

## HOMEWORK: Fortran

In this homework, write a Fortran program that demonstrates the use of modules, interfaces, types, and operator overloading.

Consider the problem of storing a sparse matrix, and the creation of operators to add two sparse matrices.

A 2D matrix of size  $n \times m$  has  $mn$  elements  $a_{ij}$  where  $i = 1, \dots, m$  and  $j = 1, \dots, n$ . This matrix is sparse if most of its elements are zero. Note that the matrix is not necessarily a square matrix.

We need two integer variables: `nr=m` and `nc=n` (not necessarily equal). We will not store the full matrix, since with  $m = n = 10^6$ , would require memory of  $10^{12}$  floats, which is more than you have available on your desktop computers. Instead, we will simply track each non-zero element by its row, column and array value at that location.

This matrix will be defined by the Fortran 90 type:

```
type sparse
  integer :: nr, nc      ! number of rows and columns
  integer :: nel         ! number of nonzero elements

  ! row (ia) and column (ja) of each nonzero element
  integer, dimension(:), pointer :: ia, ja

  ! double precision: nel elements
  real(8), dimension(:), pointer :: a
end type sparse
```

To better understand the storage format, consider the matrix of `real(8)`

$$A = \begin{pmatrix} 0. & 2. & 5. & 0. & 0. & 3. \\ 0. & 0. & 1. & 2. & 0. & 4. \\ 1. & 5. & 0. & 0. & 2. & 1. \end{pmatrix}$$

Instead of storing  $18 \text{ real}(8) = 144$  bytes, we will represent the matrix with three arrays. First, `a` is a 1D array whose size is `nel`, equal to the number of nonzero elements of  $A$ , written out in the same order of appearance as found in  $A$  (scanning along rows).

$$a = (2., 5., 3., 1., 2., 4., 1., 5., 2., 1.)$$

Second, the columns of each nonzero element of  $A$  are stored in `ja`, also of size `nel`:

$$ja = (2, 3, 6, 3, 4, 6, 1, 2, 5, 6)$$

Finally for each of the three rows of  $A$ , we identify the first nonzero element: row 1 gives 2, row two gives 1, and row 3 gives 1. Each of these elements is found in the array  $\mathbf{a}$ , and its position is stored in array  $\mathbf{ia}$ :

$$\mathbf{ia} = (1, 4, 7, 11)$$

The size of  $\mathbf{ia}$  is  $\mathbf{nr}+1$ , and the last value of  $\mathbf{ia}$  is  $\mathbf{nel}+1=11$ . In this example,  $\mathbf{nel}=10$ . So we have stored 10 real(8) in  $\mathbf{a}$ , 10 integers in  $\mathbf{ja}$  and 4 integers in  $\mathbf{ia}$ , for a total of  $(10*8+10*4+4*4=136)$  bytes. We have already saved 8 bytes. Not much. But in this case, there are 10 nonzero elements in a matrix of size 18. In the homework, the matrix will be of size  $10^7$ , and there will be many less nonzero elements. Thus the savings are much more significant.

Consider row  $i$  (where  $i = 1, 2, 3$ ). The nonzero elements of  $A$  can be found in  $\mathbf{a}(\mathbf{ia}(i))$  to  $\mathbf{a}(\mathbf{ia}(i+1)-1)$ . Thus for row 2,  $\mathbf{ia}(2)=4$  and  $\mathbf{ia}(3)=7$ . Therefore, the nonzero elements of  $A$  are  $\mathbf{a}(4)=3$ ,  $\mathbf{a}(5)=4$ , and  $\mathbf{a}(6)=6$ . The columns of these three non-zero elements are  $\mathbf{ja}(4)=3$ ,  $\mathbf{ja}(5)=4$ , and  $\mathbf{ja}(6)=6$ .

In the case that  $i$ -th row is full of zeros, we have  $\mathbf{ia}(i) = \mathbf{ia}(i+1)$  =the number of nonzeros up to the  $i$ -th row+1 Example for

$$A = \begin{pmatrix} 0 & 0 & 0 \\ 6 & 0 & 9 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\mathbf{a} = (6, 9)$$

$$\mathbf{ja} = (1, 3)$$

$$\mathbf{ia} = (1, 1, 3, 3)$$

. There are more examples later.

