2.29 Numerical Fluid Mechanics
Spring 2015 – **Lecture 9**

REVIEW Lecture 8:

- **Direct Methods for solving (linear) algebraic equations**
  - Gauss Elimination
  - LU decomposition/factorization
  - Error Analysis for Linear Systems and Condition Numbers
  - Special Matrices (Tri-diagonal, banded, sparse, positive-definite, etc)

- **Iterative Methods:**

$$\mathbf{x}^{k+1} = \mathbf{B}\,\mathbf{x}^{k} + \mathbf{c} \qquad k = 0, 1, 2, \ldots$$

"Stationary" methods:

- **Jacobi's method**

$$\mathbf{x}^{k+1} = -\mathbf{D}^{-1}(\mathbf{L} + \mathbf{U})\,\mathbf{x}^{k} + \mathbf{D}^{-1}\mathbf{b}$$

- **Gauss-Seidel iteration**

$$\mathbf{x}^{k+1} = -(\mathbf{D} + \mathbf{L})^{-1}\mathbf{U}\,\mathbf{x}^{k} + (\mathbf{D} + \mathbf{L})^{-1}\mathbf{b}$$

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REVIEW Lecture 8, Iterative Methods Cont'd:

– **Convergence: Necessary and sufficient condition**

$$\rho(\mathbf{B}) = \max_{i=1\ldots n} |\lambda_i| < 1, \quad \text{where } \lambda_i = \text{eigenvalue}(\mathbf{B}_{n\times n})$$ (ensures suffic. ||**B**||<1)

- Jacobi's method
- Gauss-Seidel iteration

Sufficient conditions:
- Both converge if **A** stricly diagonally dominant
- Gauss-Seidel also convergent if **A** sym. positive definite

– **Stop Criteria, e.g.:**

$$\begin{cases} i \le n_{\max} \\ \|x_i - x_{i-1}\| \le \varepsilon \\ \|r_i - r_{i-1}\| \le \varepsilon, \quad where \ r_i = Ax_i - b \\ \|r_i\| \le \varepsilon \end{cases}$$

– **Example**

– **Successive Over-Relaxation Methods:** (decrease $\rho(\mathbf{B})$ for faster convergence)

$$\mathbf{x}_{i+1} = (\mathbf{D} + \omega\mathbf{L})^{-1}[-\omega\mathbf{U} + (1-\omega)\mathbf{D}]\mathbf{x}_i + \omega(\mathbf{D} + \omega\mathbf{L})^{-1}\mathbf{b}$$

"Adaptive" methods:

– **Gradient Methods** $\mathbf{x}_{i+1} = \mathbf{x}_i + \alpha_i \mathbf{v}_i$

$$\begin{cases} \dfrac{dQ(\mathbf{x})}{d\mathbf{x}} = \mathbf{A}\mathbf{x} - \mathbf{b} = -\mathbf{r} \\ \mathbf{r}_i = \mathbf{b} - \mathbf{A}\mathbf{x}_i \ (\text{residual at iteration } i) \end{cases}$$

- Steepest decent

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \left(\frac{\mathbf{r}_i^T \mathbf{r}_i}{\mathbf{r}_i^T \mathbf{A} \mathbf{r}_i} \right) \mathbf{r}_i$$

- Conjugate gradient

TODAY (Lecture 9)

- End of (Linear) Algebraic Systems
  - Gradient Methods and Krylov Subspace Methods
  - Preconditioning of $\mathbf{Ax=b}$
- FINITE DIFFERENCES
  - Classification of Partial Differential Equations (PDEs) and examples with finite difference discretizations
  - Error Types and Discretization Properties
    - Consistency, Truncation error, Error equation, Stability, Convergence
  - Finite Differences based on Taylor Series Expansions
    - Higher Order Accuracy Differences, with Example
    - Taylor Tables or Method of Undetermined Coefficients
  - Polynomial approximations
    - Newton's formulas, Lagrange/Hermite Polynomials, Compact schemes

References and Reading Assignments

- Chapter 14.2 on “Gradient Methods”, Part 8 (PT 8.1-2), Chapter 23 on “Numerical Differentiation” and Chapter 18 on “Interpolation” of “Chapra and Canale, Numerical Methods for Engineers, 2006/2010/2014.”
- Chapter 3 on “Finite Difference Methods” of “J. H. Ferziger and M. Peric, Computational Methods for Fluid Dynamics. Springer, NY, 3rd edition, 2002”
- Chapter 3 on “Finite Difference Approximations” of “H. Lomax, T. H. Pulliam, D.W. Zingg, *Fundamentals of Computational Fluid Dynamics (Scientific Computation).* Springer, 2003”

Conjugate Gradient Method

- Derivation provided in lecture
- Check CGM_new.m

- Definition: "**A**-conjugate vectors" or "Orthogonality with respect to a matrix (metric)":

  if $\mathbf{A}$ is symmetric & positive definite,

$$\text{For } \; i \neq j \; \text{ we say } \; v_i, v_j \; \text{ are orthogonal with respect to } \mathbf{A}, \text{ if } \; v_i^T \mathbf{A} v_j = 0$$

- Proposed in 1952 (Hestenes/Stiefel) so that directions v_i are generated by the orthogonalization of residuum vectors (search directions are **A**-conjugate)
  - Choose new descent direction as different as possible from old ones, within **A**-metric
- Algorithm:

