AMath 483/583 — Lecture 20 — May 11, 2011

Today:

- Heat equation and discretization
- Iterative methods

Friday:

- Iterative methods

Read: Class notes and references

$CLASSHG/codes/openmp/jacobi1.f90

$CLASSHG/codes/openmp/jacobi2_omp.f90

$CLASSHG/codes/mpi/jacobi2_mpi.f90

Heat Equation / Diffusion Equation

Partial differential equation for $u(x,t)$ in one space dimension and time.

u represents temperature in a 1-dimensional metal rod, for example.

Or concentration (density) of a chemical diffusing in a tube of water.

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Or concentration (density) of a chemical diffusing in a tube of water.

The PDE is

$$u_t(x,t) = Du_{xx}(x,t) + f(x,t)$$

where subscripts represent partial derivatives,

$D =$ diffusion coefficient,

$f(x,t) =$ source term.

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 $u_t = 0$.)

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

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

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

Boundary conditions:

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

Steady state diffusion

More generally: Take $D = 1$ or absorb in f,

$$u_{xx}(x) = -f(x) \qquad \text{for } 0 \le x \le 1,$$

Boundary conditions:

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

Can be solved exactly if we can integrate f twice and use boundary conditions to choose the two constants of integration.

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Example: $f(x) = 0, \quad \alpha = 20, \quad \beta = 60$:

Solution: $u(x) = \alpha + x(\beta - \alpha)$.

No heat source $\implies$ linear variation in steady state ($u_{xx} = 0$).

Steady state diffusion

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Boundary conditions:

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

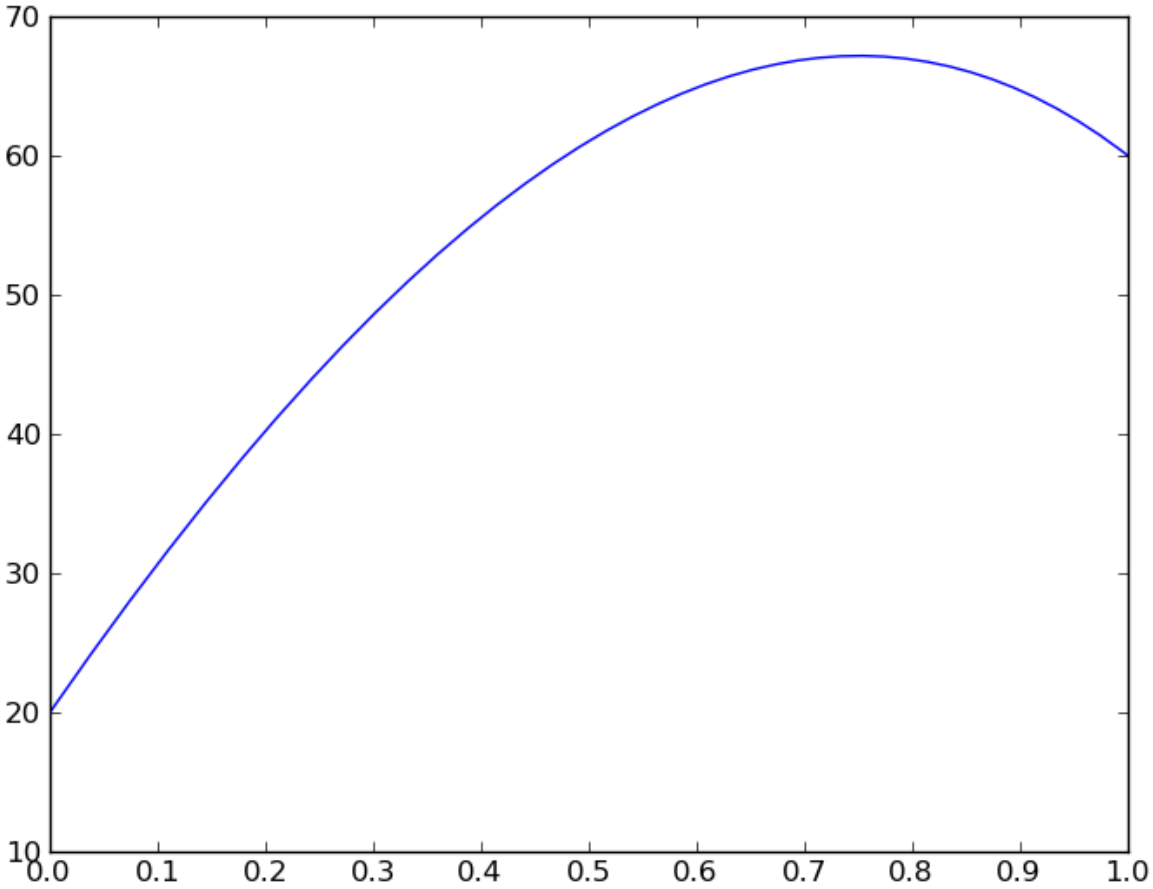
Can be solved exactly if we can integrate f twice and use boundary conditions to choose the two constants of integration.

