Fortran - Arrays

Arrays, Multidimensional Array, Dynamic Arrays

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a definition

a data structure, the array, which stores a fixed-size sequential collection of elements of the same type. An array is used to store a collection of data, but it is often more useful to think of an array as a collection of variables of the same type.



An example

```
program array1
implicit none
integer :: i
real, dimension(5) :: A = (/ 1, 2, 3, 4, 5 /)

do i=1,5
    print *, A(i)
end do
end program array1
```

What's different from C/C++?

- index starts at 1
- () 's instead of [] 's
- explicit declarations require '/' at the beginning and end of the series



Reading and writing

```
program array2
implicit none
integer :: i, n=5
real, dimension(n) :: A

do i=1,5
   A(i) = i*i
end do

do i=1,5
   print *, A(i)
end do

print *, A
end program array2
```

What's different from C/C++?

- index starts at 1
- () 's instead of [] 's
- explicit declarations require '/' at the beginning and end of the series
- you can reference an array by the array variable.
- size of an array can be a parameter



Exercise 1.

Write a program that creates an array of 100 random numbers between 0 and 100 Run the following code, modify it so it meets the exercise criteria

```
// this code generates an array of 100 random numbers
program test_random_number
implicit none
real, dimension(100) :: r
    call random_number(r)
    print *, r
end program
```



As an argument to a Function

```
program with fct
                                            real function average(n, x)
                                            integer :: n, i
implicit none
                                            real, dimension(n) :: x
integer, parameter :: n = 10
                                            real
                                                              :: sum
real, dimension (n) :: a
                                            sum = 0.
! Calculate Average
aver = average(n, a) ! Function
                                            do i=1, n
                          call
                                              sum = sum + x(i)
! Read more data (n, a2)
                                            enddo
open ...; read ...; close ...
                                            average = sum / real(n)
! Calculate Average again
                                            end function average
aver2 = average(n, a2)
                                            end program
contains
```



Exercise 2.

Using your random array generators,
Write 2 functions that take an array as an argument

- one function that finds the maximum value and the index of the maximum value
- one function that finds the minimum value and the index of minimum value



Exercise 3.

Using your random array generator, Write a function that takes an array and 2 index locations and swaps the values of the array at the 2 index locations.



Exercise 4.

Using your random array generator,
Write a function that will sort your randomly generated array from smallest to largest,
by traversing your array and swapping values of adjacent indices if a(i) > a(i+1)

How can you test that your array is sorted?



Exercise 5.

Using Exercise 4, write a test function which will take your "sorted" array as an argument and tests it to verify that the array is indeed sorted, this function will return a logical.



the definition from C/C++ (Row major)

int a [3] [4];

Row 0

Row 1

Row 2

Column 0	Column 1	Column 2	Column 3
a[0][0]	a[0][1]	a[0][2]	a[0][3]
a[1][0]	a[1][1]	a[1][2]	a[1][3]
a[2][0]	a[2][1]	a[2][2]	a[2][3]



Run this code.

```
program array3
implicit none
integer :: i, j, k=0
integer, dimension(5,5) :: A

do i=1, 5
    do j=1, 5
        k = k + 1
        A(i,j) = k
    end do
end do

print *, A

end program array3
```

You might think it'd print all of Row 1, then Row 2, then Row 3, all unformatted.



Run this code.

```
you should see something like:
program array3
implicit none
integer :: i, j, k=0
                                                           11
                                                                   16
integer, dimension(5,5) :: A
                                                  12 17 22
18 23 4
24 5 10
                                          13
                                                                                    14
                                          19
                                                                            15
                                                                                    20
do i=1, 5
                                          25
  do j=1, 5
   k = k + 1
    A(i,j) = k
  end do
end do
print *, A
end program array3
```



Run this code.

```
you should see something like:
program array3
implicit none
integer :: i, j, k=0
integer, dimension(5,5) :: A
                                                   12 17 22 3
18 23 4 9
24 5 10 15
                                             13
                                                                                           14
                                             19
                                                                                           20
do i=1, 5
                                             25
  do j=1, 5
    k = k + 1
     A(i,j) = k
                                             What is this telling us?
  end do
end do
print *, A
end program array3
```



Run this code.

```
you should see something like:
program array3
implicit none
integer :: i, j, k=0
integer, dimension(5,5) :: A
                                                      12 17 22
18 23 4
24 5 10
                                             13
                                                                                           14
                                             19
                                                                                  15
                                                                                           20
do i=1, 5
                                             25
   do j=1, 5
     k = k + 1
                                             What is this telling us?
     A(i,j) = k
                                             Fortran is Column major!
  end do
end do
                                                                        16
                                                                                  21
                                                                                  22
                                                                        17
print *, A
                                                     8 13
                                                                                  23
                                                                        19
                                                                                  24
end program array3
                                                               1.5
                                                                         20
                                                                                  25
```



More about arrays, multi-dimension arrays.