$v_0 = r_0 = b - A x_0$

do

$\alpha_i = (v_i^\top r_i)/(v_i^\top A v_i)$	Step length
$x_{i+1} = x_i + \alpha_i v_i$	Approximate solution
$r_{i+1} = r_i - \alpha_i A v_i$	New Residual
$\beta_i = -(v_i^\top A r_{i+1})/(v_i^\top A v_i)$	Step length &
$v_{i+1} = r_{i+1} + \beta_i v_i$	new search direction

until a stop criterion holds

Note: $A\, v_i$ = one matrix vector multiply at each iteration

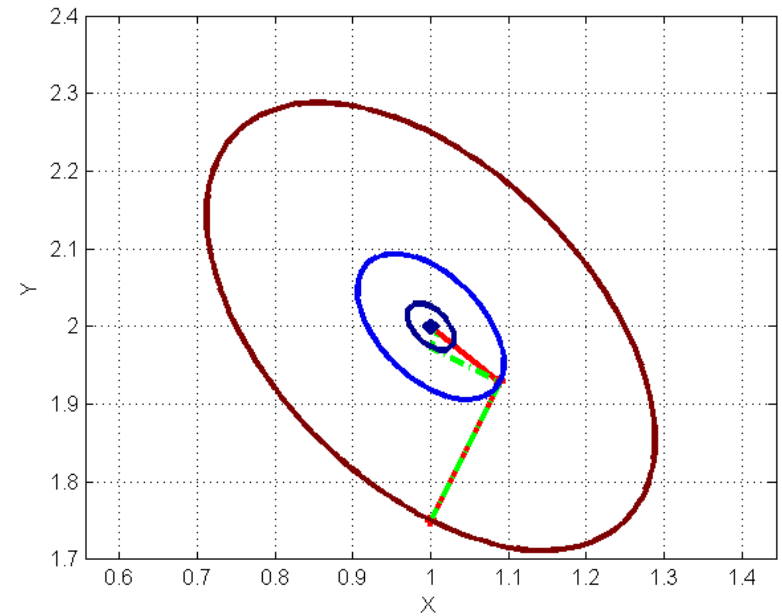

Figure indicates solution obtained using Conjugate gradient method (red) and steepest descent method (green).

•

– solution with "n" iterations, but decent accuracy with much fewer

–

–

• $\mathbf{Ax}=\mathbf{b}$

– $\mathbf{b}, \mathbf{A}\,\mathbf{b}, \mathbf{A}^2\,\mathbf{b}, \cdots$

– $n_s \le n$ $\mathcal{K}_{n_s} = \text{span}\left\{\mathbf{b}, \mathbf{A}\,\mathbf{b}, \cdots, \mathbf{A}^{n_s - 1}\,\mathbf{b}\right\}$

–

–

–

n_s

– An iteration to do this is the "Arnoldi's iteration" which is a stabilized Gram

– n n_s

-
  -
  - x_n are in $\mathcal{K}_n = \text{span}\left\{\begin{matrix}\mathbf{b}, \mathbf{A}\,\mathbf{b}, \\ \cdots, \mathbf{A}^{n-1}\,\mathbf{b}\end{matrix}\right\}$
-
  - Based on the idea of projecting the "$\mathbf{Ax}=\mathbf{b}$ problem" into the

    n $\mathbf{Ax}=\mathbf{b}$
  -
    - $\mathbf{A}$
      - $\mathbf{Ax}=\mathbf{b}$ $\mathbf{x}_n \in \mathcal{K}_n$

        $\mathbf{Ax_n} - \mathbf{b}$
    -
    -
  -
    -

Preconditioning of $\mathbf{A\,x = b}$

- Pre-conditioner approximately solves $\mathbf{A\,x = b}$.

  Pre-multiply by the inverse of a non-singular matrix $\mathbf{M}$, and solve instead:

  $$\mathbf{M}^{-1}\mathbf{A\,x} = \mathbf{M}^{-1}\,\mathbf{b} \qquad \text{or} \qquad \mathbf{A\,M}^{-1}\,(\mathbf{M\,x}) = \mathbf{b}$$

  – Convergence properties based on $\mathbf{M}^{-1}\mathbf{A}$ or $\mathbf{A\,M}^{-1}$ instead of $\mathbf{A}$!

  – Can accelerate subsequent application of iterative schemes

  – Can improve conditioning of subsequent use of non-iterative schemes: GE, LU, etc

- Jacobi preconditioning:
  – Apply Jacobi a few steps, usually not efficient
- Other iterative methods (Gauss-Seidel, SOR, SSOR, etc):
  – Usually better, sometimes applied only once
- Incomplete factorization (incomplete LU) or incomplete Cholesky
  – LU or Cholesky, but avoiding fill-in of already null elements in A
- Coarse-Grid Approximations and Multigrid Methods:
  – Solve $\mathbf{A\,x = b}$ on a coarse grid (or successions of coarse grids)
  – Interpolate back to finer grid(s)