More interesting example:

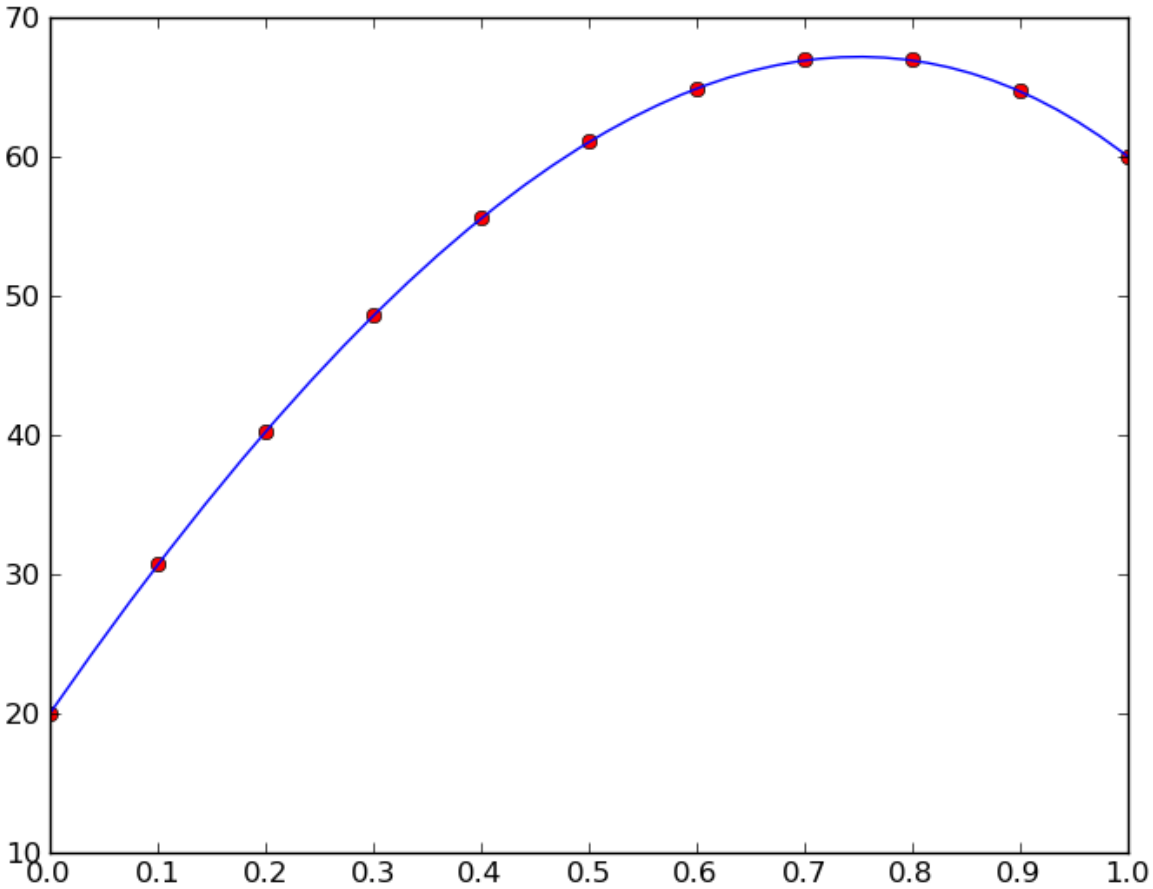
Example: $f(x) = 100e^x, \quad \alpha = 20, \quad \beta = 60$:

Solution: $u(x) = -100e^x + (100e - 60)x + 120.$

Steady state diffusion



Steady state diffusion



For more complicated equations, numerical methods must generally be used, giving approximations at discrete points.

