

Outline:

- Heat equation and discretization
- OpenMP and MPI for iterative methods
- Jacobi, Gauss-Seidel, SOR

Notes and Sample codes:

- Class notes: Linear algebra software
- `$UWHPSC/codes/openmp/jacobi1d_omp1.f90`
- `$UWHPSC/codes/openmp/jacobi1d_omp2.f90`
- `$UWHPSC/codes/mpi/jacobi1d_mpi.f90`

Steady state diffusion

If $f(x, t) = f(x)$ does not depend on time and if the boundary conditions don't depend on time, then $u(x, t)$ will converge towards steady state distribution satisfying

$$0 = Du_{xx}(x) + f(x)$$

(by setting $u_t = 0$.)

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This is now an **ordinary differential equation (ODE)** for $u(x)$.

We can solve this on an interval, say $0 \leq x \leq 1$ with

Boundary conditions:

$$u(0) = \alpha, \quad u(1) = \beta.$$

Finite difference method

$$U_i \approx u(x_i)$$

$$u_x(x_{i+1/2}) \approx \frac{U_{i+1} - U_i}{\Delta x}$$

$$u_x(x_{i-1/2}) \approx \frac{U_i - U_{i-1}}{\Delta x}$$

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So we can **approximate second derivative** at x_i by:

$$\begin{aligned} u_{xx}(x_i) &\approx \frac{1}{\Delta x} \left(\frac{U_{i+1} - U_i}{\Delta x} - \frac{U_i - U_{i-1}}{\Delta x} \right) \\ &= \frac{1}{\Delta x^2} (U_{i-1} - 2U_i + U_{i+1}) \end{aligned}$$

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This gives coupled system of n linear equations:

$$\frac{1}{\Delta x^2} (U_{i-1} - 2U_i + U_{i+1}) = -f(x_i)$$

for $i = 1, 2, \dots, n$. With $U_0 = \alpha$ and $U_{n+1} = \beta$.

Coupled system of n linear equations:

$$(U_{i-1} - 2U_i + U_{i+1}) = -\Delta x^2 f(x_i)$$

for $i = 1, 2, \dots, n$. With $U_0 = \alpha$ and $U_{n+1} = \beta$.

Iterative method starts with initial guess $U^{[0]}$ to solution and then improves $U^{[k]}$ to get $U^{[k+1]}$ for $k = 0, 1, \dots$

Note: Generally does not involve modifying matrix A .

Do not have to store matrix A at all, only know about stencil.

Jacobi iteration

$$(U_{i-1} - 2U_i + U_{i+1}) = -\Delta x^2 f(x_i)$$

Solve for U_i :

$$U_i = \frac{1}{2} (U_{i-1} + U_{i+1} + \Delta x^2 f(x_i)) .$$

Note: With no heat source, $f(x) = 0$,
the temperature at each point is average of neighbors.

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Suppose $U^{[k]}$ is a approximation to solution. Set

$$U_i^{[k+1]} = \frac{1}{2} \left(U_{i-1}^{[k]} + U_{i+1}^{[k]} + \Delta x^2 f(x_i) \right) \quad \text{for } i = 1, 2, \dots, n.$$

Repeat for $k = 0, 1, 2, \dots$ until convergence.

Can be shown to converge (eventually... **very slow!**)

Jacobi iteration in Fortran

```
uold = u ! starting values before updating
do iter=1,maxiter
  dumax = 0.d0
  do i=1,n
    u(i) = 0.5d0*(uold(i-1) + uold(i+1) + dx**2*f(i))
    dumax = max(dumax, abs(u(i)-uold(i)))
  enddo

  ! check for convergence:
  if (dumax .lt. tol) exit

  uold = u ! for next iteration
enddo
```

Note: we must use old value at $i - 1$ for Jacobi.

Otherwise we get the **Gauss-Seidel** method.

$$u(i) = 0.5d0*(u(i-1) + u(i+1) + dx**2*f(i))$$

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Note: we must use old value at $i - 1$ for Jacobi.

