Introduction to High Performance Scientific Computing

Autumn, 2016

Lecture 17

Project Part 1

- Random walks in 1-D
- Consider equations of the form:

  X(t+dt) = X(t) + F[X(t),dt]

- Here, X and F, are both random variables
- Simplest example: F = +/- dx based on flip of a coin → random walk

Compute several *realizations*, X1(t), X2(t),… XM(t) and then compute statistics over these M realizations

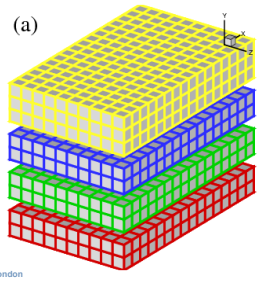
These statistics (the mean and stdev) will generally depend on time

Random walk on a network follows same idea

Send/Recv and domain decomposition

A parallel computation computes a potential field, *f(x,y,z,t)* on four processors.
P0, P1, P2, P3 solve for *f* in separate subdomains

(a)



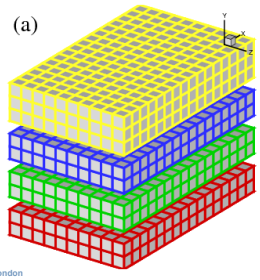
- How would you compute the gradient?

$$\nabla f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right)$$

- No problems with x and z directions
- But what about y?

Last time: Send/Recv

A parallel computation computes a potential field, *f(x,y,z,t)* on four processors.
P0, P1, P2, P3 solve for *f* in separate subdomains



- Send and Recv *must* be paired:
  - If yellow sends to blue, blue must recv from yellow
- Yellow and blue should not send to each other simultaneously
- Instead:

Yellow → Blue
Blue → Green
Green → Red
Red → Yellow (if periodic)

and then the reverse

Parallel differentiation example

```
!-------------------------------------------------------------
!Send data at top boundary up to next processor
!i.e. send f(nlocal+1) to myid+1 and store it there as f(1)
!data from myid=numprocs-1 is sent to myid=0
!-------------------------------------------------------------
    if (myid<numprocs-1) then
        receiver = myid+1
    else
        receiver = 0
    end if

    if (myid>0) then
        sender = myid-1
    else
        sender = numprocs-1
    end if

    call MPI_SEND(f(Nlocal+1),1,MPI_DOUBLE_PRECISION,receiver,0,
                                                  MPI_COMM_WORLD,ierr)
    call MPI_RECV(f(1) 1,MPI_DOUBLE_PRECISION,sender,MPI_ANY_TAG,
                                    MPI_COMM_WORLD,status,ierr)
```


Today

Solving the (steady) 2D heat equation

Heat equation

Task: Compute temperature distribution in a room

Governing equation: Heat equation (diffusion equation):

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T + S(\mathbf{x}, t)$$

$$T(\mathbf{x}, t = 0) = f(\mathbf{x})$$ Initial condition

Here, S is a ***heat source.*** Boundary conditions should also be specified as appropriate.

Problem: given the source, initial condition, and boundary conditions, solve for the temperature distribution, T(**x**,t)

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1-D (steady) heat equation

First consider steady problem, e.g., S = S(x), a and b are constants:

$$\frac{\partial^2 T}{\partial x^2} + S(x) = 0$$ Poisson equation

Numerical method:
1. Discretize the derivative:

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2}$$ 2nd-order, centered scheme

$$x_i = i * \Delta x,\ i = 0, 1, 2, ..., N+1$$
$$(N+1) * \Delta x = 1$$

With boundary conditions: $T_0 = T_a,\ T_N = T_b$

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Programming example

Equation for T_i: $\frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2} = -S_i$

In matrix form: AT = b

$$A = \begin{bmatrix} -2 & 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 & -2 & 1 \\ 0 & \dots & 0 & 0 & 0 & 1 & -2 \end{bmatrix}, \quad b = \frac{1}{\Delta x^2} \begin{bmatrix} -\Delta x^2 T_a - S_1 \\ -S_2 \\ \vdots \\ -S_i \\ \vdots \\ -S_{N-1} \\ -\Delta x^2 T_b - S_N \end{bmatrix}$$

