Numerical Methods for Partial Differential Equations: an Overview

math652_Spring2009@colorstate

PDEs are mathematical models of physical phenomena

Heat conduction

$$u_t = \kappa\, u_{xx}, \qquad 0 < x < L, \quad t > 0,$$
$$u(x,0) = u_0(x), \quad 0 \le x \le L,$$
$$u(0,t) = 1, \quad u(L,t) = 0, \quad t \ge 0.$$

$u(x,t)$: temperature at position x and time t

κ: heat conductivity coefficient

u_0: given function

Wave motion

$$u_{tt} - \alpha^2\, u_{xx} = f(x,t), \qquad 0 < x < L, \quad t > 0,$$
$$u(x,0) = u_0(x), \qquad u_t(x,0) = u_1(x), \qquad 0 \le x \le L,$$
$$u(0,t) = g_1(t), \qquad u(L,t) = g_2(t), \qquad t \ge 0.$$

$u(x,t)$: displacement at position x and time t

α: 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: Schrodinger equation
- Chemical reaction rate: Schrodinger equation
- Semiconductor: Schrodinger-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
- Schrodinger-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)

$$-\triangle u = -\sum_{i=1}^{d} u_{x_i x_i} = f(\mathbf{x}), \qquad\qquad -u_{xx} = f(x).$$

Heat equation

$$u_t - \triangle u = 0, \qquad\qquad u_t - u_{xx} = 0.$$

Wave equation

$$u_{tt} - \triangle u = 0, \qquad\qquad u_{tt} - u_{xx} = 0.$$

Helmholtz equation, Telegraph equation, ……

Different Types of PDEs

Nonlinear scalar PDE

Nonlinear Poisson equation

$$-\triangle u = f(u), \qquad\qquad -u_{xx} = f(u).$$

Nonlinear convection-diffusion equation

$$u_t + f(u)_x = \nu u_{xx}, \qquad \nu > 0.$$

Korteweg-de Vries (KdV) equation

$$u_t + u\, u_x + u_{xxx} = 0.$$

Eikonal equation, Hamilton-Jacobi equation, Klein-Gordon equation,
Nonlinear Schrodinger equation, Ginzburg-Landau equation, …….

Different Types of PDEs

Linear systems

Navier system -- linear elasticity

$$\mu \triangle \mathbf{u} + (\lambda + \mu)\mathrm{grad}(\mathrm{div}\ \mathbf{u}) = \mathbf{0}.$$

Stokes equations

$$\begin{aligned} \mathbf{u}_t + \nabla p &= \nu \triangle \mathbf{u}, \\ \nabla \cdot \mathbf{u} &= 0. \end{aligned}$$

Maxwell equations

$$\begin{aligned} \nabla \times \mathbf{E} + \partial_{\mathbf{t}} \mathbf{B} &= \mathbf{0} \\ \nabla \times \mathbf{B} - \partial_{\mathbf{t}} \mathbf{E} &=: \mathbf{J} \\ \nabla \cdot \mathbf{E} &=: \rho \\ \nabla \cdot \mathbf{B} &= 0 \end{aligned}$$

Different Types of PDEs

Nonlinear systems

Reaction-diffusion system

$$\mathbf{u}_t - \triangle \mathbf{u} = \mathbf{F}(\mathbf{u}).$$

System of conservation laws (Euler Equations …)

$$\mathbf{u}_t + \operatorname{div} \mathbf{F}(\mathbf{u}) = \mathbf{0}.$$

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

$$u_{xx} = f(x), \qquad a < x < b.$$

Boundary conditions (BC)

Dirichlet boundary condition

$$u(a) = \alpha, \qquad u(b) = \beta;$$

Neumann boundary condition

$$u'(a) = \alpha, \qquad u'(b) = \beta;$$

Robin boundary condition

$$u'(a) + \gamma_1 u(a) = \alpha, \qquad u'(b) + \gamma_2 u(b) = \beta.$$

Periodic boundary condition

$$u(a) = u(b), \qquad u'(a) = u'(b).$$

For a specific problem

Initial condition – time-dependent problem

For $$u_t = \cdots$$
$$u(\mathbf{x}, 0) = u_0(\mathbf{x}).$$

For $$u_{tt} = \cdots$$
$$u(\mathbf{x}, 0) = f(\mathbf{x}),$$
$$u_t(\mathbf{x}, 0) = g(\mathbf{x}).$$

