Introduction to Fortran

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Session 1

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?

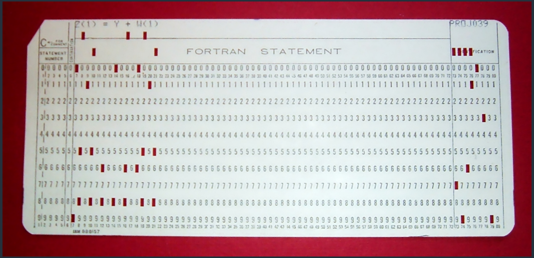
- old language! 1956 – 62 years old
  - oldest "high-level" language
  - many versions over the years, latest is 2018! And next one is being worked on as we speak
- some parts feel outdated
  - backwards compatibility is important
  - but original reasons for some features no longer hold
- but still 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
- Further revisions:
  - Fortran 95
  - Fortran 2003
  - Fortran 2008
  - Fortran 2018

Why Fortran?

- Built for efficient mathematical calculations
- Multidimensional arrays are first-class objects
- 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)

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
- We would much prefer to write in a human language
- Source code is human-readable set of instructions for computer
- 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

Fundamentals

- 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!

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 `!`
- 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

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!
- 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

Cover literals here

FIXME: later

- Writing `real`s:

```
2.
0.3
4.6E4
0.02e-3
```

- Note: `real` literals are single-precision by default
  - more on this later

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
  - Other languages, like Python, we can change our minds
- Variables are declared like:

```
<type> :: <name>
```

- Note: `::` not always needed, but never hurts!
- Note: names must start with a letter, and are limited to ASCII lower/uppercase, numbers and underscore
- 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`

Hello world again

```fortran
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
- Line 6: `read*,`: read a variable from stdin/command line
- Line 9: `&`: line continuation for long lines

What's this `implicit none`?

- Always, always `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 tpyo 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

Whitespace, lines and capitalisation

Some points on Fortran grammar

FIXME

examples

Whitespace

- Mostly doesn't matter

Lines

- Statements must be on a single line unless you use a &, *line continuation*
- Optional to put & at start of next line
- Maximum of 256 lines (i.e. 255 &)

Capitalisation

- Fortran is completely case-insensitive
- Originally didn't have lower-case characters at all!

Initialisation

- Can initialise in the declaration, but WARNING!
- This unfortunately adds extra semantics that you may not intend
    - Will cover when we get onto functions

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*

```
real :: x, y
print*, 3 * 4
print*, 12 / 4
print*, 3.6e-1 + 3.6e0
x = 42.
y = 6.
print*, (x / 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 should 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
    - Don't forget `real` literals are single precision by default!
- `5 / real(2) == 2.5`
- `5. / 2 == 2.5`
- `5._real64 / real(2, kind=real64) == 2.5_real64`

Logical/relational operations

- `<`, `<=`, `>`, `>=`, `==`, `/=`
  - 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.`

Prefer `<` over `.lt.`, etc.!

`/=`, `.ne.` is not equals (part of reason why `a *= b` doesn't exist!)

```fortran
program logical_operators
  implicit none
  integer :: a = 4, b = 5
  print*, a == b
  print*, a < b
  print*, a * b /= a + b
end program logical_operators
```

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

Control flow

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

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

or 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

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 evaluates *both* conditions. may be important later...
- note difference between `.eq.` and `.eqv.`
  - `.eqv.` must be used for `logical`s

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
   ...
end do

do while (<logical-expression>)
   ...
end do

do <index> = <lower-bound>, <upper-bound>
   ...
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, and does the loop *at least once*
- Last form does `<upper-bound> - <lower-bound> + 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!

```fortran
integer :: x = 0
do
  print*, x
  x = x + 1
end do
```

exit

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

```fortran
integer :: x = 0
do
  print*, x
  x = x + 1
  if (x >= 10) exit
end do
```

do while

- Equivalent to using `exit` at start of loop

```
integer :: x = 0
do while(x < 10)
  print*, x
  x = x + 1
end do
```

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

```
integer :: x = 10
do while(x < 10)
  print*, x
  x = x + 1
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*:

```
integer :: i
do i = 0, 9
  print*, i
end do
```

do <counter> = <start>, <stop>, [<stride>]

- There is an optional `stride`:

```
integer :: i
do i = 0, 9, 2
  print*, i
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:

```fortran
integer :: i
do i = 9, 0, -2
  print*, i
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 2

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:

```
real(kind=wp), dimension(3) :: vector
! Could also declare it like so:
! real(kind=wp) :: vector(3)
vector = [1.0_wp, 2.0_wp, -4.0_wp]
```

- Fortran can natively handle multidimensional arrays:

```
real(kind=wp), dimension(3, 3) :: matrix
! or
! real(kind=wp) :: matrix(3, 3)
```

- `matrix` has 3x3 = 9 elements

Arrays

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

```
print*, vector(1)
print*, vector(2)
print*, vector(3)

do i = 1, 3
  print*, vector(1)
end do
```

Arrays

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

