2.29 Numerical Fluid Mechanics
Fall 2011 – Lecture 11

REVIEW Lecture 10:

- 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:

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

  - 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 10, Iterative Methods Cont'd:

- Convergence: $\rho(\mathbf{B}) = \max_{i=1...n} |\lambda_i| < 1, \quad \text{where } \lambda_i = \text{eigenvalue}(\mathbf{B}_{n\times n})$ (ensures ||**B**||<1)
  - Jacobi's method
  - Gauss-Seidel iteration

  Sufficient conditions:
  - Both converge if **A** diagonally dominant
  - Gauss-Seidel also convergent if **A** positive definite
- Stop Criteria:

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

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

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

- Gradient Methods $\mathbf{x}_{i+1} = \mathbf{x}_i + \alpha_{i+1}\mathbf{v}_{i+1}$
  - Steepest decent

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

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

  - Conjugate gradient

TODAY (Lecture 11)

- End of (Linear) Algebraic Systems
  - Gradient Methods and Krylov Subspace Methods
  - Preconditioning of **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

Gradient Methods

- Applicable to physically important matrices: "symmetric and positive definite" ones
- Construct the equivalent optimization problem

$$Q(x) = \frac{1}{2} x^T A x - x^T b$$

$$\frac{dQ(x)}{dx} = Ax - b$$

$$\frac{dQ(x_{opt})}{dx} = 0 \Rightarrow x_{opt} = x_e, \quad where \quad Ax_e = b$$

- Propose step rule

$$x_{i+1} = x_i + \alpha_{i+1} v_{i+1}$$

- Common methods
  - Steepest descent
  - Conjugate gradient

Steepest Descent Method

- Move exactly in the negative direction of Gradient

$$\frac{dQ(x)}{dx} = Ax - b = -(b - Ax) = -r$$

$$r : residual, \quad r_i = b - Ax_i$$

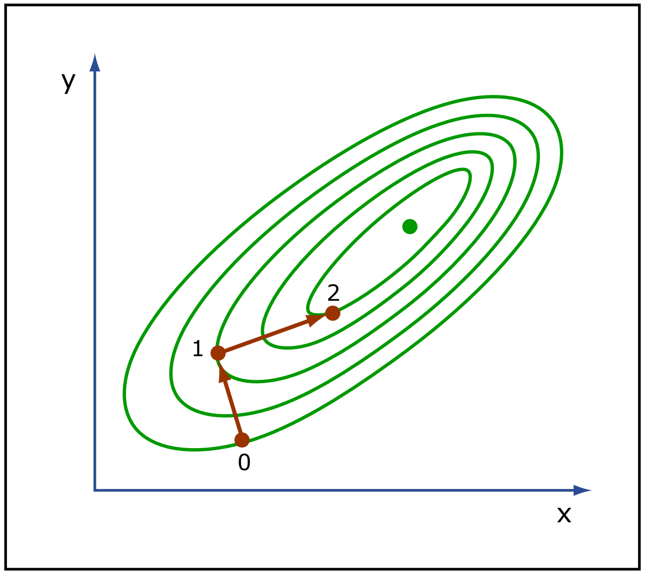


Image by MIT OpenCourseWare.

Graph showing the steepest descent method.

- Step rule

$$x_{i+1} = x_i + \frac{r_i^T r_i}{r_i^T A r_i} r_i$$

- Q(x) reduces in each step, but not as effective as conjugate gradient method

Conjugate Gradient Method

- 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:

$$\boldsymbol{v}_0 = \boldsymbol{r}_0 = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_0$$

do

$$\alpha_i = (\boldsymbol{v}_i^\top \boldsymbol{r}_i)/(\boldsymbol{v}_i^\top \boldsymbol{A}\boldsymbol{v}_i)$$ Step length

$$\boldsymbol{x}_{i+1} = \boldsymbol{x}_i + \alpha_i \boldsymbol{v}_i$$ Approximate solution

$$\boldsymbol{r}_{i+1} = \boldsymbol{r}_i - \alpha_i \boldsymbol{A}\boldsymbol{v}_i$$ New Residual

