Today:

- OpenMP and MPI versions of Jacobi iteration
- Gauss-Seidel and SOR iterative methods

Next week:

- More MPI
- Debugging and totalview
- GPU computing

Read: Class notes and references

$\text{CLASSHG/codes/openmp/jacobi1.f90}$

$\text{CLASSHG/codes/openmp/jacobi2_omp.f90}$

$\text{CLASSHG/codes/mpi/jacobi2_mpi.f90}$
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.
(\(U_{i-1} - 2U_i + U_{i+1}\)) = -\(\Delta x^2 f(x_i)\)

Solve for \(U_i\):

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

Suppose \(U^{[k]}\) is a approximation to solution. Set

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

Repeat for \(k = 0, 1, 2, \ldots\) until convergence.

Can be shown to converge (eventually... very slow!)
General Approach:

- Fork threads only once at start of program.
- Each thread is responsible for some portion of the arrays, from \( i=\text{istart} \) to \( i=\text{iend} \).
- Each iteration, must copy \( u \) to \( u_{\text{old}} \), update \( u \), check for convergence.
- Convergence check requires coordination between threads to get global \( d_{\text{umax}} \).
- Print out final result after leaving parallel block.

See code in the repository or the notes:

\[ \$\text{CLASSHG/codes/openmp/jacobi2_omp.f90} \]
Jacobi with MPI

Each process is responsible for some portion of the arrays, from \( i=\text{istart} \) to \( i=\text{iend} \).

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

**Updating formula:**
\[
  u(i) = 0.5d0 \times (\text{uold}(i-1) + \text{uold}(i+1) + \text{dx}^2 \times f(i))
\]

Need to exchange values at boundaries:
- Updating at \( i=\text{istart} \) requires \( \text{uold}(\text{istart}-1) \)
- Updating at \( i=\text{iend} \) requires \( \text{uold}(\text{istart}+1) \)

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

- **Process 0 has** \( \text{istart} = 1, \text{iend} = 5 \)
- **Process 1 has** \( \text{istart} = 6, \text{iend} = 9 \)
Other issues:

- Convergence check requires coordination between processes to get global $d_{u \text{max}}$. Use \texttt{MPI\_ALLREDUCE} so all process check same value.

- Part of final result must be printed by each process (into common file \texttt{heatsoln.txt}), in proper order.

See code in the repository or the notes:

\texttt{$CLASSHG/codes/mpi/jacobi2_mpi.f90}$
real(kind = 8), dimension(:), allocatable :: f, u, uold

... 

points_per_task = \( \frac{n + ntasks - 1}{ntasks} \)

call mpi_comm_rank(MPI_COMM_WORLD, me, ierr)

istart = me * points_per_task + 1

iend = \( \min((me + 1)*\text{points}_\text{per}_\text{task}, n) \)

allocate(f(istart-1:iend+1), u(istart-1:iend+1), &
         uold(istart-1:iend+1))

Note that each process works on only a part of the array.

Distributed memory model, so no large shared array.

Includes “ghost cells” to store boundary values from neighboring processes.
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: \texttt{uold(istart)} from \texttt{me+1} goes into \texttt{uold(iend+1)}:
\texttt{uold(iend)} from \texttt{me-1} goes into \texttt{uold(istart-1)}:

\begin{verbatim}
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
\end{verbatim}
Jacobi with MPI — Convergence test

```
do iter = 1, maxiter

  ! Send and receive boundary data (previous slides)
  dumax_task = 0.d0

  ! Jacobi update:
  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

  ! Take global maximum of dumax values
  call mpi_allreduce(dumax_task, dumax_global, 1, &
    MPI_DOUBLE_PRECISION, &
    MPI_MAX, MPI_COMM_WORLD, ierr)

  if (dumax_global < tol) exit

enddo
```
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.
Jacobi with MPI — Writing solution in order

Want to write table of values \( x(i), u(i) \) in \texttt{heatsoln.txt}.

