace

- Whitespace mostly doesn't matter:

```
1 program                                bad_whitespace
2     implicit none
3     integer::x=1
4     print      *,x
5     endprogram bad_whitespace
```

- But very important for readability!

```
1 program good_whitespace
2     implicit none
3     integer :: x = 1
4     print*, x
5     end program good_whitespace
```

Some points on Fortran grammar: whitespace

- Matter of personal taste, but go for readability over prettiness
- Prefer one space around operators (+, *, =, etc.)
- Prefer one space after “punctuation” (:, ,)
- Vertical whitespace also affects readability
- Also note: tabs are not standard Fortran! Use spaces for indentation

Some points on Fortran grammar

Lines

- Statements must be on a single line unless you use a `&`, *line continuation*

```
if (some_very_long_and_complicated_condition > some_other_very_long)
```

can be rewritten as

```
if (some_very_long_and_complicated_condition &  
    > some_other_very_long_and_complicated_condition) then
```

- Optional to put `&` at start of next line
- Maximum of 256 lines (i.e. 255 `&`)
- Prefer to put operators at the beginning of lines

Some points on Fortran grammar

Capitalisation

- Fortran is (almost) completely case-insensitive
 - Inside strings matters, but keywords and variable names don't

```
iF (eNeRgY > cRiTICaL_eNeRgY) tHen
```

is *identical* to

```
if (energy > critical_energy) then
```

but one is easier to read

- Originally didn't have lower-case characters at all!
- Prefer lower-case keywords
- Careful with names!
- You may prefer `snake_case` for variable names

Some points on Fortran grammar

File names

- The standard doesn't mention source files **at all**
- Linux also doesn't care about file extensions
- Early, fixed-form sources files used `.f` file extension
- With Fortran 90, people started using `.f90` for free-form source files
- Some people thought that `.f95`, `.f03`, etc. should be used for later standards
- Not the case!
- Just use `.f90` and you'll be fine

Arithmetic operations

- Usual mathematical operators: `+`, `-`, `*`, `/`
- Plus `**` for exponentiation
 - Careful you only use integers unless you mean it
- BODMAS/PEDMAS and left-to-right, but use `()` to clarify
 - Don't forget, make it **readable**

```
3  real :: x, y
4  print*, 3 * 4
5  print*, 12 / 4
6  print*, 3.6e-1 + 3.6e0
7  x = 42.
8  y = 6.
9  print*, x + 2. / 4. * y ** 2
10 print*, x + ((2. / 4.) * (y ** 2))
```

Mixed-type operations

- Not uncommon to want to mix types in arithmetic, e.g.
 - `integer :: n` points of `real :: grid_spacing`
- This will *promote* the different types to be the same type/kind
- Result may end being *demoted* to fit the result type
- Possible to lose information this way, but compiler *may* warn you!

Integer division

- When dividing two `integer`s, the result is an `integer` truncated towards zero
- This may be surprising!
- `5 / 2 == 2`
- Therefore, if you need the result to be a `real`, either convert (at least) one operand to `real`, or use a `real` literal

```
3  integer :: x = 5
4  print*, 5 / 2
5  print*, x / 2
6  print*, x / real(2)
7  print*, x / 2.
```

Logical/relational operations

- `<` `>`: Less/greater than
- `<=` `>=`: Less/greater than or equal to
- `==`: Equal to
- `/=`: Not equal to
 - Note the inequality operator! Might look odd if you come from C-like languages or Python
 - This operator is essentially why Fortran doesn't have short-hand operators like `a *= b`
- Also wordier versions:
 - `.lt.`, `.le.`, `.gt.`, `.ge.`, `.eq.`, `.ne.`
 - But don't use these!

```
3 integer :: a = 4, b = 5
4 print*, a == b
5 print*, a < b
6 print*, (a * b) /= (a + b)
```

Intrinsic functions

- Built-in to language
- Lots of maths!
 - `sin`, `cos`, etc.
 - F2008 has things like `hypot`, `bessel_j0`, `erf`, `norm2`
- Use them if they exist – can be heavily optimised by compiler
 - Difficult to detect if they are available of course

```
3  real :: pi = 2.0 * acos(0.0)
4  print*, sin(pi / 4.)**2 + cos(pi / 4.)**2
5  print*, hypot(3., 4.)
6  print*, len("This sentence is forty-two characters long")
```

Control flow

- Often need to change exactly what happens at runtime
- `if` statement allows us to take one of a number of *branches* depending on the value of its *condition*

```
if (<logical-expression>) then
    ! do something
end if
```

- If `<logical-expression>` evaluates to `.true.` then the statements inside the *construct* are executed
- Otherwise, we carry on executing after the `end if`

Control flow

- More generally:

```
if (<logical-expression-1>) then
  ! do something 1
else if (<logical-expression-2>) then
  ! do something 2
else
  ! do something 3
end if
```

- Bare `else` must be last
- Also note that brackets `()` are mandatory here

Control flow

- Conditions are checked from the top:

```
3  integer :: x
4  print*, "Pick any number"
5  read*, x
6  if (x >= 0) then
7      print*, "You picked a positive number"
8  else if (x > 1) then
9      print*, "This can never be reached!"
10 else
11     print*, "You picked a negative number"
12 end if
```

Logical/boolean operations

- `.and.`, `.or.`, `.not.`

```
3 integer :: x = 5
4 if ((x >= 0) .and. (x < 10)) then
5     print*, "x is between 0 and 10"
6 else
7     print*, "x not between 0 and 10"
8 end if
```

- Note for those familiar with other languages: Fortran does not have shortcut logical operations
 - Line 4 above **may** evaluate **both** conditions!
- Also note that **logicals** must be compared with `.eqv.` and not `==` or `.eq.`
 - But you will probably never use this!

Loops

- Often want to repeat some bit of code/instructions for multiple values
 - Could write everything out explicitly
- `do` loops are a way of doing this
- three slight variations:

```
do
  ! do something
end do
```

```
do while (<logical-expression>)
  ! do something
end do
```

```
do <index> = <lower-bound>, <upper-bound>
  ! do something
end do
```

Loops

- All three forms essentially equivalent
- Bare `do` needs something in body to `exit` loop
- `do while` loops *while* the condition is true
- Last form does $\langle \text{upper-bound} \rangle - \langle \text{lower-bound} \rangle + 1$ loops
 - loop variable (`<index>`) must be pre-declared
 - lower and upper bounds are your choice

Bare do

- Notice nothing to say when loop is done!

```
3  integer :: x = 0
4  do
5      print*, x
6      x = x + 1
7  end do
```

exit

- We can use `exit` to leave a loop
- Leaves current loop entirely

```
3  integer :: x = 0
4  do
5      print*, x
6      x = x + 1
7      if (x >= 10) exit
8  end do
```

do while

- Equivalent to using `exit` at start of loop

```
3  integer :: x = 0
4  do while(x < 10)
5      print*, x
6      x = x + 1
7  end do
```

- Unlike C++, `do while` checks the condition at the *beginning* of the loop:

```
3  integer :: x = 10
4  do while(x < 10)
5      print*, x
6      x = x + 1
7  end do
```

do <counter> = <start>, <stop> {, <stride>}

- Most common form of the `do` loop is with a counter
- Must be an integer and declared before-hand
- `start` and `stop` are required, `counter` goes from `start` to `stop` *inclusive*:

```
3  integer :: i
4  do i = 0, 9
5      print*, i
6  end do
```


do <counter> = <start>, <stop> {, <stride>}

- There is an optional `stride`:

```
3 integer :: i
4 do i = 0, 9, 2
5     print*, i
6 end do
```

- Note that `stop` might not be included if `stride` would step over it

A couple of points on `do`

- It's ok for `stop` < `start`: just won't be executed
- `stride` can be negative:

```
3 integer :: i
4 do i = 9, 0, -2
5     print*, i
6 end do
```

- You cannot change the value of the loop `counter` inside a loop
- Value of `counter` not defined outside loop
 - Likely to take on last value after loop, but absolutely do not rely on it!
 - Compiler free to optimise it away

