Introduction to Modern Fortran

Procedures

Nick Maclaren

nmm1@cam.ac.uk

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Sub-Dividing The Problem

- Most programs are thousands of lines
Few people can grasp all the details

- You often use similar code in several places

- You often want to test parts of the code

- Designs often break up naturally into steps

Hence, all sane programmers use procedures

What Fortran Provides

There must be a single main program
There are subroutines and functions
All are collectively called procedures

A subroutine is some out–of–line code
There are very few restrictions on what it can do
It is always called exactly where it is coded

A function's purpose is to return a result
There are some restrictions on what it can do
It is called only when its result is needed

Example – Cholesky (1)

We saw this when considering arrays
It is a very typical, simple subroutine

```
SUBROUTINE CHOLESKY (A)
    IMPLICIT NONE
    INTEGER :: J, N
    REAL :: A(:, :), X
    N = UBOUND(A, 1)
    DO J = 1, N
        . . .
    END DO
END SUBROUTINE CHOLESKY
```

Example – Cholesky (2)

And this is how it is called

```
PROGRAM MAIN
    IMPLICIT NONE
    REAL, DIMENSION(5, 5) :: A = 0.0
    REAL, DIMENSION(5) :: Z
        . . .
    CALL CHOLESKY (A)
        . . .
END PROGRAM MAIN
```

We shall see how to declare it later

Example – Variance

```
FUNCTION Variance (Array)
    IMPLICIT NONE
    REAL :: Variance, X
    REAL, INTENT(IN), DIMENSION(:) :: Array
    X = SUM(Array)/SIZE(Array)
    Variance = SUM((Array-X)**2)/SIZE(Array)
END FUNCTION Variance

    REAL, DIMENSION(1000) :: data
        . . .
    Z = Variance(data)
```

We shall see how to declare it later

Example – Sorting (1)

This was the harness of the selection sort
Replace the actual sorting code by a call

```
PROGRAM sort10
      IMPLICIT NONE
      INTEGER, DIMENSION(1:10) :: nums
      . . .
! --- Sort the numbers into ascending order of magnitude
      CALL SORTIT (nums)
! --- Write out the sorted list
      . . .
END PROGRAM sort10
```

Example – Sorting (2)

```
SUBROUTINE SORTIT (array)
    IMPLICIT NONE
    INTEGER :: temp, array(:), J, K
L1:     DO J = 1, UBOUND(array,1)-1
L2:         DO K = J+1, UBOUND(array,1)
                IF(array(J) > array(K)) THEN
                    temp = array(K)
                    array(K) = array(J)
                    array(J) = temp
                END IF
            END DO L2
        END DO L1
END SUBROUTINE SORTIT
```

CALL Statement

The CALL statement evaluates its arguments
The following is an over–simplified description

- Variables and array sections define memory
- Expressions are stored in a hidden variable

It then transfers control to the subroutine
Passing the locations of the actual arguments

Upon return, the next statement is executed

SUBROUTINE Statement

Declares the procedure and its arguments
These are called dummy arguments in Fortran

The subroutine's interface is defined by:

- The SUBROUTINE statement itself
- The declarations of its dummy arguments
- And anything that those use (see later)

```
SUBROUTINE SORTIT (array)
INTEGER :: [ temp, ] array(:) [ , J, K ]
```

Subroutines With No Arguments

You aren't required to have any arguments
You can omit the parentheses if you prefer
Preferably either do or don't, but you can mix uses

```
SUBROUTINE Joe ( )

SUBROUTINE Joe


CALL Joe ( )

CALL Joe
```

Statement Order

A SUBROUTINE statement starts a subroutine
Any USE statements must come next
Then IMPLICIT NONE
Then the rest of the declarations
Then the executable statements
It ends at an END SUBROUTINE statement

PROGRAM and FUNCTION are similar

There are other rules, but you may ignore them

Dummy Arguments

- Their names exist only in the procedure

They are declared much like local variables

Any actual argument names are irrelevant

Or any other names outside the procedure

- The dummy arguments are associated with the actual arguments

Think of association as a bit like aliasing

Argument Matching

Dummy and actual argument lists must match
The number of arguments must be the same
Each argument must match in type and rank

That can be relaxed in several ways
See under advanced use of procedures

We shall come back to array arguments shortly
Most of the complexities involve them
This is for compatibility with old standards

Functions

Often the required result is a single value
It is easier to write a FUNCTION procedure

E.g. to find the largest of three values:

- Find the largest of the first and second
- Find the largest of that and the third

Yes, I know that the MAX function does this!