Example of Convergence Studies for Linear Solvers

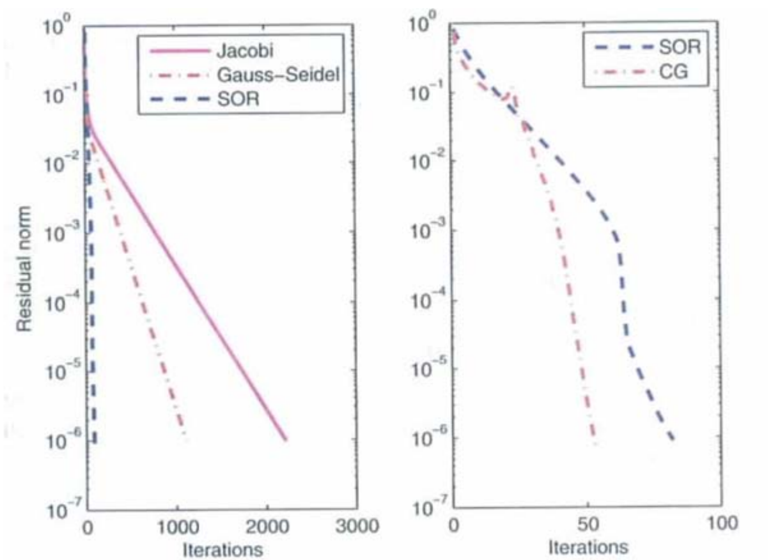

Fig 7.5: Example 7.10, with system of size 961x961: convergence behavior of various iterative schemes for the discretized Poisson equation.

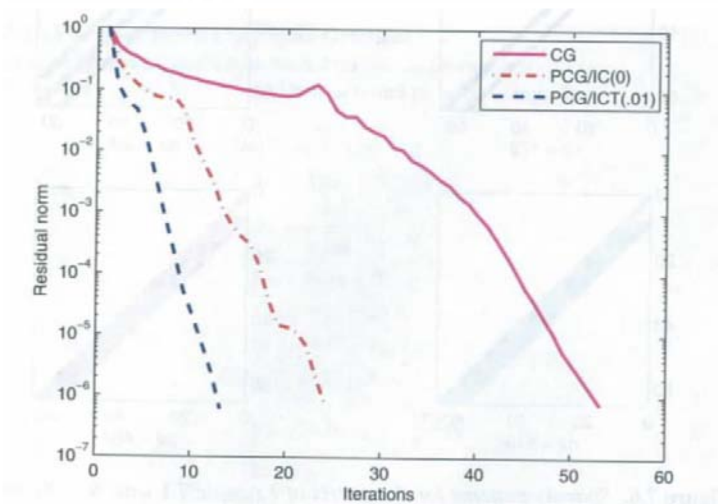

Fig 7.7: Iteration progress for CG, PCG with the IC(0) preconditioner and PCG with the IC preconditioner using drop tolerance tol=0.01

IC(0): is incomplete Cholesky factorization. This is Cholesky as we have seen it, but a non-zero entry in the factorization is generated only if A was not zero there to begin with.

IC: same, but non-zero entry generated if it is ≥ tol

PCG: Preconditioned conjugate gradient

Ascher and Greif (SIAM-2011)

Review of/Summary for Iterative Methods

Table removed due to copyright restrictions. Useful reference tables for this material: Tables PT3.2 and PT3.3 in Chapra, S., and R. Canale. *Numerical Methods for Engineers*. 6th ed. McGraw-Hill Higher Education, 2009. ISBN: 9780073401065.

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FINITE DIFFERENCES - Outline

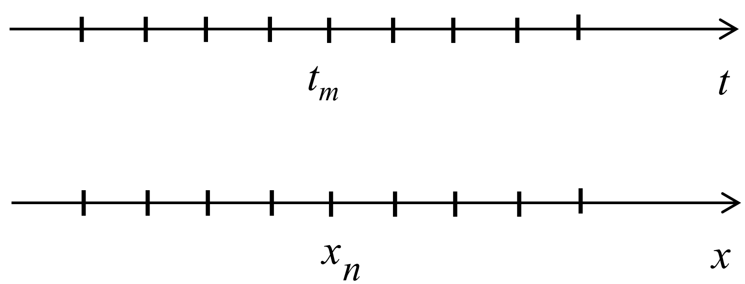
- Classification of Partial Differential Equations (PDEs) and examples with finite difference discretizations
  - Elliptic PDEs
  - Parabolic PDEs
  - Hyperbolic PDEs
- Error Types and Discretization Properties
  - Consistency, Truncation error, Error equation, Stability, Convergence
- Finite Differences based on Taylor Series Expansions
- Polynomial approximations
  - Equally spaced differences
    - Richardson extrapolation (or uniformly reduced spacing)
    - Iterative improvements using Roomberg's algorithm
  - Lagrange polynomial and un-equally spaced differences
  - Compact Difference schemes

Continuum Model

$$\frac{\partial w}{\partial t} + c\frac{\partial w}{\partial x} = 0$$

Sommerfeld Wave Equation (c= wave speed). This radiation condition is sometimes used at open boundaries of ocean models.