$$\beta_i = -(\boldsymbol{v}_i^\top \boldsymbol{A}\boldsymbol{r}_{i+1})/(\boldsymbol{v}_i^\top \boldsymbol{A}\boldsymbol{v}_i)$$ Improved step length &

$$\boldsymbol{v}_{i+1} = \boldsymbol{r}_{i+1} + \beta_i \boldsymbol{v}_i$$ new search direction

until a stop criterion holds

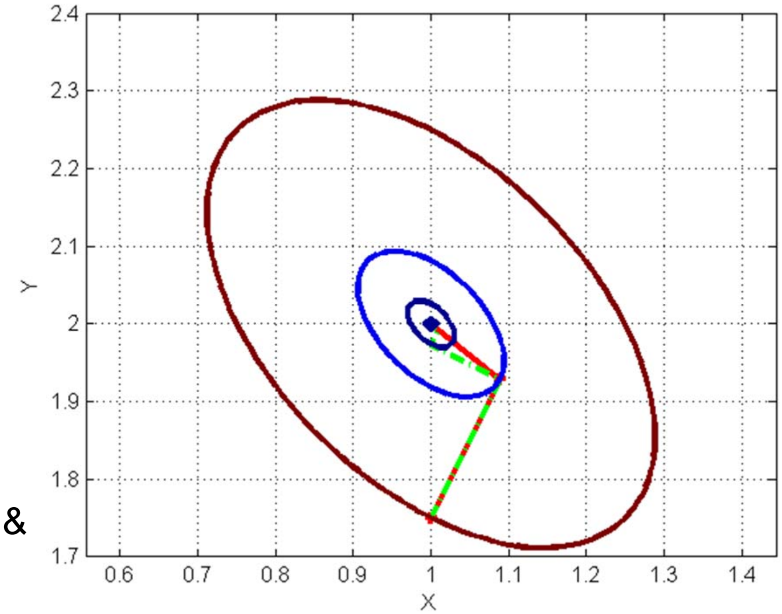


Figure indicates solution obtained using Conjugate gradient method (red) and steepest descent method (green).

Conjugate Gradient (CG) Method and Krylov Subspace Methods

- Conjugate Gradient Properties
  - Accurate solution with "n" iterations, but decent accuracy with much fewer number of iterations
  - Only matrix or vector products
  - Is a special case of Krylov subspace algorithms for symmetric PD matrices
- Krylov Subspaces for $\mathbf{Ax}=\mathbf{b}$: Definitions and Properties
  - Krylov sequence: the set of vectors $\mathbf{b}, \mathbf{A}\,\mathbf{b}, \mathbf{A}^2\,\mathbf{b}, \cdots$
  - Krylov subspace of size n is: $K_n = \text{span}\left\{\mathbf{b}, \mathbf{A}\,\mathbf{b}, \cdots, \mathbf{A}^{n-1}\,\mathbf{b}\right\}$
  - The sequence converges towards the eigenvector with the largest eigenvalue
  - Vectors become more and more linearly dependent
  - Hence, if one extracts an orthogonal basis for the subspace, one would likely get good approximations of the top eigenvectors with the n largest eigenvalues
  - An iteration to do this is the "Arnoldi's iteration" which is a stabilized Gram-Schmidt procedure (e.g. see Trefethen and Bau, 1997)

Conjugate Gradient (CG) Method and Krylov Subspace Methods

- CG method is a Krylov Subspace method for PD matrices:
  - The search/residual vectors of CG span the Krylov subspace
  - Hence, intermediate solutions of CG method x_n are in $K_n = \text{span}\left\{ \begin{matrix} \mathbf{b}, \mathbf{A}\,\mathbf{b}, \\ \cdots, \mathbf{A}^{n-1}\,\mathbf{b} \end{matrix} \right\}$
- Krylov Subspace methods
  - Based on the idea of projecting the "$\mathbf{Ax}=\mathbf{b}$ problem" into the Krylov subpace of smaller dimension n
  - Provide variations of CG for non-symmetric non-singular matrices
    - Generalized Minimal Residual (GMRES) or MINRES (for sym. but non P.D. $\mathbf{A}$)
      - Approximates the solution $\mathbf{Ax}=\mathbf{b}$ by the vector $\mathbf{x}_n \in K_n$ that minimizes the norm of the residual $\mathbf{Ax_n} - \mathbf{b}$
    - (Stabilized) bi-conjugate gradients (BiCGstab)
    - Quasi-minimal residual
  - See Trefethen and Bau, 1997, Asher and Grief, 2011; and other refs
    - This field is full of acronyms!