The function name defines a local variable

- Its value on return is the result returned

The RETURN statement does not take a value

Example (1)

```
FUNCTION largest_of (first, second, third)
    IMPLICIT NONE
    INTEGER :: largest_of
    INTEGER :: first, second, third
    IF (first > second) THEN
        largest_of = first
    ELSE
        largest_of = second
    END IF
    IF (third > largest_of) largest_of = third
END FUNCTION largest_of
```

Example (2)

```
INTEGER :: trial1, trial2 ,trial3, total, count
total = 0 ;    count = 0
DO
    PRINT *, 'Type three trial values:'
    READ *, trial1, trial2, trial3
    IF (MIN(trial1, trial2, trial3) < 0) EXIT
        count = count + 1
        total = total + &
          largest_of(trial1, trial2, trial3)
END DO
PRINT *, 'Number of trial sets = ', count, &
    ' Total of best of 3 = ',total
```

Functions With No Arguments

You aren't required to have any arguments
You must not omit the parentheses

```
FUNCTION Fred ( )
   INTEGER :: Fred

X = 1.23 * Fred ( )
CALL Alf ( Fred ( ) )
```

In the following, Fred is a procedure argument

```
CALL Alf ( Fred )
```

Internal Procedures (1)

Procedures can contain internal procedures
These can be SUBROUTINEs and FUNCTIONs
The statement order is as follows:

PROGRAM, SUBROUTINE or FUNCTION
    All of the code of the actual procedure
CONTAINS
    Any number of internal procedures
END PROGRAM, SUBROUTINE or FUNCTION

- Internal procedures may not themselves contain internal procedures

Internal Procedures (2)

- Warning: that order takes some getting used to

The procedure can use the internal procedures
And one of them can call any other

Most useful for small, private auxiliary ones
You can include any number of internal procedures

- They are visible only in the outer procedure

Won't clash with the same name elsewhere

Internal Procedures (3)

```
PROGRAM main
    REAL, DIMENSION(10) :: vector
    PRINT *, 'Type 10 values'
    READ *, vector
    PRINT *, 'Variance = ', Variance(vector)
CONTAINS
    FUNCTION Variance (Array)
        REAL :: Variance, X
        REAL, INTENT(IN), DIMENSION(:) :: Array
        X = SUM(Array)/SIZE(Array)
        Variance = SUM((Array-X)**2)/SIZE(Array)
    END FUNCTION Variance
END PROGRAM main
```

Name Inheritance (1)

Everything accessible in the enclosing procedure
can also be used in the internal procedure

This includes all of the local declarations
And anything imported by USE (covered later)

Internal procedures need only a few arguments
Just the things that vary between calls
Everything else can be used directly

Name Inheritance (2)

A local name takes precedence

```
PROGRAM main
    REAL :: temp = 1.23
    CALL pete (4.56)
CONTAINS
    SUBROUTINE pete (temp)
        PRINT *, temp
    END SUBROUTINE pete
END PROGRAM main
```

Will print 4.56, not 1.23
Avoid doing this – it's very confusing

Using Procedures

Use this technique for solving test problems

- It is one of the best techniques for real code

There is another, equally good one, under modules

And there are yet others that you may need to use

INTENT (1)

You can make arguments read−only

```
SUBROUTINE Summarise (array, size)
    INTEGER, INTENT(IN) :: size
    REAL, DIMENSION(size) :: array
```

That will prevent you writing to it by accident
Or calling another procedure that does that
It may also help the compiler to optimise

- Strongly recommended for read−only args

INTENT (2)