Discrete Model



$$t_m = t_0 + m\Delta t\ ,\quad m = 0, 1, \ldots M-1$$
$$x_n = x_0 + n\,\Delta x\ ,\quad n = 0, 1, \ldots N-1$$

$$\frac{\partial w}{\partial t} \simeq \frac{\Delta w}{\Delta t},\qquad \frac{\partial w}{\partial x} \simeq \frac{\Delta w}{\Delta x}$$

p parameters, e.g. variable c

Differential Equation

$$L(p, w, x, t) = 0$$

"Differentiation"
"Integration"

Difference Equation

$$L_{mn}(p_{mn}, w_{mn}, x_n, t_m) = 0$$

System of Equations

$$\sum_{j=0}^{N-1} F_i(w_j) = B_i$$

Linear System of Equations

$$\sum_{j=0}^{N-1} A_{ij} w_j = B_i$$

"Solving linear equations"

Eigenvalue Problems

$$\overline{\overline{\mathbf{A}}}\mathbf{u} = \lambda\mathbf{u} \Leftrightarrow (\overline{\overline{\mathbf{A}}} - \lambda\overline{\overline{\mathbf{I}}})\mathbf{u} = \mathbf{0}$$

Non-trivial Solutions

$$\det(\overline{\overline{\mathbf{A}}} - \lambda\overline{\overline{\mathbf{I}}}) = 0$$

"Root finding"

Consistency/Accuracy and Stability => Convergence
(Lax equivalence theorem for well-posed linear problems)

Classification of Partial Differential Equations

(2D case, 2nd order PDE)

Quasi-linear PDE for $\phi(x, y)$

$$A\phi_{xx} + B\phi_{xy} + C\phi_{yy} = F(x, y, \phi, \phi_x, \phi_y)$$

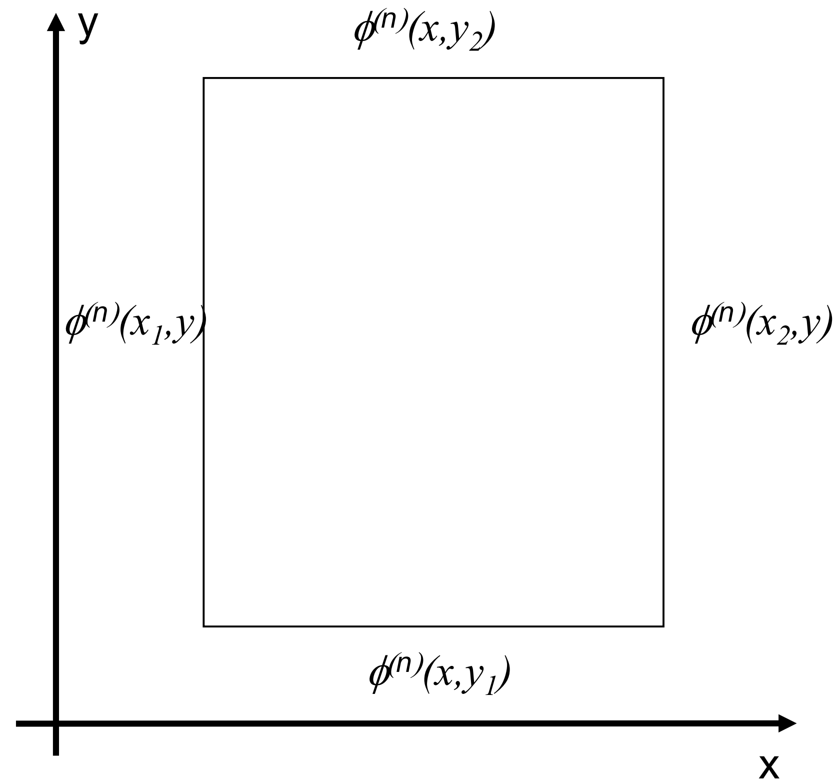
A,B and C Constants

$$B^2 - 4AC > 0 \quad \text{Hyperbolic}$$

$$B^2 - 4AC = 0 \quad \text{Parabolic}$$

$$B^2 - 4AC < 0 \quad \text{Elliptic}$$

(Only valid for two independent variables: x,y)



- In general: A, B and C are function of: $x, y, \phi, \phi_x, \phi_y$
- Equations may change of type from point to point if A, B and C vary with x, y, etc.
- Navier-Stokes, incomp., const. viscosity: $\dfrac{D\mathbf{u}}{Dt} = \dfrac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\,\mathbf{u} = -\dfrac{1}{\rho}\nabla p + \nu\,\nabla^2 \mathbf{u} + \mathbf{g}$

Classification of Partial Differential Equations

(2D case, 2nd order PDE)

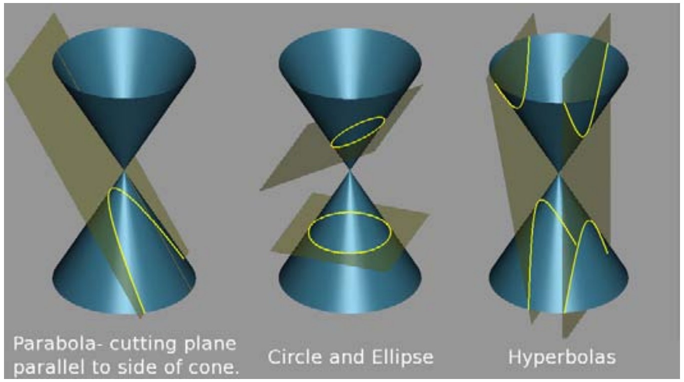
Meaning of Hyperbolic, Parabolic and Elliptic