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)
- 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

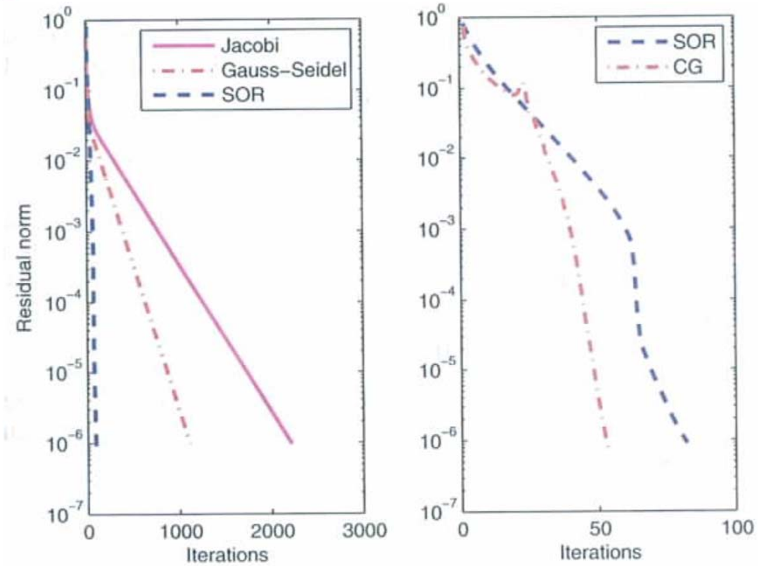


Fig 7.5: Example 7.10, with N=3: convergence behavior of various iterative schemes for the discretized Poisson equation.

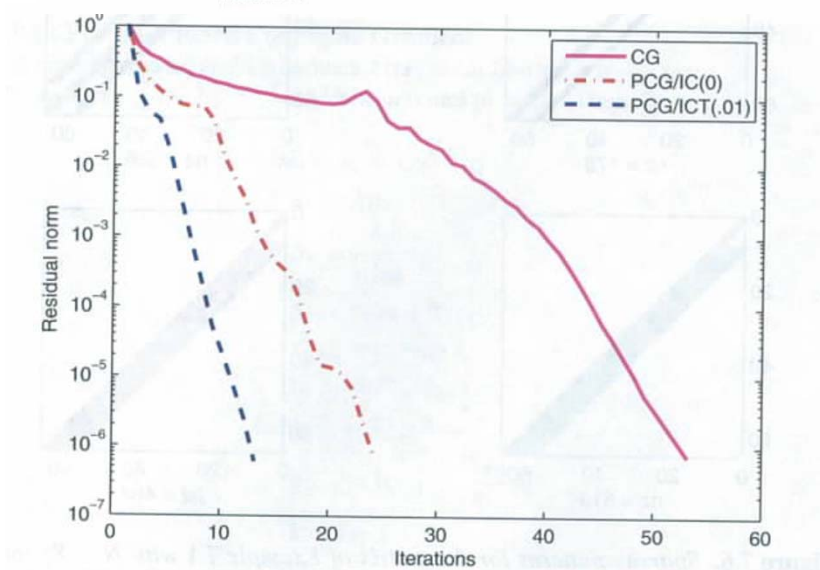


Fig 7.7: Iteration progress for CG, PCG with the IC(0) preconditioner and PCG with the IC preconditioner using drop tolerance tol=0.01

Ascher and Greif, Siam-2011

Review of/Summary for Iterative Methods

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.