Session 3

Overview

- Arrays
- Parameters
- Kinds
- Procedures (functions and subroutines)

Arrays

- Arrays are one of the “killer features” of Fortran
 - Big reason why it’s lasted so long!
- Vector in 3D space could be 1D array of 3 elements:

```
3 integer, dimension(3) :: vector1
4 ! Or equivalently:
5 integer :: vector2(3)
```

- Fortran can natively handle multidimensional arrays:

```
3 integer, dimension(3, 3) :: matrix1
4 ! Or equivalently:
5 integer :: matrix2(3, 3)
```

- `matrix1` has $3 \times 3 = 9$ elements

Array indexing

- We can *index* an array using an integer:

```
9  do i = 1, 3
10     vector1(i) = i
11 end do
12
13 print*, "vector1(1):", vector1(1)
```

- We can even take a *slice* using the `:` notation:

```
14 print*, "vector1(2:3):", vector1(2:3)
```

- We can optionally leave off the lower and/or upper bounds:

```
16  ! All of first row:
17  print*, matrix1(1, :)
18  ! First two columns, last two rows:
19  print*, matrix1(:2, 2:)
```

Arrays

- **Note:** By default, Fortran indices start at 1!
- Can change this:

```
3 integer, dimension(-1:1) :: array
4 integer :: i
5
6 array(-1) = 12
7 array(0) = 42
8 array(1) = -18
```

- 1D array, 3 values with indices -1, 0, 1
- Note array bounds separated with :, dimensions (or *ranks*) with ,:

```
real, dimension(-1:1, 3:5) :: stress_tensor
```

- Still 3x3, but first dimension has indices -1, 0, 1, and second has 3, 4, 5

Literal arrays

- Just like scalar types have literals, so do arrays
- Wrap the scalar values in square brackets [`<values>...`]
 - Older style is (`/<values>.../`)
- Can use this to initialise or assign to arrays:

```
5 integer, dimension(3) :: array1 = [1, 2, 3]
```

- Or even pass to functions:

```
15 print*, sin([1., 2., 3., 4.])
```

- Unfortunately, only works for 1D arrays! Multidimensional arrays need to use `reshape`

Literal multidimensional arrays

```
5      integer :: matrix2(3, 3)

21     matrix2 = reshape([ &
22         9, 8, 7, &
23         6, 5, 4, &
24         3, 2, 1], shape(matrix2))
```

- Second argument to `reshape` is shape of result
- For assigning to arrays, we can just use `shape` intrinsic to get the right answer

Constructing arrays

- How to fill an array with 10 values between 0 and 2π ?
- Could do:

```
array(1) = 0.  
array(2) = 2. * pi * (1. / 10.)  
array(3) = 2. * pi * (2. / 10.)  
...  
! or  
do i = 1, 10  
    array(i) = 2. * pi * (real(i - 1) / 10.)  
end do
```

- This can be written a bit more compactly using an *implied do*:

```
array2 = [(2. * pi * (real(i - 1) / 10.), i=1, 10)]
```

- Not always the best tool, but sometimes very useful!

Operations with arrays

- We can do element-wise operations on arrays very simply:

```
18 print*, "42 + vector1:", 42 + vector1
19 print*, "2 * vector1:", 2 * vector1
20 print*, "vector1 + vector2:", vector1 + vector2
21 print*, "vector1 - vector2:", vector1 - vector2
22 print*, "vector1 * vector2:", vector1 * vector2
23 print*, "vector1 / vector2:", vector1 / vector2
```

- Notice how we can use both scalars and arrays in these operations?
- These whole-array operations make Fortran very powerful:

```
pressure = density * temperature
```

- Assuming all three variables are the same shape, this just does the right thing

Conformability

- When working with multiple arrays, need to make sure shapes *conform* (i.e. match exactly)
 - Useful intrinsic, `shape`, to tell you the shape!
- Scalars conform with everything
- Slices with the same shape conform (even if upper/lower bounds don't match)

```
4 integer, dimension(3) :: vector1 = [(i, i=1, 3)]
5 integer, dimension(3, 3) :: matrix1 = reshape(&
6     [(i, i=1, 9)], shape(matrix1))
7 integer, dimension(4) :: vector2 = [(i, i=1, 4)]
8 integer, dimension(3, 4) :: matrix2 = reshape(&
9     [(i, i=1, 12)], shape(matrix2))
10
11 print*, "shape(vector1):", shape(vector1)
12 print*, "shape(matrix1):", shape(matrix1)
```

Conformability

```
19      ! Won't work, different sizes
20      ! print*, vector1 + vector2
21
22      ! Ok, can use a slice of vector2
23      print*, vector1 + vector2(:3)
24
25      ! Won't work because the ranks don't match
26      ! print*, vector1 + matrix1
27
28      ! Ok, shape(matrix1(:, 1)) == shape(vector1)
29      print*, vector1 + matrix1(:, 1)
```

Memory layout

- Brief aside into computer architecture
- Computer memory is indexed by a linear series of addresses
- Usually written in hexadecimal
 - e.g. `0x07FFAB43`
- When we want to store multidimensional arrays, need to store them “flattened”
- Also need to pick which is the “fastest” dimension, i.e. which is stored first in memory

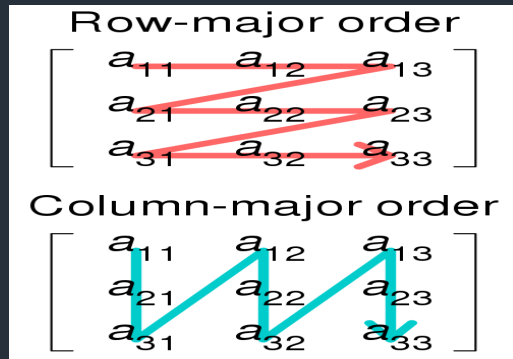
Memory layout

- Maths matrix:

$$\begin{matrix} & \begin{matrix} 1 & 2 & \dots & n \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ \vdots \\ \vdots \\ \vdots \end{matrix} & \left[\begin{array}{cccc} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ a_{31} & a_{32} & \dots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \end{array} \right] \end{matrix}$$

Memory layout

- Two choices:
- $a_{11}, a_{12}, \dots, a_{1n}$, then a_{21}, a_{22}, \dots
- or $a_{11}, a_{21}, \dots, a_{m1}$, then a_{12}, a_{22}, \dots
- *Row-major* or *column-major*



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Memory layout

- What does this mean in practice?
- Nested loops over multidimensional arrays should have the inner-most loop go over the left-most rank:

```
integer :: i, j, k  
real(real64), dimension(3, 3, 3) :: matrix
```

```
do k = 1, 3  
  do j = 1, 3  
    do i = 1, 3  
      matrix(i, j, k) = i + j + k  
    end do  
  end do  
end do
```

Memory layout

- Assuming no loop-dependencies, answer is identical to reversing order of loops
- But performance can be very different!
 - order of magnitude!
- This is different from C-like languages

```
15  call cpu_time(start_time)
16
17  do iteration = 1, max_iteration
18      do k = 1, nz
19          do j = 1, ny
20              do i = 1, nx
21                  matrix1(i, j, k) = i + j + k
22              end do
23          end do
24      end do
25  end do
26
```

Useful intrinsics

- The basic mathematical intrinsic functions also work on arrays:
- `sin`, `cos`, `tan`, `sqrt`, `exp`, `log`, etc.

```
6  real, dimension(N) :: x = [(2.*pi * real(i)/N, i=1, N)]
7
8  print*, x
9  print*, sin(x)
10 print*, cos(x)
11 print*, abs(sin(x))
12 print*, exp(-(x - pi)**2 / (pi / 4.))
```

Useful intrinsics

There are many useful functions for working with arrays built in to Fortran

Many of these intrinsics take an optional `dim` argument to take the function just along that dimension

Working with vectors/matrices

- `dot_product(vector_a, vector_b)`: Returns the dot product of two 1D arrays of the same size
- `matmul(matrix_a, matrix_b)`: Returns the matrix multiplication of two matrices
- `product(array)`: Return the product of all the elements
- `sum(array)`: Return the sum of all the elements
- `norm2(array)`: Return the L_2 norm, essentially `sqrt(array**2)`

Useful intrinsics

Logical inquiries

- `all(mask)`: Returns true if all the elements in the logical array `mask` are true, otherwise returns false
 - `mask` can be an expression like: `all(array > 0)`
- `any(mask)`: True if any of the elements in `mask` are true
- `count(mask)`: Returns how many elements in `mask` are true (an integer)

Useful intrinsics

Finding elements and values

- `maxval(array)`: Returns the maximum value in `array`
- `minval(array)`: Returns the minimum value in `array`
- `maxloc(array [, mask])`: Returns the *location* of the maximum value
- `minloc(array [, mask])`: Returns the *location* of the minimum value
 - Get the element closest to `value`: `minloc(abs(array - value))`
- `findloc(array, value)`: Return the location of `value` in `array`
 - Note that this is not so useful for `real` arrays!