You can also make them write–only
Less useful, but still very worthwhile

```
SUBROUTINE Init (array, value)
    IMPLICIT NONE
    REAL, DIMENSION(:), INTENT(OUT) :: array
    REAL, INTENT(IN) :: value
    array = value
END SUBROUTINE Init
```

As useful for optimisation as INTENT(IN)

INTENT (3)

The default is effectively INTENT(INOUT)

- But specifying INTENT(INOUT) is useful

It will trap the following nasty error

```
SUBROUTINE Munge (value)
    REAL, INTENT(INOUT) :: value
    value = 100.0*value
    PRINT *, value
END SUBROUTINE Munge

CALL Munge(1.23)
```

Example

```
SUBROUTINE expsum(n, k, x, sum)
    IMPLICIT NONE
    INTEGER, INTENT(IN) :: n
    REAL, INTENT(IN) :: k, x
    REAL, INTENT(OUT) :: sum
    INTEGER :: i
    sum = 0.0
    DO i = 1, n
        sum = sum + exp(-i*k*x)
    END DO
END SUBROUTINE expsum
```

Aliasing

Two arguments may overlap only if read–only
Also applies to arguments and global data

- If either is updated, weird things happen

Fortran doesn't have any way to trap that
Nor do any other current languages – sorry

Use of INTENT(IN) will stop it in many cases

- Be careful when using array arguments

Including using array elements as arguments

PURE Functions

You can declare a function to be PURE

All data arguments must specify INTENT(IN)
It must not modify any global data
It must not do I/O (except with internal files)
It must call only PURE procedures
Some restrictions on more advanced features

Generally overkill – but good practice
Most built–in procedures are PURE

Example

This is the cleanest way to define a function

```
PURE FUNCTION Variance (Array)
    IMPLICIT NONE
    REAL :: Variance, X
    REAL, INTENT(IN), DIMENSION(:) :: Array
    X = SUM(Array)/SIZE(Array)
    Variance = SUM((Array-X)**2)/SIZE(Array)
END FUNCTION Variance
```

Most safety, and best possible optimisation

ELEMENTAL Functions

Functions can be declared as ELEMENTAL
Like PURE, but arguments must be scalar

You can use them on arrays and in WHERE
They apply to each element, like built–in SIN

```
ELEMENTAL FUNCTION Scale (arg1, arg2)
    REAL, INTENT(IN) :: arg1, arg2
    Scale = arg1/sqrt(arg1**2+arg2**2)
END FUNCTION Scale

REAL, DIMENSION(100) :: arr1, arr2, array
array = Scale(arr1, arr2)
```

Keyword Arguments (1)

```
SUBROUTINE AXIS (X0, Y0, Length, Min, Max, Intervals)
     REAL, INTENT(IN) :: X0, Y0, Length, Min, Max
     INTEGER, INTENT(IN) :: Intervals
 END SUBROUTINE AXIS

 CALL AXIS(0.0, 0.0, 100.0, 0.1, 1.0, 10)
```

- Error prone to write and unclear to read

And it can be a lot worse than that!

Keyword Arguments (2)

Dummy arg. names can be used as keywords
You don't have to remember their order

```
SUBROUTINE AXIS (X0, Y0, Length, Min, Max, Intervals)
    . . .

CALL AXIS(Intervals=10, Length=100.0, &
     Min=0.1, Max=1.0, X0=0.0, Y0=0.0)
```

- The argument order now doesn't matter

The keywords identify the dummy arguments

Keyword Arguments (3)

Keywords arguments can follow positional
The following is allowed

```
SUBROUTINE AXIS (X0, Y0, Length, Min, Max, Intervals)
    . . .

CALL AXIS(0.0, 0.0, Intervals=10, Length=100.0, &
     Min=0.1, Max=1.0)
```

- Remember that the best code is the clearest

Use whichever convention feels most natural

Keyword Reminder

Keywords are not names in the calling procedure
They are used only to map to dummy arguments
The following works, but is somewhat confusing

```
SUBROUTINE Nuts (X, Y, Z)
    REAL, DIMENSION(:) :: X
    INTEGER :: Y, Z
END SUBROUTINE Nuts

INTEGER :: X
REAL, DIMENSION(100) :: Y, Z
CALL Nuts (Y=X, Z=1, X=Y)
```