- In 1-D, this is just a tridiagonal system of equations
- Easy to solve directly (with, say, ***DGTSV***)

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Jacobi iteration

- Basic idea: rewrite Ax=b as $A_1x = A_2x + b$
- *Choose* A_1 so that it is easy to invert, then solve iterative system:
- $A_1x^{k+1} = A_2x^k + b$
  - Requires guess, x^0
- *Jacobi iteration*: Choose A_1 to be diagonal matrix (main diagonal of A):

$$\frac{T_{i+1}^{k-1} - 2T_i^k + T_{i-1}^{k-1}}{\Delta x^2} = -S_i$$

$$T_i^k = \frac{\Delta x^2}{2} S_i + \frac{1}{2}\left(T_{i+1}^{k-1} + T_{i-1}^{k-1}\right)$$

Main algorithm, easy to code!

Jacobi iteration in Fortran

- One Fortran trick: set variables to be dimension(0:N+1)
  - x(0)=0, x(N+1)=1, T(0)=a, T(N+1)=b
  - Then, easy to compute T_1 using:

$$T_i^k = \frac{\Delta x^2}{2} S_i + \frac{1}{2}\left(T_{i+1}^{k-1} + T_{i-1}^{k-1}\right)$$

Core part of code (see *jacobi1s.f90*):

```
do k1=1,kmax
   Tnew(1:n) = S(1:n)*dx2f + 0.5d0*(T(0:n-1) + T(2:n+1)) !Jacobi
   deltaT(k1) = maxval(abs(Tnew(1:n)-T(1:n))) !compute relative error
   T(1:n)=Tnew(1:n)    !update variable
   if (deltaT(k1)<tol) exit !check convergence criterion
end do
```


Parallel Jacobi

Let's now parallelize the solver with OpenMP

- Look for loops that can be parallelized
- Look for vectorized operations that can be converted to loops that can be parallelized

Parallel:

```
dmax=0.d0
!$omp parallel do reduction(max:dmax)
do i1=1,n
    Tnew(i1) = S(i1)*dx2f + 0.5d0*(T(i1-1) + T(i1+1))
    dmax = max(dmax,abs(Tnew(i1)-T(i1)))
end do
!$omp end parallel do
deltaT(k1) = dmax
```

2-D (steady) heat equation

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + S(x,y) = 0$$ **Poisson equation**

2-D (steady) heat equation

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + S(x,y) = 0$$ **Poisson equation**

Numerical method:
1. Discretize the derivative:

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_{i,j} \approx \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2}$$

$$\left(\frac{\partial^2 T}{\partial y^2}\right)_{i,j} \approx \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{\Delta y^2}$$

$$\Delta x = \Delta y = \Delta$$

2nd-order, centered scheme

2-D (steady) heat equation

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$$\Delta x = \Delta y = \Delta$$

2nd-order, centered scheme

With boundary conditions: $T(x=0,y) = L(y),\ T(x=1,y) = R(y)$

$T(x,y=0) = D(x),\ T(x,y=1) = U(x)$

2-D (steady) heat equation

Numerical method:
1. Discretize the derivative:

$$\left(\frac{\partial^2 T}{\partial x^2}\right)_{i,j} \approx \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2}$$

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$$\Delta x = \Delta y = \Delta$$

2nd-order, centered scheme

Final equation:

$$\frac{T_{i+1,j} + T_{i,j+1} - 4T_{i,j} + T_{i-1,j} + T_{i,j-1}}{\Delta^2} = -S_i$$

$$x_i = i * \Delta,\ i = 0, 1, 2, ..., N+1$$
$$y_j = j * \Delta,\ j = 0, 1, 2, ..., N+1$$

With b.c.'s imposed at i=0, i=N+1 **and** j=0, j=N+1

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2-D (steady) heat equation

We now have system of n^2 linear equations, AT = B:

$$A = \begin{bmatrix} M & I & 0 & 0 & 0 & \dots & 0 \\ I & M & I & 0 & 0 & \dots & 0 \\ 0 & I & M & I & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & I & M & I \\ 0 & \dots & 0 & 0 & 0 & I & M \end{bmatrix}$$