- The general 2nd order PDE in 2D:

$$A\phi_{xx} + B\phi_{xy} + C\phi_{yy} = F$$

is analogous to the equation for a conic section:

$$Ax^2 + Bxy + Cy^2 = F$$



- Conic section:
  - Is the intersection of a right circular cone and a plane, which generates a group of plane curves, including the circle, ellipse, hyperbola, and parabola
  - One characterizes the type of conic sections using the discriminant $B^2 - 4AC$
- PDE:
  - $B^2 - 4AC > 0$ (Hyperbolic)
  - $B^2 - 4AC = 0$ (Parabolic)
  - $B^2 - 4AC < 0$ (Elliptic)

Examples

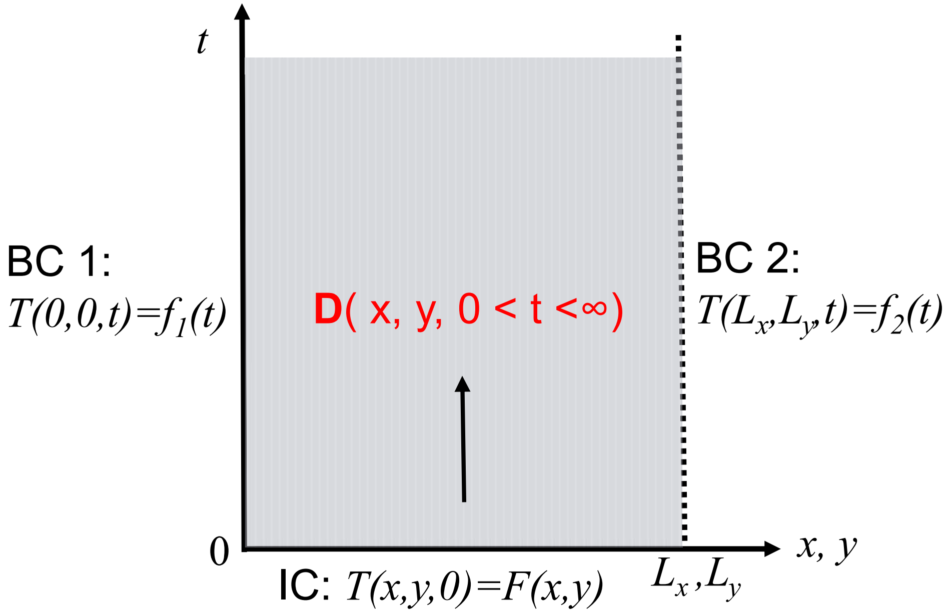
$$\frac{\partial T}{\partial t} = \frac{\kappa}{\rho c}\nabla^2 T + f\,, \quad (\alpha = \frac{\kappa}{\rho c})$$

Heat conduction equation, forced or not (dominant in 1D)

$$\frac{\partial \mathbf{u}}{\partial t} = \nu\,\nabla^2 \mathbf{u} + \mathbf{g}$$

Unsteady, diffusive, small amplitude flows or perturbations (e.g. Stokes Flow)

- Usually smooth solutions ("diffusion effect" present)
- "Propagation" problems
- Domain of dependence of solution is domain **D** (x, y, and 0 < t < ∞):
- Finite Differences/Volumes, Finite Elements



Partial Differential Equations
Parabolic PDE - Example

Heat Conduction Equation

$$\kappa T_{xx}(x,t) = \rho c T_t(x,t), 0 < x < L, 0 < t < \infty$$

Initial Condition

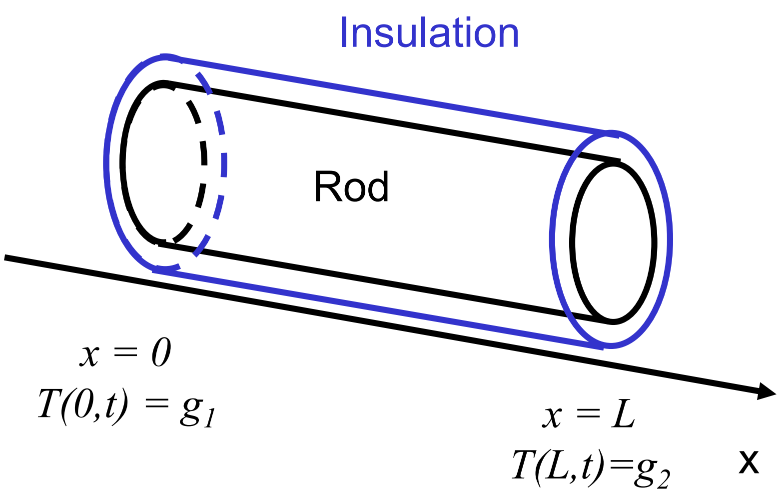
$$T(x,0) = f(x), 0 \le x \le L$$

Boundary Conditions

$$T(0,t) = g_1, 0 < t < \infty$$

$$T(L,t) = g_2, 0 < t < \infty$$

κ Thermal conductivity
c Specific heat capacity
ρ Density
T Temperature



IVP in one dimension (t), BVP in the other (x)
Time Marching, Explicit or Implicit Schemes