Model problems

Boundary-value problem (BVP)

$$u_{xx} = f(x), \qquad a < x < b,$$
$$u(a) = \alpha, \qquad u(b) = \beta.$$

Model problem

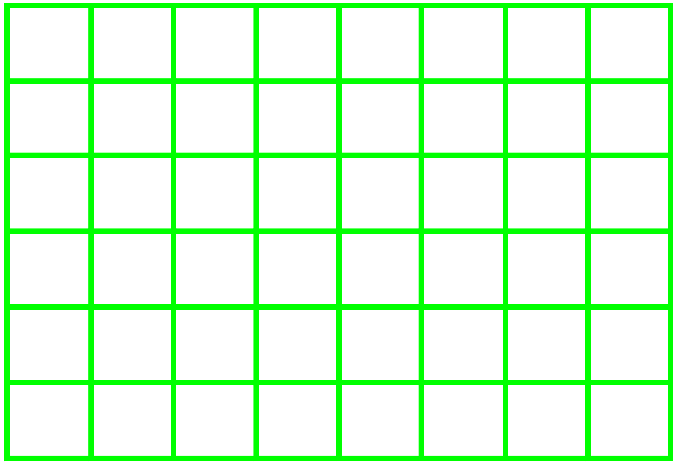
Initial value problem – Cauchy problem

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

Initial boundary value problem (IBVP)

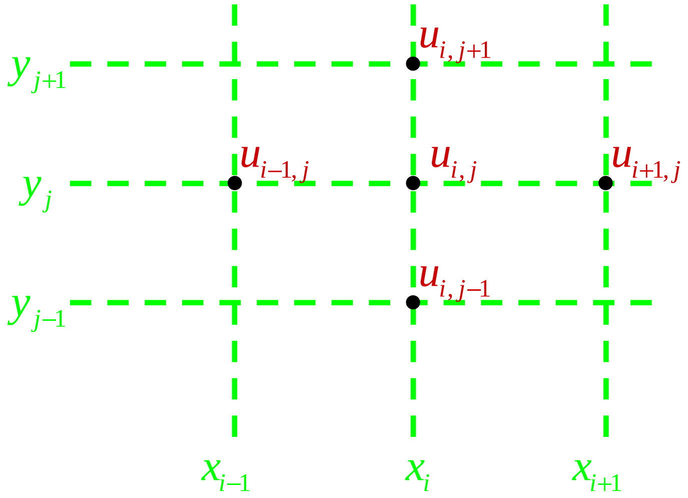
$$u_t + \alpha\, u_x = \nu\, u_{xx}, \qquad a < x < b, \quad \nu > 0,$$
$$u(a,t) = g_1(t), \qquad u(b,t) = g_2(t), \qquad t \geq 0,$$
$$u(x,0) = u_0(x), \qquad a \leq x \leq b.$$

Major numerical methods for PDEs



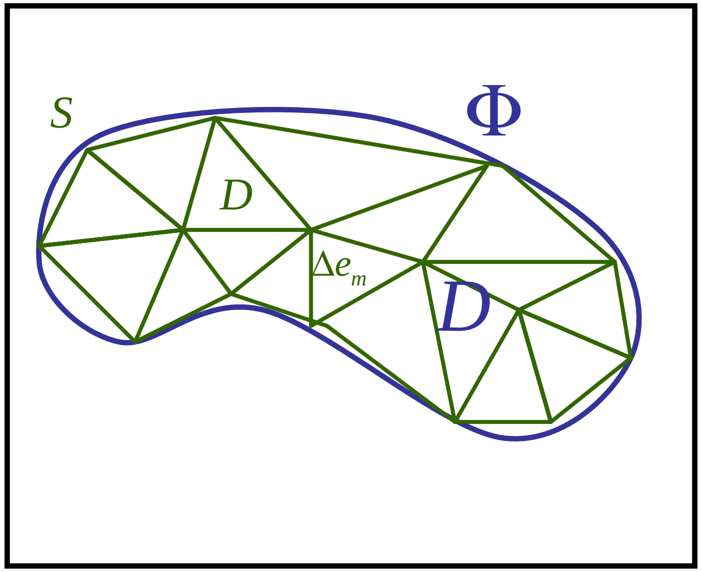
- Finite difference method (FDM)
  - ✓ Pros
    - Simple and easy to design the scheme
    - Flexible to deal with the nonlinear problem
    - Widely used for elliptic, parabolic and hyperbolic equations
    - Most popular method for simple geometry, ….
    - Easy to program
  - ✓ Cons
    - Not easy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