Finite difference method

Define grid points $x_i = i\Delta x$ in interval $0 \le x \le 1$, where

$$\Delta x = \frac{1}{n+1}$$

So $x_0 = 0,\ x_{n+1} = 1$, and the n grid points $x_1,\ x_2,\ \ldots,\ x_n$ are equally spaced inside the interval.

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Let $U_i \approx u(x_i)$ denote approximate solution.

We know $U_0 = \alpha$ and $U_{m+1} = \beta$ from boundary conditions.

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Idea: Replace differential equation for $u(x)$ by system of n algebraic equations for U_i values ($i = 1,\ 2,\ \ldots,\ n$).

Finite difference method

$$U_i \approx u(x_i)$$

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

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

Finite difference method

$U_i \approx u(x_i)$

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

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

So we can approximate second derivative at x_i by:

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

Finite difference method

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

This gives coupled system of n linear equations:

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

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

Tridiagonal linear system

For $n = 5$:

$$\begin{bmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \\ U_5 \end{bmatrix} = -\Delta x^2 \begin{bmatrix} f(x_1) \\ f(x_2) \\ f(x_3) \\ f(x_4) \\ f(x_5) \end{bmatrix} - \begin{bmatrix} \alpha \\ 0 \\ 0 \\ 0 \\ \beta \end{bmatrix}.$$

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General $n \times n$ system requires $O(n^3)$ flops to solve.

Tridiagonal $n \times n$ system requires $O(n)$ flops to solve.

Could use LAPACK routine `dgtsv`.

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 $0 \le x \le 1, \;\; 0 \le y \le 1$.

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We will only consider rectangle $0 \le x \le 1, \;\; 0 \le y \le 1$.

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

$$u_{xx}(x, y) + u_{yy}(x, y) = -f(x, y)$$

Finite difference equations in 2D

Let $U_{ij} \approx u(x_i, y_j)$.

Replace differential equation

$$u_{xx}(x, y) + u_{yy}(x, y) = -f(x, y)$$

by algebraic equations

$$\frac{1}{\Delta x^2}\left(U_{i-1,j} - 2U_{i,j} + U_{i+1,j}\right) + \frac{1}{\Delta y^2}\left(U_{i,j-1} - 2U_{i,j} + U_{i,j+1}\right) = -f(x_i, y_j)$$

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

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

Finite difference equations in 2D

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

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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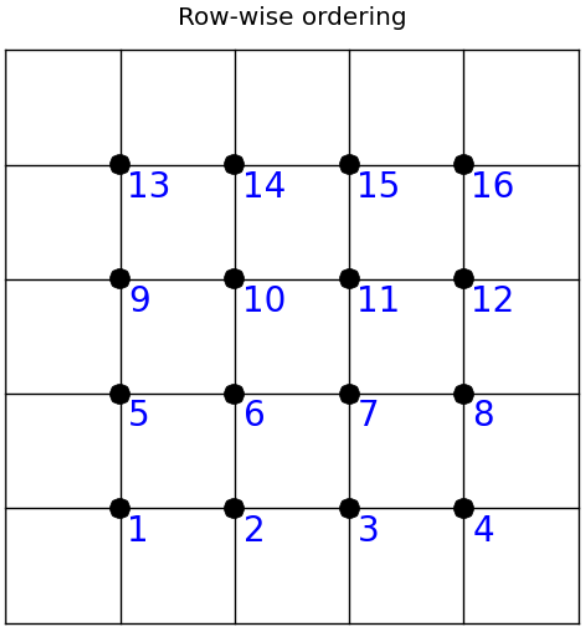
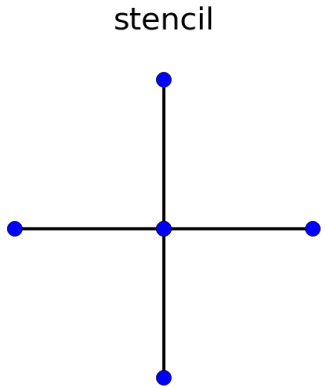
Contains $(10,000)^2 = 100,000,000$ elements.

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

Finite difference equations in 2D





Matrix has block tridiagonal structure:

$$A = \frac{1}{h^2}\begin{bmatrix} T & I & & \\ I & T & I & \\ & I & T & I \\ & & I & T \end{bmatrix} \qquad T = \begin{bmatrix} -4 & 1 & & \\ 1 & -4 & 1 & \\ & 1 & -4 & 1 \\ & & 1 & -4 \end{bmatrix}$$

Iterative methods

Back to one space dimension first...