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

References and Reading Assignments

- Part 8 (PT 8.1-2), Chapter 23 on "Numerical Differentiation" and Chapter 18 on "Interpolation" of "Chapra and Canale, Numerical Methods for Engineers, 2010/2006."
- 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"

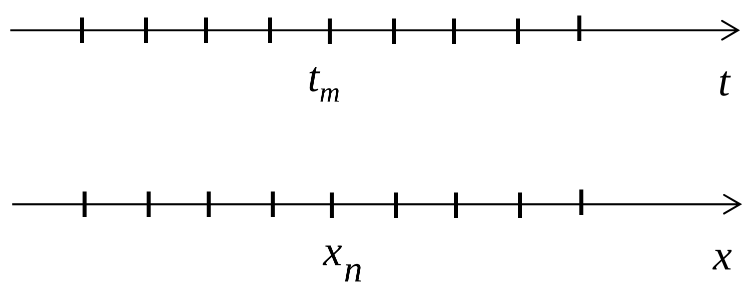
From Mathematical Models to Numerical Simulations

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



$$t_m = t_0 + m\Delta t \;, \quad m = 0, 1, \ldots M-1$$

$$x_n = x_0 + n\,\Delta x \;, \quad n = 0, 1, \ldots N-1$$

$$\frac{dw}{dx} \simeq \frac{\Delta w}{\Delta x} \,, \quad \frac{dw}{dt} \simeq \frac{\Delta w}{\Delta t}$$

p parameters

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)

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

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

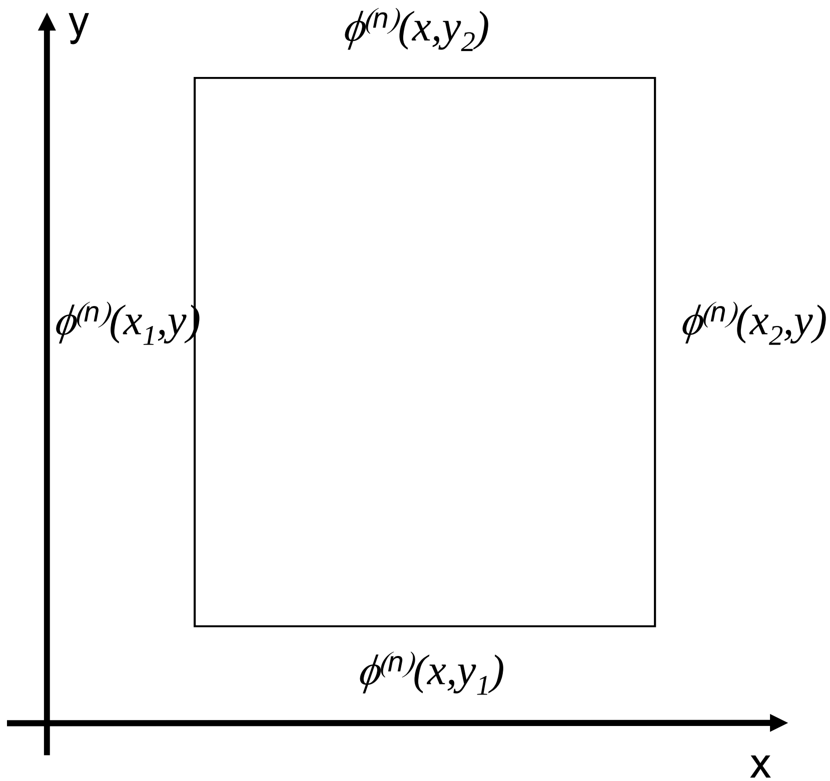
A,B and C Constants

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

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

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

(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: $\frac{D\mathbf{u}}{Dt} = \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\,\mathbf{u} = -\frac{1}{\rho}\nabla p + \nu\, \nabla^2 \mathbf{u} + \mathbf{g}$

Classification of Partial Differential Equations

(2D case, 2^{nd} order)