Useful intrinsics

Array size and shape inquiries

- `lbound(array)`: Return a 1D array of the lower bounds of `array`
- `ubound(array)`: Return a 1D array of the upper bounds of `array`
- `shape(array)`: Return a 1D array of the size of each dimension
- `size(array)`: Return a scalar of the total size of `array` (i.e. `product(shape(array))`)

Useful intrinsics

Making new arrays

- `merge(tsource, fsource, mask)`: Return `tsource` where `mask` is true and `fsource` where `mask` is false
- `spread(source, dim, ncopies)`:
- `transpose(array)`: Returns the transpose of a 2D array
- `reshape(source, shape [, pad] [, order])`: Returns a copy of `source` with `shape`. `pad` can be used to fill in values if the result is larger than `source`. `order` can be used to do a general n -D transpose

Allocatable arrays

- If size of array not known until some time into the program execution, can use `allocatable` arrays to dynamically size them

! These two are equivalent:

```
real(kind=wp), dimension(:), allocatable :: array1
```

```
real(kind=wp), allocatable :: array2(:)
```

! 3D array:

```
real(kind=wp), dimension(:, :, :), allocatable :: array3
```

- The number of dimensions/rank must be known at compile time
 - Size of each dimension must be just :
- After declaration, we must use `allocate` before first use:

```
real(kind=wp), dimension(:, :), allocatable :: array
```

```
allocate(array(10, 5))
```

! array is now 10x5

Allocatable arrays

- `array` is now `allocated`, but *uninitialised*
 - i.e. if we index it we will get nonsense
 - same state as a non-allocatable array before we fill it
- When finished with the array, we can `deallocate` it and free up the memory:

```
deallocate(array)
```

- Less important than C-like languages due to *automatic* variables and scope – will cover this later
- It is an error to `deallocate` an unallocated array, so:

```
if (allocated(array)) deallocate(array)
```

Guarding `allocate`

- Possible to request more memory than available
- Good practice to always check `allocate` succeeds using `stat` argument
- Value of `stat` is non-portable and might not even be documented!
- Combine with `errmsg`:

```
9  allocate(bigarray(bignumber), stat=status, errmsg=errmsg)
10
11  if (status /= 0) then
12      print*, trim(errmsg)
13      print*, status
14      ! Note non-constant stop code is technically F2018
15      error stop status
16  end if
```

Guarding `allocate`

- Note `errmsg` may not always be accurate. . .
- Bare `allocate` will terminate on error, possibly with more useful error message
- If you use `stat=` keyword, **always** check it!
 - otherwise program will continue and be wrong

Aside: heap and stack

- Two (main) areas of memory in the computer: the heap and the stack
 - Only a model, not necessarily physically separate!
- The stack is first-in, first-out, like a stack of plates
- Program uses this for passing arguments to functions, local variables, where to return to, etc.
- Stack is only a limited size, so very large arrays as local variables may *overflow* the stack
- The heap is just a big pile of memory
- Slower to find what you want, but there's more of it
- `allocate` puts variables on the heap instead of the stack
- So even if you know the size, can be useful to `allocate`

parameter

- sometimes want a variable that can't be modified at runtime, e.g. `pi`
- or have lots of arrays of fixed size

```
real, dimension(10) :: x_grid_spacing, y_grid_spacing  
real, dimension(10) :: x_grid, y_grid  
real, dimension(10, 10) :: density
```

- What if you now need a 20x20 grid?
- use a `parameter`!
- fixed at compile time
 - has to be made of literals, other `parameters`, `intrinsic`s
- names are great!
- attribute (now we definitely need `::`)
- super useful for things like `pi`, `speed_of_light`, `electron_mass`, etc.

parameter examples

```
1  program parameters
2      use, intrinsic :: iso_fortran_env, only : real64
3      implicit none
4      integer, parameter :: wp = real64
5      real(kind=wp), parameter :: pi = 4._wp*atan(1._wp)
6      integer, parameter :: grid_size = 4
7      integer, dimension(grid_size), parameter :: x_grid = [1, 2, 3, 4]
8
9      print*, pi
10     print*, x_grid
11 end program parameters
```

character parameters

- It can be a quite annoying to keep the `len` of a `character` in sync with how long it is
- For `character parameters` though, we can use `len=*`

```
character(len=*), parameter :: filename = "output.log"
```

- Only works for `parameters` and dummy `intent(in)` arguments (see later) though!
- Non-constant `characters` can be `allocatable` with `len=:` though!

character examples

```
3  character(len=*), parameter :: fixed_string = "output.log"
4  character(len=:), allocatable :: flexible_string
5
6  print*, len(fixed_string), fixed_string
7
8  flexible_string = "first time"
9  print*, len(flexible_string), flexible_string
10
11 flexible_string = "second time"
12 print*, len(flexible_string), flexible_string
```

Kinds of types

- Most important for `reals`
 - Sometimes important for `integers`
- Floating point representation
- Doing lots of maths with floating point numbers can lose precision => need more precision in our `reals`
- Default `real` kind is (normally) 32-bit (4 bytes) (`float` in C)
 - Can represent numbers $\pm 3.4 \times 10^{38}$ to about 7 decimal places
- Using 64-bits (8 bytes) we can represent numbers $\pm 1.7 \times 10^{308}$ to about 15 decimal places

Kinds of types

- Different ways to specify the kind
- Three old styles:
 - `double precision`: use twice the number of bytes as for `real`
 - Standard! but vague
 - `real*8`: use 8 bytes
 - Non-standard! never use this
 - You'll see it a bunch in old codes though
 - `real(8)` or `real(kind=8)`: use real of `kind` 8
 - Standard but non-portable!
 - What number represents what `kind` is entirely up to the compiler

Kinds of types

- Don't use those! Use either this:

```
! Get the kind number that can give us 15 digits of precision and 300  
! orders of magnitude of range  
integer, parameter :: wp = selected_real_kind(15, 300)  
! Declare a variable with this kind  
real(kind=wp) :: x  
! Use a literal with this range  
x = 1.0_wp
```

Kinds of types

iso_fortran_env

- Even better! F2008 feature, but use this and complain if stuck on a previous standard (upgrade compilers!)

```
use, intrinsic :: iso_fortran_env, only : real64
real(real64) :: x
x = 1.0_real64
```

- Can combine this with a parameter:

```
use, intrinsic :: iso_fortran_env, only : real64
integer, parameter :: wp = real64
real(kind=wp) :: x
x = 1.0_wp
```

- We will cover what the `use` line means later

Kinds of types

- `real` literals are single precision by default, so need `kind` identifier

```
4  real, parameter :: pi = 3.141592653589793238462643383
5  real(real64), parameter :: pi_wrong = 3.141592653589793238462643383
6  real(real64), parameter :: pi_right = 3.141592653589793238462643383_real64
```

- Mixed-kind operations will convert like mixed-type operations
- Lots of intrinsics take a `kind` argument:
 - `5._real64 / real(2, kind=real64) == 2.5_real64`