Coupled system of n linear equations:

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

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

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

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:

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

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

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

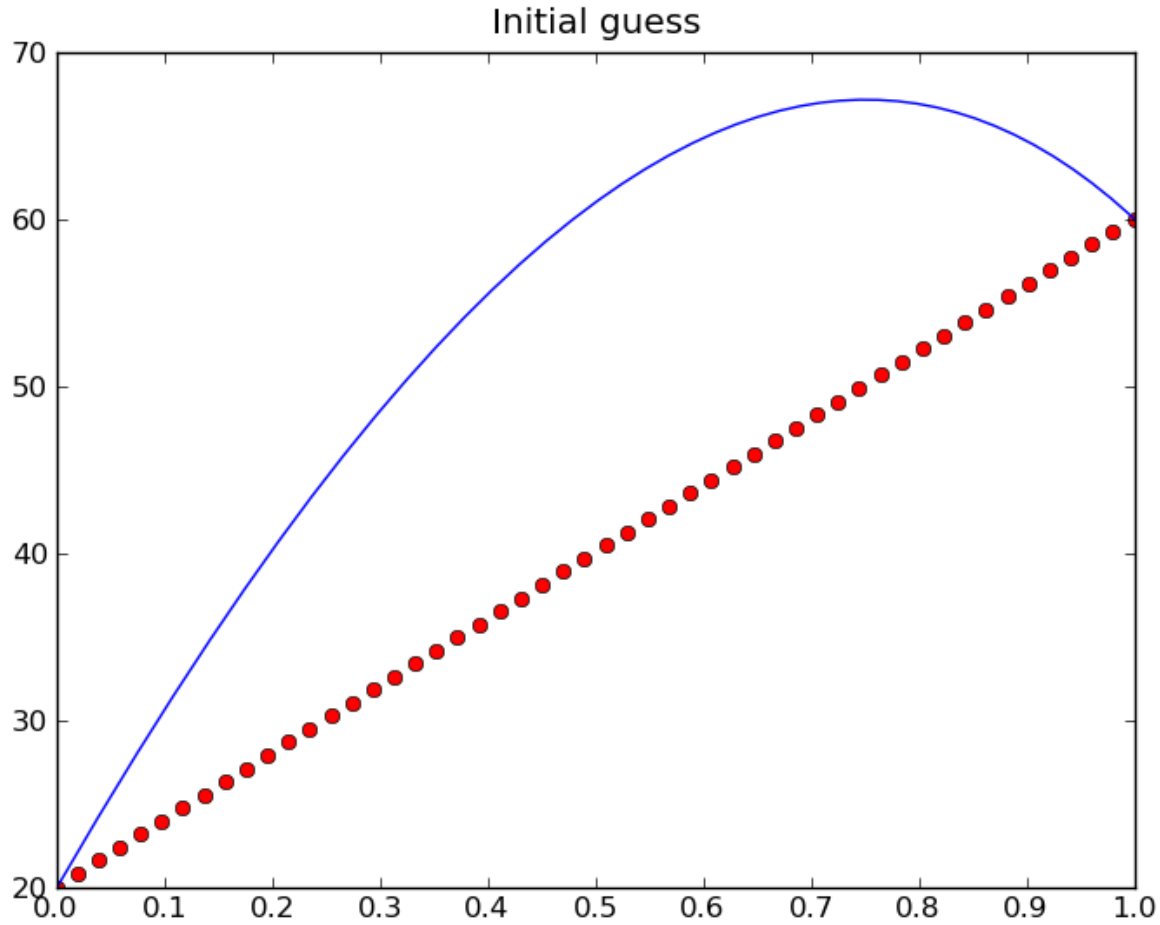
Suppose $U^{[k]}$ is a approximation to solution. Set