Otherwise we get the **Gauss-Seidel** method.

$$u(i) = 0.5d0*(u(i-1) + u(i+1) + dx**2*f(i))$$

This actually converges faster!

Jacobi with OpenMP – coarse grain

General Approach:

- Fork threads only once at start of program.
- Each thread is responsible for some portion of the arrays, from `i=istart` to `i=iend`.
- Each iteration, must copy `u` to `uold`, update `u`, check for convergence.
- Convergence check requires coordination between threads to get global `dumax`.
- Print out final result after leaving parallel block

See code in the repository or the notes:

[\\$UWHPSC/codes/openmp/jacobi1d_omp2.f90](#)

Jacobi with MPI

Each process is responsible for some portion of the arrays,
from $i=i_{\text{start}}$ to $i=i_{\text{end}}$.

No shared memory: each process only has part of array.

Updating formula:

$$u(i) = 0.5d0*(uold(i-1) + uold(i+1) + dx**2*f(i))$$

Need to exchange values at boundaries:

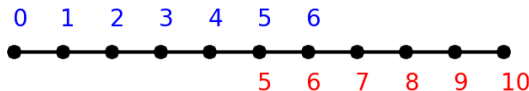
Updating at $i=i_{\text{start}}$ requires $uold(i_{\text{start}}-1)$

Updating at $i=i_{\text{end}}$ requires $uold(i_{\text{start}}+1)$

Example with $n = 9$ interior points (plus boundaries):

Process 0 has $i_{\text{start}} = 1$, $i_{\text{end}} = 5$

Process 1 has $i_{\text{start}} = 6$, $i_{\text{end}} = 9$



Jacobi with MPI — Sending to neighbors

```
call mpi_comm_rank(MPI_COMM_WORLD, me, ierr)
...
do iter = 1, maxiter
  uold = u

  if (me > 0) then
    ! Send left endpoint value to "left"
    call mpi_isend(uold(istart), 1, MPI_DOUBLE_PRECISION,
                  me - 1, 1, MPI_COMM_WORLD, req1, ierr)
  end if

  if (me < ntasks-1) then
    ! Send right endpoint value to "right"
    call mpi_isend(uold(iend), 1, MPI_DOUBLE_PRECISION,
                  me + 1, 2, MPI_COMM_WORLD, req2, ierr)
  end if
end do
```

Note: Non-blocking `mpi_isend` is used,

Different tags (1 and 2) for left-going, right-going messages.

Jacobi with MPI — Receiving from neighbors

Note: `uold(istart)` from `me+1` goes into `uold(iend+1)`:
`uold(iend)` from `me-1` goes into `uold(istart-1)`:

```
do iter = 1, maxiter
  ! mpi_send's from previous slide
  if (me < ntasks-1) then
    ! Receive right endpoint value
    call mpi_recv(uold(iend+1), 1, MPI_DOUBLE_PRECISION,
                 me + 1, 1, MPI_COMM_WORLD, mpistatus, ierr)
  end if

  if (me > 0) then
    ! Receive left endpoint value
    call mpi_recv(uold(istart-1), 1, MPI_DOUBLE_PRECISION,
                 me - 1, 2, MPI_COMM_WORLD, mpistatus, ierr)
  end if

  ! Apply Jacobi iteration on my section of array
  do i = istart, iend
    u(i) = 0.5d0*(uold(i-1) + uold(i+1) + dx**2*f(i))
    dumax_task = max(dumax_task, abs(u(i) - uold(i)))
  end do
end do
```

Jacobi with MPI

Other issues:

- Convergence check requires coordination between processes to get global `dumax`.
Use `MPI_ALLREDUCE` so all process check same value.
- Part of final result must be printed by each process (into common file `heatsoln.txt`), in proper order.

See code in the repository or the notes:

[\\$UWHPSC/codes/mpi/jacobi1d_mpi.f90](#)

Jacobi with MPI — Writing solution in order

Want to write table of values $x(i), u(i)$ in `heatsoln.txt`.