IVP: Initial Value Problem
BVP: Boundary Value Problem

Partial Differential Equations
Parabolic PDE - Example

Heat Conduction Equation

$$T_t(x,t) = \alpha T_{xx}(x,t), 0 < x < L, 0 < t < \infty$$

$$\alpha = \frac{\kappa}{\rho c}$$

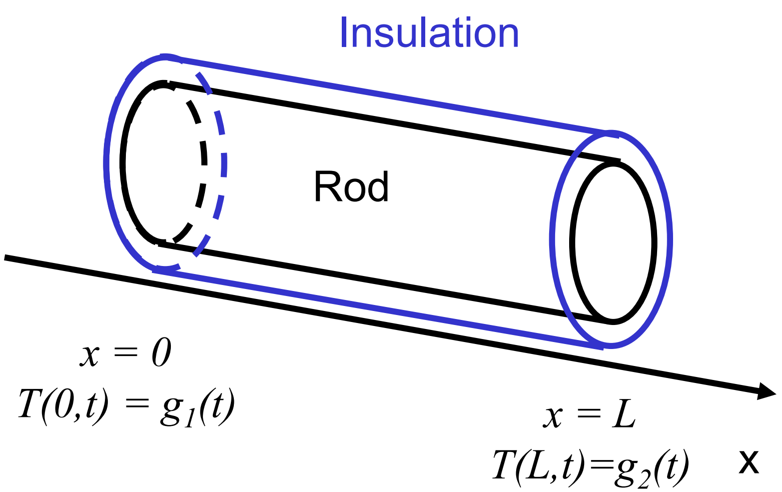
Initial Condition

$$T(x,0) = f(x), 0 \le x \le L$$

Boundary Conditions

$$T(0,t) = g_1(t), 0 < t < \infty$$

$$T(L,t) = g_2(t), 0 < t < \infty$$



Partial Differential Equations
Parabolic PDE - Example

Equidistant Sampling

$$h = L/n$$
$$k = T/m$$

Discretization

$$x_i = (i-1)h, \; i = 2, \dots, n-1$$
$$t_j = (j-1)k, \; j = 1, \dots, m$$

Forward (Euler) Finite Difference in time

$$T_t(x,t) = \frac{T(x_i, t_{j+1}) - T(x_i, t_j)}{k} + O(k)$$

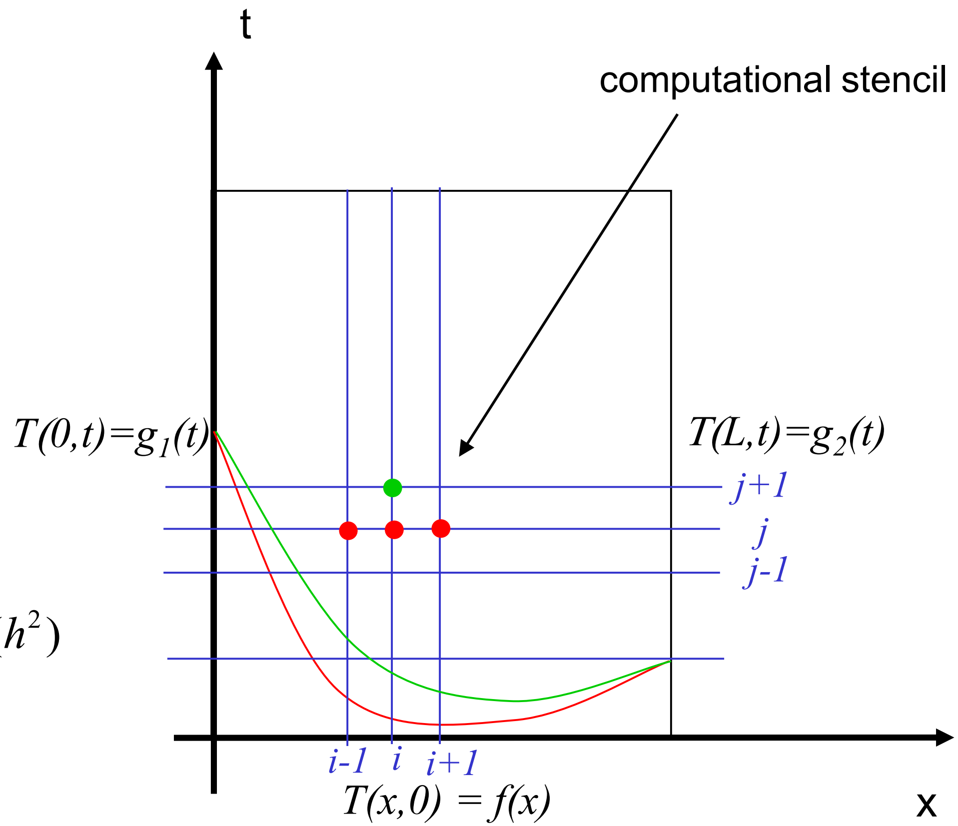
Centered Finite Difference in space

$$T_{xx}(x,t) = \frac{T(x_{i-1}, t_j) - 2T(x_i, t_j) + T(x_{i+1}, t_j)}{h^2} + O(h^2)$$

$$T_{i,j} = T(x_i, t_j)$$

Finite Difference Equation

$$\frac{T_{i,j+1} - T_{i,j}}{k} = \alpha \frac{T_{i-1,j} - 2T_{i,j} + T_{i+1,j}}{h^2}$$