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

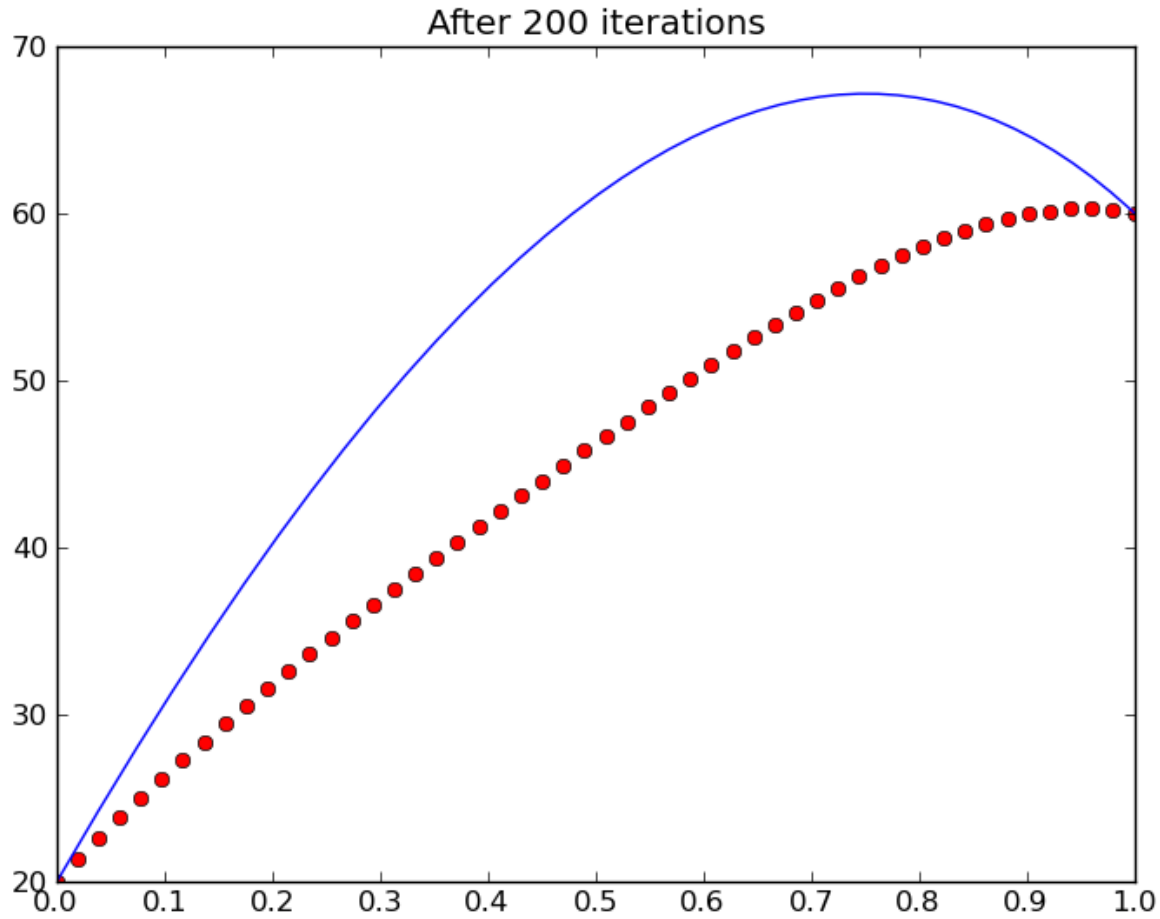
Repeat for $k = 0,\ 1,\ 2,\ \ldots$ until convergence.