Kinds of types

- Similar story for `integers`
- Default kind is usually 32-bit again
- Can represent the numbers -2^{31} to $2^{31} - 1$
- A 64-bit `integer` can represent -2^{63} to $2^{63} - 1$
- Can choose this kind with either:

! Get the kind that can represent an integer with 18 digits

```
integer, parameter :: ip = selected_real_kind(18)
integer(ip) :: x
```

! or, better:

```
use, intrinsic :: iso_fortran_env, only : int64
integer(int64) :: y
```

Breaking up programs

- Large **programs** become difficult to understand and *maintain*
- Quickly come across chunks of code we want to reuse
- Therefore very good idea to break programs up into building blocks
- This gives us reusable components
 - Reduce copy-paste errors
 - Repeat tasks multiple times
 - Use same task in multiple contexts
 - Gives names to parts of code
- Names are an often over-looked advantage!
 - Important to choose names wisely
- Two ways of breaking **programs** in Fortran:
 - Procedures
 - Modules
 - Cover later

Procedures

- Two types of procedures:
 - `functions`
 - `subroutines`
- Generically called *procedures* or *subprograms*
- May also refer to them both as *functions* – will make it clear when I mean `functions` in particular

Benefits of procedures

- Testing
 - Can test individual parts of the code in isolation
- Reuse
 - Same function can be used in different contexts
 - Can even build up a *library* of functions
- Maintainability
 - Code can be easier to understand
 - Can fix implementation without touching rest of code
- Abstraction
 - Can now think of chunk of code as a thing itself
 - Good names help here!
- Encapsulation
 - Hide internal details from other parts of the `program`
 - Program against the *interface*

Functions

- Takes arguments and returns a single result (may be array)
- Always returns a value
- Intrinsic functions, e.g. `sin(x)`, `sqrt(x)`
- syntax:

```
function <name>(<input>)  
  implicit none  
  <type>, intent(in) :: <input>  
  <type> :: <name>  
  ! body  
  <name> = ! result  
end function <name>
```

Functions

- Result has the same name as the function, by default
- Can change this with `result` keyword

```
1 function kronecker_delta(i, j) result(delta)
2   integer, intent(in) :: i, j
3   integer :: delta
4   if (i == j) then
5     delta = 1
6   else
7     delta = 0
8   end if
9 end function kronecker_delta
```

Functions

- Functions in `programs` go after a `contains` statement:

```
1 program basic_function
2   implicit none
3
4   print*, kronecker_delta(1, 2)
5   print*, kronecker_delta(2, 2)
6
7 contains
8   function kronecker_delta(i, j) result(delta)
9     integer, intent(in) :: i, j
```

Functions

- Use function like `y = function(x)`
- Use `()` even if a function requires no arguments: `x = function()`
- As long as `implicit none` is in your `program` (or `module`, see later), not necessary in procedures
 - Some people advise as good practice though!
 - I will be skipping this from examples for space reasons

Subroutines

- Essentially functions that don't need to return anything
- Can still return things via out-arguments
 - Could be multiple out-arguments
 - Not always a good idea!
- Syntax:

```
subroutine <name>(<input>, <output>)  
  implicit none  
  <type>, intent(in) :: <input>  
  <type>, intent(out) :: <output>  
  ! body  
end subroutine <name>
```

- Subroutines are used via the `call` statement:

```
call <name>(<arguments>)
```

Subroutine example

```
10  subroutine increment_x_by_y(x, y)
11      integer, intent(inout) :: x
12      integer, intent(in) :: y
13      x = x + y
14  end subroutine increment_x_by_y
```

used like:

```
5  print*, x
6  call increment_x_by_y(x, 3)
7  print*, x
```


Recursion

- Due to historical reasons, procedures are not recursive by default: they cannot call themselves directly or indirectly
- Need to use `result` keyword to change name of function result
- Use `recursive` keyword:

```
recursive function factorial(n) result(res)  
    ...  
end function factorial
```

Local variables

- Variables declared inside procedures are *local* to that routine
 - Also called *automatic* variables
- Their *scope* is the immediate procedure
- Cannot be accessed outside the routine, except via:
 - function result
 - `intent(out)` or `intent(inout)` dummy arguments (see later)
- Local `allocatable` variables are automatically `deallocated` on exit from a procedure
 - not the case for dummy arguments (see later), or variables accessed from a different scope (also see later!)

Local variables

```
3   integer :: x = 4
4   print*, add_square(x), x
5   contains
6   function add_square(number) result(res)
7       integer, intent(in) :: number
8       integer :: res
9       integer :: x
10      x = number * number
11      res = number + x
12  end function add_square
```

`x` in the main program and `x` within `add_square` are different variables

More on scope

- Possible for procedures to access variables in the containing scope
 - Technically called *host association*
- Generally not a great idea!

```
1  print*, add_square(x), x
2  contains
3  function add_square(number) result(res)
4      integer, intent(in) :: number
5      integer :: res
6      x = number * number
7      res = number + x
8  end function add_square
```

- This is surprising, despite the `intent(in)`!
- Also hard to see where `x` comes from
- There are uses for this, but prefer to explicitly pass in variables via arguments

Initialising local variables

- A word of warning when initialising local variables
- Giving a variable a value on the same line it is declared gives it an implicit `save` attribute
- This `saves` the value of the variable between function calls
- Initialisation is then *not done* on subsequent calls:

```
13  subroutine increment_count_implicit()  
14      integer :: count = 0  
15      count = count + 1  
16      print*, "Called implicit version", count, "times"  
17  end subroutine increment_count_implicit
```

intent

- When writing programs, can be very useful to tell the compiler as much information as you can
- One useful piece of info is the *intent* of arguments to procedures
- This can help avoid certain classes of bugs
- There are three `intents`:
- `intent(in)`: this is for arguments which should not be modified in the routine, only provide information **to** the procedure
- `intent(out)`: for arguments which are the *result* of the routine. these are *undefined* on entry to the routine: don't try to read them!
- `intent(inout)`: for arguments are to be modified by the procedure
 - if you don't explicitly provide an `intent`, this is the default
- These are essentially equivalent to read-only, write-only and read-write
- Prefer `functions` over `subroutines` with `intent(out)` arguments
 - Easier to read!

Dummy arguments

- *Dummy* arguments are the *local* names of the procedure arguments
- *Actual* arguments are the names at the calling site
 - *actual* arguments are said to be *associated* with the *dummy* arguments
- The routine doesn't care or know what the names of the actual arguments are
 - type, kind, rank and order have to match though!

Dummy arguments

```
1 program dummy_arguments
2   implicit none
3   integer :: x = 1, y = 2
4   real :: z = 3.0
5
6   call print_three_variables(x, y, z)
7 contains
8   subroutine print_three_variables(a, b, c)
9     integer, intent(in) :: a, b
10    real, intent(in) :: c
11    print*, "a is ", a, "; b is ", b, "; c is ", c
12  end subroutine print_three_variables
13 end program dummy_arguments
```

■ x becomes associated with a; y with b; z with c

Keyword arguments

- Another nifty feature of Fortran is keyword arguments:

```
6  call print_three_variables(b=y, c=z, a=x)
7  contains
8  subroutine print_three_variables(a, b, c)
```

- Lets us change the order of the arguments
- **Very** useful as documentation at the calling site!
 - especially when lots of arguments (but don't)
 - or multiple arguments with same type next to each other

```
call calculate_position(0.345, 0.5346)
```

! or

```
call calculate_position(radius=0.345, angle=0.5346)
```

Dummy arguments and arrays

Three choices for passing arrays:

- `dimension(n, m, p)`: explicit size
 - Need to pass `n`, `m`, `p` as well (or get them from elsewhere)
 - Actual argument has to be exactly this size
 - Compiler can only check size is correct if it knows the size at compile time
- `dimension(n, m, *)`: *assumed size* – old, don't use!
 - Compiler doesn't know the size of the array, so you better index it correctly!
- `dimension(:, :, :)`: *assumed shape*
 - Compiler now **does** know the size of the actual array passed
 - Can check if you go out-of-bounds (may need compiler flag!)
 - Indices now always start at 1
- `dimension(n:, m:, p:)`: assumed shape with lower bounds
 - Compiler still knows the correct size
 - but remaps indices to match your provided lower bounds
 - `n`, `m`, `p` need to be passed in (or got from elsewhere)

Pure procedures

- It turns out to be very useful for the compiler to know if a function has *side-effects*
 - Does it modify any arguments except those marked `intent(out|inout)`?
 - Does it modify any variables from a different scope?
 - Does it have a local variable with `save`?
 - Does it attempt to `read` or `write` anything?
- A *pure* procedure has no side-effects
 - `functions` must only return values
 - `subroutines` can have `intent(out)` arguments
- Given the same input, you will always get the same output
 - e.g. `abs(-0.5)` always returns `0.5`
- Useful documentation!
- Compiler can catch more bugs/mistakes
- Compiler may be able to apply some more aggressive optimisations

Elemental procedures

- We saw some intrinsics can handle scalars or arrays
- It is also possible to write our own functions that can operate on both scalars and arrays
- These functions apply the function to each element, so they are called *elemental*
- Elemental functions must be `pure` or marked `impure`

```
4  integer, dimension(3) :: x = [1, 2, 3]
5  print*, double(x)
6
7  contains
8      elemental integer function double(x)
9          integer, intent(in) :: x
10         double = 2 * x
11     end function double
```

Returning `allocatable` variables from functions

- Both `functions` and `subroutines` can `allocate` variables
- Returning an `allocatable` from a `function` can be quite convenient, because it will automatically reallocate the assignee

```
15 function make_grid(grid_size)
16     integer, intent(in) :: grid_size
17     real, dimension(:), allocatable :: make_grid
18     integer :: i
19
20     make_grid = [(real(i) / grid_size, i=1, grid_size)]
21 end function make_grid
```

Use like:

```
9 grid = make_grid(grid_size)
```

Session 5

Overview

- More control flow
- Input and output
- Characters

Choosing an option: `select case`

- When comparing series of mutually exclusive values, order is not important
- `case` construct can be useful:

```
select case (<expression>)
case (<case-1>)
    ! do something 1
case (<case-2>)
    ! do something 2
{case default}
    ! do something 3
end select
```

- `case default` matches when nothing else does
 - Not necessary, but absence might hide bugs!

select case

- The expression in the `select case` must be an `integer`, `logical` or `character` scalar variable
- Can specify value or range:
 - `value`
 - `:upper_bound`
 - `lower_bound:`
 - `lower:upper`
- Ranges must be of same type
- Case must be known at compile time
 - i.e. literals, `parameters`, and expressions using them only
- Cases may not overlap!
 - Compare to multiple `if` statements

select case

```
8  select case(number)
9  case (42)
10     print*, "You picked exactly forty-two"
11  case (:10)
12     print*, "You picked a number less than or equal to ten"
13  case (50:)
14     print*, "You picked a number more than or equal to fifty"
15  case (11:20)
16     print*, "You picked a number between eleven and twenty"
17  case default
18     print*, "You picked a number between twenty and fifty,&
19             & excluding forty-two"
20  end select
```

select case with characters

- Neat thing about `select case` in Fortran: works with strings!

```
8  select case (animal)
9  case ("cat")
10     print*, "meow!"
11  case ("dog")
12     print*, "woof!"
13  case ("pig")
14     print*, "oink!"
15  case default
16     print*, "<generic animal noise>"
17  end select
```

- Can be useful for parsing user arguments
 - careful not to overdo it though, this is expensive!

Selective array expressions: `where`

- It can be very useful to perform operations on an array only on certain elements
 - e.g. taking `log` of non-zero elements
- The `where` construct does exactly this:

```
where (<array-logical-expression>)  
  ! do something on "true" elements  
elsewhere  
  ! do something on "false" elements  
endwhere
```

- Equivalent of `do` loop and `if/else` construct acting on every element
- The `where` mask must conform to the array(s) used in the construct body
- Not very common, but useful to have when you need it

where example

```
7  where (pressure > 0)
8    log_pressure = log(pressure)
9  elsewhere
10   log_pressure = -1.e20
11 end where
```

is the same as:

```
15 do i = 1, 6
16   if (pressure(i) > 0) then
17     log_pressure(i) = log(pressure(i))
18   else
19     log_pressure(i) = -1.e20
20   end if
21 end do
```

Loop labels

- Many constructs in Fortran can be given labels
- Useful as a form of documentation: what does this loop **do**?
- Also useful when you need to jump out of a nested loop:

```
5  outer: do i = 1, 5
6      inner: do j = 1, 5
7          if ((i + j) == 7) exit outer
8          print*, i, "+", j, "=", i + j
9      end do inner
10 end do outer
```

Skip an iteration: `cycle`

- Sometimes need to skip a loop iteration, but keep looping
- Other languages use `continue`: unfortunately, this is an old keyword for `end do`!
- Fortran uses `cycle` instead

```
5  do i = 1, 5
6      if (i == 3) cycle
7      print*, i
8  end do
```

Skip an iteration: `cycle`

- Like `exit`, can also give `cycle` a loop label:

```
5  outer: do i = 1, 5
6      inner: do j = 1, 5
7          if ((i + j) == 7) cycle outer
8          print*, i, "+", j, "=", i + j
9      end do inner
10 end do outer
```


Formatted I/O

- What does the `*` mean in `print`, `read`?
- Why is it `print` and `read`?
- Why does Fortran put great big spaces between variables in `print`?

Formatted I/O

- `print*`, is essentially short for `write(*, *)`
- `read*`, is essentially short for `read(*, *)`
- Note lack of trailing commas!
- One step closer
- `write(*, *)` is short for `write(unit=*, fmt=*)`
- A bit closer!

What do those stars mean

- First argument, `unit`, tells program **where** to `read/write`
 - `*` means `stdout` – *standard out* for `write`
 - usually “screen”, but could be redirected somewhere else
 - `*` means `stdin` – *standard in* for `read`
 - usually keyboard, but could be something else redirected
 - Similar to file descriptor/handle in other languages
- Second argument, `fmt`, short for *format*, tells program *how* to `read/write`
 - `*` means “read/write everything, separated by spaces”
 - Also called *list-directed I/O*

Formatted I/O

- Instead of star, can give a *format string*
 - (technically *data edit descriptor*, but yeesh)
- Basic form is '`(<something>)`', where `<something>` is a comma-separated list of format codes
- `write(*, '(a, i0, a)') "I have ", number_of_cats, " cats"`
 - `a` means `character`
 - `i0` means `integer`, the `0` is “make it as wide as it needs to be”
- Can also stick text in there:
- `write(*, '("I have ", i0, " cats")') number_of_cats`
- Lots of format codes: use your favourite search engine!

