Discretization of PDEs and Tools for the Parallel Solution of the Resulting Systems

Stan Tomov

Innovative Computing Laboratory
Computer Science Department
The University of Tennessee

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Topics

Projection in Scientific Computing
(lecture 1)

Sparse matrices, parallel implementations
(lecture 3)

PDEs, Numerical solution, Tools, etc.
(lecture 2)

Iterative Methods
(lectures 4 and 5)
Part I
Partial Differential Equations

Part II
Mesh Generation and Load Balancing

Part III
Tools for Numerical Solution of PDEs
Part I

Partial Differential Equations
Mathematical Model:

- a representation of the essential aspects of an existing system which presents knowledge of that system in usable form (Eykhoff, 1974)

**Navier-Stokes equations:**

\[
\begin{align*}
\nabla \cdot u &= 0 \\
\frac{\partial u}{\partial t} &= -(u \cdot \nabla)u - \frac{1}{\rho} \nabla p + \nu \nabla^2 u + f \\
B.C. & , \ etc.
\end{align*}
\]
We are interested in models that are

- **Dynamic**
  i.e. account for changes in time

- **Heterogeneous**
  i.e. account for heterogeneous systems

Typically represented with

- **Partial Differential Equations**
Mathematical Modeling

How can we model for e.g. Heat Transfer?

- **Heat**
  * a form of energy (thermal)

- **Heat Conduction**
  * transfer of thermal energy from a region of higher temperature to a region of lower temperature

- **Some notations**

  \[ Q : \text{amount of heat} \]
  \[ k : \text{material conductivity} \]
  \[ T : \text{temperature} \]
  \[ A : \text{area of cross-section} \]
The Law of Heat Conduction

\[ \frac{\Delta Q}{\Delta t} = k \ A \frac{\Delta T}{\Delta x} \]

Change of heat is proportional to the gradient of the temperature and the area \( A \) of the cross-section.

\( Q \): amount of heat
\( k \): material conductivity
\( T \): temperature
\( A \): area of cross-section
Consider 1-D heat transfer in a thin wire

- so thin that $T$ is piecewise constant along the slides, i.e. $T_0(t), T_1(t), T_2(t)$, etc.
- ideally insulated

Let us write a balance for the temperature at $T_1$ for time $t + \Delta t$

$$T_1(t + \Delta t) =?$$
\[ T_1(t + \Delta t) \approx T_1(t) + k\Delta t \frac{(T_2(t) - T_1(t))}{(\Delta x)^2} + k\Delta t \frac{(T_0(t) - T_1(t))}{(\Delta x)^2} \]

\[ = T_1(t) + k\Delta t \frac{T_2(t) - 2T_1(t) + T_0(t)}{(\Delta x)^2} \]

Take \( \lim_{\Delta x, \Delta t \to 0} \)

\[ \Rightarrow \quad \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} \quad (Exercise) \]
Heat Transfer

Extend to 2-D and put a source term $f$ to easily get

$$\frac{\partial T}{\partial t} = k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + f \equiv k \Delta T + f$$

Known as the Heat equation
Other Important PDEs

- Poisson equation (elliptic)
  \[ \Delta u = f \]

- Heat equation (parabolic)
  \[ \frac{\partial T}{\partial t} = k \, \Delta T + f \]

- Wave equation (hyperbolic)
  \[ \frac{1}{\nu^2} \frac{\partial^2 u}{\partial t^2} = \Delta u + f \]
Classification of PDEs

For a general second-order PDE in 2 variables:

\[ Au_{xx} + Bu_{xy} + Cu_{yy} + \cdots = 0 \]

**Elliptic:**
- if \( B^2 - 4AC < 0 \)
- process in equilibrium (no time dependence)
- easy to discretize but challenging to solve

**Parabolic:**
- if \( B^2 - 4AC = 0 \)
- processes evolving toward steady state

**Hyperbolic:**
- if \( B^2 - 4AC > 0 \)
- not evolving toward steady state
- difficult to discretize (support discontinuities) but easy to solve in characteristic form
How do we solve them?