Meaning of Hyperbolic, Parabolic and Elliptic

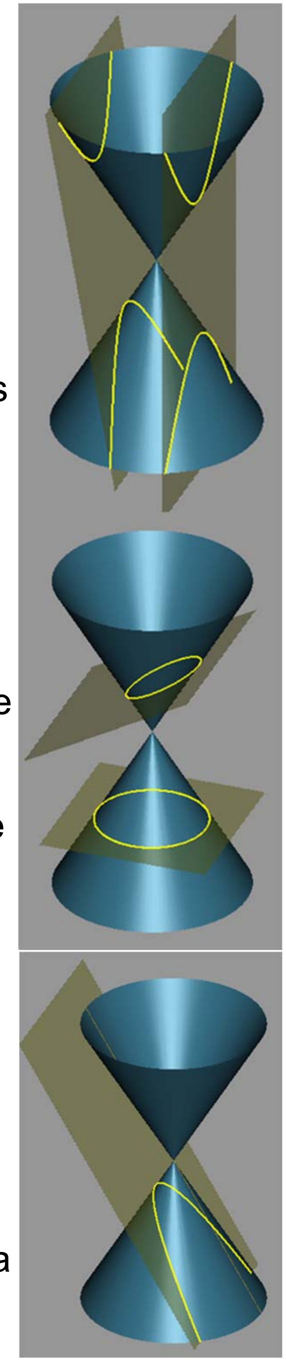
- The general 2^{nd} order PDE in 2D:

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

  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 $B^2\text{-}4AC$
- PDE:
  - $B^2\text{-}4AC > 0$ (Hyperbolic)
  - $B^2\text{-}4AC = 0$ (Parabolic)
  - $B^2\text{-}4AC < 0$ (Elliptic)



Partial Differential Equations
Parabolic PDE: $B^2 - 4AC = 0$

Examples

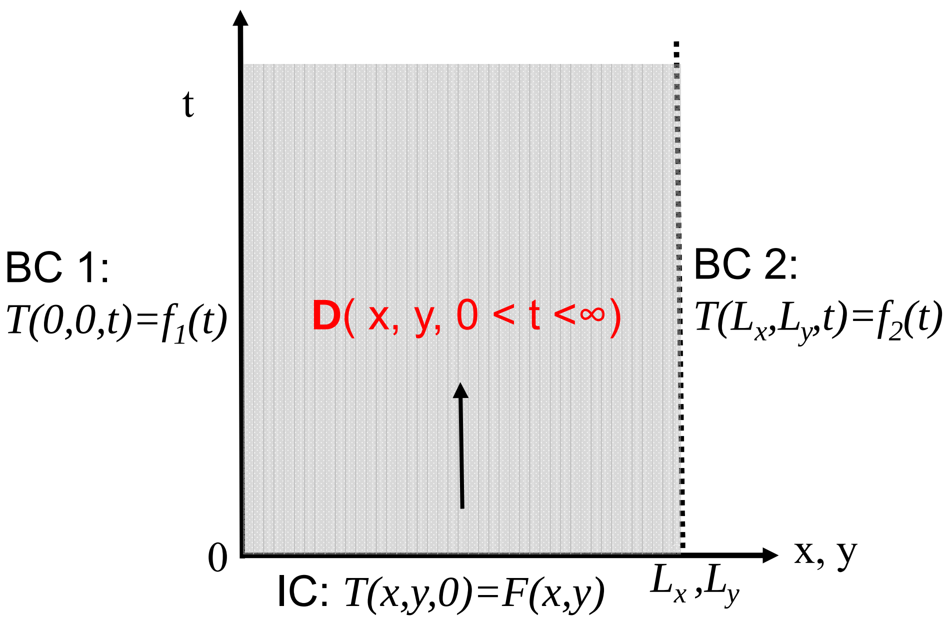
$$\frac{\partial T}{\partial t} = \frac{\kappa}{\sigma\rho}\nabla^2 T + f \,, \quad (\alpha = \frac{\kappa}{\sigma\rho})$$

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 u is domain **D** (x, y, 0 < t < ∞):
- Finite Differences/Volumes, Finite Elements