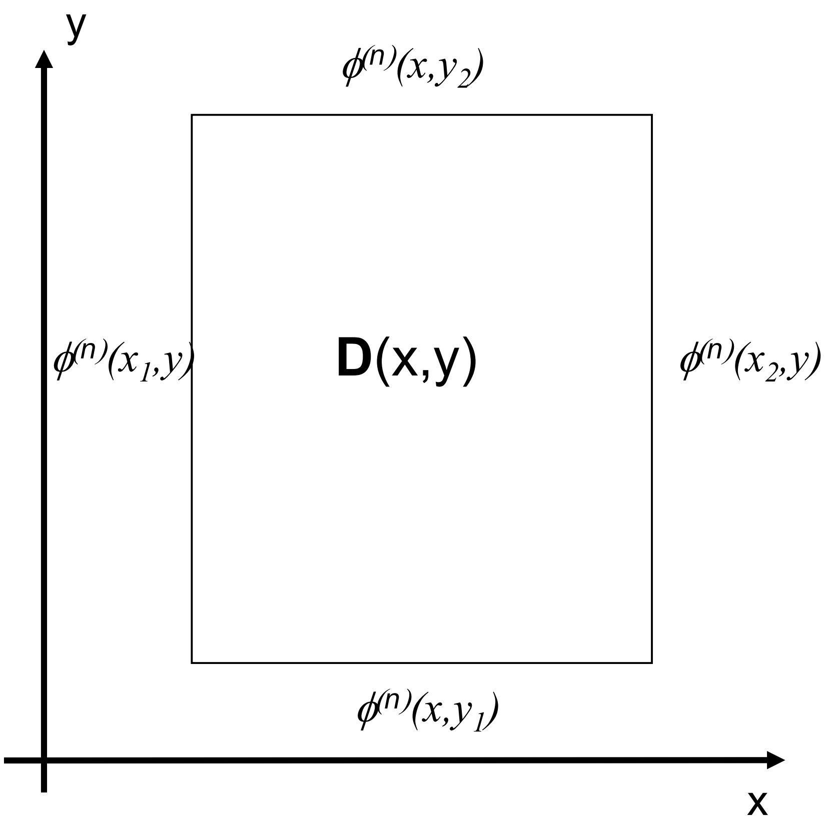
Partial Differential Equations
ELLIPTIC: $B^2 - 4AC < 0$

Quasi-linear PDE for $\phi(x, y)$

$$A\phi_{xx} + B\phi_{xy} + C\phi_{yy} = F(x, y, \phi, \phi_x, \phi_y)$$

A,B and C Constants

$B^2 - 4AC > 0$	Hyperbolic
$B^2 - 4AC = 0$	Parabolic
$B^2 - 4AC < 0$	Elliptic



Partial Differential Equations
Elliptic PDE

Laplace Operator $\nabla^2 \equiv u_{xx} + u_{yy}$

Examples:

$$\nabla^2 \phi = 0$$

Laplace Equation – Potential Flow

$$\nabla^2 \phi = g(x,y)$$

Poisson Equation
- Potential Flow with sources
- Steady heat conduction in plate + source

$$\nabla^2 u + f(x,y) u = 0$$

Helmholtz equation – Vibration of plates

$$\mathbf{U} \cdot \nabla \mathbf{u} = \nu \nabla^2 \mathbf{u}$$

Steady Convection-Diffusion

- Smooth solutions ("diffusion effect")
- Very often, steady state problems
- Domain of dependence of u is the full domain **D**(x,y) => "global" solutions
- Finite differ./volumes/elements, boundary integral methods (Panel methods)