- **1D: A was tridiagonal**
- **2D: A is now *block* tridiagonal**
- **M is a** n x n **tridiagonal matrix**

$$M = \begin{bmatrix} -4 & 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & -4 & 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & -4 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 & -4 & 1 \\ 0 & \dots & 0 & 0 & 0 & 1 & -4 \end{bmatrix}$$

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2-D (steady) heat equation

We now have system of n^2 linear equations, AT = B:

$$T = \begin{bmatrix} T_{11} \\ T_{21} \\ \vdots \\ T_{n1} \\ T_{12} \\ \vdots \\ T_{n2} \\ \vdots \\ T_{1n} \\ \dots \\ T_{nn} \end{bmatrix} \quad B = \begin{bmatrix} S_{11}\Delta^2 - T_{01} - T_{10} \\ S_{21}\Delta^2 - T20 \\ \vdots \\ S_{n1}\Delta^2 - T_{n0} - T_{n+1,1} \\ S_{12}\Delta^2 - T_{02} \\ \vdots \\ S_{n2}\Delta^2 - T_{n+1,2} \\ \vdots \\ S_{n1}\Delta^2 - T_{n+1,1} \\ \vdots \\ S_{nn}\Delta^2 - T_{n+1,n} - T_{n,n+1}] \end{bmatrix}$$

Boundary conditions appear in appropriate elements of B

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2-D (steady) heat equation

We now have system of n^2 linear equations, AT = B

- Direct solution of n x n matrix: $O(n^3)$ operations (LU decomposition of A + back-substitution with B)
- We have n^2 x n^2 matrix, so on 100 x 100 grid, matrix is 1e4 x 1e4 and contains 1e8 elements (in double precision, that's 800 mb!)
- So, in 2D (and 3D) direct solution becomes expensive and memory-intensive

2-D (steady) heat equation

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- Direct solution of n x n matrix: $O(n^3)$ operations (LU decomposition of A + back-substitution with B)
- We have n^2 x n^2 matrix, so on 100 x 100 grid, matrix is 1e4 x 1e4 and contains 1e8 elements (in double precision, that's 800 mb!)
- So, in 2D (and 3D) direct solution becomes expensive and memory-intensive
- But the matrix, A, is *sparse*, so iterative method will only need to store $O(n^2)$ elements (rather than n^4)
- A good iterative method (SOR, conjugate gradient, multigrid) will be faster as well
- Jacobi iteration is *inefficient,* but a good starting point for looking at iterative methods

2-D (steady) heat equation

Jacobi iteration:

$$T_{i,j}^{k+1} = \frac{\Delta^2}{4} S_i + \frac{1}{4}\left(T_{i+1,j}^{k} + T_{i,j+1}^{k} + T_{i-1,j}^{k} + T_{i,j-1}^{k}\right)$$

- New temperature = Source contribution + average of surrounding temperatures
- How do we convert 1D code → 2D?

2-D (steady) heat equation

Jacobi iteration:

$$T_{i,j}^{k+1} = \frac{\Delta^2}{4} S_i + \frac{1}{4}\left(T_{i+1,j}^k + T_{i,j+1}^k + T_{i-1,j}^k + T_{i,j-1}^k\right)$$

- New temperature = Source contribution + average of surrounding temperatures
- How do we convert 1D code → 2D?
- Plan:
  1. Need 2D variables: x, y, S, T
  2. Intialize 2D field and apply boundary conditions
  3. During iterations, average in two dimensions rather than one

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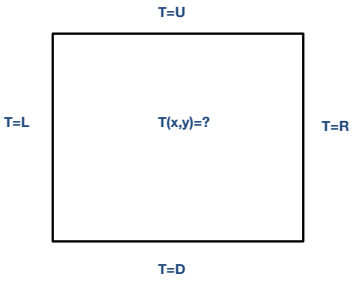
2-D (steady) heat equation

Final problem: Use Jacobi iteration to find T(x,y) on unit square with fixed temperature on boundaries and prescribed source, S(x,y)