Hiatus

That is most of the basics of procedures
Except for arrays and CHARACTER

Now might be a good time to do some examples
The first few questions cover the material so far

Assumed Shape Arrays (1)

- The best way to declare array arguments
You must declare procedures as above

- Specify all bounds as simply a colon (':')
The rank must match the actual argument
The lower bounds default to one (1)
The upper bounds are taken from the extents

```
REAL, DIMENSION(:) :: vector
REAL, DIMENSION(:, :) :: matrix
REAL, DIMENSION(:, :, :) :: tensor
```

Example

```
SUBROUTINE Peculiar (vector, matrix)
    REAL, DIMENSION(:), INTENT(INOUT) :: vector
     REAL, DIMENSION(:, :), INTENT(IN) :: matrix
     . . .
END SUBROUTINE Peculiar

REAL, DIMENSION(20:1000), :: one
REAL, DIMENSION(−5:100, −5:100) :: two
CALL Peculiar (one(101:160), two(21:, 26:75) )
```

vector will be DIMENSION(1:60)
matrix will be DIMENSION(1:80, 1:50)

Assumed Shape Arrays (2)

Query functions were described earlier

SIZE, SHAPE, LBOUND and UBOUND

So you can write completely generic procedures

```
SUBROUTINE Init (matrix, scale)
    REAL, DIMENSION(:, :), INTENT(OUT) :: matrix
    INTEGER, INTENT(IN) :: scale
    DO N = 1, UBOUND(matrix,2)
        DO M = 1, UBOUND(matrix,1)
            matrix(M, N) = scale*M + N
        END DO
    END DO
END SUBROUTINE Init
```

Cholesky Decomposition

```
SUBROUTINE CHOLESKY(A)
    IMPLICIT NONE
    INTEGER :: J, N
    REAL, INTENT(INOUT) :: A(:, :), X
    N = UBOUND(A, 1)
    IF (N < 1 .OR. UBOUND(A, 2) /= N)
      CALL Error("Invalid array passed to CHOLESKY")
    DO J = 1, N
          . . .
  END DO
END SUBROUTINE CHOLESKY
```

Now I have added appropriate checking

Setting Lower Bounds

Even when using assumed shape arrays
you can set any lower bounds you want

- You do that in the called procedure

```
SUBROUTINE Orrible (vector, matrix, n)
    REAL, DIMENSION(2*n+1:) :: vector
    REAL, DIMENSION(0:, 0:) :: matrix
    . . .
END SUBROUTINE Orrible
```

Warning

Argument overlap will not be detected
Not even for assumed shape arrays

- A common cause of obscure errors

No other language does much better

Explicit Array Bounds

In procedures, they are more flexible
Any reasonable integer expression is allowed

Essentially, you can use any ordinary formula
Using only constants and integer variables
Few programmers will ever hit the restrictions

The most common use is for workspace
But it applies to all array declarations

Automatic Arrays (1)

Local arrays with run–time bounds are called
automatic arrays

Bounds may be taken from an argument
Or a constant or variable in a module

```
SUBROUTINE aardvark (size)
USE sizemod    ! This defines worksize
INTEGER, INTENT(IN) :: size

REAL, DIMENSION(1:worksize) :: array_1
REAL, DIMENSION(1:size*(size+1)) :: array_2
```

Automatic Arrays (2)

Another very common use is a ‘shadow’ array
i.e. one the same shape as an argument

```
SUBROUTINE pard (matrix)
REAL, DIMENSION(:, :) :: matrix

REAL, DIMENSION(UBOUND(matrix, 1), &
        UBOUND(matrix, 2)) :: &
    matrix_2, matrix_3
```

And so on – automatic arrays are very flexible

Explicit Shape Array Args (1)

We cover these because of their importance
They were the only mechanism in Fortran 77

- But, generally, they should be avoided

In this form, all bounds are explicit
They are declared just like automatic arrays
The dummy should match the actual argument
Making an error will usually cause chaos