Partial Differential Equations
Elliptic PDE - Example

$$0 \leq x \leq a \ , \ \ 0 \leq y \leq b;$$

Equidistant Sampling

$$h = a/(n-1)$$
$$h = b/(m-1)$$

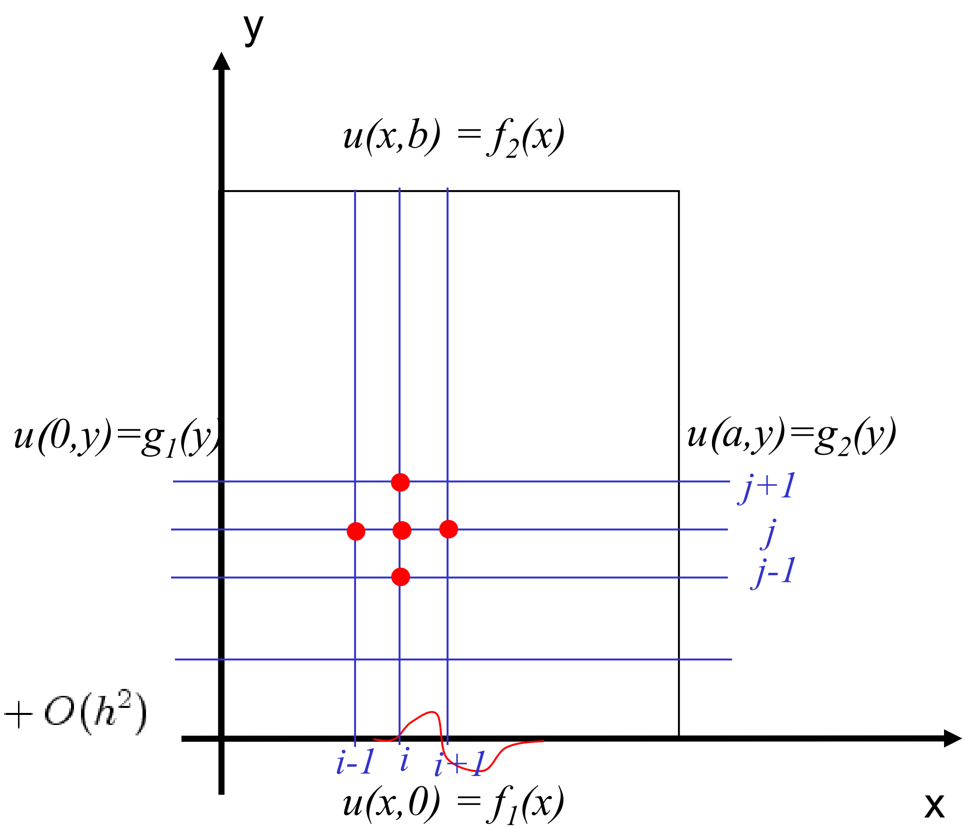
Discretization

$$x_i = (i-1)h, \ i = 1, \ldots, n$$
$$y_j = (j-1)h, \ j = 1, \ldots, m$$

Finite Differences

$$u_{xx}(x,t) = \frac{u(x_{i-1}, y_j) - 2u(x_i, y_j) + u(x_{i+1}, y_j)}{h^2} + O(h^2)$$

$$u_{yy}(x,t) = \frac{u(x_i, y_{j-1}) - 2u(x_i, y_j) + u(x_i, y_{j+1})}{h^2} + O(h^2)$$



Dirichlet BC

Partial Differential Equations
Elliptic PDE - Example

Discretized Laplace Equation

$$\nabla^2 u = \frac{u(x_{i-1}, y_j) + u(x_i, y_{j-1}) - 4u(x_i, y_j) + u(x_{i+1}, y_j) + u(x_i, y_{j+1})}{h^2} = 0$$

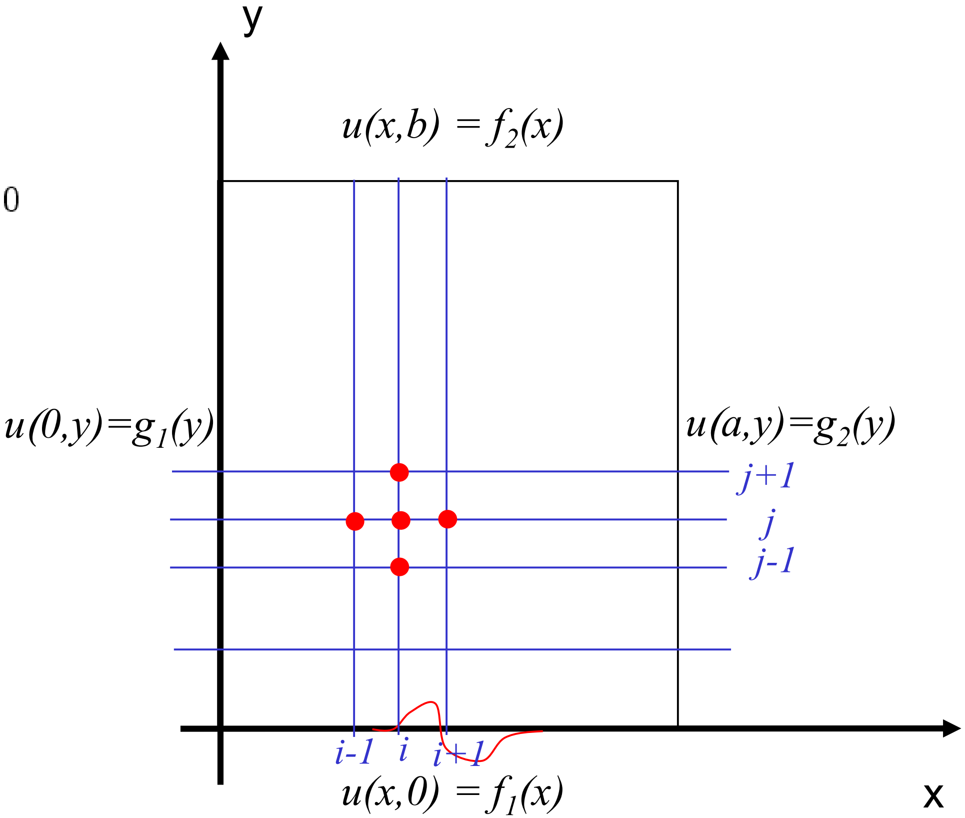
$$u_{i,j} = u(x_i, t_j)$$

Finite Difference Scheme

$$u_{i+1,j} + u_{i-1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j} = 0$$

Boundary Conditions

$$\begin{aligned} u(x_1, y_j) &= u_{1,j}\ ,\quad 2 \le j \le m-1 \\ u(x_n, y_j) &= u_{n,j}\ ,\quad 2 \le j \le m-1 \\ u(x_i, y_1) &= u_{i,1}\ ,\quad 2 \le i \le n-1 \\ u(x_i, y_n) &= u_{i,n}\ ,\quad 2 \le i \le n-1 \end{aligned}$$



Global Solution Required