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Jacobi iteration in Fortran

1D:

```
do k1=1,kmax
   Tnew(1:n) = S(1:n)*dx2f + 0.5d0*(T(0:n-1) + T(2:n+1)) !Jacobi
   deltaT(k1) = maxval(abs(Tnew(1:n)-T(1:n))) !compute relative error
   T(1:n)=Tnew(1:n)    !update variable
   if (deltaT(k1)<tol) exit !check convergence criterion
end do
```

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Jacobi iteration in Fortran

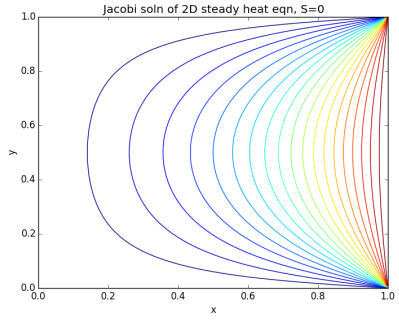
2D (see *jacobi2s.f90*):

```
do k1=1,kmax
        Tnew(1:n,1:n) = S(1:n,1:n)*del2f +
0.25*(T(2:n+1,1:n) + T(0:n-1,1:n) + T(1:n,0:n-1) + T(1:n,2:n+1)) !Jacobi
deltaT(k1) = maxval(abs(Tnew(1:n,1:n)-T(1:n,1:n))) !compute relative
error
        T(1:n,1:n)=Tnew(1:n,1:n)    !update variable
        if (deltaT(k1)<tol) exit !check convergence criterion
    end do
```

- **Run code with** U=D=L=0, R=1
- $S = S_0 \sin(\pi x) \sin(\pi y)$

2-D (steady) heat equation

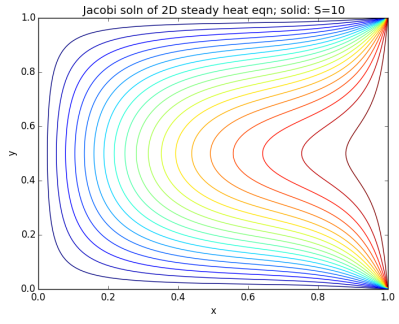
Homogeneous solution (S=0):



The hot wall sets the temperature distribution

2-D (steady) heat equation

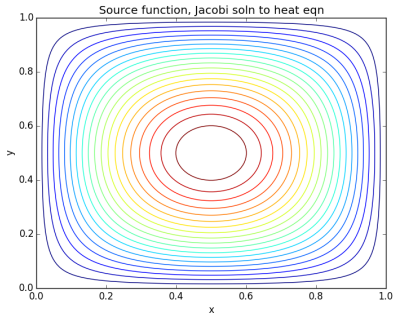
Particular solution (S=10):



Source in middle of room shifts temperature distribution

2-D (steady) heat equation

Source function:



Source in middle of room shifts temperature distribution

2-D (steady) heat equation

Parallelize with OpenMP:

- **Essentially the same as in 1D**
- **Parallel loop iterates across rows of** A
- **Reduction of deltaT to check for convergence**

2-D (steady) heat equation

1D:

```
dmax=0.d0
!$omp parallel do reduction(max:dmax)
do i1=1,n
    Tnew(i1) = S(i1)*dx2f + 0.5d0*(T(i1-1) + T(i1+1))
    dmax = max(dmax,abs(Tnew(i1)-T(i1)))
end do
!$omp end parallel do
deltaT(k1) = dmax
if (deltaT(k1)<tol) exit !check convergence criterion

!$omp parallel do
do i1=1,n
    T(i1) = Tnew(i1)
end do
!$omp end parallel do
```

2-D (steady) heat equation

2D (*see jacobi2s_omp.f90*):

```
dmax = 0.0
!$OMP parallel do reduction(max:dmax)
do j1=1,n
    Tnew(1:n,j1) = S(1:n,j1)*del2f + 0.25*(T(2:n+1,j1) +
  T(0:n-1,j1) + T(1:n,j1-1) + T(1:n,j1+1))!Jacobi iteration
    dmax = max(dmax,maxval(abs(Tnew(1:n,j1)-T(1:n,j1))))
end do
!$OMP end parallel do
deltaT(k1) = dmax
if (deltaT(k1)<tol) exit !check convergence criterion
!$OMP parallel do
do j1=1,n
    T(1:n,j1) = Tnew(1:n,j1)
end do
!$OMP end parallel do
```

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2-D (steady) heat equation

- Moving from 1D serial to 2D parallel (with OpenMP) is straightforward
- Much more difficult if solving equations directly
- What about MPI?

