Introduction to Modern Fortran

Advanced Use Of Procedures

Nick Maclaren

Computing Service

nmm1@cam.ac.uk, ext. 34761

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Summary

We have omitted some important concepts. They are complicated and confusing.

There are a lot of features we have omitted. Mostly because they are hard to use correctly. And sometimes because they are inefficient.

This lecture covers some of the most important concepts.

- Refer to this when you need to.
Association (1)

Fortran uses argument association in calls. Dummy arguments refer to the actual ones.

- You don’t need to know exactly how it is done. It may be aliasing or copy-in/copy-out.

Expressions are stored in a hidden variable. The dummy argument is associated with that.
- It obviously must not be updated in any way.

Using INTENT is strongly recommended.
Association (2)

REAL, DIMENSION(1:10, 1:20, 1:3) :: data
CALL Fred (data(:, 5:15, 2), 1.23*xyz )

SUBROUTINE Fred (array, value)
REAL, DIMENSION(:, :) :: array
REAL, INTENT(IN) :: value

array in fred refers to data(:, 5:15, 2)
value refers to a location containing 1.23*xyz
Updating Arguments (1)

A **dummy argument** must not be updated if:

- The actual argument is an expression
- It **overlaps** another argument in any way

```fortran
REAL, DIMENSION(1:20, 1:3) :: data
CALL Fred (data(5:15, 2), data(17::, 2))

SUBROUTINE Fred (arr1, arr2)
REAL, DIMENSION(:) :: arr1, arr2
arr1 = 1.23 ; arr2 = 4.56
```

- The above works as you expect
Updating Arguments (2)

REAL, DIMENSION(1:20, 1:3) :: data
CALL Fred (data(5:15, 2), data(1:10, 2))

SUBROUTINE Fred (arr1, arr2)
REAL, DIMENSION(:) :: arr1, arr2
arr2(1, 1) = 4.56

• The above is not allowed
Because arr1 and arr2 overlap

Even though arr2(1, 1) is not part of arr1
Updating Arguments (3)

REAL :: X
CALL Fred (X + 0.0)

SUBROUTINE Fred (Y)
Y = 4.56

• The above is not allowed – obviously

• That also applies to array expressions
Vector indexing behaves like an expression
Warning for C/C++ People

REAL, DIMENSION(1:20) :: data
CALL Fred (data(2), data)

SUBROUTINE Fred (var, array)
REAL :: var
REAL, DIMENSION(:) :: array
array = 4.56

• The above is **not** allowed, either

Even **array elements** are **associated**
Using Functions

**Functions** are called just like built-in ones.
They may be **optimised** in similar ways.

```fortran
REAL :: scale, data(1000)
  
  READ *, scale  ! assume that this reads 0.0
  Z = Variance(data)/(scale+Variance(data))
```

**Variance** may be called 0, 1 or 2 times.
Impure Functions

Pure functions have defined behaviour
• Whether they are declared PURE or not

Impure functions occasionally misbehave
Generally, because they are over-optimised

There are rules for safety in practice
But they are too complicated for this course

• Ask if you need help with this
FUNCTION Result Variable

The function name defines the result variable
You can change this if you prefer

FUNCTION Variance_of_an_array (Array) RESULT(var)
    REAL :: var
    REAL, INTENT(IN), DIMENSION(:) :: Array
    var = SUM(Array)/SIZE(Array)
    var = SUM((Array-var)**2)/SIZE(Array)
END FUNCTION Variance_of_an_array

REAL, DIMENSION(1000) :: data
    ...
Z = Variance_of_an_array(data)
PURE Subroutines

You can declare a subroutine to be PURE

Like functions, but with one fewer restriction
INTENT(OUT) and INTENT(INOUT) are allowed

PURE SUBROUTINE Init (array, value)
REAL, DIMENSION(:), INTENT(OUT) :: array
REAL, INTENT(IN) :: value
array = value
END SUBROUTINE Init

They can be declared as ELEMENTAL, too
Recursion

Fortran 90 allowed this for the first time

Recursive procedures must be declared as such

• If you don’t, recursion may cause chaos

\[
\text{RECURSIVE SUBROUTINE Chop (array, value)}
\]

• Avoid it unless you actually need it

• Check all procedures in the recursive loop
OPTIONAL Arguments

• Use **OPTIONAL** for setting **defaults** only
  On entry, check and copy **ALL** args
  Use **ONLY** local copies thereafter
  Now, all variables are well defined when used

• Can do the converse for optional **results**
  Just before returning, check and copy back

• Beyond this should be done only by **experts**
OPTIONAL Example (1)

