A Prototype Finite Difference Model

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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
- Examples
  - geco.mines.edu/workshop

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

$$\psi = 0$$

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

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

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

$$L_x = L_y = 2000Km$$

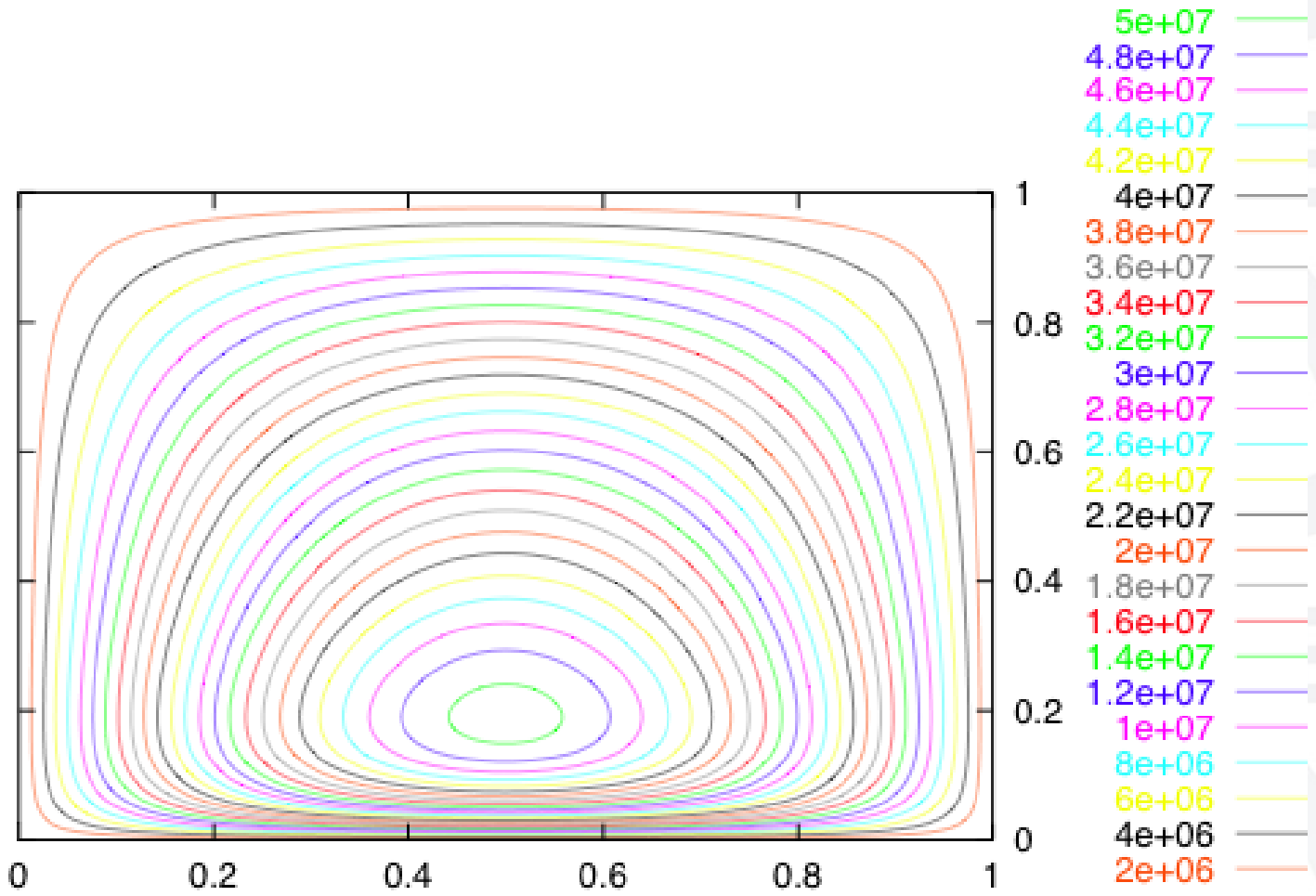
$$\gamma = 3 * 10^{(-6)}$$

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

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

$$\psi = 0$$

The steady state solution



Domain Discretization

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

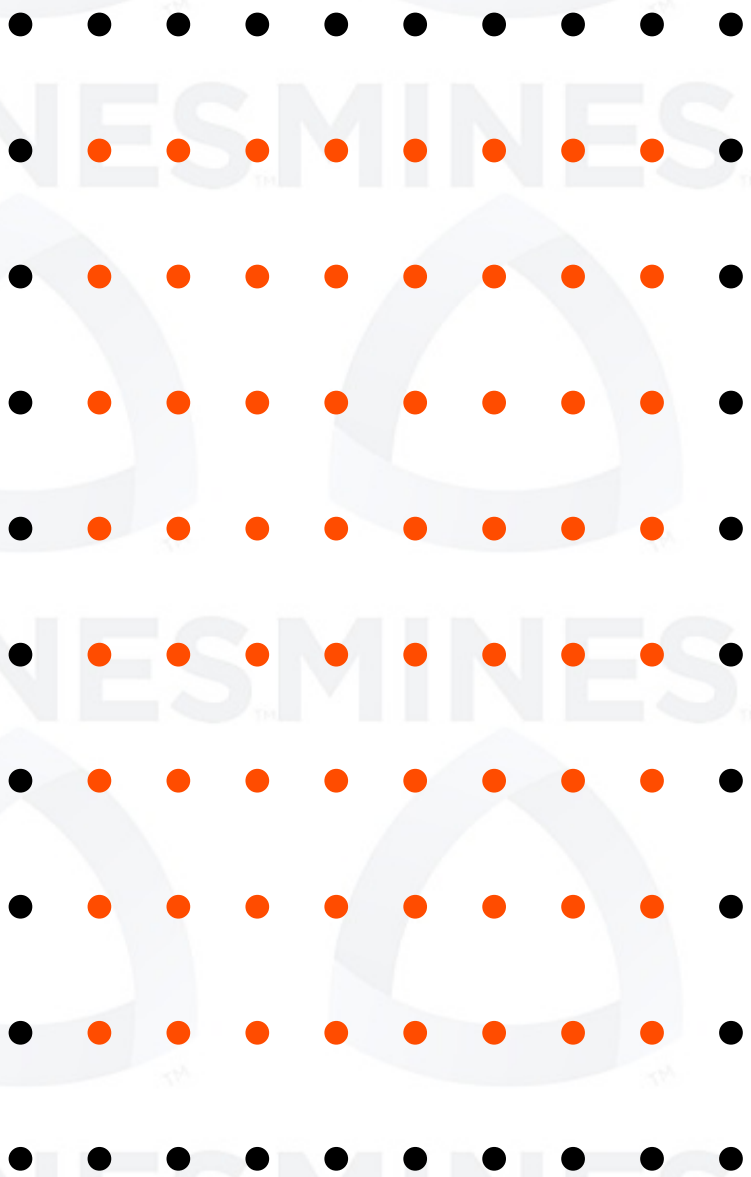
$$x_i = i\Delta x, i = 0, 1, ..., nx+1$$

$$y_j = j\Delta y, j = 0, 1, ..., ny+1$$