Partial Differential Equations
Parabolic PDE

Heat Flow Equation

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

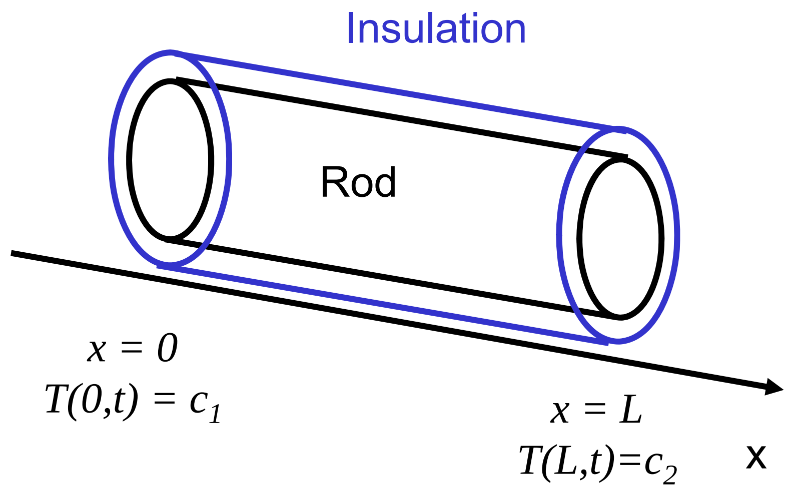
Initial Condition

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

Boundary Conditions

$$T(0,t) = c_1, 0 < t < \infty$$

$$T(L,t) = c_2, 0 < t < \infty$$



κ Thermal conductivity
σ Specific heat
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

