Outline:

- Linear systems: LU factorization and condition number
- Heat equation and discretization
- Iterative methods

Sample codes:

- $UWHPSC/codes/openmp/jacobi1d_omp1.f90
- $UWHPSC/codes/openmp/jacobi1d_omp2.f90
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**
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• Heat equation and discretization
• Iterative methods

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DGESV — Solves a general linear system

SUBROUTINE DGESV( N, NRHS, A, LDA, IPIV, B, LDB, INFO )

NRHS = number of right hand sides

B = matrix whose columns are right hand side(s) on input solution vector(s) on output.

LDB = leading dimension of B.

INFO = integer returning 0 if successful.

A = matrix on input, L,U factors on output,

IPIV = Returns pivot vector (permutation of rows)
       integer, dimension(N)
       Row I was interchanged with row IPIV(I).
If $A$ is nonsingular it can be factored as

$$PA = LU$$

where

$P$ is a permutation matrix (rows of identity permuted),

$L$ is lower triangular with 1’s on diagonal,

$U$ is upper triangular.

After returning from `dgesv`:

- $A$ contains $L$ and $U$ (without the diagonal of $L$),
- $IPIV$ gives ordering of rows in $P$. 
Gaussian elimination as factorization

Example:

\[
A = \begin{bmatrix}
2 & 1 & 3 \\
4 & 3 & 6 \\
2 & 3 & 4
\end{bmatrix}
\]

\[
\begin{bmatrix}
0 & 1 & 0 \\
0 & 0 & 1 \\
1 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
2 & 1 & 3 \\
4 & 3 & 6 \\
2 & 3 & 4
\end{bmatrix}
= \begin{bmatrix}
1 & 0 & 0 \\
1/2 & 1 & 0 \\
1/2 & -1/3 & 1
\end{bmatrix}
\begin{bmatrix}
4 & 3 & 6 \\
0 & 1 & 0 \\
0 & 0 & 1/3
\end{bmatrix}
\]

\(\text{IPIV } = (2,3,1)\)

and \(A\) comes back from \texttt{DGESV} as:

\[
\begin{bmatrix}
4 & 3 & 6 \\
1/2 & 1.5 & 1 \\
1/2 & -1/3 & 1/3
\end{bmatrix}
\]
See $UWHPSC/codes/lapack/random.

Sample codes that solve the linear system $Ax = b$ with a random $n \times n$ matrix $A$, where the value $n$ is run-time input.

`randomsys1.f90` is with static array allocation.

`randomsys2.f90` is with dynamic array allocation.
See $UWHPSC/codes/lapack/random$.

Sample codes that solve the linear system $Ax = b$ with a random $n \times n$ matrix $A$, where the value $n$ is run-time input.

randomsys1.f90 is with static array allocation.
randomsys2.f90 is with dynamic array allocation.
randomsys3.f90 also estimates condition number of $A$.

$$\kappa(A) = \|A\| \|A^{-1}\|$$

Can bound relative error in solution in terms of relative error in data using this:

$$Ax^* = b^* \text{ and } A\tilde{x} = \tilde{b} \implies \frac{\|\tilde{x} - x^*\|}{\|x^*\|} \leq \kappa(A) \frac{||\tilde{b} - b^*||}{\|b^*\|}$$
Heat Equation / Diffusion Equation

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

$u$ represents temperature in a 1-dimensional metal rod.

Or concentration of a chemical diffusing in a tube of water.

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

where subscripts represent partial derivatives,
$D =$ diffusion coefficient (assumed constant in space & time),
$f(x,t) =$ source term (heat or chemical being added/removed).

Also need initial conditions $u(x,0)$ and boundary conditions $u(x_1,t)$, $u(x_2,t)$. 

R.J. LeVeque, University of Washington
AMath 483/583, Lecture 23
Heat Equation / Diffusion Equation

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

$u$ represents temperature in a 1-dimensional metal rod. Or concentration 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 (assumed constant in space & time),

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Also need initial conditions $u(x, 0)$ and boundary conditions $u(x_1, t), u(x_2, t)$. 
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 \( u(x) \).
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 \( u(x) \).

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

**Boundary conditions:**

\[
u(0) = \alpha, \quad u(1) = \beta.
\]
More generally: Take $D = 1$ or absorb in $f$,

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

Boundary conditions:

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

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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Boundary conditions:

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

Example: $\alpha = 20, \quad \beta = 60, \quad f(x) = 0$ (no heat source)

Solution: $u(x) = \alpha + x(\beta - \alpha) \quad \implies \quad u''(x) = 0.$

No heat source $\implies$ linear variation in steady state ($u_{xx} = 0$).
More generally: Take $D = 1$ or absorb in $f$,

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

Boundary conditions:

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

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

**Solution:** $u(x) = (100e - 60)x + 120 - 100e^x$. 
For more complicated equations, numerical methods must generally be used, giving approximations at discrete points.
Steady state diffusion

For more complicated equations, numerical methods must generally be used, giving approximations at discrete points.
Define grid points $x_i = i \Delta x$ in interval $0 \leq x \leq 1$, 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.
Define grid points \( x_i = i\Delta x \) in interval \( 0 \leq x \leq 1 \), 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.

