A Prototype Finite Difference Model

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Examples at

http://hpc.mines.edu/examples

or enter the commands:

```
mkdir examples
cd examples
wget http://hpc.mines.edu/examples/examples.tgz
```

For this session go to the "stommel" directory

A Prototype Model

- We will introduce a finite difference model that will serve to demonstrate what a computational scientist needs to do to take advantage of Distributed Memory computers using MPI
- The model we are using is a two dimensional solution to a model problem for Ocean Circulation, the Stommel Model

The Stommel Problem

- Wind-driven circulation in a homogeneous rectangular ocean under the influence of surface winds, linearized bottom friction, flat bottom and Coriolis force.

- Solution: intense crowding of streamlines towards the western boundary caused by the variation of the Coriolis parameter with latitude

Governing Equations Model Constants

$$\psi = 0$$

$$\psi = 0 \qquad \psi = 0$$

$$\gamma\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right) + \beta \frac{\partial \psi}{\partial x} = f$$

$$f = -\alpha \sin\left(\frac{\pi y}{2L_y}\right)$$

$$L_x = L_y = 2000 Km$$

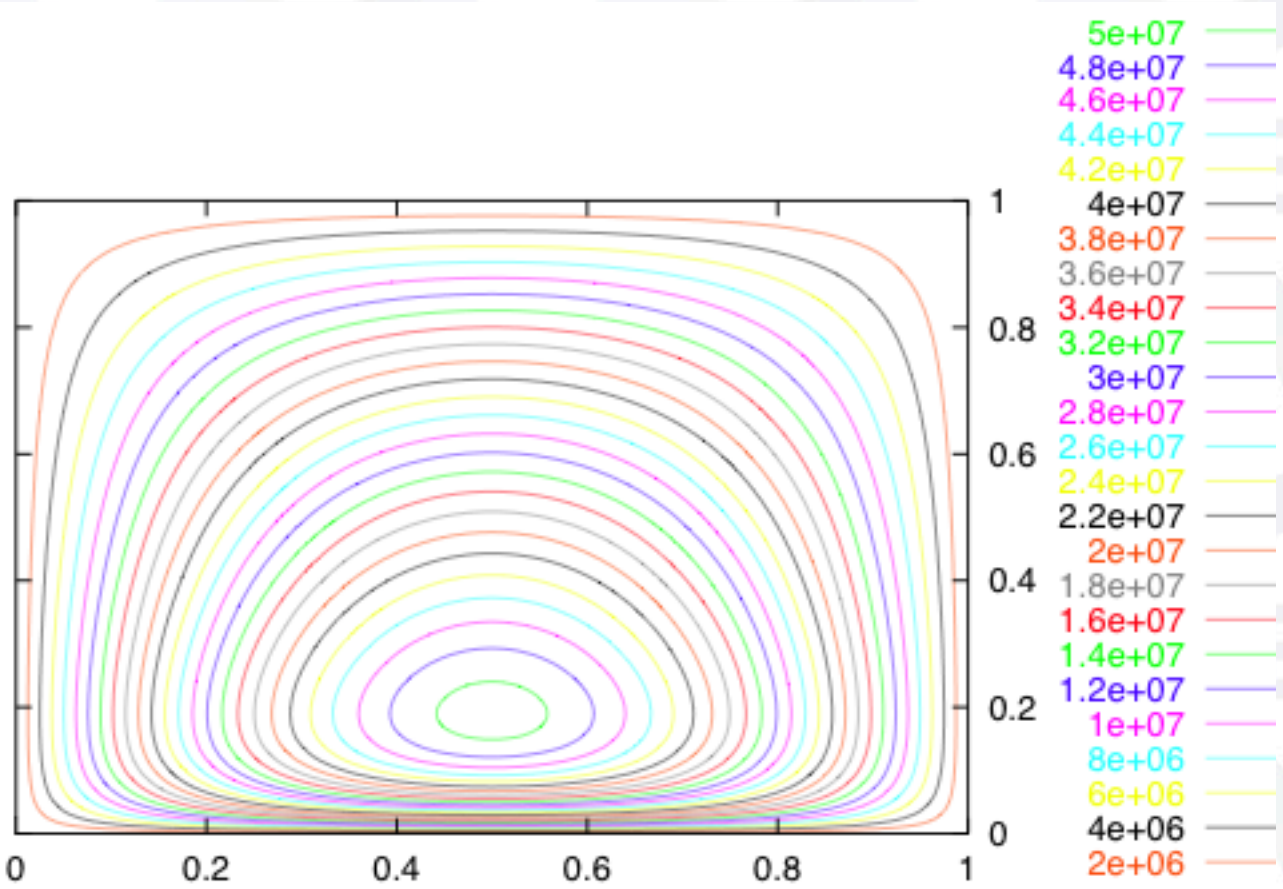
$$\gamma = 3 * 10^{(-6)}$$

$$\beta = 2.25 * 10^{(-11)}$$

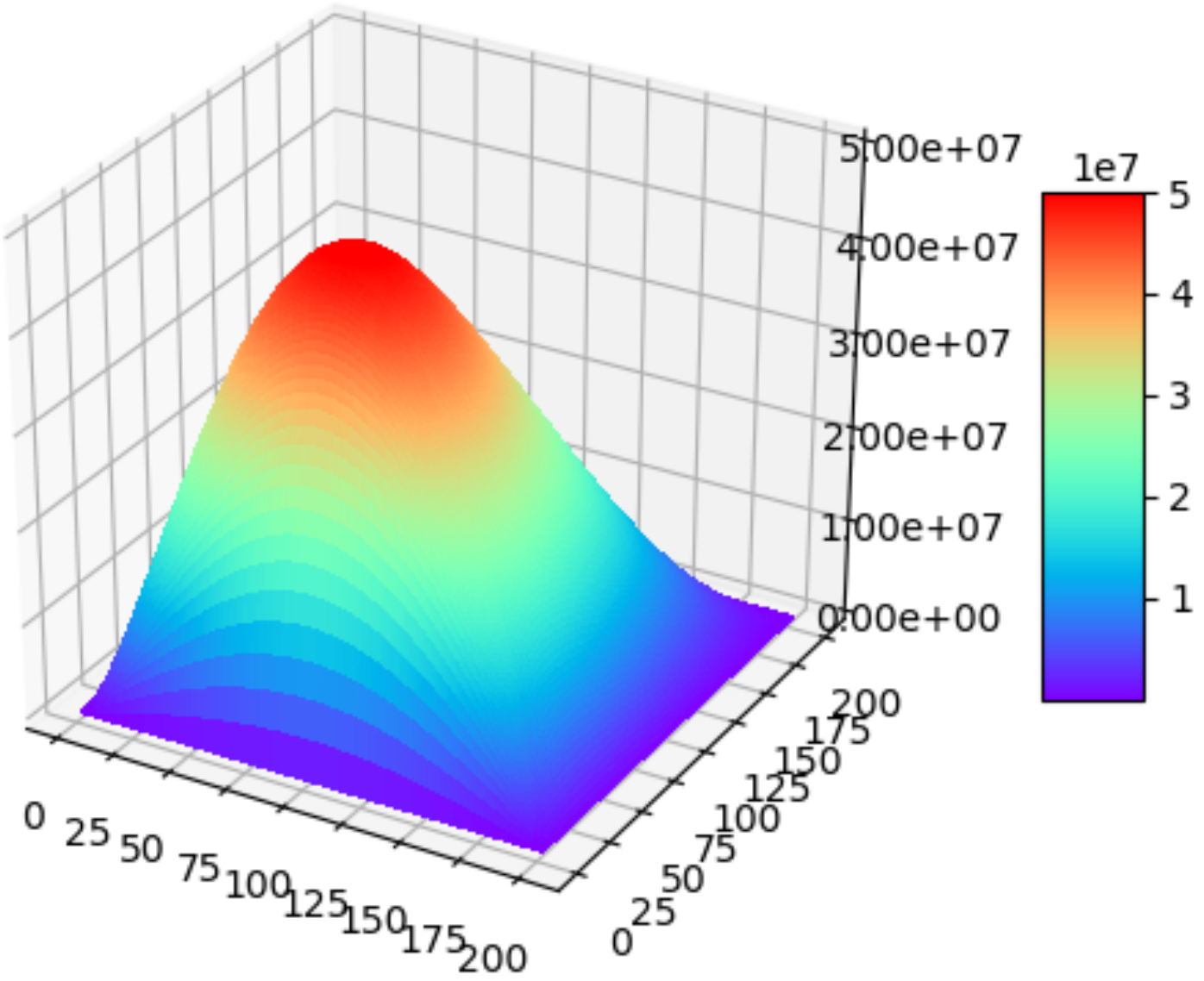
$$\alpha = 10^{(-9)}$$

$$\psi = 0$$

The steady state solution



The steady state solution

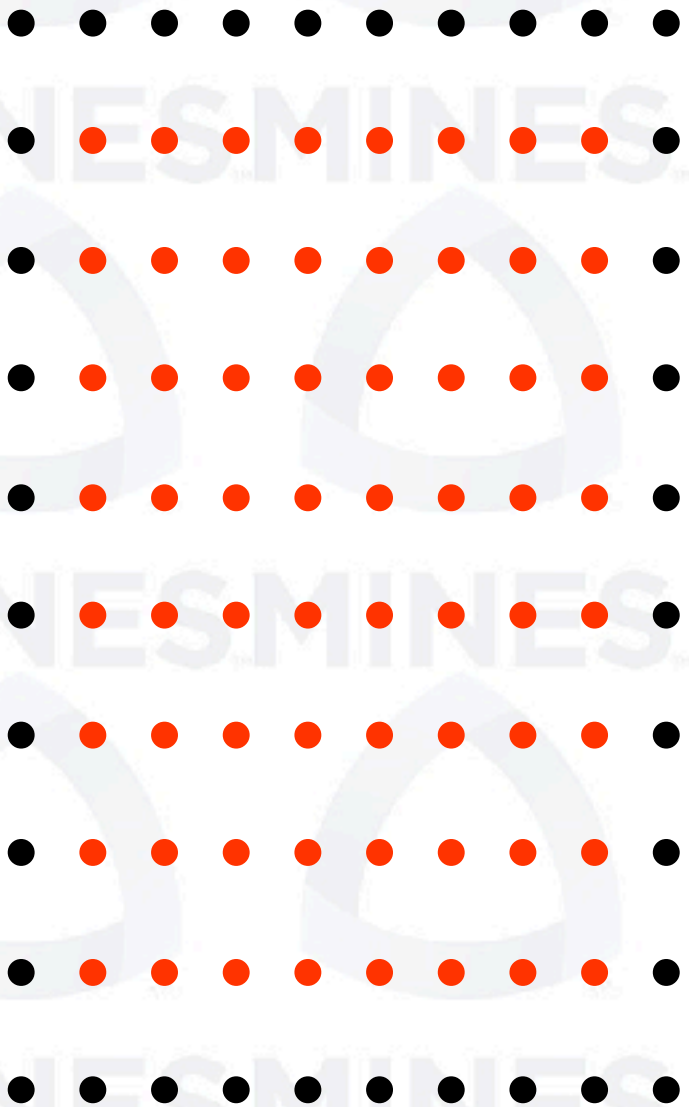


Domain Discretization

Define a grid consisting of points (x_i, y_j) given by

$$x_i = i\Delta x, i = 0,1,\ldots\ldots,nx+1$$
$$y_j = j\Delta y, j = 0,1,\ldots\ldots,ny+1$$
$$\Delta x = L_x/(nx+1)$$
$$\Delta y = L_y/(ny+1)$$

Domain Discretization



Seek to find an approximate solution

$\psi(x_i, y_j)$ at points (x_i, y_j):

$$\psi i, j \approx \psi(x_i, y_j)$$

Centered Finite Difference Scheme for the Derivative Operators

$$\frac{\partial \psi}{\partial x} \approx \frac{\psi_{i+1,j} - \psi_{i-1,j}}{2\Delta x}$$

$$\frac{\partial^2 \psi}{\partial x^2} \approx \frac{\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j}}{(\Delta x)^2}$$

$$\frac{\partial^2 \psi}{\partial y^2} \approx \frac{\psi_{i,j+1} - 2\psi_{i,j} + \psi_{i,j-1}}{(\Delta y)^2}$$

Governing Equation Finite Difference Form

$$\psi_{i,j} = a_1\psi_{i+1,j} + a_2\psi_{i-1,j} + a_3\psi_{i,j+1} + a_4\psi_{i,j-1} - a_5 f_{i,j}$$

$$a_1 = \frac{\Delta y^2}{2(\Delta x^2 + \Delta y^2)} + \frac{\beta \Delta x^2 \Delta y^2}{4\gamma \Delta x(\Delta x^2 + \Delta y^2)}$$