Need them to be in proper order, so Process 0 must write to this file first, then Process 1, etc.

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Approach:

Each process m_e waits for a message from m_e-1 indicating that it has finished writing its part. (Contents not important.)

Each process must open the file (without clobbering values already there), write to it, then close the file.

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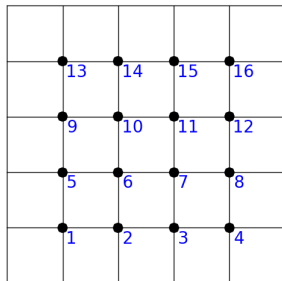
Each process must open the file (without clobbering values already there), write to it, then close the file.

Assumes all processes share a file system!

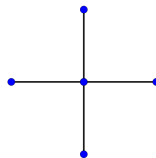
On cluster or supercomputer, need to either:
send all results to single process for writing, or
write distributed files that may need to be combined later
(some visualization tools handle distributed data!)

Jacobi in 2D

Row-wise ordering



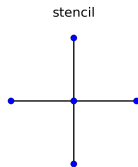
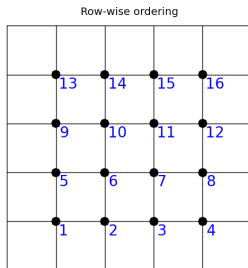
stencil



Updating point 7 for example (u_{32}):

$$U_{32}^{[k+1]} = \frac{1}{4}(U_{22}^{[k]} + U_{42}^{[k]} + U_{21}^{[k]} + U_{41}^{[k]} + h^2 f_{32})$$

Jacobi in 2D using MPI



With two processes: Could partition unknown into

Process 0 takes grid points 1–8

Process 1 takes grid points 9–16

Each time step:

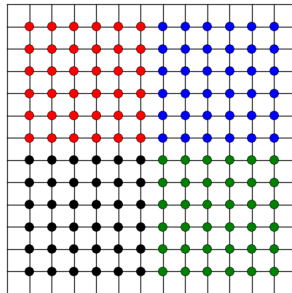
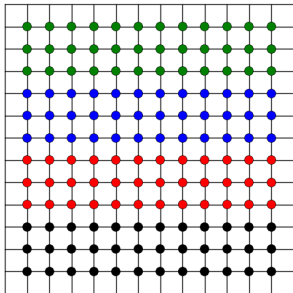
Process 0 sends top boundary (5–8) to Process 1,

Process 1 sends bottom boundary (9–12) to Process 0.

Jacobi in 2D using MPI

With more grid points and processes...

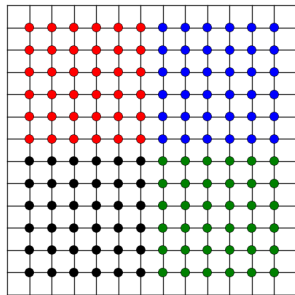
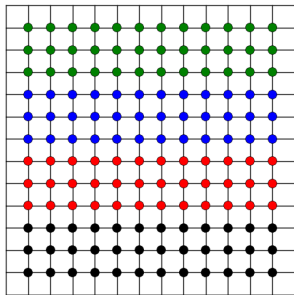
Could partition several different ways, e.g. with 4 processes:



Jacobi in 2D using MPI

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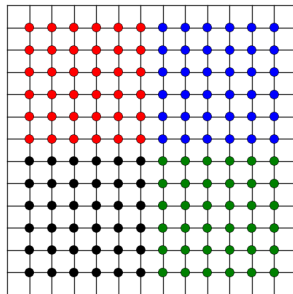
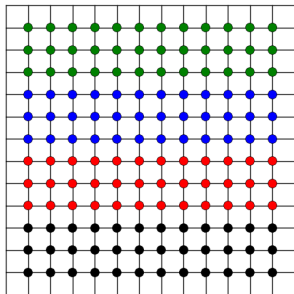
The partition on the right requires less communication.

