Numerical Methods for Partial Differential Equations: an Overview

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PDEs are mathematical models of physical phenomena

Heat conduction
\[ u_t = \kappa u_{xx}, \quad 0 < x < L, \quad t > 0, \]
\[ u(x, 0) = u_0(x), \quad 0 \leq x \leq L, \]
\[ u(0, t) = 1, \quad u(L, t) = 0, \quad t \geq 0. \]

\( u(x, t) \): temperature at position \( x \) and time \( t \)
\( \kappa \): heat conductivity coefficient
\( u_0 \): given function

Wave motion
\[ u_{tt} - \alpha^2 u_{xx} = f(x, t), \quad 0 < x < L, \quad t > 0, \]
\[ u(x, 0) = u_0(x), \quad u_t(x, 0) = u_1(x), \quad 0 \leq x \leq L, \]
\[ u(0, t) = g_1(t), \quad u(L, t) = g_2(t), \quad t \geq 0. \]

\( u(x, t) \): displacement at position \( x \) and time \( t \)
\( \alpha \): constant
\( u_0, u_1, g_1 \) and \( g_2 \): given functions
PDEs are mathematical models of

**Chemical Phenomena**
- Mixture problems
- Motion of electron, atom: Schrödinger equation
- Chemical reaction rate: Schrödinger equation
- Semiconductor: Schrödinger-Poisson equations

**Biological Phenomena**
- Population of a biological species
- Biomolecular electrostatics: Poisson-Boltzmann equation
- Calcium dynamics, ion diffusion: Nernst-Planck equation
- Cell motion and interaction
- Blood flow: Navier-Stokes equation
PDEs are mathematical models of

Engineering
- Fluid dynamics
  - Euler equations
  - Navier-Stokes Equations
- Electromagnetic
  - Poisson equation
  - Helmholtz’s equation
  - Maxwell equations
- Elasticity dynamics (structure of foundation)
  - Navier system
- Material Sciences
PDEs are mathematical models of

Semiconductor industry
  • Drift-diffusion equations
  • Euler-Poisson equations
  • Schrödinger-Poisson equations

Plasma physics
  • Vlasov-Poisson equations
  • Zakharov system

Financial industry
  • Black-Scholes equations

Economics, Medicine, Life Sciences, Social Sciences
Numerical PDEs with Applications

- Computational Mathematics: Scientific computing/numerical analysis
- Computational Physics
- Computational Chemistry
- Computational Biology
- Computational Fluid Dynamics
- Computational Engineering
- Computational Materials Sciences
- Computational Social Sciences: Computational sociology
Different Types of PDEs

**Linear scalar PDE**

Poisson equation (Laplace equation)

\[- \Delta u = - \sum_{i=1}^{d} u_{x_i x_i} = f(x), \quad -u_{xx} = f(x).\]

Heat equation

\[u_t - \Delta u = 0, \quad u_t - u_{xx} = 0.\]

Wave equation

\[u_{tt} - \Delta u = 0, \quad u_{tt} - u_{xx} = 0.\]

Helmholtz equation, Telegraph equation, ……
Different Types of PDEs

Nonlinear scalar PDE

Nonlinear Poisson equation

\[- \Delta u = f(u), \quad -u_{xx} = f(u).\]

Nonlinear convection-diffusion equation

\[u_t + f(u)_x = \nu u_{xx}, \quad \nu > 0.\]

Korteweg-de Vries (KdV) equation

\[u_t + uu_x + u_{xxx} = 0.\]

Eikonal equation, Hamilton-Jacobi equation, Klein-Gordon equation, Nonlinear Schrodinger equation, Ginzburg-Landau equation, ……
Different Types of PDEs

Linear systems

Navier system -- linear elasticity

\[ \mu \Delta \mathbf{u} + (\lambda + \mu)\text{grad(\text{div } \mathbf{u})} = \mathbf{0}. \]

Stokes equations

\[ \mathbf{u}_t + \nabla p = \nu \Delta \mathbf{u}, \]

\[ \nabla \cdot \mathbf{u} = 0. \]

Maxwell equations

\[ \nabla \times \mathbf{E} + \partial_t \mathbf{B} = 0 \]

\[ \nabla \times \mathbf{B} - \partial_t \mathbf{E} = J \]

\[ \nabla \cdot \mathbf{E} = \rho \]

\[ \nabla \cdot \mathbf{B} = 0 \]
Different Types of PDEs

Nonlinear systems

Reaction-diffusion system

\[ u_t - \Delta u = F(u). \]

System of conservation laws (Euler Equations …)

\[ u_t + \text{div} \ F(u) = 0. \]

Navier-Stokes equations
Classification of PDEs

For scalar PDE

Elliptic equations:
- Laplace equation, Poisson equation, …

Parabolic equations
- Heat equations, …

Hyperbolic equations
- Conservation laws, ….

