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
$CLASSHG/codes/openmp/jacobi1.f90
$CLASSHG/codes/openmp/jacobi2_omp.f90
$CLASSHG/codes/mpi/jacobi2_mpi.f90

Jacobi iteration

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

Solve for \(U_i\):
\[U_i = \frac{1}{2} \left( U_{i-1} + U_{i+1} + \Delta x^2 f(x_i) \right).\]

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

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

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

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 \(i=\text{istart}\) to \(i=i\text{end}\).
- Each iteration, must copy \(u\) to \(u\text{old}\), update \(u\), check for convergence.
- Convergence check requires coordination between threads to get global \(\text{dumax}\).
- Print out final result after leaving parallel block

See code in the repository or the notes:
$CLASSHG/codes/openmp/jacobi2_omp.f90

Jacobi with MPI

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

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

Updating formula:
\[u(i) = 0.5d0*(u\text{old}(i-1) + u\text{old}(i+1) + \Delta x^2*2*f(i))\]

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

Example with \(n = 9\) interior points (plus boundaries):
- Process 0 has \(\text{istart} = 1, \text{iend} = 5\)
- Process 1 has \(\text{istart} = 6, \text{iend} = 9\)
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:
$CLASSHG/codes/mpi/jacobi2_mpi.f90

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Jacobi with MPI — splitting up arrays

```fortran
real(kind=8),dimension(:), allocatable :: f, u, uold

... points_per_task = (n + ntasks - 1)/ntasks
call mpi_comm_rank(MPI_COMM_WORLD, me, ierr)
istart = me * points_per_task + 1
iend = min((me + 1)*points_per_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.

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Jacobi with MPI — Sending to neighbors

```fortran
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, 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, 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.

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Jacobi with MPI — Receiving from neighbors

```fortran
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
```

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Jacobi with MPI — Convergence test

```fortran
! 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
```

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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!)

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Heat equation in 2 dimensions

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 \(0 \leq x \leq 1, 0 \leq y \leq 1\).

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

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

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Finite difference equations in 2D

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

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.

Matrix is **sparse**: each row has at most 5 nonzeros out of \(n^2\) elements! But structure is no longer tridiagonal.

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Finite difference equations in 2D

Matrix has block tridiagonal structure:

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

\[
T = \begin{bmatrix}
-4 & 1 & & \\
1 & -4 & 1 & \\
& 1 & -4 & 1 \\
& & 1 & -4 \\
\end{bmatrix}
\]

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.

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.
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

```fortran
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,nuold = 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
endo
```

Note: Now $u(i)$ depends on value of $u(i-1)$ that has already been updated for previous $i$.

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.

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

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:

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

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

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.

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 \(1 < \omega < 2\).

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

Convergence rates

Red-Black SOR in 1D

```fortran
     do iter=1,maxiter
       dumax = 0.0d0
       ! 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))
       enddo
       ! 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))
       enddo
     ! check for convergence...
     note that uold, ugs must be private!
```

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