$$\Delta x = L_x / (nx + 1)$$

$$\Delta y = L_y / (ny + 1)$$

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

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

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

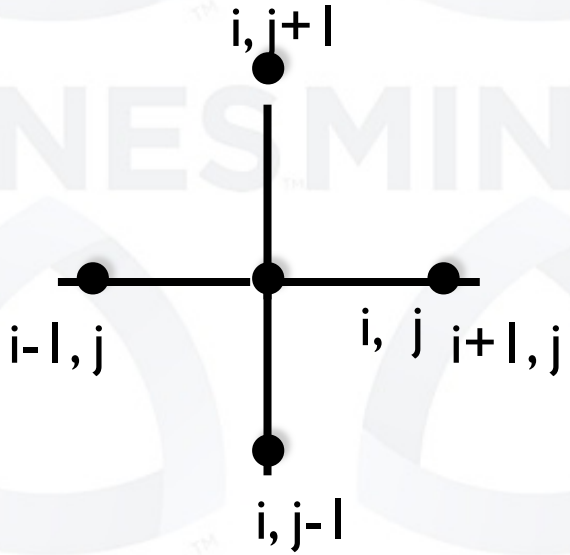
$$a_2 = \frac{\Delta y^2}{2(\Delta x^2 + \Delta y^2)} - \frac{\beta \Delta x^2 \Delta y^2}{4\gamma \Delta x(\Delta x^2 + \Delta y^2)}$$

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

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

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

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

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

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

end do

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

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;
}
```