Introduction to Modern Fortran

Advanced Array Concepts

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Summary

This will describe some advanced array features
Use them only when you need their facilities

It will also cover some aspects of array use
Important for correctness and performance

There is a lot more on both
- Please ask if you need any help
Higher Rank Constructors

Constructors create only rank one arrays.
We shall now see how to construct higher ranks.

It is done by constructing a rank one array
And then mapped using the RESHAPE function.

This is very easy, but looks a bit messy.
The RESHAPE Intrinsic (1)

This allows arbitrary restructuring of arrays
The following is only its very simplest use

RESHAPE (source, shape)

source provides the data in array element order
shape specifies the shape of array to deliver
The RESHAPE Intrinsic (2)

REAL, DIMENSION(3, 4) :: array

array = RESHAPE( (/ 1.1, 2.1, 3.1, 1.2, 2.2, &
   3.2, 1.3, 2.3, 3.3, 1.4, 2.4, 3.4 /), (/ 3, 4 /) )

Is functionally equivalent to:

DO m = 1, 3
   DO n = 1, 4
      array(m, n) = m+0.1*n
   END DO
END DO
The RESHAPE Intrinsic (3)

It can be used in initialisation expressions

```
REAL, DIMENSION(3, 4) :: array = &
RESHAPE( (/ 1.1, 2.1, 3.1, 1.2, 2.2, &
 3.2, 1.3, 2.3, 3.3, 1.4, 2.4, 3.4 /), (/ 3, 4 /))
```

It also allows arbitrary reordering
And padding with copies of an array

See the references for more details
Example

Create the zero vector, and the three unit vectors

\[
\text{REAL, DIMENSION(1:3), PARAMETER :: } & \\
\text{vec\_0 = (/ 0.0, 0.0, 0.0 /), } & \\
\text{vec\_i = (/ 1.0, 0.0, 0.0 /), } & \\
\text{vec\_j = (/ 0.0, 1.0, 0.0 /), } & \\
\text{vec\_k = (/ 0.0, 0.0, 1.0 /)}
\]

Create the identity matrix

\[
\text{REAL, DIMENSION(1:3, 1:3), PARAMETER :: } & \\
\text{identity = RESHAPE( (/ vec\_i, vec\_j, vec\_k /), (/ 3, 3 /) )}
\]
RESHAPE More Generally

It isn’t restricted to multi-dim. constants
You can use it for fancy array restructuring

• Study the specification before doing that
Restructuring arrays is dangerous territory

• And there are several other such intrinsics
I.e. ones with important uses but no simple uses
Vector Indexing (1)

Vectors may be used as indices

INTEGER, DIMENSION(1:5) :: &
    j = (/ 3, 1, 5, 2, 4 /), k = (/ 2, 3, 2, 1, 3 /)
REAL, DIMENSION(1:5) :: x, &
    y = (/ 1.2, 2.3, 3.4, 4.5, 5.6 /)
x(j) = y(k)
PRINT *, y(k)
PRINT *, x

2.3000000  3.4000001  2.3000000  1.2000000  3.4000001
3.4000001  1.2000000  2.3000000  3.4000001  2.3000000
Vector Indexing (2)

Using vector indices is a bit like sections. There are important differences – be careful.

You can them for reading arrays quite safely. Elements must be distinct if updating.

- NOT recommended for use in arguments. If used in arguments, those must not be updated. And it forces the compiler to copy the array.
Masked Assignment (1)

Set all negative values in an array A to zero

REAL, DIMENSION(20, 30) :: array

DO j = 1,30
    DO k = 1,20
        IF (array(k,j) < 0.0) array(k,j) = 0.0
    END DO
END DO

But the WHERE statement is more convenient

WHERE (array < 0.0) array = 0.0
Masked Assignment (2)

It has a **statement construct** form, too

```fortran
WHERE (array < 0.0)
  array = 0.0
ELSE WHERE
  array = 0.01*array
END WHERE
```

**Masking expressions** are **LOGICAL** arrays
You can use an actual array there, if you want
Masks and assignments need the same **shape**
Masked Assignment (3)

Fortran 2003 extends it considerably

Don’t use LHS arrays in non-elemental functions
The following is asking for trouble:

WHERE (arr1 < arr2)
  arr1 = 1.0
ELSE WHERE
  arr2 = sum(arr1)
END WHERE

• Don’t bother with the FORALL statement
Memory Efficiency (1)

Local arrays can be implemented in many ways. Only a few Ada compilers handle them properly.

You can exhaust your program’s stack with them. Too big, or too many due to deep recursion.
- It will usually cause a truly horrible crash.

Allocatable arrays always go on the ‘heap’. Automatic arrays often go on the ‘heap’. That is less efficient, but is handled much better.