- Only the very simplest uses are covered

There are more details in the extra slides

Explicit Shape Array Args (2)

You can use constants

```
SUBROUTINE Orace (matrix, array)
    INTEGER, PARAMETER :: M = 5, N = 10
    REAL, DIMENSION(1:M, 1:N) :: matrix
    REAL, DIMENSION(1000) :: array
    . . .
END SUBROUTINE Orace

INTEGER, PARAMETER :: M = 5, N = 10
REAL, DIMENSION(1:M, 1:N) :: table
REAL, DIMENSION(1000) :: workspace
CALL Orace(table, workspace)
```

Explicit Shape Array Args (3)

It is common to pass the bounds as arguments

```
SUBROUTINE Weeble (matrix, m, n)
    INTEGER, INTENT(IN) :: m, n
    REAL, DIMENSION(1:m, 1:n) :: matrix
    . . .
END SUBROUTINE Weeble
```

You can use expressions, of course

- But it is not really recommended

Purely on the grounds of human confusion

Explicit Shape Array Args (4)

You can define the bounds in a module
Either as a constant or in a variable

```
SUBROUTINE Wobble (matrix)
    USE sizemod    ! This defines m and n
    REAL, DIMENSION(1:m, 1:n) :: matrix
    . . .
END SUBROUTINE Weeble
```

- The same remarks about expressions apply

Assumed Size Array Args

The last upper bound can be *

I.e. unknown, but assumed to be large enough

```
SUBROUTINE Weeble (matrix, n)
    REAL, DIMENSION(n, *) :: matrix
    . . .
END SUBROUTINE Weeble
```

- You will see this, but generally avoid it

It makes it very hard to locate bounds errors

It also implies several restrictions

Warnings

The size of the dummy array must not exceed
the size of the actual array argument

- Compilers will rarely detect this error

There are also some performance problems when
passing assumed shape and array sections
to explicit shape or assumed size dummies

That is in the advanced slides on procedures
Sorry – but it's complicated to explain

Example (1)

We have a subroutine with an interface like:

```
SUBROUTINE Normalise (array, size)
INTEGER, INTENT(IN) :: size
REAL, DIMENSION(size) :: array
```

The following calls are correct:

```
REAL, DIMENSION(1:10) :: data

CALL Normalise (data, 10)
CALL Normalise (data(2:5), SIZE(data(2:5)))
CALL Normalise (data, 7)
```

Example (2)

```
SUBROUTINE Normalise (array, size)
INTEGER, INTENT(IN) :: size
REAL, DIMENSION(size) :: array
```

The following calls are not correct:

```
INTEGER, DIMENSION(1:10) :: indices
REAL :: var, data(10)

CALL Normalise (indices, 10)    ! wrong base type
CALL Normalise (var, 1)    ! not an array
CALL Normalise (data, 10.0)    ! wrong type
CALL Normalise (data, 20)    ! dummy array too big
```

Character Arguments

Few scientists do anything very fancy with these
See the advanced foils for anything like that

People often use a constant length
You can specify this as a digit string

Or define it using PARAMETER
That is best done in a module

Or define it as an assumed length argument

Explicit Length Character (1)

The dummy should match the actual argument
You are likely to get confused if it doesn't

```
SUBROUTINE sorter (list)
    CHARACTER(LEN=8), DIMENSION(:) :: list
    . . .
END SUBROUTINE sorter

CHARACTER(LEN=8) :: data(1000)
. . .
CALL sorter(data)
```

Explicit Length Character (2)

```
MODULE Constants
    INTEGER, PARAMETER :: charlen = 8
END MODULE Constants

SUBROUTINE sorter (list)
    USE Constants
  CHARACTER(LEN=charlen), DIMENSION(:) :: list
    . . .
END SUBROUTINE sorter

USE Constants
CHARACTER(LEN=charlen) :: data(1000)
CALL sorter(data)
```