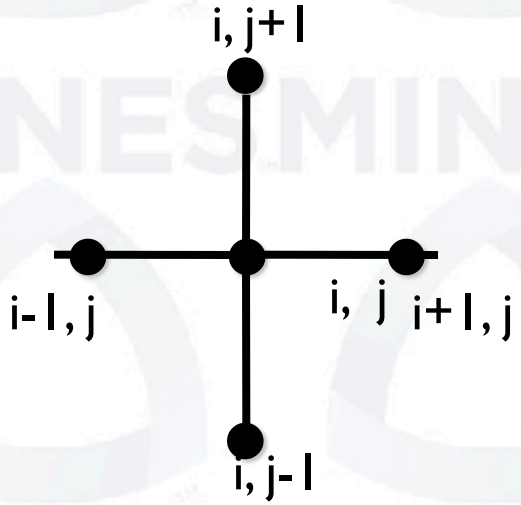
$$a_2 = \frac{\Delta y^2}{2(\Delta x^2 + \Delta y^2)} - \frac{\beta \Delta x^2 \Delta y^2}{4\gamma \Delta x(\Delta x^2 + \Delta y^2)}$$

$$a_3 = \frac{\Delta x^2}{2(\Delta x^2 + \Delta y^2)}$$

$$a_4 = \frac{\Delta x^2}{2(\Delta x^2 + \Delta y^2)}$$

$$a_5 = \frac{\Delta x^2 \Delta y^2}{2\gamma(\Delta x^2 + \Delta y^2)}$$

Five-point Stencil Approximation



interior grid points: i=1,nx;
j=1,ny

boundary points:

(i,0) & (i,ny+1) ; i=0,nx+1

(0,j) & (nx+1,j) ; j=0,ny+1

$$\psi_{i,j} = a_1\psi_{i+1,j} + a_2\psi_{i-1,j} + a_3\psi_{i,j+1} + a_4\psi_{i,j-1} - a_5 f_{i,j}$$

$$\psi_{i,0} = \psi_{i,ny+1} = 0; \quad \psi_{0,j} = \psi_{nx+1,j} = 0;$$

Jacobi Iteration

Start with an initial guess for $(\psi_{i,j})$

Repeat the process

do i = 1, nx; j = 1, ny

$$(\psi_{i,j})\_new = a_1(\psi_{i+1,j}) + a_2(\psi_{i-1,j}) + a_3(\psi_{i,j+1}) + a_4(\psi_{i,j-1}) - a_5 f_{i,j}$$

end do

$$(\psi_{i,j}) = (\psi_{i,j})\_new$$

Our Examples

File	Comment
ccalc.c	parallel
stc_03.c	parallel
pcalc.py	parallel
stp_00.py	serial
stp.py	parallel
tiny.in	tiny input file
small.in	small input file
st.in	regular input file

We have a finite difference model that will serve to demonstrate what a computational scientist needs to do to take advantage of Distributed Memory computers using MPI.
The model we are using is a two dimensional solution to a model problem for Ocean Circulation, the Stommel Model. It has Wind-driven circulation in a homogeneous rectangular ocean under the influence of surface winds, linearized bottom friction, flat bottom and Coriolis force.
Solution: intense crowding of streamlines towards the western boundary caused by the variation of the Coriolis parameter with latitude.
For a description of the Fortran and C versions of this program see:
http://geco.mines.edu/prototype/Show_me_some_local_HPC_tutorials/stoma.pdf
http://geco.mines.edu/prototype/Show_me_some_local_HPC_tutorials/stomb.pdf
The python version, stp.py, follows this C version except it does a 1d decomposition.
The C version is 1500x faster than the python version.
pcalc.py and ccalc.c are similar except they create a new communicator that contains N-1 tasks. These tasks do the calculation and pass data to the remaining task to be plotted. Thus we can have "C" do the heavy calculation and python do plotting.