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

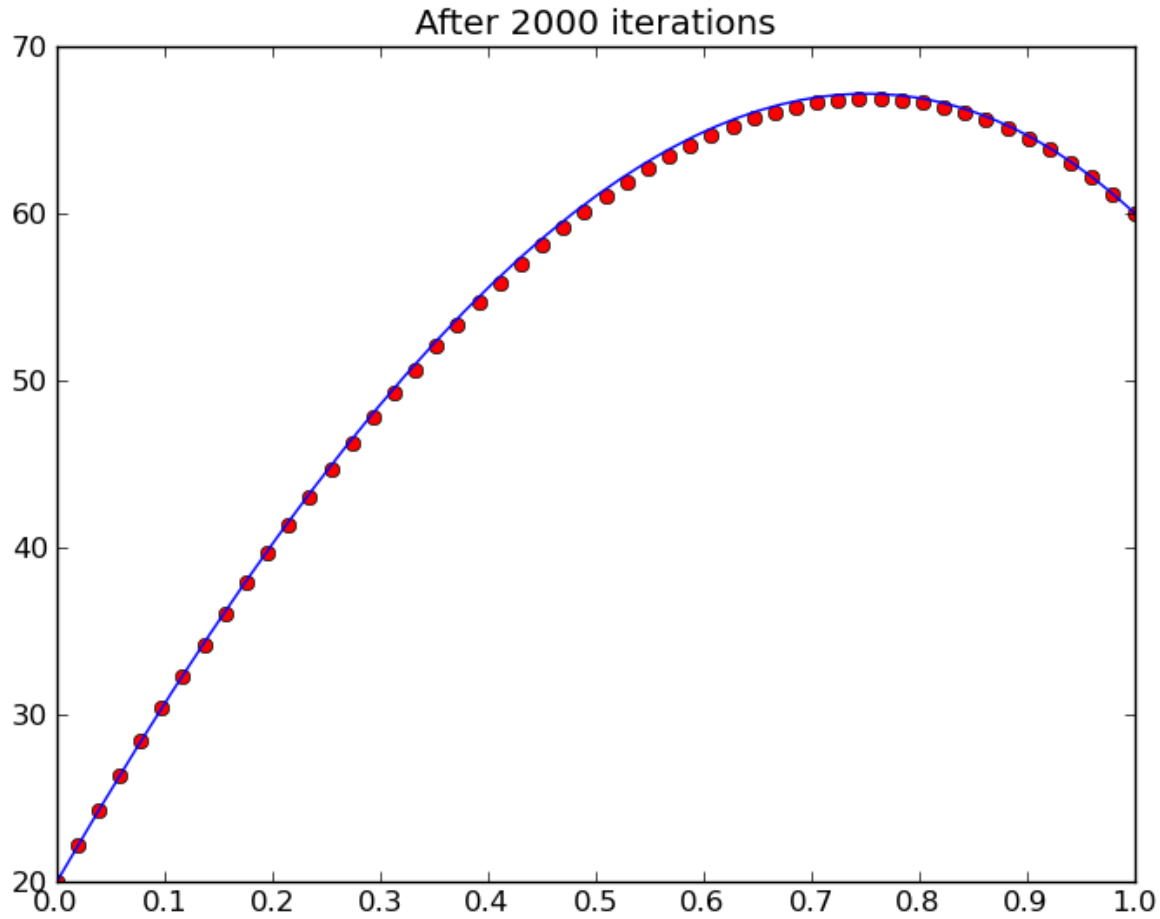
Slow convergence of Jacobi



Slow convergence of Jacobi



Slow convergence of Jacobi



Iterative methods

Jacobi iteration is about the worst possible iterative method.

But it's very simple, and useful as a test for parallelization.

Better iterative methods:

- Gauss-Seidel
- Successive Over-Relaxation (SOR)
- Conjugate gradients
- Preconditioned conjugate gradients
- Multigrid