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

We know \( U_0 = \alpha \) and \( U_{n+1} = \beta \) from boundary conditions.
Define grid points $x_i = i \Delta x$ in interval $0 \leq x \leq 1$, where

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

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

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

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:

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

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

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

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 \( i = 1, 2, \ldots, n \). With \( U_0 = \alpha \) and \( U_{n+1} = \beta \).
Tridiagonal linear system

\[
\alpha - 2U_1 + U_2 = -\Delta x^2 f(x_1) \quad (i = 1)
\]
\[
U_1 - 2U_2 + U_3 = -\Delta x^2 f(x_2) \quad (i = 2)
\]
Etc.

For \( n = 5 \):
\[
\begin{bmatrix}
-2 & 1 & 0 & 0 & 0 \\
1 & -2 & 1 & 0 & 0 \\
0 & 1 & -2 & 1 & 0 \\
0 & 0 & 1 & -2 & 1 \\
0 & 0 & 0 & 1 & -2 \\
\end{bmatrix}
\begin{bmatrix}
U_1 \\
U_2 \\
U_3 \\
U_4 \\
U_5 \\
\end{bmatrix}
= -\Delta x^2
\begin{bmatrix}
f(x_1) \\
f(x_2) \\
f(x_3) \\
f(x_4) \\
f(x_5) \\
\end{bmatrix}
- \begin{bmatrix}
\alpha \\
0 \\
0 \\
0 \\
\beta \\
\end{bmatrix}.
\]
Tridiagonal linear system

\[ \begin{align*}
\alpha - 2U_1 + U_2 &= -\Delta x^2 f(x_1) \quad (i = 1) \\
U_1 - 2U_2 + U_3 &= -\Delta x^2 f(x_2) \quad (i = 2) \\
\text{Etc.}
\end{align*} \]

For \( n = 5 \):

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

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 \texttt{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 $0 \leq x \leq 1, \ 0 \leq y \leq 1$. 
Heat equation in 2 dimensions

One-dimensional equation generalizes to

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

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

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

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

This is a PDE in two spatial variables. (Poisson Problem)
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 \(D = 1\)):**

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

This is a PDE in two spatial variables. **(Poisson Problem)**

**Laplace’s equation** if \(f(x, y) \equiv 0\).

\[ \nabla^2 = (\partial_x^2 + \partial_y^2) \] is the Laplacian operator.
Finite difference equations for 2D Poisson problem

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

\[
\begin{align*}
  \frac{1}{\Delta x^2} (U_{i-1,j} - 2U_{i,j} + U_{i+1,j}) \\
  + \frac{1}{\Delta y^2} (U_{i,j-1} - 2U_{i,j} + U_{i,j+1}) = -f(x_i, y_j)
\end{align*}
\]
Finite difference equations for 2D Poisson problem

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

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

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

$$\frac{1}{h^2} (U_{i-1,j} + U_{i+1,j} + U_{i,j-1} + U_{i,j+1} - 4U_{i,j}) = -f(x_i, y_j).$$
Finite difference equations for 2D Poisson problem

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

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

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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.
Finite difference equations for 2D Poisson problem

Row-wise ordering

Matrix has block tridiagonal structure:

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

\[ T = \begin{bmatrix}
-4 & 1 \\
1 & -4 \\
1 & -4 \\
\end{bmatrix} \]
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 $U_{n+1} = \beta$.

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

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 \(U_i\):

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

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

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

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

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

R.J. LeVeque, University of Washington  AMath 483/583, Lecture 23
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
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)
endo
Jacobi iteration in Fortran

```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.

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

\[ u(i) = 0.5d0*(u(i-1) + u(i+1) + dx**2*f(i)) \]

This actually converges faster!
Jacobi with OpenMP \texttt{parallel do} (fine grain)

See: 
$\$UWHPSC/codes/openmp/jacobi1d_omp1.f90$

\begin{verbatim}

uold = u ! starting values before updating

do iter=1,maxiter

dumax = 0.d0

!$omp parallel do reduction(max : dumax)
do i=1,nu
    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

\end{verbatim}

Note: Forking threads twice each iteration.
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 \( \text{dumax} \).
- Print out final result after leaving parallel block

See code in the repository or the notes:

\$UWHPSU/codes/openmp/jacobi1d_omp2.f90