Formatted I/O

Basic format codes

- `a`: `character`
- `i`: `integer`
- `f`: `real`
- `e`: `real`, but using scientific notation

Widths

- `cw.d`:
 - `c`: code (e.g. `i`, `f`, `e`)
 - `w`: width of whole field
 - `d`: number of digits after decimal place for `real`, minimum number of digits (pad with leading zeros) for `integer`

Formatted I/O

```
12  print*, "integer formats:"
13  write(*, '( "      |12345678|")')
14  write(*, '("i0:   |", i0, "|")') grid_size
15  write(*, '("i4:   |", i4, "|")') grid_size
16  write(*, '("i4.4: |", i4. 4, "|")') grid_size
17  write(*, '("i0:   |", i0, "|")') 23249425
18  write(*, '("i4:   |", i4, "|")') 23249425

24  write(*, '( "      |000000000111111111|")')
25  write(*, '( "      |123456789012345678|")')
26  write(*, '("f3.1:  |", f3.1, "|")') 2. * pi
27  write(*, '("f8.4:  |", f8.4, "|")') 2. * pi
28  write(*, '("f2.1:  |", f2.1, "|")') 2. * pi
```

Formatted I/O

- Can repeat chunks:

```
write(*, '(2(i0, 2(f8.3)))') ...
```

- expands to:

```
write(*, '(i0, f8.3, f8.3, i0, f8.3, f8.3)') ...
```

- More complicated example:

8

```
write(*, '(3("[", 3(i0, ", "), "], ")))' array
```

- This means:

- three lots of square brackets surrounding:
- three lots of `integer` separated by commas

Formatted I/O

- The I/O control statement will consume stuff from *transfer list* to fill up the format string:
 - `write` writes a newline every time it “fills up” the format string
 - `read` similar, but ignores everything until after next newline
- This will print the whole of `array`, two elements per line:

1

```
write(*, '("|", i2.1, " ", i2.1, "|")') array
```


Formatted I/O

Other notes:

- Compiler will check types, but unfortunately only at runtime
 - This is because format string can be built dynamically!
- Nice tip: can put format string into a `character`
 - Good if reusing the same format a lot
- If the format string is too small for the data, program will print stars (`****`) taking up the full space instead

Unformatted I/O

- Formatted I/O is about writing variables as text
- Fine for small amounts of data
- But can rapidly become bottleneck at large amounts
- For example, printing a `real` as text: sign, leading digit, decimal point, 8 digits, exponent symbol, exponent sign, 2 exponent digits: total 15 characters
- Assuming ASCII, then 1 byte per character: 15 bytes vs 4 for internal binary representation
- Almost 4x larger!
- Plus additional cost of converting
- Possible rounding errors as well

Unformatted I/O

- When we `open` a file (next section), can choose to open it `form='unformatted'`
- Avoids problems from before
- Now can `read/write` directly the internal representation
- Good for checkpoints, etc.
- **Much** faster than writing text
- **Can** be read by other programs, but technically not portable
 - i.e. don't rely on it!
- For serious HPC programs, better to use a library such as NetCDF

open - File I/O

- Open a file called `<filename>` for reading/writing:

```
open(newunit=<unit>, file=<filename>)
```

- Now we can't just use `*` for the unit, as we need a "handle" to give to `read/write`
- `<unit>` is an `integer` (that you've already declared)
- `newunit` will make sure it's unique (and negative)
- `newunit` is F2008. On older versions you need to manage the unit numbers yourself:

```
integer, parameter :: rectangle_unit = 11  
open(unit=rectangle_unit, file="rectangle.shape")
```

- There are some pre-declared units, so use values > 10 to be safe

open arguments

Lots of possible arguments, but two useful ones are `status` and `action`:

`status`

- Can be one of the following:
- `"old"`: must already exist
- `"new"`: must not exist
- `"replace"`: overwrite any existing file
- `"scratch"`: remove file after `close` or end of program
- `"unknown"`: you don't care!

open arguments

action

- Can be one of the following:
- "read": open the file for read only
- "write": open the file for write only
- "readwrite": allow both read and write

read

- Once you've got a file with a `unit`, you can read from it into variables

```
read(unit=<unit>, fmt=<fmt>) <transfer-list>
```

- `<unit>` must be already `opened` unit
- `unit=*, fmt=*` is same as `read(*,*)`
- The `intrinsic` module `iso_fortran_env` has `input_unit` for `stdin`

write

- Similarly, once you've got a file with a `unit`, you can write into it from variables or expressions

```
write(unit=<unit>, fmt=<fmt>) <transfer-list>
```

- `<unit>` must be already `opened` unit
- `unit=*, fmt=*` is same as `write(*,*)`
- The `intrinsic` module `iso_fortran_env` has `output_unit` for `stdout`

close

- Need to `close` files after we're done to ensure contents get written to disk properly

```
close(unit=<unit>)
```

- If `<unit>` is not an `opened` unit, `close` does nothing

Error checking I/O: `iostat`

- All the file I/O commands can take an `iostat` argument
- Should be integer you've already declared
- Error if `iostat /= 0`
- Best practice is to check value of `iostat`

```
integer :: iostat  
open(newunit=unit_num, file="filename", iostat=iostat)  
if (iostat /= 0) error stop "Error opening file"
```

- Worst practice is to use `iostat` and not check it!

Error checking I/O: `iomsg`

- Any I/O operation errors will cause abort unless `iostat` is used
- `iostat == 0` means success – any other value is compiler dependent
- Use `iomsg` to get a nice human readable message!
- Unfortunately, no spec on how long it should be

```
integer :: iostat
character(len=200) :: error_msg
open(newunit=unit_num, file="filename", iostat=iostat &
     iomsg=error_msg)
if (iostat /= 0) then
    print*, error_msg
    error stop
end if
```

Working with files example

```
10  open(newunit=file_unit, file="rectangle.shape", status="old", &
11      action="read", iostat=iostat, iomsg=error_message)
12
13  if (iostat /= 0) then
14      print*, "Something went wrong opening the file!"
15      print*, error_message
16      error stop iostat
17  end if
18
19  read(unit=file_unit, fmt='(f5.3, f5.3)') height, width
20
21  close(unit=file_unit)
22
23  write(output_unit, output_format) height, width, height * width
```

Namelist

- Another nifty feature of Fortran
- Great for simple things, not so great for more complicated things
- Similar to list/record-based I/O above: give a list of variables to read from/write to file
- But now with reading, have a bit more flexibility

```
namelist /<name>/ <variable1> {, <variable2> ...}
```

```
read(<unit>, nml=<name>)
```

and the input file looks like:

```
&<name>  
  <variable1> = <value1>      ! Comment  
  <variable2> = <value2>  
/
```

Namelist

- Can also write namelists
 - useful for recording what inputs were actually used
- Variables can be in any order
- Can even miss variables! useful for default values
- Extra ones not in the `namelist` statement is an error though
- Also, `logicals` can be T/F, `.true./false.`
- Variables need to be declared first
- Comments are allowed (and are ignored), case insensitive (as usual), and whitespace is mostly ignored (except within names, as usual)
- Unfortunately, `namelists` are not quite *first-class entities*
 - Meaning you cannot put them in a variable of any kind, pass them to a function, etc.
 - This becomes a pain if you want to do more complicated things, e.g. have multiple ion species, each with identical namelists

Namelist example

```
4  integer :: height = 2, width = 3
5  integer :: file_unit
6
7  namelist /rectangle/ height, width
8
9  open(newunit=file_unit, file="rectangle.nml")
10 read(file_unit, rectangle)
11 close(file_unit)
12
13 print*, "area = ", height * width
14 print*, ""
15
16 write(output_unit, nml=rectangle)
```

Working with `characters`

- `characters` of a fixed length are terminated by *blanks*, i.e. spaces
- so `character(len=10) :: cat = "ziggy "`
- `characters` can be indexed similarly to arrays, with one restriction: the colon (`:`) is **required**:

```
character(len=10) :: cat = "Ziggy      "  
cat(:3) == "Zig"  
cat(4:4) == "g"  
cat(5:) == "y      "
```


Working with `characters`

- We can stick two `characters` together with the *concatenation operator*, `//`:

```
character(len=*), parameter :: cat1 = "Ziggy", cat2 = "Lana"  
character(len=*), parameter :: both_cats = cat1 // " and " // cat2
```

- This is the easiest way to build up a string dynamically
- But we can also `write` to a `character`!
- Just use the variable in place of the `unit` argument

Writing to a character

```
4  character(len=7) :: run_name
5  integer :: run_number
6
7  run_number = 456
8  write(run_name, '(A, I4.4)') "run", run_number
9  print*, run_name
10
11  ! Too long for the character!
12  run_number = 89988
13  write(run_name, '(A, I4.4)') "run", run_number
14  print*, run_name
```

Useful intrinsics for `characters`

- `len(string)`: How long is `string`, including the trailing spaces
- `len_trim(string)`: How long is `string`, **excluding** the trailing spaces
- `trim`: Remove all trailing spaces
- `adjustl(string)`, `adjustr(string)`: “Adjust” the string left/right, moving leading/trailing spaces to the end/beginning
- `index(string, substring)`: Return the starting position of `substring` within `string`, or zero if it's not found.
- `new_line(a)`: Get the new line `character` of the same kind as `a`
 - This is the equivalent of `\n` in C, Python, etc.