For system of PDEs
For a specific problem

Physical domains

\[ u_{xx} = f(x), \quad a < x < b. \]

Boundary conditions (BC)

Dirichlet boundary condition

\[ u(a) = \alpha, \quad u(b) = \beta; \]

Neumann boundary condition

\[ u'(a) = \alpha, \quad u'(b) = \beta; \]

Robin boundary condition

\[ u'(a) + \gamma_1 u(a) = \alpha, \quad u'(b) + \gamma_2 u(b) = \beta. \]

Periodic boundary condition

\[ u(a) = u(b), \quad u'(a) = u'(b). \]
For a specific problem

Initial condition – time-dependent problem

For \( u_t = \cdots \)
\[ u(x, 0) = u_0(x). \]

For \( u_{tt} = \cdots \)
\[ u(x, 0) = f(x), \quad u_t(x, 0) = g(x). \]

Model problems

Boundary-value problem (BVP)
\[ u_{xx} = f(x), \quad a < x < b, \]
\[ u(a) = \alpha, \quad u(b) = \beta. \]
Model problem

Initial value problem – Cauchy problem

\[ u_t + a \, u_x = 0, \quad \text{or} \quad u_t + f(u)_x = 0, \quad -\infty < x < \infty, \]
\[ u(x, 0) = u_0(x), \quad -\infty < x < \infty. \]

Initial boundary value problem (IBVP)

\[ u_t + \alpha \, u_x = \nu \, u_{xx}, \quad a < x < b, \quad \nu > 0, \]
\[ u(a, t) = g_1(t), \quad u(b, t) = g_2(t), \quad t \geq 0, \]
\[ u(x, 0) = u_0(x), \quad a \leq x \leq b. \]
Major numerical methods for PDEs

- Finite difference method (FDM)
  - Pros
    - Simple and easy to design the scheme
    - Flexible to deal with the nonlinear problem
    - Widely used for elliptic, parabolic and hyperbolic equations
    - Most popular method for simple geometry, ….
    - Easy to program
  - Cons
    - Not easy to deal with complex geometry
    - Not easy for complicated boundary conditions
Major numerical methods for PDEs

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Major numerical methods for PDEs

• Finite element method (FEM)
  ✓ Pros
    - Flexible to deal with problems with complex geometry and complicated boundary conditions
    - Rigorous mathematical theory for analysis
    - Widely used in mechanical structure analysis, heat transfer, electromagnetics
  ✓ Cons
    - Need more mathematical knowledge to formulate a good and equivalent variational form
    - Appears hard to program
Major numerical methods for PDEs

- Finite element method: complex geometry
Major numerical methods for PDEs

- Finite element method: adaptivity
Major numerical methods for PDEs

- **Spectral method (Math676 Fall 2008)**
  - High (spectral) order of accuracy
  - Usually restricted for problems with regular geometry
  - Widely used for linear elliptic and parabolic equations on regular geometry
  - Widely used in quantum physics, quantum chemistry, material sciences, …
  - Not easy to deal with nonlinear problem
  - Not easy to deal with hyperbolic problem
  - Not easy to deal with complex geometry
Major numerical methods for PDEs

• Finite volume method (FVM)
  ✓ Flexible to deal with problems with complex geometry and complicated boundary conditions
  ✓ Keep physical laws in the discretized level
  ✓ Widely used in CFD
• Boundary element method (BEM)
  ✓ Reduce a problem in one less dimension
  ✓ Restricted to linear elliptic and parabolic equations
  ✓ Need more mathematical knowledge to find a good and equivalent integral form
  ✓ Very efficient fast Poisson solver when combined with the fast multipole method (FMM), ….
At the end of the course, you shall be able to

✓ Generate your own code of standard 2D FD, FV and FEM
✓ Understand the pathway of algorithm formulation
✓ Understand the error analysis of FEM
✓ Understand various requirements of PDEs on numerical methods
✓ Read papers on numerical analysis of PDEs, carry out research