- Ordered collection of elements
- Each element has an index
- Index may start at any integer number, not only 1
- Array element may be of intrinsic or derived type
- Array size refers to the number of elements
- The number of dimensions is the rank
- The size along a dimension is called an extent
- Array shape is the sequence of extents

```
size of a: 21
rank of a: 2
extent of a, first dimension: 3
shape of a: (3,7)

size of b:96
rank of b:3
extent of b, first dimension: 3
shape of b: (3,4,8)
```



recall from C++

```
int main ()
#include <iostream>
                                                                 int a[3][4];
using namespace std;
                                                                 for ( int i = 0; i < 3; i++ )
int multiplyByC(int arr[][4], int rows, int cols, int C)
                                                                    for ( int j = 0; j < 4; j++ )
                                                                        a[i][j] = i+j;
  for (int i = 0; i < rows; i++)
                                                                 multiplyByC(a, 3, 4, 5);
     for (int j = 0; j < cols; j++)
                                                                 for ( int i = 0; i < 3; i++ )
                                                                    for ( int j = 0; j < 4; j++ ) {
         arr[i][j] *= C;
                                                                        cout << a[i][j]<< endl;</pre>
  return 0;
                                                                 return 0;
```



in Fortran as a Subroutine

```
program mArray
                                                          contains
implicit none
integer :: i, j
                                                          subroutine multiplyByC(arr, ans, rows, cols, C)
integer, dimension(3,4) :: a, b
                                                          implicit none
                                                          integer :: rows, cols, C
do i=1, 3
  do j=1, 4
                                                          integer, dimension(rows, cols) :: arr, ans
     A(i,j) = i+j
  end do
                                                             ans = arr * C
end do
                                                          end subroutine
call multiplyByC(a, b, 3, 4, 5);
                                                          end program
print *, b
```



in Fortran as a Function

```
program mArray
                                                          contains
implicit none
integer :: i, j
                                                          function multiplyByC(arr,rows, cols, C)
integer, dimension(3,4) :: a, b
                                                          implicit none
                                                          integer :: rows, cols, C
do i=1, 3
  do j=1, 4
                                                          integer, dimension(rows, cols) :: arr, multiplyByC
     A(i,j) = i+j
   end do
                                                             multiplyByC = arr * C
end do
                                                          end function
b = multiplyByC(a, 3, 4, 5);
                                                          end program
print *, b
```



Exercise 6.

Write a subroutine or function that creates a 100x100 identity matrix, a matrix where the diagonal values are 1's and the rest of the values - the upper and lower triangles - are 0's



Exercise 7.

- Using your random number generator, create 2 random 100x100 matrices.
- Write a subroutine or function that multiplies the 2 matrices together and puts the result in a third matrix.
- Test your matrix multiplication subroutine by multiplying your random matrix with the same size identity matrix, the result will be the same as the original matrix.

Matrix Multiplication Algorithm:

- Input: matrices A and B
- Let C be a new matrix of the appropriate size
- For i from 1 to n:
 - o For j from 1 to p:
 - Let sum = 0
 - For k from 1 to m:
 - Set sum ← sum + A[i][k] × B[k][j]
 - Set C[i][j] ← sum
- Return C



- Variables on the left and the right have to be conformable in size and shape i.e. number of elements and rank
- Scalars are conformable
- Strides can be used