With m^2 processes on grid with n^2 points:

$2(m^2 - 1)n$ boundary points on left,

$4(m - 1)n$ boundary points on right.

Jacobi in 2D using MPI



For partition on left: Natural to number processes 0,1,2,3 and pass boundary data from Process k to $k \pm 1$.

For $m \times m$ array of processors as on right: How do we figure out the neighboring process numbers?

Creating a communicator for Cartesian blocks

```
integer dims(2)
logical isperiodic(2), reorder

ndim = 2          ! 2d grid of processes
dims(1) = 4       ! for 4x6 grid of processes
dims(2) = 6
isperiodic(1) = .false.    ! periodic in x?
isperiodic(2) = .false.    ! periodic in y?
reorder = .true.          ! optimize ordering

call MPI_CART_CREATE(MPI_COMM_WORLD, ndim, &
                     dims, isperiodic, reorder, comm2d, ierr)
```

Create communicator [comm2d](#). See also:

[MPI_CART_CREATE](#), [MPI_CART_SHIFT](#), [MPI_CART_COORDS](#).

Gauss-Seidel iteration in Fortran

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do iter=1,maxiter
  dumax = 0.d0
  do i=1,n
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    dumax = max(dumax, abs(u(i)-uold))
  enddo

  ! check for convergence:
  if (dumax .lt. tol) exit

enddo
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Good news: This converges about twice as fast as Jacobi!

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But... loop carried dependence! Cannot parallelize so easily.

Red-black ordering

We are free to write equations of linear system in any order...
reordering rows of coefficient matrix, right hand side.

Can also number unknowns of linear system in any order...
reordering elements of solution vector.

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reordering elements of solution vector.

Red-black ordering: Iterate through points with odd index first ($i = 1, 3, 5, \dots$) and then even index points ($i = 2, 4, 6, \dots$).

Then all black points can be updated in any order,
all red points can then be updated in any order.

Same asymptotic convergence rate as natural ordering.



Red-Black Gauss-Seidel

```
do iter=1,maxiter
  dumax = 0.d0

  ! UPDATE ODD INDEX POINTS:
  !$omp parallel do reduction(max : dumax) &
  !$omp private(uold)
  do i=1,n,2
    uold = u(i)
    u(i) = 0.5d0*(u(i-1) + u(i+1) + dx**2*f(i))
    dumax = max(dumax, abs(u(i)-uold))
  enddo

  ! UPDATE EVEN INDEX POINTS:
  !$omp parallel do reduction(max : dumax) &
  !$omp private(uold)
  do i=2,n,2
    uold = u(i)
    u(i) = 0.5d0*(u(i-1) + u(i+1) + dx**2*f(i))
    dumax = max(dumax, abs(u(i)-uold))
  enddo

  ! check for convergence:
  if (dumax .lt. tol) exit
enddo
```

Gauss-Seidel method in 2D

If $\Delta x = \Delta y = h$:

$$\frac{1}{h^2} (U_{i-1,j} + U_{i+1,j} + U_{i,j-1} + U_{i,j+1} - 4U_{i,j}) = -f(x_i, y_j).$$

Solve for $U_{i,j}$ and iterate:

$$u_{i,j}^{[k+1]} = \frac{1}{4} (u_{i-1,j}^{[k+1]} + u_{i+1,j}^{[k]} + u_{i,j-1}^{[k+1]} + u_{i,j+1}^{[k]} - h^2 f_{i,j})$$

Again no need for matrix A .

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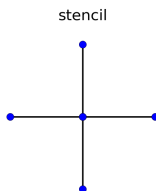
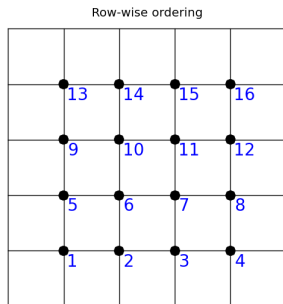
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Note: Above indices for old and new values assumes we iterate in the **natural row-wise order**.