Python Version

```
#!/usr/bin/env python
from math import pi,sin
from math import fabs as abs
#from Numeric import empty
from numpy import empty
import numpy
from time import time as walltime
global vals,cons
global psi,new_psi,forf
import sys
global a1,a2,a3,a4,a5,a6,dx,dy
global r1,r2
global ttol
```

Python Version

```
class constants:
   a1,a2,a3,a4,a5,a6,dx,dy=(0.0,0.0,0.0,0.0,0.0,0.0,0.0,0.0)
   def __init__(this,inputs):
      dx=inputs.lx/(inputs.nx+1.0)
      dy=inputs.ly/(inputs.ny+1.0)
      dx2=dx*dx
      dy2=dy*dy
      bottom=2.0*(dx2+dy2)
      a1=(dy2/bottom)+(inputs.beta*dx2*dy2)/(2.0*inputs.gamma*dx*bottom)
      a2=(dy2/bottom)-(inputs.beta*dx2*dy2)/(2.0*inputs.gamma*dx*bottom)
      a3=dx2/bottom
      a4=dx2/bottom
      a5=dx2*dy2/(inputs.gamma*bottom)
      a6=pi/(inputs.ly)
      this.dx=dx
      this.dy=dy
      this.a1=a1
      this.a2=a2
      this.a3=a3
      this.a4=a4
      this.a5=a5
      this.a6=a6
   def getCons(this):
      return(this.a1,this.a2,this.a3,this.a4,this.a5,this.a6,this.dy,this.dx)
```

Python Version

```
class input:
   nx,ny=(50 , 50)
   lx,ly=(2000000 , 2000000)
   alpha,beta,gamma=(1.0e-9 , 2.25e-11 , 3.0e-6)
   steps=5000
   def __init__(this):
      pass
   def getInput(this):

return(this.nx,this.ny,this.lx,this.ly,this.alpha,this.bet
a,this.gamma,this.steps)
```

Python Version

```
def do_force(forf,i1,i2,j1,j2):
   def force(y):
      global cons,vals
      return(-vals.alpha*sin(y*cons.a6))
   for i in range(i1-1,i2+2):
      for j in range(j1-1,j2+2):
         y=j*cons.dy
         forf[i,j]=force(y)
```

```
def bc(psi,i1,i2,j1,j2):
   psi[i1-1,:]=0.0
   psi[i2+1,:]=0.0
   psi[:,j1-1]=0.0
   psi[:,j2+1]=0.0
```

Python Version

```
def do_jacobi(psi,new_psi,i1,i2,j1,j2):
# does a single Jacobi iteration step
# input is the grid and the indices for the interior cells
# new_psi is temp storage for the the updated grid
# output is the updated grid in psi and diff which is
# the sum of the differences between the old and new grids
   global cons
   global forf
   global ttot
   global a1,a2,a3,a4,a5,a6,dx,dy
   diff=0.0
   ts=walltime()
   for j in r2:
      for i in r1:
         new_psi[i,j]=a1*psi[i+1,j] + a2*psi[i-1,j] + \
         a3*psi[i,j+1] + a4*psi[i,j-1] - \
         a5*forf[i,j]
         diff=diff+abs(new_psi[i,j]-psi[i,j])
   psi[:,:]=new_psi[:,:]
   te=walltime()
   ttot=ttot+(te-ts)
   return (diff)
```

Python Version

```
#get the input.  see above for typical values
vals=input()

#set the indices for the interior of the grid
i1=1
i2=vals.nx
j1=1
j2=vals.ny
# allocate the grid to size nx * ny plus the boundary cells
t1=walltime()
psi=empty(((i2-i1)+3,(j2-j1)+3),"d")
new_psi=empty(((i2-i1)+3,(j2-j1)+3),"d")
forf=empty(((i2-i1)+3,(j2-j1)+3),"d")
#calculate the constants for the calculations
cons=constants(vals)
(a1,a2,a3,a4,a5,a6,dx,dy)=cons.getCons()

# set initial guess for the value of the grid
psi[:,:]=1.0
do_force(forf,i1,i2,j1,j2)
#set boundary conditions
bc(psi,i1,i2,j1,j2)
```

Python Version

```
new_psi[:,:]=psi[:,:]
iout=vals.steps//100
if(iout  == 0):
   iout=1
r1=range(i1,i2+1)
r2=range(j1,j2+1)
ttot=0
for i in range(0,vals.steps):
   diff=do_jacobi(psi,new_psi,i1,i2,j1,j2)
   if ((i+1) % iout) == 0 :
      print(i+1,diff)
t2=walltime()
write_it(psi,i1,i2,j1,j2,i2,j2)
print("total time=",t2-t1, "  time spent in do_jacobi=",ttot)
```