```
integer, dimension(-1:1) :: array
```

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

```
real(real64), dimension(-1:1, 3:5) :: stress_tensor
```

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

Arrays

- Can index an entire dimension via a *slice* with `:`

```
real(kind=wp), dimension(3) :: vector
real(kind=wp), dimension(3, 3) :: matrix
vector = [1.0_wp, 2.0_wp, -4.0_wp]
matrix(1, :) = vector
matrix(2, :) = 2.0_wp * vector
matrix(3, :) = 3.0_wp * vector
```

- Note `vector(:)` is the same as `vector`

Array inquiry functions

FIXME

- Later, probably

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

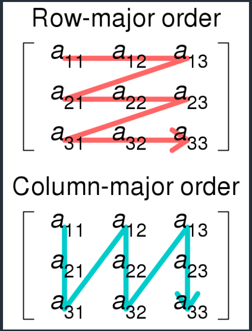
Memory layout

- Maths matrix:

$$
\begin{array}{c c}
 & \begin{array}{cccc} 1 & 2 & \dots & n \end{array} \\
\begin{array}{c} 1 \\ 2 \\ 3 \\ \vdots \\ m \end{array} &
\begin{bmatrix}
a_{11} & a_{12} & \dots & a_{1n} \\
a_{21} & a_{22} & \dots & a_{2n} \\
a_{31} & a_{32} & \dots & a_{3n} \\
\vdots & \vdots & \vdots & \vdots \\
a_{m1} & a_{m2} & \dots & a_{mn}
\end{bmatrix}
\end{array}
$$

Memory layout

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



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
  - Matlab is also column-major

Example

Speed difference

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

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`:

```fortran
program bigarray_prog
  use, intrinsic :: iso_fortran_env, only : real64, int64
  implicit none
  integer(int64), parameter :: bignumber = huge(1) * 2
  real(real64), dimension(:), allocatable ::bigarray
  integer :: stat
  character(len=200) :: errmsg

  allocate(bigarray(bignumber), stat=stat, errmsg=errmsg)

  if (stat /= 0) then
```

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 `parameter`s, intrinsics
- names are great!
- attribute (now we definitely need `::`)
- super useful for things like `pi`, `speed_of_light`, `electron_mass`, etc.

parameter examples

```fortran
program parameters
  use, intrinsic :: iso_fortran_env, only : real64
  implicit none
  integer, parameter :: wp = real64
  real(kind=wp), parameter :: pi = 4._wp*atan(1._wp)
  integer, parameter :: grid_size = 4
  integer, dimension(grid_size), parameter :: x_grid = [1, 2, 3, 4]

  print*, pi
  print*, x_grid
end program parameters
```

Kinds of types

- Most important for `real`s
- Floating point representation
- Doing lots of maths with floating point numbers can lose precision => need more precision in our `real`s
- 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 these:

```fortran
! Get the kind number that can give us 15 digits of precision and 300
! orders of magntitude 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
```

Procedures

- Break programs up into building blocks
- Reusable components
  - Repeat tasks multiple times
  - Use same task in multiple contexts
- Procedures:
  - Functions
  - Subroutines
- Modules
  - Cover later
- Procedures are good:
  - easier to test
  - reuse
  - maintainability
  - abstraction
  - collaboration
- Encapsulation: hide internal details from other parts of the program. Program against the *interface*

Procedures

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

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

Functions

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- Always returns a value
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- syntax:

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

Functions

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

```fortran
function kronecker_delta(i, j) result(delta)
  integer, intent(in) :: i, j
  integer :: delta
  if (i == j) then
    delta = 1
  else
    delta = 0
  end if
end function kronecker_delta
```

Functions

- Functions in `program`s go after a `contains` statement:

```fortran
program basic_function
  implicit none

  print*, kronecker_delta(1, 2)
  print*, kronecker_delta(2, 2)

contains
  function kronecker_delta(i, j) result(delta)
    integer, intent(in) :: i, j
```

- 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 may advise as good practice though

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

- Subroutines are used via the `call` statement:

```
call my_subroutine(argument)
```

Subroutine example

```
subroutine increment_x_by_y(x, y)
  integer, intent(inout) :: x
  integer, intent(in) :: y
  x = x + y
end subroutine increment_x_by_y
```

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 `deallocate`d 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

```fortran
  integer :: x = 4
  print*, add_square(x), x
contains
  function add_square(number) result(res)
    integer, intent(in) :: number
    integer :: res
    integer :: x
    x = number * number
    res = number + x
  end function add_square
```

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

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 `save`s the value of the variable between function calls
- Initialisation is then *not done* on subsequent calls:

```
subroutine increment_count_implicit()
  integer :: count = 0
  count = count + 1
  print*, "Called implicit version", count, "times"
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 `intent`s:
- `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 `function`s over `subroutine`s 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

```fortran
program dummy_arguments
  implicit none
  integer :: x = 1, y = 2
  real :: z = 3.0

  call print_three_variables(x, y, z)
contains
  subroutine print_three_variables(a, b, c)
    integer, intent(in) :: a, b
    real, intent(in) :: c
    print*, "a is ", a, "; b is ", b, "; c is ", c
  end subroutine print_three_variables
end program dummy_arguments
```