FUNCTION fred (alf, bert)
REAL :: fred, alf, mybert
REAL, OPTIONAL, INTENT(IN) :: bert
IF (PRESENT(bert)) THEN
    mybert = bert
ELSE
    mybert = 0.0
END IF

Now use mybert in rest of procedure
OPTIONAL Example (2)

SUBROUTINE fred (alf, bert)
REAL :: alf
REAL, OPTIONAL, INTENT(OUT) :: bert
...
IF (PRESENT(bert)) bert = ...
END SUBROUTINE fred
Fortran 2003

Adds potentially useful `VALUE` attribute
See [OldFortran](#) course for information

And the **PROCEDURE** declaration statement
A cleaner and more modern form of `EXTERNAL`
Its usage is not what you would expect, though

And probably more ...
Arrays and CHARACTER

We have over-simplified these so far
No problem, if you use only recommended style

• You need to know more if you go beyond that

• We start by describing what you can do
Including some warnings about efficient use

And then continue with how it actually works
Array Valued Functions

Arrays are **first-class objects** in Fortran
Functions can return array results

- In practice, doing so always needs a **copy**
  However, don’t worry too much about this

Declare the **function** just as for an **argument**
The constraints on the **shape** are similar

- If it is too slow, ask for advice
Example

This is a bit futile, but shows what can be done

```fortran
FUNCTION operate (mat1, mat2, mat3)
  IMPLICIT NONE
  REAL, DIMENSION(:, :), INTENT(IN) :: &
    mat1, mat2, mat3
  REAL, DIMENSION(UBOUND(mat1, 1), &
    UBOUND(mat2, 2)) :: operate
  ! Checking omitted, again
  operate = MATMUL(mat1, mat2) + mat3
END FUNCTION operate
```
Array Functions and Copying

The result need not be copied on return
The interface provides enough information
In practice, don’t bet on it …

Array functions can also fragment memory
Ask if you want to know how and why

• Generally a problem only for HPC
  I.e. when either time or memory are bottlenecks
What Can Be Done

- Just use array functions regardless
  If you don’t have a problem, why worry?

- Time and profile your program
  Tune only code that is a bottleneck

- Rewrite array functions as subroutines
  I.e. turn the result into an argument

- Use ALLOCATABLE results (sic)

- Ask for further advice with tuning
CHARACTER And Copying

In this respect, \texttt{CHARACTER} \equiv \texttt{array}
Most remarks about arrays apply, unchanged

- But it is \textit{only rarely} important

Fortran is \textit{rarely} used for heavy character work
It works fairly well, but it isn’t ideally suited
Most people find it \textit{very} tedious for that

- If you need to, ask for advice
Character Valued Functions (1)

Earlier, we considered just one form
Almost anything more needs a copy
Some compilers will copy even those

• Often, the cost of that does not matter

You are not restricted to just that form
Declare the function just as for an argument
The constraints on the shape are similar

• If it is too slow, ask for advice
Character Valued Functions (2)

The result length can be taken from an argument

FUNCTION reverse_word (word)
   IMPLICIT NONE
   CHARACTER(LEN=*) , INTENT(IN) :: word
   CHARACTER(LEN=LEN(word)) :: reverse_word
   INTEGER :: I , N
   N = LEN(word)
   DO I = 1 , N
      reverse_word(I:I) = word(N+1-I:N+1-I)
   END DO
END FUNCTION reverse_word
Character Valued Functions (3)

This is a bit futile, but shows what can be done
The result length is a non-trivial expression

FUNCTION interleave (text1, count, text2)
  IMPLICIT NONE
  CHARACTER(LEN=*) , INTENT(IN) :: text1 , text2
  INTEGER , INTENT(IN) :: count
  CHARACTER(LEN=LEN(text1)+count+ &
            LEN(text2)) :: interleave
  interleave = text1 // REPEAT(’ ’ , count) // text2
END FUNCTION interleave
Explicit/Assumed Size/Shape (1)

- The good news is that everything works. Can mix assumed and explicit ad lib.