- Making all big arrays allocatable isn’t stupid.
Memory Efficiency (2)

As always, every solution has its own problems
Lots of allocation and deallocation isn’t ideal

- Each (de)allocation costs some CPU time
  Not generally a problem for Fortran programs

- Poor compilers may have memory leaks
  Most Fortran compilers don’t have them badly

Both because of the language’s restrictions
Memory Efficiency (3)

• The big problem is memory fragmentation. Describing how and why is beyond this course. Luckily, in AD 2007, there is a simple solution.

• Best one is to use 64-bit addressing. Gets rid of the worst of the problems, painlessly. I do that, even on systems with 2 GB of memory.

• Please ask if you want to know more.
Order of Evaluation (1)

Array assignments etc. are like implicit loops. But, except in I/O, no order of evaluation implied. Also the behaviour is different when modifying:

- Each pass of a loop is executed in order.
- Array assignments do it all “in parallel”.

- You should avoid code where it matters. The compiler may have to copy the array. It risks confusion when tuning your code.
Order of Evaluation (2)

INTEGER, DIMENSION(5) :: array = (/ 1, 2, 3, 4, 5 /)
array(2:5) = array(1:4)
PRINT *, array
array = (/ 1, 2, 3, 4, 5 /)
DO k = 1, 4
    array(k+1) = array(k)
END DO
PRINT *, array

1 1 2 3 4
1 1 1 1 1
Performance (1)

- Efficient use of arrays is critical
  This course has **NOT** taught any of that
  It covers quite enough without adding it!

- **Generally,** follow this procedure:

  Start by writing **clean and clear** code
  Get it working, and test it fairly thoroughly
  If too slow, use a **profiler** to see where
  And only then tune **only those** aspects
You get **most gain** by using **faster methods**
Followed by the following aspects:

- Improve the **layout** and **access patterns**
  This is **locality** (improved cache usage etc.)

- Avoid unnecessary **array copying**
  Compilers often have to do that for some codes
  Some compilers copy when they **don’t** need to

- Improve the actual **CPU efficiency**
  This is getting into advanced tuning
Memory Locality (1)

Things *used together* should be *stored together*
Remember that “*first index varies fastest*”

REAL, DIMENSION(3000, 5000) :: array
DO n = 1, 5000
  DO m = 1, 3000
    array(m, n) = m+0.1*n
  END DO
END DO

- Note that the first index varies fastest
Memory Locality (2)

Sections and masking can cause trouble

```fortran
REAL, DIMENSION(1000, 1000) :: array
CALL FRED(array(123, :))
```

The elements of the vector are a long way apart
A problem if FRED accesses it a lot

- Consider making a temporary copy of it
Access Patterns

- **Sequential access** is generally efficient. Avoid non-sequential access wherever possible.

- This can be much slower than sequential.

```fortran
REAL, DIMENSION(1000) :: arr1, arr2
INTEGER, DIMENSION(1000) :: random
arr1(random) = arr2(random)
```
Unnecessary Copying (1)

It is hard to describe when this may occur
It helps if you can mentally compile the code

- Avoiding using the LHS array on the RHS
  Except when the uses are purely elemental

- Generally, sections do not need a copy
  Unlike arguments with vector indexed arrays

- Compilers often do unnecessary copying
  In a very bad case, even for CALL Fred(data(:))
Example

INTEGER :: arr1(1:50), arr2(1:100), arr3(1:100)
REAL, DIMENSION(20, 20) :: mat1, mat2, mat3

These shouldn’t require a copy

\[
\begin{align*}
arr1 &= arr1 + arr2(1:50) + arr3(arr2(51:100)) \\
mat1 &= \text{MATMUL}(mat2, \text{mat3})
\end{align*}
\]

But these almost certainly will

\[
\begin{align*}
arr1 &= arr1(:,:, -1) + arr2(1:50) \\
mat1 &= \text{MATMUL}(\text{mat1}, \text{mat2})
\end{align*}
\]
Unnecessary Copying (2)

And, while this shouldn’t, ...

\[
mat1 = mat1 + \text{MATMUL}(mat2, mat3)
\]

There is more on this under procedures

- Generally, don’t worry unless you have to
  If your program runs fast enough, who cares?

- If not, time and profile it first
  Ask for advice if you have problems
High-Performance Problems

There are some other problems some people hit
Too complicated to even describe here

- Ignore them until you have problems
Then ask for help with tackling them

Buzzwords and phrases include:
  - TLB thrashing
  - Cache conflicts
  - False sharing
  - Memory banking
Reminder

- You don’t have to remember all of this
- Start by using the simplest features only
- Use the fancy ones only when you need them
  If you know they exist, you can look them up