- Variables on the left and the right have to be conformable in size and shape i.e. number of elements and rank
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- Strides can be used



```
real
                                                        What's being done on each line?
real, dimension(10) :: a, b
real, dimension(10,10) :: c, d
       = b
       = d
a(1:10) = b(1:10)
a(2:3) = b(4:5)
a(1:10) = c(1:10,2)
       = X
       = X
a(1:3) = b(1:5:2)
a = c(:,1)
a = c(:,5)
a = c(1,:)
a = c(5,:)
```



best practices

- Always access slices as V(:, 1), V(:, 2), or V(:, :, 1), e.g. the colons should be on the left.
 - That way the stride is contiguous and it will be faster.
 - When you need some slice in your algorithm, always setup the array in a way, so that you call it as above. If you put the colon on the right, it will be slow.

```
dydx = matmul(C(:, :, i), y) ! fast 
 <math>dydx = matmul(C(i, :, :), y) ! slow
```



best practices

- the "fortran storage order" is:
 - smallest/fastest changing/innermost-loop index first,
 - largest/slowest/outermost-loop index last ("Inner-most are left-most.").
 - So the elements of a 3D array A(N1,N2,N3) are stored, and thus most efficiently accessed as:

```
do i3 = 1, N3
    do i2 = 1, N2
        do i1 = 1, N1
             A(i1, i2, i3)
        end do
    end do
end do
```



Exercise 8.

- Create a 100x100 matrices
 - set all elements initially equal to 1
 - slice your matrix such that
 - elements in rows 1 through 50 and column 1 through 50 are set to 1
 - elements in rows 1 through 50 and column 51 through 100 are set to 2
 - elements in rows 51 through 50 and column 1 through 100 are set to 3
 - elements in rows 51 through 100 and column 51 through 100 are set to 4



Sometimes you need to allocate memory for an array that is not static in size.

new declaration option: allocatable

new command: allocate, deallocate



```
program alloc_array
implicit none

real, dimension(:), allocatable :: x_1d ! Attribute
real, dimension(:,:), allocatable :: x_2d ! allocatable

...
read n, m
...

allocate(x_1d(n), stat=ierror) ! Check the
if (ierror /= 0) stop 'error x_1d' ! error status

allocate(x_2d(n,m), stat=ierror)
if (ierror /= 0) stop 'error x_2d'

deallocate(x) ! optional
```

- Declaration and allocation in two steps
- Declare an array as allocatable
 Use colons (:) as placeholders
- Allocate/deallocate in the executable part



```
subroutine sub(n)
                                                      What are your thoughts here?
real, dimension(:), allocatable :: x_1d
                                                      What happens to the allocated memory space
allocate(x_1d(n), stat=ierror)
                                    ! Check the
                                                      when you leave the subroutine?
if (ierror /= 0) stop 'error x 1d'
                                    ! error status
                                                      Does this work or does it produce a memory
                                                      leak?
end
```



```
subroutine sub(n)
                                                       What are your thoughts here?
real, dimension(:), allocatable :: x_1d
                                                       Dynamically allocated arrays are automatically
allocate(x_1d(n), stat=ierror)
                                     ! Check the
                                                       deallocated, when you leave the scope
if (ierror /= 0) stop 'error x 1d'
                                     ! error status
                                                       Nevertheless, it does not hurt to put a
deallocate(x_1d)
                                                       deallocate statement yourself
end
```



```
program main
                                                           What about this problem?
real, dimension(:), allocatable :: x_1d
allocate(x_1d(100000000), state=ierror)
                                                           We have an array being dynamically allocated, we
if (ierror /= 0) stop 'error x 1d'
                                                           don't know the size, but we want to pass it to an
                                                           function or subroutine
call sub(x_1d)
contains
subroutine sub(x_1d)
end subroutine
end program
```



```
program main
                                                          What about this problem?
real, dimension(:), allocatable :: x 1d
allocate(x_1d(100000000), state=ierror)
                                                          We have an array being dynamically allocated, we
if (ierror /= 0) stop 'error x 1d'
                                                          don't know the size, but we want to pass it to an
                                                          function or subroutine
call sub(x_1d)
                                                          We allow the program to assume the size using (:)
contains
                                                          and proceed as normal.
subroutine sub(x_1d)
real, dimension(:) :: x
end subroutine
end program
```



Exercise 9.

- Using modules and interfaces
 - o read in 1 or 2 integers
 - if the the user enters 1 integer, n
 - dynamically allocate an array to build a *square* (nxn) matrix
 - if the the user enters 2 integers, n and m,
 - dynamically allocate an array to build an n x m matrix
 - Fill your array using random numbers
 - if the random number is even make the element = zero.
 - if the random number is odd make the element = one.
 - o using nested do-loops, print out the matrix in an easy to read format