Session 7

Overview

- Modules
- Derived types
- Interfaces

Modules

- Very big programs become difficult to develop and maintain
- Becomes useful to split up into separate files
 - Can group related functions together
- May want to reuse functions between projects
- Early versions of Fortran just stuck subprograms into separate files and linked them altogether
 - Still works!
 - But don't do it!
- But compiler doesn't know what procedures are in what files, or what the interfaces look like (number and type of arguments)
- Solution is **modules**

Modules

- Modules are their own scope
 - Names in one `module` do not clash with names in another
 - Similar to *namespaces* in other languages
- Compiler gets access to same information about procedures as if they were inside the `program`
- Always, **always** use `modules` when using multiple files
- `modules` can also contain variables as well as procedures
 - Try to avoid though, except for `parameters`
- Can choose what entities in a `module` to make `public` or `private`
 - `module` is a bit like a single instance of an object

Modules

- Syntax looks very similar to `program`:

```
module <name>
  implicit none
  ! variables, types, parameters
contains
  ! functions, subroutines
end module <name>
```

- Just like `programs`, `implicit none` applies to the whole `module`

Modules

- But note that `module` body before `contains` cannot include executable statements!

```
module badbad
  implicit none
  print*, "This won't compile!"
end module badbad
```

Using modules

- Using a `module` is simple:

```
program track_particles
  use particle_properties
  implicit none
```

- This makes everything in `particle_properties` available to the whole `program`
 - Equivalent to `from particle_properties import *` in Python
- Only one module per `use`:

```
program track_particles
  use file_utilities
  use particle_properties
  use physical_constants
  implicit none
```

Using modules

- Usually better practice to `use modules` only in the particular functions that need them
- We can also just `use` certain things from a `module`:

```
subroutine push_particle
```

```
  use particle_properties, only : kinetic_energy, coulomb_force  
  use physical_parameters, only : electron_mass, electron_charge
```

- These can be either variables or procedures
- This is great!
 - More obvious where things come from
 - Doesn't bring in unneeded names
 - Can even rename things if they clash locally

```
subroutine push_particle
```

```
  use physical_parameters, only : c => speed_of_light
```

- Note: `use` statements must come before `implicit none`

Module visibility

- Plain `use <module>` brings in **everything** from `<module>` to the local scope
 - This is called *use association*
- Sometimes we want to have some variable or procedure that is used “internally” to a module, and don’t want to be able to access it from outside that module
- We can use `public` and `private` statements and attributes to control which names are available to be `used`
- `private` entities (i.e. variables or functions) won’t be visible outside the module
- `private/public` statement by itself marks the default visibility
- By default, `public` is assumed
- Then can add either as an attribute to individual entities
- Entities `used` from other modules can also have visibility attributes applies to them

Module visibility syntax

- As an attribute on a variable:

```
<type>, <visibility-spec> {, <other-attributes>} :: <variable>
```

! For example:

```
integer, dimension(2, 2), parameter, private :: internal_array = ...
```

- Or a separate visibility specification statement:

```
<visibility-spec> :: <entity>
```

! For example:

```
public :: some_public_thing
```

Module visibility

```
1 module particle_properties
2   use, intrinsic :: iso_fortran_env, only : real64
3   use physical_constants, only : proton_mass, speed_of_light
4   implicit none
5   private ! Marks all entities as private by default
6   ! Public attribute on a variable
7   real(real64), parameter, public :: deuterium_mass = 1.99955249 * proton_m
8   ! Separate attribute for procedure
9   public :: kinetic_energy
10  ! Separate attribute for entity used from another module
11  public :: proton_mass
12 contains
13  function kinetic_energy(mass, velocity)
14    use, intrinsic :: iso_fortran_env, only : real64
```

Compiling modules

- Compiling a `module` results in a `.mod` file as well as the built object file (`.o`)
 - (Actual file extensions may vary)
- This file describes the names in the `module` as well interfaces to the functions, and is similar (though very different!) to a C header file
- Slightly unfortunately, `.mod` files are not portable, even between versions of the same compiler!
 - This is essentially the *Application Binary Interface* (ABI) and is a Hard Problem to maintain backwards compatibility while still adding new features

Compiling modules

- Getting an executable that you can run is (essentially) two step process:
 - *Compile* source code to *object files*
 - *Link* object files to *executable*
- Compiler normally takes care of both compiling and linking for us
- If we tell the compiler about all the files we want to compile and link together in one go, we don't need to do anything special
- Modules are not executable, so if we don't want to compile everything at once, need to tell compiler to stop at the object file stage
- To link the final executable, we then need to tell the linker about all the object (`.o`) and module (`.mod`) files

Compiling modules

- For `gfortran`, use the `-c` flag to just compile and not link:

```
# Creates my_module.o and my_module.mod
```

```
$ gfortran -c my_module.f90
```

```
# Just creates my_program.o
```

```
$ gfortran -c my_program.f90
```

- To link, we can use `gfortran` again:

```
# Link together the object files
```

```
$ gfortran my_module.o my_program.o -o my_program
```

- Note that `gfortran` looks in the current directory for the `.mod` files
 - Don't need to explicitly list the `.mod` files
- Can use `-I<directory>` to tell `gfortran` to look somewhere else

Modules in practice

- Cannot have circular dependencies
 - `module_A` uses `module_B` which uses `module_A`
 - This won't work!
 - Ways round it using `submodules`: not covered here!
- Some trickiness: there is now an order in which you have to compile files:
 - If `module_A` uses `module_B` which uses `module_C`, then:
 - need to compile `module_C` then `module_B` then `module_A`
- Can do it manually, but quickly gets out of hand
- Some compilers can sort this out (but need two passes)
- There are tools available, e.g. `fortdepend`
- Also build systems such as `CMake` can take care of this for you

Derived types

- Not uncommon to need to call a set of functions with the same few arguments
- Or we may have some variables that we need to keep in sync
- One solution to these problems is a *derived type*
 - Other languages call these *structs* or *classes*
- A derived type contains *components* (or *members*) which can be intrinsic types or other derived types
- Fortran does have the ability to do some *object-oriented programming*
 - Will only cover a little bit here

FIXME

Derived types – basic syntax

```
type :: <name>  
    <type> :: <component name>  
    ...  
end type <name>
```

Use like

```
type(<name>) :: <variable name>
```

Derived types – example

```
type :: particle
  real(real64) :: mass
  real(real64), dimension(3) :: velocity
end type
```

Accessing components of derived types

- Refer to component with %

```
type(particle) :: proton
```

```
proton%mass = 1._real64
```

```
proton%velocity = [2._real64, -1._real64, 1.5_real64]
```

Derived type inheritance

FIXME

particle with mass, charge, energy

type-bound procedures

- Can associate a procedure with a type
 - But procedure can remain as a *free function*
- Called *methods* in other languages
- Slightly annoying in that definition still needs to be in the `contains` section of the `program` or `module`

FIXME

- example

Private/Public

- Just like `modules` can have declare the visibility of their entities, `types` can specify visibility of their members
- This is very useful if there's some member that needs to be kept in sync with the state of the type
 - e.g. a particle might store its energy, instead of recalculating it every time
 - Or a container might store how many items it holds
- These are called *invariants*
- Can make the invariant `private` and then provide `public` methods to get or set the value
- Visibility is at the `module` scope

FIXME

- example

Optional arguments

- Common to have a function that only sometimes needs a particular argument
- Can make these arguments `optional`
- We've met a few intrinsics with optional arguments
- Need to check that an `optional` argument is `present` before we can use it
 - Except to pass it to other functions
- Require a bit of special handling if we want to give `optional` arguments default values

Optional arguments

```
8  subroutine greet(name, politely)
9      character(len=*), intent(in) :: name
10     logical, intent(in), optional :: politely
11
12     character(len=:), allocatable :: greeting
13
14     greeting = "Hey, "
15
16     if (present(politely)) then
17         if (politely) then
18             greeting = "Good morning, "
19         end if
20     end if
21
22     print*, greeting, name
23 end subroutine greet
```

Optional arguments

```
4  call greet("Peter")
5  call greet("Peter", politely=.true.)
```

Also notice that we need to check if `politely` is `present` before trying to use it at all:

```
16  if (present(politely)) then
17      if (politely) then
```

The following is dangerous, because standard doesn't mandate short-circuiting:

```
if (present(politely) .and. politely) then
...