There are some potential performance problems:
- Passing assumed to explicit forces a copy.
- It can be a problem calling some libraries. Especially ones written in old Fortran.
- Write clean code, and see if it is fast enough. If you find that it isn’t, ask for advice.
Explicit/Assumed Size/Shape (2)

This code is not a problem:

SUBROUTINE Weeble (matrix)
   REAL, DIMENSION(:, :) :: matrix
END SUBROUTINE Weeble

SUBROUTINE Burble (space, M, N)
   REAL, DIMENSION(M, N) :: space
   CALL Weeble(space)
END SUBROUTINE Burble

REAL, DIMENSION(100,200) :: work
CALL Burble(work, 100, 200)
Explicit/Assumed Size/Shape (3)

Nor even something as extreme as this:

SUBROUTINE Weeble (matrix)
  REAL, DIMENSION(:, :) :: matrix
END SUBROUTINE Weeble

SUBROUTINE Burble (space, N, J1, K1, J2, K2)
  REAL, DIMENSION(N, *) :: space
  CALL Weeble(space(J1:K1, J2:K2))
END SUBROUTINE Burble

REAL, DIMENSION(100, 200) :: work
CALL Burble(work, 100, 20, 80, 30, 70)
Explicit/Assumed Size/Shape (4)

But this code forces a copy:

SUBROUTINE Bubble (matrix, M, N)
    REAL, DIMENSION(M, N) :: matrix
END SUBROUTINE Bubble

SUBROUTINE Womble (space)
    REAL, DIMENSION(:, :) :: space
    CALL Bubble(space, UBOUND(space, 1), &
                UBOUND(space, 2))
END SUBROUTINE Womble

REAL, DIMENSION(100,200) :: work
CALL Womble(work)
Example – Calling LAPACK

LAPACK is written in Fortran 77
It cannot handle assumed shape arrays
So here is how to call SPOTRF (Cholesky)

SUBROUTINE Chol (matrix, info)
  REAL, DIMENSION(:,:), INTENT(INOUT) :: matrix
  INTEGER, INTENT(INOUT) :: info
  CALL SPOTRF(’L’, UBOUND(matrix, 1), &
             matrix, UBOUND(matrix, 1), info)
END SUBROUTINE Chol

matrix will be copied on call and return
Sequence Association (1)

Have covered assumed shape and char. length
And explicit shape and char. length
but only when the dummy and actual match

• That constraint is not required (nor checked)

You need to know an extra concept to go further
That is called sequence association

• You are recommended to go cautiously here
Don’t do it until you are confident with Fortran
Sequence Association (2)

Explicit shape and assumed size arrays only
If the dummy and actual bounds do not match

Argument is flattened in array element order
And is given a shape by the dummy bounds
Exactly the way the RESHAPE intrinsic works

There are important uses of this technique
• Or you can shoot yourself in the foot
Example

SUBROUTINE operate_1 (vector, N)
  REAL, DIMENSION(N) :: vector
  ...
SUBROUTINE operate_2 (matrix, M, N)
  REAL, DIMENSION(M, N) :: matrix
  ...

REAL, DIMENSION(1000000) :: workspace
  ...
IF (cols = 0) THEN
  CALL operate_1(workspace, rows)
ELSE
  CALL operate_2(workspace, rows, cols)
END IF
Sequence Association (3)

The same holds for explicit length CHARACTER. Everything is concatenated and then reshaped.

Character lengths are like an extra dimension. Naturally, it varies faster than the first index.

One restriction needed to make this work: Assumed shape arrays of CHARACTER need assumed length or matching lengths.
Example

SUBROUTINE operate (fields, N)
    CHARACTER(LEN=8), DIMENSION(10, N) :: fields
END SUBROUTINE operate

CHARACTER(LEN=80), DIMENSION(1000) :: lines

! Read in N lines
CALL operate(lines, N)
Implicit Interfaces (1)

Calling an undeclared procedure is allowed
The actual arguments define the interface

- I strongly recommend not doing this
Mistyped array names often show up as link errors

REAL, DIMENSION(1000) :: lines

... lines(5) = lones(7)

Undefined symbol lones_ in file test.o
Implicit Interfaces (2)

Only Fortran 77 interface features can be used.
The args and result must be exactly right.
Must declare the result type of functions.

\[
\text{REAL, DIMENSION(KIND=dp) :: DDOT} \\
\ldots \\
X = \text{DDOT(array)}
\]

- This is commonly done for external libraries.
  I.e. ones that are written in Fortran 77, C etc.

- Interface modules are a better way.
EXTERNAL

This declares an external procedure name

It’s essential only when passing as argument
I.e. if the procedure name is used but not called

• I recommend it for all undeclared procedures
  More as a form of documentation than anything else

• But explicit interfaces are always better
Example

Here is the **LAPACK** example again

SUBROUTINE Chol (matrix, info)
   REAL, DIMENSION(:,:), INTENT(INOUT) :: matrix
   INTEGER, INTENT(INOUT) :: info
   EXTERNAL :: SPOTRF
   CALL SPOTRF('L', UBOUND(matrix, 1), &
               matrix, UBOUND(matrix, 1), info)
END SUBROUTINE Chol