Major numerical methods for PDEs



- 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

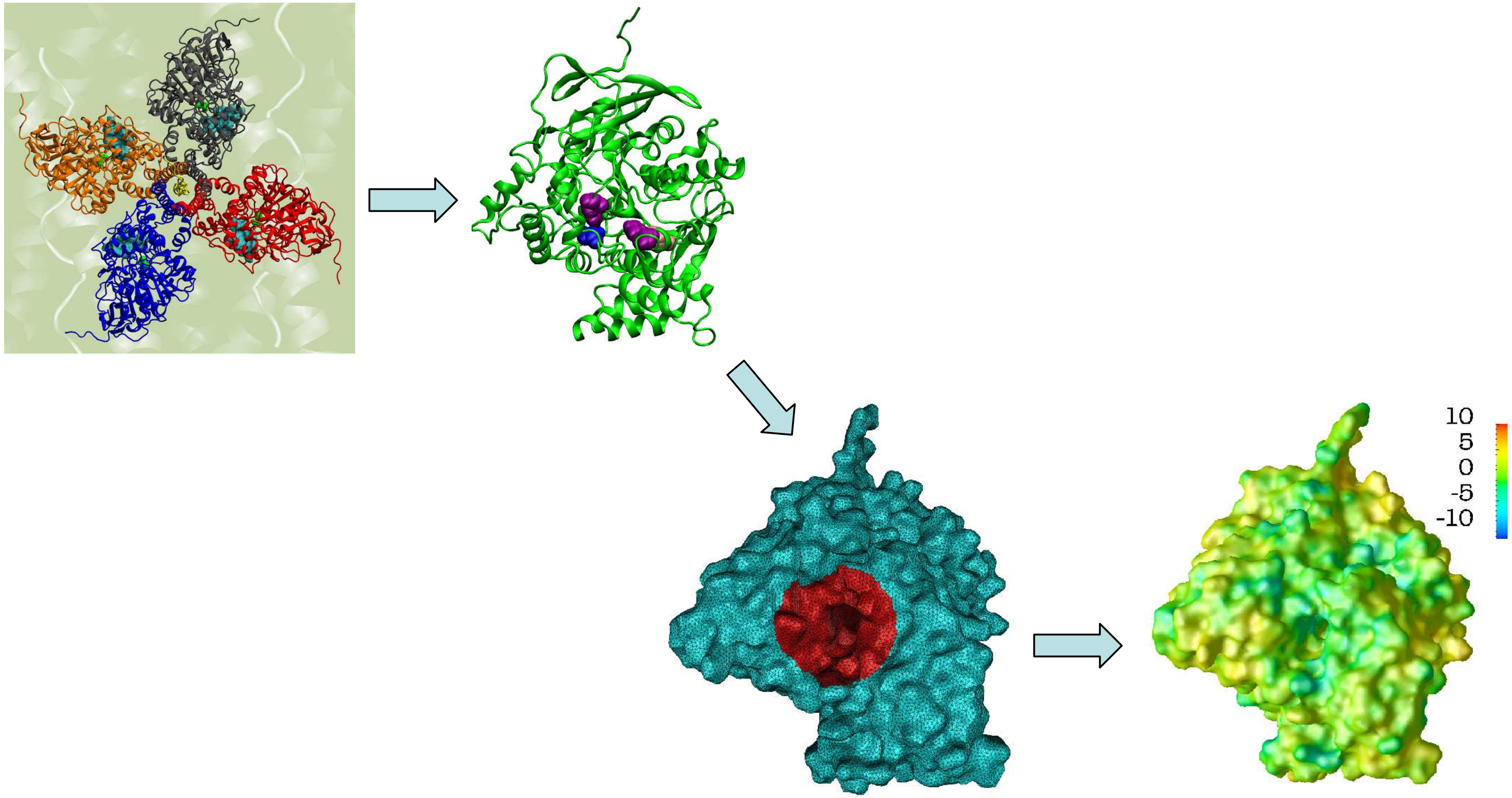
Major numerical methods for PDEs



- 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