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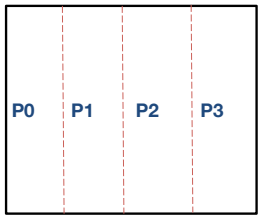
2-D (steady) heat equation

What is best domain decomposition?

If we have four processors, can try:



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2-D (steady) heat equation

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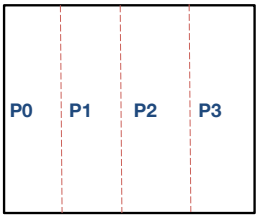


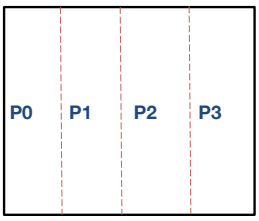
Then, parallelization is essentially same as differentiation example:

- Loop across rows
- At "boundary" rows, send/recv data needed to compute second derivative
- Reduce max(|deltaT|)

2-D (steady) heat equation

What is best domain decomposition?

If we have four processors, can try:

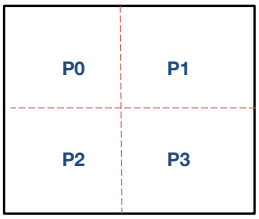


- But is the 1D decomposition the best?
- Want to minimize communication
- M "layers": of a n x n grid:
  - (M-1)*n boundary points

2-D (steady) heat equation

What is best domain decomposition?

If we have four processors, can also try:

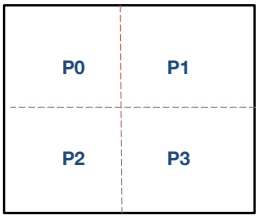


- But is the 1D decomposition the best?
- Want to minimize communication
- M "boxes": of a n x n grid:
  - Each interior box has 2n/sqrt(M) boundary points
  - Total: 2n*(sqrt(M)-1) boundary points

2-D (steady) heat equation

What is best domain decomposition?

If we have four processors, can also try:



- But is the 1D decomposition the best?
- Want to minimize communication
- M "boxes": of a n x n grid:
  - Each box has 2n/sqrt(M) boundary points
  - Total: 2n*(sqrt(M) -1) boundary points
- Boxes: less communication, but more difficult to implement!

2-D (steady) heat equation

- MPI provides tools for creating and managing complex "topologies"
- For example, to create a 4 x 3 "grid" of processes:

```
call MPI_cart_create(MPI_COMM_WORLD, ndims, dims, periods, reorder,
                     new_comm, ierr)
```

with: ndims = 2, dims = (/4,3/), periods = (/.false.,/.true/), reorder = .false.

- Here, periods sets periodic boundary conditions along the three columns

2-D (steady) heat equation

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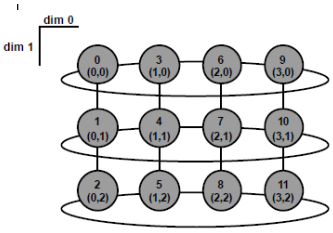
- Here, periods sets periodic boundary conditions along the three columns
- Other useful commands with the new communicator, new_comm:
  - MPI_Cart_coords: given process id, provides (i,j) coordinate
  - MPI_Cart_rank: given (i,j), provides id (0, 1, 2, …, numprocs)
- Most useful: MPI_Cart_shift: provides id of neighboring processes in horizontal or vertical direction
  - Use to set up send/recv sequences needed for exchanging boundary data.

2-D (steady) heat equation

- **Most useful:** MPI_Cart_shift**: provides id of neighboring processes in horizontal or vertical direction**
  - **Use to set up send/recv sequences needed for exchanging boundary data.**
- **How to decide on process grid dimensions?**
- MPI_Dims_create:
Given number number of processes and dimensions, outputs process grid Dimensions (4,3 in picture →)
- **e.g. 400 x 300 grid points:**
4 x 3 process grid with
100 x 100 points on each grid



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