Heat Flow Equation

$$T_t\left(x,t\right)=c^2T_{xx}\left(x,t\right),0<x<L,0<t<\infty$$

$$c=\sqrt{\frac{\kappa}{\rho\sigma}}$$

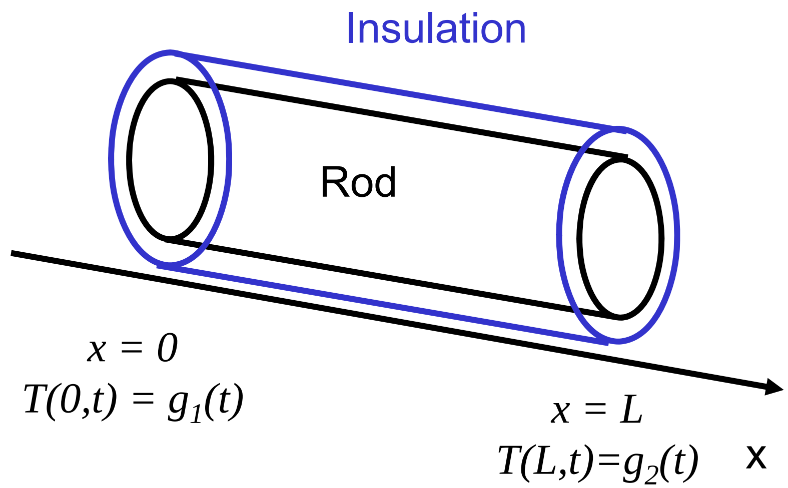
Initial Condition

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

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

Equidistant Sampling

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

Discretization

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

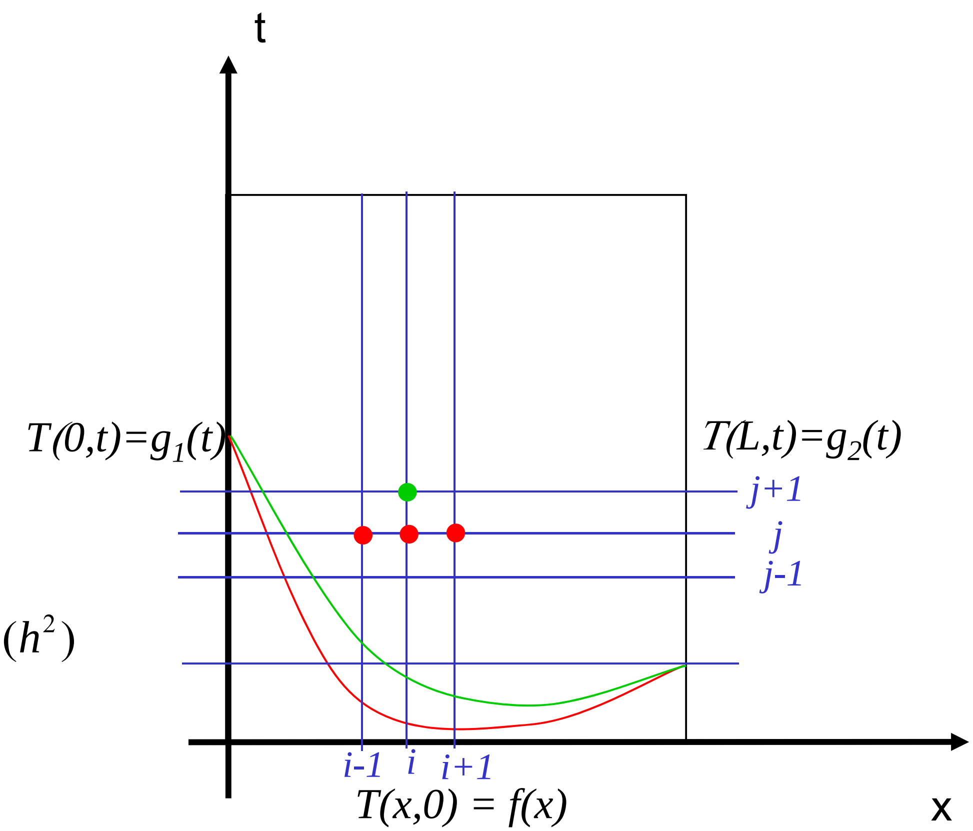
Forward (Euler) Finite Difference

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

Centered Finite Difference

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

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



Finite Difference Equation

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

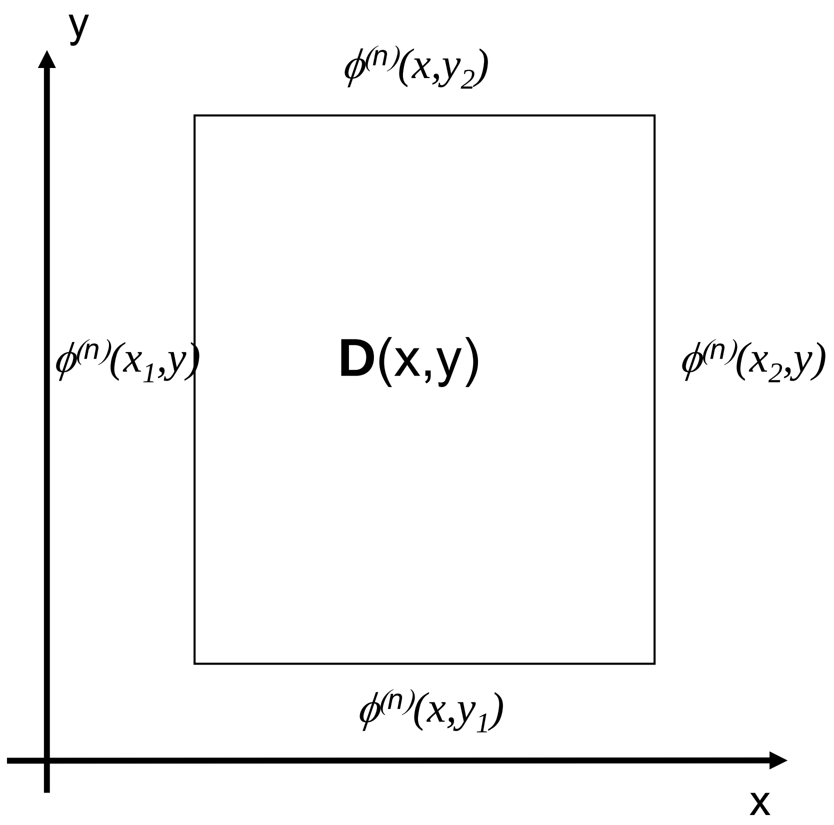
Partial Differential Equations
ELLIPTIC: $B^2 - 4AC < 0$

Quasi-linear PDE

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

A,B and C Constants

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



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