- `x` becomes associated with `a`; `y` with `b`; `z` with `c`

dummy arguments and arrays

- Three choices for passing arrays:
- `dimension(n, m, p)`: explicit size
  - Actual argument has to be exactly this size
  - Compiler can only check 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

Keyword arguments

- Another nifty feature of Fortran is keyword arguments:

```
  call print_three_variables(b=y, c=z, a=x)
contains
  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)
```

More on scope

- possible for procedures to access variables in the containing scope
- generally not a great idea

```fortran
  print*, add_square(x), x
contains
  function add_square(number) result(res)
    integer, intent(in) :: number
    integer :: res
    x = number * number
    res = number + x
  end function add_square
```

- this is surprising, despite the `intent(in)`!
- also hard to see where `x` comes from

`case`

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

```
select case (x)
case (1)
  print*, "x is 1"
case (2:4)
  print*, "x is between 2 and 4"
case default
  print*, "x is neither 1 nor between 2 and 4"
end select
```

- The expression in the `select case` must be an `integer`, `logical` or `character` scalar variable
- Ranges must be of same type
- `:upper_bound`

cycle

- skip to next loop iteration

```
integer :: i
do i = 1, 5
  if (i == 3) cycle
  print*, i
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:

```
integer :: i, j
outer: do i = 1, 5
  inner: do j = 1, 5
    if ((i + j) == 9) exit outer
    print*, i, j
```

Session 4

open - File I/O

- Open a file for reading/writing:

```
open(newunit=unit_num, file="filename")
```

- unit_num is integer (that you've already declared)
- compiler will make sure it's unique (and negative)
- newunit is F2008. Older versions:

```
open(unit=unit_num, file="rectangle.shape")
```

- unit_num must already have a value (choose >=10)
- Lots of other arguments:
- status
- action
- iostat

read

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

```
read(unit=unit_num, fmt=*) height, width
```

- `unit_num` must be already `open`ed file
- `unit=*`, `fmt=*` is same as `read(*,*)`

write

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

```
write(unit=unit_num, fmt=*) height, width
```

- `unit_num` must be already `open`ed file
- `unit=*`, `fmt=*` is same as `write(*,*)`

`close`

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

```
close(unit=unit_num)
```

- `unit_num` must be already `open`ed file

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

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

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

modules

- very big programs become difficult to develop and maintain
- becomes useful to split up into separate files
- early versions of Fortran just stuck subprograms into separate files and compiled 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 `module`s
- compiler generates interfaces for you
- *always* use `module`s when using multiple files
- `module`s can also contain variables as well as procedures
  - try to avoid though, except for `parameter`s
- 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, type, parameters

contains

  ! functions, subroutines

end module <name>
```

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

```
module badbad
  implicit none
```

Using modules

- Using a `module` is simple:

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

- or even better, just certain things:

```
subroutine push_particle
  use particle_properties, only : electron_mass
```

- this is great!
  - more obvious where `electron_mass` comes from
  - doesn't bring in extra names
  - can rename things

```
subroutine push_particle
  use particle_properties, only : electron_mass => mass
```

Modules

- Compiling a `module` results in a `.mod` file as well as the built object
- This is essentially an interface file, 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 "Application Binary Interface" (ABI) and is a Hard Problem

Modules in practice

- Cannot have circular dependencies
  - A uses B which uses A
  - This won't work!
  - Ways round it (may cover `submodule`s later)
- Some trickiness: there is now an order in which you have to compile files
- If A uses B which uses C, need to compile C then B then 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

private/public

optional arguments

formatted i/o

good practice

Missed bits

array constructors

elemental functions

namelists

`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

```fortran
integer :: x = 1
print*, x

block
  real :: x = 3.142
  print*, x
end block

print*, x
```

interoperability with C/python

Coarrays

where

C++ course

Session 1

- suggested reading
- history of C/C++
- pros/cons of C++
- computer basics
  - bits and bytes
  - integers and floats
  - how CPU works
- what is programming
- how to write a program
- hello world
  - compiling and running
  -
    - reading
- whitespace + variable names

session 2

- maths operators
- literals
- types
- variables
- integer division/mixed type operations
- floating point maths
- intrinsics
- branching – if/else
- relational operators
- logical operators
- shortcut evaluation
- scope

session 3

- select case
- iteration
  - do/while
  - exit
  - cycle
- file handling

session 4

- functions
  - void/non-void
  - recursive
  - pass-by-value, -ref
    - intent
  - default arguments (optional)
- const and static (parameter and save)
- enums
- arrays
  - multidimensional arrays
- pointers

session 5

- heap and stack
- memory allocation
- i/o formatting

session 6

- preprocessor
- larger projects

session 7

- OOP
  - structs/classes
  - methods
  - accessors
  - const-ness
  - ctors
  - dtors