Python Version

```
def write_it(psi,i1, i2, j1, j2,nx,ny):
   from numpy import empty
   myid=100
   if(i1==1):
      i0=0
   else :
      i0=i1
   if(i2==nx):
      i3=nx+1
   else :
      i3=i2
   if(j1==1):
      j0=0
   else :
      j0=j1
   if(j2==ny):
      j3=ny+1
   else :
      j3=j2
      fname="out"+str(myid)
      eighteen=open(fname,"w")
      aline=(str(i3-i0+1)+" , "+str(j3-j0+1)+"
   "+str(psi.shape))
      eighteen.write(aline+"\n")
      for i in range(i0,i3+1) :
         for j in range(j0,j3+1) :
            xout=str(psi[i][j])
            eighteen.write(xout)
            if(j != j3):
               eighteen.write(" ")
         eighteen.write("\n")
      eighteen.close()
```

A Prototype Finite Difference Model (Philosophy)

Overview

- Model written in Fortran 90
- Uses many new features of F90
  - Free format
  - Modules instead of commons
  - Module with kind precision facility
  - Interfaces
  - Allocatable arrays
  - Array syntax

http://inside.mines.edu/~tkaiser/fortran//

http://inside.mines.edu/~tkaiser/fortran/new/

Free Format

- Statements can begin in any column
- ! Starts a comment
- To continue a line use a "&" on the line to be continued

Modules instead of commons

- Modules have a name and can be used in place of named commons
- Modules are defined outside of other subroutines
- To "include" the variables from a module in a routine you "use" it
- The main routine stommel and subroutine jacobi share the variables in module "constants"

```
module constants
    real dx,dy,a1,a2,a3,a4,a5,a6
end module
…
program stommel
    use constants
…
end program
```

```
subroutine jacobi
    use constants
…
end subroutine jacobi
```

Kind precision facility

Instead of declaring variables

```
real*8 x,y
```

We use

```
real(b8) x,y
```

Where b8 is a constant defined within a module

```
module numz
 integer,parameter::b8=selected_real_kind(14)
end module
program stommel
    use numz
    real(b8) x,y
    x=1.0_b8
...
```

Kind precision facility Why?

Legality
Portability
Reproducibility
Modifiability

Declaring variables “double precision” will give us 16 byte reals on some machines

```
integer,parameter::b8=selected_real_kind(14)
real(b8) x,y
x=1.0_b8
```

Allocatable arrays

- We can declare arrays to be allocatable
- Allows dynamic memory allocation
- Define the size of arrays at run time

```
real(b8),allocatable::psi(:,:)     ! our calculation grid
real(b8),allocatable::new_psi(:,:) ! temp storage for the grid
```

```
! allocate the grid to size nx * ny plus the boundary cells
 allocate(psi(0:nx+1,0:ny+1))
 allocate(new_psi(0:nx+1,0:ny+1))
```

Interfaces

- Similar to C prototypes
- Can be part of the routines or put in a module
- Provides information to the compiler for optimization
- Allows type checking

```
module face
  interface bc
    subroutine bc (psi,i1,i2,j1,j2)
      use numz
      real(b8),dimension(i1:i2,j1:j2):: psi
      integer,intent(in):: i1,i2,j1,j2
    end subroutine
  end interface
end module
program stommel
    use face
...
```

Array Syntax

Allows assignments of arrays without do loops

```
! allocate the grid to size nx * ny plus the boundary cells
    allocate(psi(0:nx+1,0:ny+1))
    allocate(new_psi(0:nx+1,0:ny+1))


! set initial guess for the value of the grid
    psi=1.0_b8


! copy from temp to main grid
    psi(i1:i2,j1:j2)=new_psi(i1:i2,j1:j2)
```

Program Outline (1)

- Module NUMZ - defines the basic real type as 8 bytes
- Module INPUT - contains the inputs
  - nx,ny (Number of cells in the grid)
  - lx,ly (Physical size of the grid)
  - alpha,beta,gamma (Input calculation constants)
  - steps (Number of Jacobi iterations)
- Module Constants - contains the invariants of the calculation

Program Outline (2)