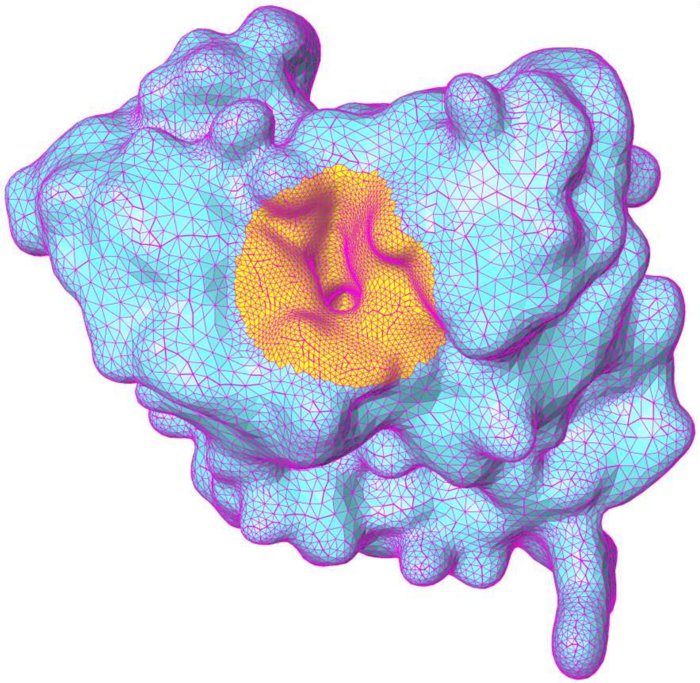
Major numerical methods for PDEs

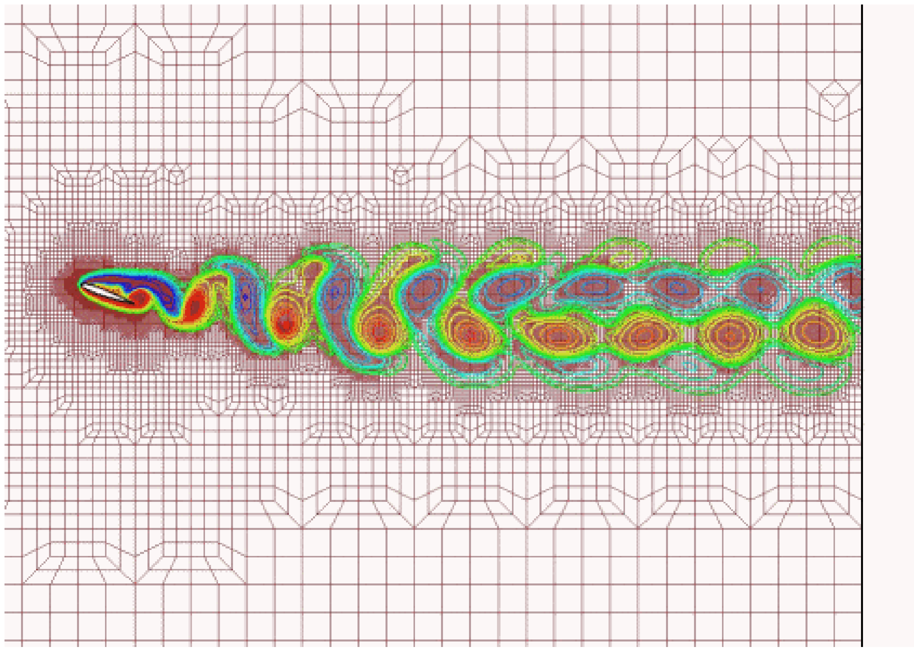
- Finite element method: complex geometry



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