Assumed Length CHARACTER

A CHARACTER length can be assumed
The length is taken from the actual argument

You use an asterisk (*) for the length
It acts very like an assumed shape array

Note that it is a property of the type
It is independent of any array dimensions

Example (1)

```
FUNCTION is_palindrome (word)
    LOGICAL :: is_palindrome
    CHARACTER(LEN=*), INTENT(IN) :: word
    INTEGER :: N, I
    is_palindrome = .False.
    N = LEN(word)
 comp: DO I = 1, (N-1)/2
        IF (word(I:I) /= word(N+1-I:N+1-I)) THEN
            RETURN
        END IF
    END DO comp
    is_palindrome = .True.
END FUNCTION is_palindrome
```

Example (2)

Such arguments do not have to be read–only

```
SUBROUTINE reverse_word (word)
    CHARACTER(LEN=*), INTENT(INOUT) :: word
    CHARACTER(LEN=1) :: c
    N = LEN(word)
    DO I = 1, (N-1)/2
        c = word(I:I)
        word(I:I) = word(N+1-I:N+1-I)
        word(N+1-I:N+1-I) = c
    END DO
END SUBROUTINE reverse_word
```

Character Workspace

The rules are very similar to those for arrays
The length can be an almost arbitrary expression
But it usually just shadows an argument

```
SUBROUTINE sort_words (words)
    CHARACTER(LEN=*) :: words(:)
    CHARACTER(LEN=LEN(words)) :: temp
    . . .
END SUBROUTINE sort_words
```

Character Valued Functions

Functions can return CHARACTER values
Fixed–length ones are the simplest

```
FUNCTION truth (value)
    IMPLICIT NONE
    CHARACTER(LEN=8) :: truth
    LOGICAL, INTENT(IN) :: value
    IF (value) THEN
        truth = '.True.'
    ELSE
        truth = '.False.'
    END IF
END FUNCTION truth
```

Example

```
SUBROUTINE diagnose (message, value)
    CHARACTER(LEN=*), INTENT(IN) :: message
    REAL :: value
    PRINT *, message, value
END SUBROUTINE diagnose
```

```
CALL diagnose("Horrible failure",determinant)
```

Static Data

Sometimes you need to store values locally
Use a value in the next call of the procedure

- You do this with the SAVE attribute

Initialised variables get that automatically
It is good practice to specify it anyway

The best style avoids most such use
It can cause trouble with parallel programming
But it works, and lots of programs rely on it

Example

This is a futile example, but shows the feature

```
SUBROUTINE Factorial (result)
    IMPLICIT NONE
    REAL, INTENT(OUT) :: result
    REAL, SAVE :: mult = 1.0, value = 1.0
    mult = mult+1.0
    value = value*mult
    result = value
END SUBROUTINE Factorial
```

Warning

Omitting SAVE will usually appear to work
But even a new compiler version may break it
As will increasing the level of optimisation

- Decide which variables need it during design

- Always use SAVE if you want it
And preferably never when you don't!

- Never assume it without specifying it

Warning for C/C++ Users

Initialisation without SAVE initialises once
It does NOT reinitialise each time it is called

- It can't be done using Fortran initialisation

Do it using an explicit assignment statement

Delayed Until Modules

Sometimes you need to share global data
It's trivial, and can be done very cleanly

Procedures can be passed as arguments
This is a very important facility for some people
For historical reasons, this is a bit messy

- However, internal procedures can't be

They can be in Fortran 2008 – i.e. shortly

We will cover both of these under modules
It just happens to be simplest that way!

Other Features

There is a lot that we haven't covered
We will return to some of it later

- The above covers the absolute basics
Plus some other features you need to know

- Be a bit cautious when using other features
Some have been omitted because of "gotchas"

- And I have over–simplified a few areas

Extra Slides

Topics in the advanced slides on procedures

- Argument association and updating
- The semantics of function calls
- Optional arguments
- Array– and character–valued functions
- Mixing explicit and assumed shape arrays
- Array arguments and sequence association
- Miscellaneous other points

Omissions

Rather a lot has been omitted here, unfortunately
It's there in the notes, if you are interested

If you think that Fortran can't do it, look deeper
Sorry about that, but this had to be simplified