Speedup for problems like steady state heat equation

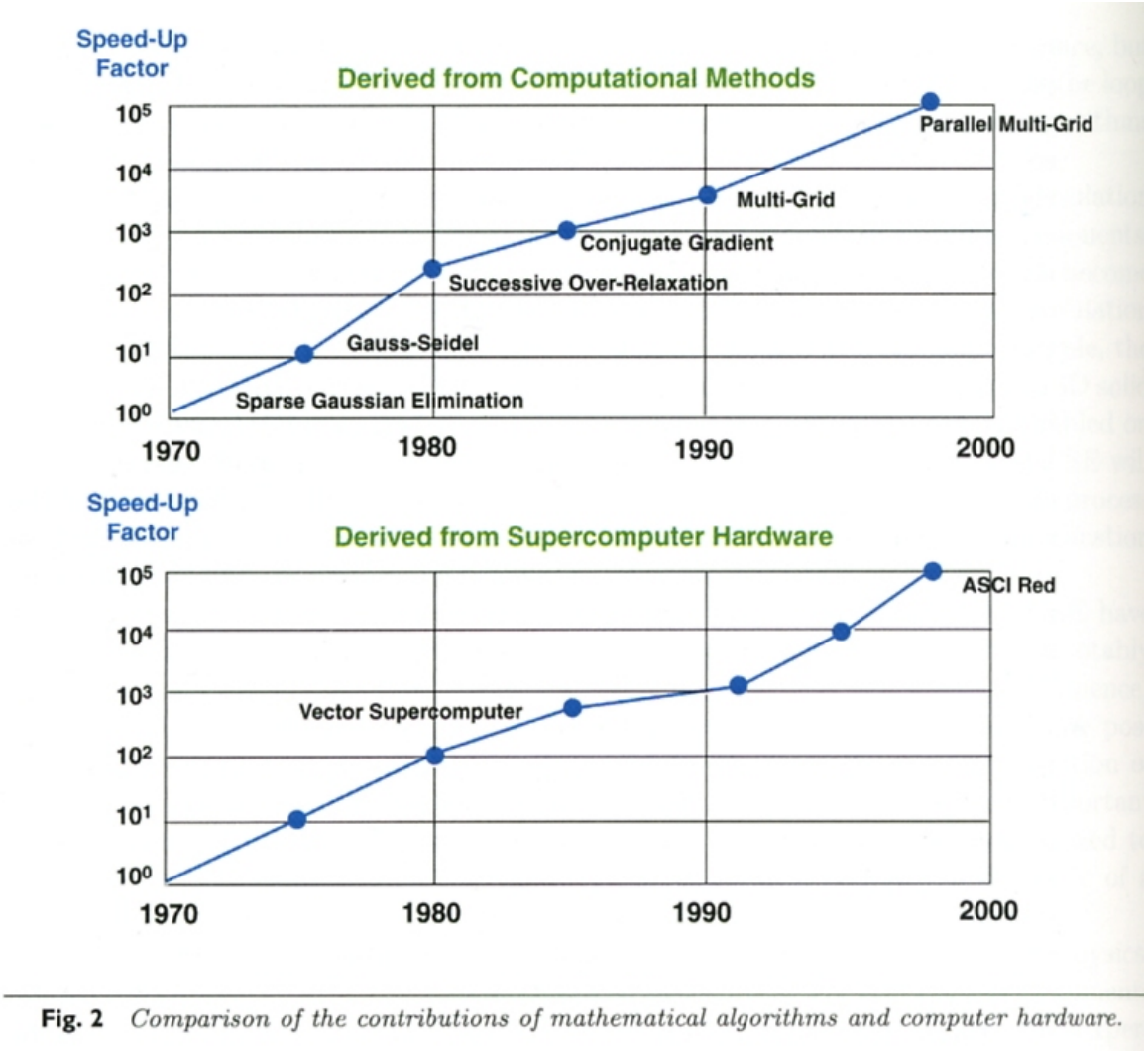


Fig. 2 *Comparison of the contributions of mathematical algorithms and computer hardware.*

Source: SIAM Review

Iterative methods – initialization

```
! allocate storage for boundary points too:
allocate(x(0:n+1), u(0:n+1), f(0:n+1))

dx = 1.d0 / (n+1.d0)

!$omp parallel do
do i=0,n+1
    ! grid points:
    x(i) = i*dx
    ! source term:
    f(i) = 100.*exp(x(i))
    ! initial guess (linear function):
    u(i) = alpha + x(i)*(beta-alpha)
    enddo
```

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.

Jacobi with OpenMP `parallel do` (fine grain)

```
uold = u  ! starting values before updating

do iter=1,maxiter

    dumax = 0.d0

    !$omp parallel do reduction(max : dumax)
    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

    !$omp parallel do
    do i=1,n
        uold(i) = u(i) ! for next iteration
        enddo
    enddo
```

Note: Forking threads twice each iteration.

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:
$CLASSHG/codes/openmp/jacobi2_omp.f90

Jacobi with MPI

Each process is responsible for some portion of the arrays,
from `i=istart` to `i=iend`.

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:

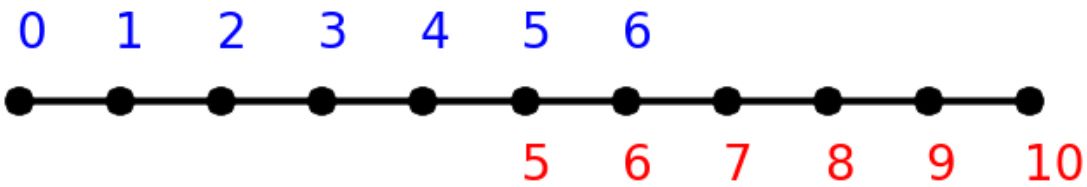
Updating at `i=istart` requires `uold(istart-1)`

Updating at `i=iend` requires `uold(istart+1)`

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

Process 0 has `istart = 1, iend = 5`

Process 1 has `istart = 6, 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

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_PRECI
            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_PRECISI
            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_PRECIS
            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_PREC
            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 — 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 `me` waits for a message from `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.

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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!)