- Module face - contains the interfaces for the subroutines
  - bc - boundary conditions
  - do_jacobi - Jacobi iterations
  - force - right hand side of the differential equation
  - Write_grid - writes the grid

Program Outline (3)

- Main Program
  - Get the input
  - Allocate the grid to size nx * ny plus the boundary cells
  - Calculate the constants for the calculations
  - Set initial guess for the value of the grid
  - Set boundary conditions using
  - Do the jacobi iterations
  - Write out the final grid

C version considerations

- To simulate the F90 numerical precision facility we:
  - #define FLT double
  - And use FLT as our real data type throughout the rest of the program
- We desire flexibility in defining our arrays and matrices
  - Arbitrary starting indices
  - Contiguous blocks of memory for 2d arrays
  - Use routines based on *Numerical Recipes in C*

Vector allocation routine

```
FLT *vector(INT nl, INT nh)
{
/* creates a vector with bounds vector[nl:nh]] */
        FLT *v;
/* allocate the space */
        v=(FLT *)malloc((unsigned) (nh-nl+1)*sizeof(FLT));
        if (!v) {
            printf("allocation failure in vector()\n");
                exit(1);
    }
/* return a value offset by nl */
        return v-nl;
}
```

Matrix allocation routine

```
FLT **matrix(INT nrl,INT nrh,INT ncl,INT nch)
/* creates a matrix with bounds matrix[nrl:nrh][ncl:nch] */
/* modified from the book version to return contiguous space */
{
 INT i;
 FLT **m;
/* allocate an array of pointers */
 m=(FLT **) malloc((unsigned) (nrh-nrl+1)*sizeof(FLT*));
 if (!m){
  printf("allocation failure 1 in matrix()\n"); exit(1);}
 m -= nrl; /* offset the array of pointers by nrl */
 for(i=nrl;i<=nrh;i++) {
  if(i == nrl){
/* allocate a contiguous block of memroy*/
   m[i]=(FLT *) malloc((unsigned) (nrh-nrl+1)*(nch-ncl+1)*sizeof(FLT));
   if (!m[i]){
     printf("allocation failure 2 in matrix()\n");exit(1); }
   m[i] -= ncl; /* first pointer points to beginning of the block */
  }
  else {
    m[i]=m[i-1]+(nch-ncl+1); /* rest of pointers are offset by stride */
  }
 }
 return m;
}
```

Digression... a 3d Volume allocation routine

Same idea but we allocate an array of slices

```
FLT ***cube(INT nslice1,INT nslice2,INT nrow1,INT nrow2,INT ncol1,INT ncol2) {
FLT **slice(INT nrow1,INT nrow2,INT ncol1,INT ncol2,FLT **temp);
     FLT *temp,***mcube;
     INT i;
     mcube=(FLT ***) malloc((unsigned) (nslice2-nslice1+1)*sizeof(FLT*));
     if (!mcube){
          printf("allocation failure at 1 in cube()\n");
          return NULL;
     }
     mcube -= nslice1;
     temp=(FLT*) malloc((unsigned) (nslice2-nslice1+1)*
                                   (nrow2-nrow1+1)*
                                   (ncol2-ncol1+1)*sizeof(FLT));
     if (*temp){
          printf("allocation failure at 2 in cube()\n");
          return NULL;
     }
     for(i=nslice1;i<=nslice2;i++) {
          mcube[i]=slice(nrow1, nrow2, ncol1, ncol2,&temp);
          if(!mcube[i]) return NULL;
          temp += (nrow2-nrow1+1)*(ncol2-ncol1+1);
     }
     return mcube;
}
```

Digression... a 3d version of this routine

Our slice allocation routine

```
FLT **slice(INT nrow1,INT nrow2,INT ncol1,INT ncol2,FLT **temp) {
    INT i;
     FLT **mslice;
     mslice=(FLT **) malloc((unsigned) (nrow2-nrow1+1)*sizeof(FLT*));
     if (!mslice){
          printf("allocation falure at 3 in slice()\n");
          return NULL;
     }
     mslice -= nrow1;
     for(i=nrow1;i<=nrow2;i++) {
         if(i == nrow1){
              mslice[i]=*temp;
              mslice[i] -= ncol1;
         }
         else {
             mslice[i]=mslice[i-1]+(ncol2-ncol1+1);
         }
     }
     return mslice;
}
```