In summary, to scan this array, scan each row:  $i = 1, \mathbf{nr}$ . For each row  $i$ , calculate  $\mathbf{ia}(i)$  and  $\mathbf{ia}(i+1)-1$ . The nonzero columns are  $\mathbf{ja}(\mathbf{ia}(i))$  through  $\mathbf{ja}(\mathbf{ia}(i+1)-1)$ , and the nonzero elements of  $A$  are  $\mathbf{A}(i, \mathbf{ja}(\mathbf{ia}(i)))$  through  $\mathbf{A}(i, \mathbf{ja}(\mathbf{ia}(i+1)-1))$ .

When adding two arrays, for each row, identify the nonzero columns and add the corresponding elements of the two arrays. Be careful: while the two matrices to be added are both sparse, the nonzero elements are not necessarily in the same locations. You should check that the addition works properly on small  $3 \times 3$  or  $4 \times 4$  matrices with nonzero elements in different locations. .

**Under non circumstances are you to store the full matrix. The matrix should on be stored in compressed format. However, you are allowed to allocate temporary storage for a single row or column if you feel that is necessary.**

- Create a module called `sparse_mod`, that defines the `sparse_matrix` type which contains all necessary information on the matrix: number of rows and columns ( $\mathbf{nr}, \mathbf{nc}$ ), number of nonzero elements, and pointers to arrays  $\mathbf{a}$ ,  $\mathbf{ia}$ ,  $\mathbf{ja}$ .
- Allocate  $\mathbf{nel}$  elements for  $\mathbf{a}$  and  $\mathbf{ja}$  and  $\mathbf{nr}+1$  elements for  $\mathbf{ia}$ .
- Create a matrix of size 1,000 by 10,000, and fill it with 10,000 elements. Use a constructor for this purpose. Thus on average, each row contains 10 elements. You should use a random number generator to assign the columns for each row, and you should use a random number generator to fill the nonzero elements of the matrix with values between 0 and 10.

- Create an operator(+) in the module to add two sparse matrices. For example, consider the two matrices  $A$  and  $B$ :

$$A = \begin{pmatrix} 0 & 3 & 0 \\ 5 & -7 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$B = \begin{pmatrix} 0 & 3 & 0 \\ 2 & -6 & 0 \\ 4 & 0 & -3 \end{pmatrix}$$

Notice that  $A$  and  $B$  matrices do not have zeros in the same elements. The sum is:

$$C = A + B = \begin{pmatrix} 0 & 6 & 0 \\ 7 & -13 & 0 \\ 4 & 0 & -2 \end{pmatrix}$$

- When adding two sparse matrices of equal dimension, it is therefore important to consider all the non-zero elements of both matrices.
- Create a main program. This main program should have a structure similar to:

```

program main
use sparse_mod
implicit none
type(sparse) :: mat1, mat2, mat3, matsum
....
! Initialize mat1, mat2, and mat3, which you can manually set their a, ia and ja.

...

matsum = mat1 + mat2 + mat3

print results      ! (e.g. the nonzero elements of rows 5 for mat1, mat2
                   !                               and matsum
end program main

```

- Test your program with the following example:

$$A = \begin{pmatrix} 0 & 0 & 0 \\ 5 & -7 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$B = \begin{pmatrix} 0 & 3 & 0 \\ 0 & -6 & 0 \\ 4 & 0 & -3 \end{pmatrix}$$

$$C = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 8 & 0 \end{pmatrix}$$

$$A + B + C = D = \begin{pmatrix} 0 & 3 & 0 \\ 5 & -13 & 0 \\ 4 & 8 & -3 \end{pmatrix}$$

Note that for matrix  $A$ ,

$$a = (5, -7)$$

```

                                 $ja = (1, 2)$ 
                                 $ia = (1, 1, 3, 3)$ 

for matrix  $B$ 
                                 $a = (3, -6, 4, -3)$ 
                                 $ja = (2, 2, 1, 3)$ 
                                 $ia = (1, 2, 3, 5)$ 

for matrix  $C$ 
                                 $a = (8)$ 
                                 $ja = (2)$ 
                                 $ia = (1, 1, 1, 2)$ 

for matrix  $D$ 
                                 $a = (3, 5, -13, 4, 8, -3)$ 
                                 $ja = (2, 1, 2, 1, 2, 3)$ 
                                 $ia = (1, 2, 4, 7)$ 

```

Your code should past this test. Please print out your test result.

- Make sure you have NOTES/README/INSTALL files to describe ideas you may have had while you were working (NOTES), what the program does (README), and what to do to get the program to run (INSTALL).
- Make sure the code is documented (you are graded on this)