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

Approach:

Each process \texttt{me} waits for a message from \texttt{me-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.
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.

**Approach:**

Each process $m$ waits for a message from $m-1$ 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.

**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!)
One-dimensional equation generalizes to

\[ u_t(x, y, t) = D(u_{xx}(x, y, t) + u_{yy}(x, y, t)) + f(x, y, t) \]

on some domain in the \( x-y \) plane, with initial and boundary conditions.

We will only consider rectangle \( 0 \leq x \leq 1, \ 0 \leq y \leq 1. \)
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We will only consider rectangle $0 \leq x \leq 1, \ 0 \leq y \leq 1$.

**Steady state problem (with $D = 1$):**

$$u_{xx}(x, y) + u_{yy}(x, y) = -f(x, y)$$
\[
\frac{1}{h^2} (U_{i-1,j} + U_{i+1,j} + U_{i,j-1} + U_{i,j+1} - 4U_{i,j}) = -f(x_i, y_j).
\]

On \( n \times n \) grid (\( \Delta x = \Delta y = 1/(n + 1) \)) this gives a linear system of \( n^2 \) equations in \( n^2 \) unknowns.

The above equation must be satisfied for \( i = 1, 2, \ldots, n \) and \( j = 1, 2, \ldots, n \).

Matrix is \( n^2 \times n^2 \),

- e.g. on 100 by 100 grid, matrix is \( 10,000 \times 10,000 \).
- Contains \((10,000)^2 = 100,000,000\) elements.
Finite difference equations in 2D

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Matrix is \textit{sparse}: each row has at most 5 nonzeros out of \( n^2 \) elements! But structure is no longer tridiagonal.
Finite difference equations in 2D

Matrix has block tridiagonal structure:

\[ A = \frac{1}{h^2} \begin{bmatrix} \begin{bmatrix} T & I \\ I & T \\ I & T \end{bmatrix} & \begin{bmatrix} I & I \\ T & T \\ I & I \end{bmatrix} \end{bmatrix} \]

\[ T = \begin{bmatrix} -4 & 1 \\ 1 & -4 & 1 \\ 1 & -4 \end{bmatrix} \]
Jacobi in 2D

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

The partition on the right requires less communication.

With \( m^2 \) processes on grid with \( n^2 \) points,
\( 2m^2n \) boundary points on left, \( 2mn \) boundary points on right.
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)

Can find neighboring processes within comm2d using
MPI_CART_SHIFT
Gauss-Seidel iteration in Fortran

```fortran
do iter=1,maxiter
    dumax = 0.d0
    do i=1,n
        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
```

**Note:** Now \( u(i) \) depends on value of \( u(i-1) \) that has already been updated for previous \( i \).
Gauss-Seidel iteration in Fortran

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**Good news:** This converges about twice as fast as Jacobi!
Gauss-Seidel iteration in Fortran

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\end{verbatim}

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

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

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

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.
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 \( A \).
Gauss-Seidel method in 2D

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$$

Again no need for matrix $A$.

**Note:** Above indices for old and new values assumes we iterate in the natural row-wise order.
Gauss-Seidel in 2D

Row-wise ordering

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.
SOR method

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

Iterates “relax” towards solution.

Successive Over-Relaxation (SOR):

Compute Gauss-Seidel approximation and then go further:

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

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

where \(1 < \omega < 2\).
SOR method

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U_{i}^{[k+1]} = U_{i}^{[k]} + \omega(U_{i}^{GS} - U_{i}^{[k]})
\]

where \(1 < \omega < 2\).

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

errors vs. iteration k

Jacobi

Gauss–Seidel

SOR

R.J. LeVeque, University of Washington

AMath 483/583, Lecture 21, May 13, 2011
do iter=1,maxiter
dumax = 0.d0

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

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

! check for convergence...

Note that _uold_, _ugs_ must be _private_!