```

Might try to read `politely` first, but it doesn't exist!

block

- Fortran requires all variables to be declared at the top of the scope, before first executable statement
 - Limitation of early compilers!
- But modern best practice is to declare variables only where you need them
- Reducing scope -> always good!
 - Easier to read
 - Reduces chances for bugs
- `block` construct allows introduction of new entities
- Names within a `block` can *shadow* or hide those outside

block example

```
3  integer :: x = 1
4  print*, x
5
6  block
7      real :: x = 3.142
8      print*, x
9  end block
10
11 print*, x
```

stop and error stop

- Sometimes want to finish a program “early”
 - Maybe some quantity has converged
 - Maybe something’s gone wrong and we can’t continue
- Two statements: `stop` and `error stop`
 - Essentially equivalent, except `error stop` always indicates an error somehow
- Can take an `integer` or `character` constant (i.e. value has to be known exactly at compile time)
 - Relaxed in Fortran 2018!

```
character(len=*), parameter :: converged = "The simulation has converged!"  
...  
stop converged
```

- Unfortunately, the standard is vague on what happens with an integer
- **Usually** is the exit code, if between 0–127
 - Can’t 100% rely on this, but mostly fine

Other useful intrinsics

FIXME

- `call execute_command_line`
- `call cpu_time`
- `call get_command_line`

Interfaces

- Early Fortran standards didn't have `contains` or `modules`
- Functions could be external to the program, e.g. in a library
- Return type for functions was `implicit`, i.e. based on first letter of name
- Type and number of arguments was completely unknown to the compiler
 - Programmer had better get them right!
- Very bug prone!

Missing interface example

External library:

```
1 integer function idouble(x)
2   integer, intent(in) :: x
3   idouble = 2 * x
4 end function idouble
5
6 integer function iadd(a, b, c)
7   integer, intent(in) :: a, b, c
8   iadd = a + b + c
9 end function iadd
```

Program:

```
1 program use_external_function
2   print*, idouble(2.0)
3   print*, iadd(2, 4)
4 end program use_external_function
```

Interfaces

- Fortran 90 introduced `contains`, `modules` and `interfaces`
- Interface is essentially the procedure minus the executable statements
- Procedures in `modules` and `programs` have *interfaces* generated by the compiler
 - Also known as *signatures* or *prototypes*
- The interface allows the compiler to give warnings/errors if arguments are wrong
- Programmers could also write an explicit `interface` block for external procedures themselves
 - Useful for legacy libraries or interoperability with other languages

Interfaces

```
3  interface
4      integer function idouble(x)
5          integer, intent(in) :: x
6      end function idouble
7
8      integer function iadd(a, b, c)
9          integer, intent(in) :: a, b, c
10     end function iadd
11 end interface
12
13 print*, idouble(2)
14 print*, iadd(2, 3, 4)
```

Now compiler knows that `idouble(2.0)` and `iadd(2, 4)` are mistakes!

Passing procedures

- With an interface, we can now pass procedures to other procedures
- Useful for writing e.g. integration routines

Let's take two functions we want to apply:

```
18  integer function double(x)
19      integer, intent(in) :: x
20      double = 2 * x
21  end function double
22
23  integer function add_two(x)
24      integer, intent(in) :: x
25      add_two = x + 2
26  end function add_two
```

Passing procedures

Using an explicit interface in the function:

```
28   integer function apply(f, x)
29       interface
30           integer function f(y)
31               integer, intent(in) :: y
32           end function f
33       end interface
34       integer, intent(in) :: x
35
36       apply = f(x)
37   end function apply
```

And calling the function:

```
10   print*, apply(double, 42)
11   print*, apply(add_two, 6)
```

Passing procedures

- This gets very verbose if we use the same function interface a lot
- Another option is to use an *abstract interface* to name a signature

```
4 abstract interface
5     integer function univariate(x)
6         integer, intent(in) :: x
7     end function univariate
8 end interface
```

- We can then declare our dummy argument to be a **procedure** of this type:

```
39 integer function apply2(f, x)
40     integer, intent(in) :: x
41     procedure(univariate) :: f
42
43     apply2 = f(x)
44 end function apply2
```

Generic interfaces

- Very common to want to have the same function for multiple types, or different sets of arguments
 - Called *overloads* in other languages, but not quite the same in Fortran
- Before Fortran 90, needed to have a different name for each function
 - e.g. `idouble` for `double` function on `integers`, `cdouble` for `complex`
- Only intrinsics could have generic names
- `interface` allows us to “group” functions or subroutines together under a common name
 - Cannot group **both** `functions` and `subroutines` together though!
- Somewhat annoyingly, can only do this for external procedures or those in `modules`, **not** those in `programs`

Generic interfaces

- For external procedures, need to write out explicit interfaces
- Don't need to repeat interface for modules, can just say

```
interface <generic-name>  
  module procedure <specific-name-1>  
  module procedure <specific-name-2>  
end interface <generic-name>
```

- Can use this to define new *constructors* for derived types, or even operators:

```
interface operator(+)  
  module procedure add_my_type  
end interface
```

Generic interfaces

In a module:

```
1  module generic_interfaces
2      implicit none
3
4      interface double
5          module procedure idouble
6          module procedure rdouble
7      end interface double
```

Using it in a program:

```
25  program generic_interfaces_prog
26      use generic_interfaces, only : double
27      implicit none
28      print*, double(2)
29      print*, double(2.0)
30  end program generic_interfaces_prog
```

Generic interfaces

- There are some rules about what can be put in a generic interface
- Mostly, the dummy arguments must be *distinguishable*:
 - Different number of arguments
 - Different types
 - Different kinds
 - Different ranks
 - `allocatable`/`pointer`
 - Procedure vs variable
- Gets a little tricky if names **and** types clash

Bad old stuff

FIXME

- `common` blocks
- `goto`
- `do; do; 10 continue`

Documentation

- Documentation is a vital but dull part of programming
- Everybody hates trying to use undocumented code
 - Even worse trying to modify someone else's!
- Comments can be used to document the code inline
- Good practice to put a comment above procedures to explain what it does and **how**
- Comments on tricky bits of code to explain **why**
- Various tools, e.g. Ford: <https://github.com/Fortran-FOSS-Programmers/ford>
- Usually special comment syntax for bits you want Ford to recognise, e.g. **!!**

Ford documentation example

```
!! Feeds your cats and dogs, if enough food is available. If not enough
!! food is available, some of your pets will get angry.
subroutine feed_pets(cats, dogs, food, angry)
    !! The number of cats to keep track of.
    integer, intent(in) :: cats
    !! The number of dogs to keep track of.
    integer, intent(in) :: dogs
    !! The ammount of pet food (in kilograms) which you have on hand.
    real, intent(inout) :: food
    !! The number of pets angry because they weren't fed.
    integer, intent(out) :: angry
    ...
end subroutine feed_pets
```

Further reading

- “Modern Fortran explained”, Metcalf, Reid, Cohen
- Fortran wiki

intrinsic modules

FIXME

Internal procedures

- `functions` and `subroutines` can `contain` other procedures
- Sometimes useful for longer functions with repeated chunks
- However: these internal procedures can use variables from their parent function
 - See above on scope!
- This makes it easier to make mistakes
- Usually better to make a separate procedure
 - Can make it `private` in a `module`