Gauss-Seidel in 2D

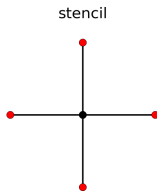
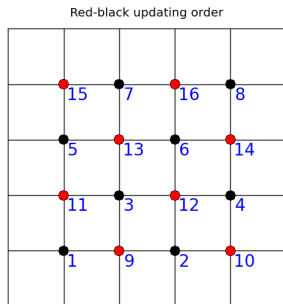


Updating point 7 for example (u_{32}):

Depends on **new values** at points 6 and 3, **old** values at points 7 and 10.

$$U_{32}^{[k+1]} = \frac{1}{4}(U_{22}^{[k+1]} + U_{42}^{[k]} + U_{21}^{[k+1]} + U_{41}^{[k]} + h^2 f_{32})$$

Red-black ordering in 2D



Again all black points can be updated in any order:

New value depends only on red neighbors.

Then all red points can be updated in any order:

New value depends only on black neighbors.

SOR method

Gauss-Seidel move solution in right direction but not far enough in general.

Iterates “relax” towards solution.

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Iterates “relax” towards solution.

Successive Over-Relaxation (SOR):

Compute Gauss-Seidel approximation and then go further:

$$U_i^* = \frac{1}{2}(U_{i-1}^{[k+1]} + U_{i+1}^{[k]} + \Delta x^2 f(x_i))$$
$$U_i^{[k+1]} = U_i^{[k]} + \omega(U_i^* - U_i^{[k]})$$

where $1 < \omega < 2$.

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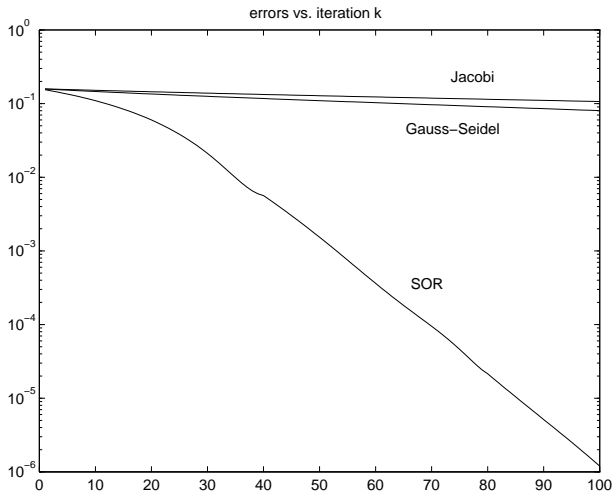
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$$U_i^{[k+1]} = U_i^{[k]} + \omega(U_i^* - U_i^{[k]})$$

where $1 < \omega < 2$.

Optimal omega (For this problem): $\omega = 2 - 2\pi\Delta x$.

Convergence rates



Red-Black SOR in 1D

```
do iter=1,maxiter
  dumax = 0.d0

  ! UPDATE ODD INDEX POINTS:
  !$omp parallel do reduction(max : dumax) &
  !$omp private(uold, ustar)
  do i=1,n,2
    uold = u(i)
    ustar = 0.5d0*(u(i-1) + u(i+1) + dx**2*f(i))
    u(i) = uold + omega*(ustar-uold)
    dumax = max(dumax, abs(u(i)-uold))
  enddo

  ! UPDATE EVEN INDEX POINTS:
  !$omp parallel do reduction(max : dumax) &
  !$omp private(uold, ustar)
  do i=2,n,2
    uold = u(i)
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    u(i) = uold + omega*(ustar-uold)
    dumax = max(dumax, abs(u(i)-uold))
  enddo

  ! check for convergence...
```

Note that `uold`, `ustar` must be **private**!

Announcements

Homework 6 is in the notes and due next **Friday**.

Quizzes for this week's lectures due next **Wednesday**.

Office hours today 9:30 – 10:20.

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Next week:

Monday: no class

Wednesday: Guest lecture —

Brad Chamberlain, Cray

Chapel: A Next-Generation Partitioned
Global Address Space (PGAS) Language