Numerical solution approaches:
- Finite difference method
- Finite element method
- Finite volume method
- Boundary element method
Finite Difference Method

- use finite differences to approximate differential operators
- one of the simplest and extensively used method in solving PDEs
- the error, called truncation error, is due to finite approximation of the Taylor series of the differential operator
Consider the 2-D Poisson equation:

\[ \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f \]

The idea, first in 1-D:

- Use Taylor series to approximate \( \frac{d^2 u}{dx^2} (x) \) with \( u(x), u(x + h), u(x - h) \)

\[
\begin{align*}
  u(x + h) &= u(x) + h \frac{du}{dx} (x) + \frac{h^2}{2} \frac{d^2 u}{dx^2} (x) + \frac{h^3}{3!} \frac{d^3 u}{dx^3} (x) + O(h^4) \\
  u(x - h) &= u(x) - h \frac{du}{dx} (x) + \frac{h^2}{2} \frac{d^2 u}{dx^2} (x) - \frac{h^3}{3!} \frac{d^3 u}{dx^3} (x) + O(h^4)
\end{align*}
\]

\[ \Rightarrow \frac{d^2 u}{dx^2} (x) = \frac{1}{h^2} (u(x + h) + u(x - h) - 2u(x)) + O(h^2) \]
Similarly in 2-D

- Use Taylor series to approximate $\Delta u(x, y)$ with $u(x, y), u(x + h, y), u(x - h, y), u(x, y + h), u(x, y - h)$.

\[
\begin{align*}
&u(x + h, y) = u(x, y) + h \frac{\partial u}{\partial x}(x, y) + \frac{h^2}{2} \frac{\partial^2 u}{\partial x^2}(x, y) + \frac{h^3}{3!} \frac{\partial^3 u}{\partial x^3}(x, y) + O(h^4) \\
&u(x - h, y) = u(x, y) - h \frac{\partial u}{\partial x}(x, y) + \frac{h^2}{2} \frac{\partial^2 u}{\partial x^2}(x, y) - \frac{h^3}{3!} \frac{\partial^3 u}{\partial x^3}(x, y) + O(h^4) \\
&u(x, y + h) = u(x, y) + h \frac{\partial u}{\partial y}(x, y) + \frac{h^2}{2} \frac{\partial^2 u}{\partial y^2}(x, y) + \frac{h^3}{3!} \frac{\partial^3 u}{\partial y^3}(x, y) + O(h^4) \\
&u(x, y - h) = u(x, y) - h \frac{\partial u}{\partial y}(x, y) + \frac{h^2}{2} \frac{\partial^2 u}{\partial y^2}(x, y) - \frac{h^3}{3!} \frac{\partial^3 u}{\partial y^3}(x, y) + O(h^4)
\end{align*}
\]

$\Rightarrow \Delta u(x, y) = \frac{1}{h^2} (u(x + h, y) + u(x - h, y) + u(x, y + h) + u(x, y - h) - 4u(x)) + O(h^2)$
A Finite Difference Method Example

Consider the 1-D equation:

$$\frac{d^2 u}{dx^2}(x) = f(x), \quad \text{for } x \in (0, 1)$$

and the Dirichlet boundary condition

$$u(0) = u(1) = 0$$

The interval $[0, 1]$ is discretized uniformly with $n + 2$ points

At any point $x_i$ we are looking for $u_i$, an approximation of the exact solution $u(x_i)$, using the approximation

$$-u_{i-1} + 2u_i - u_{i+1} = h^2 f_i,$$

and the fact that $u_0 = u_{n+1} = 0$,

we obtain a linear system of the form

$$Ax = b$$

where $b = (f_i)_{i=1,n}$ and $x = (u_i)_{i=1,n}$ and

$$A = \frac{1}{h^2} \begin{pmatrix} 2 & -1 \\ -1 & 2 & -1 \\ & -1 & 2 & -1 \\ & & & \ddots \\ & & & & -1 & 2 & -1 \\ & & & & & -1 & 2 \\ 
\end{pmatrix}$$

(slide used material from Julien Langou's presentation)
A Finite Difference Method Example

Consider the 2-D Poisson equation:

\[ \Delta u = f \]

and the Dirichlet boundary condition

\[ u(x, y) = 0 \text{ for } (x, y) \in \partial \Omega \]

The interval \([0, 1] \times [0, 1]\) is discretized uniformly with \((n + 2) \times (n + 2)\) points

\[ A = \frac{1}{h^2} \begin{pmatrix} B & -l & -1 \\ -l & B & -1 \\ & & \ddots & \ddots & \ddots \\ -l & B & -1 \\ -l & -l & B \end{pmatrix} \]

where

\[ B = \begin{pmatrix} 4 & -1 & -1 & -1 \\ -1 & 4 & -1 & \vdots \\ \vdots & \ddots & \ddots & \vdots \\ -1 & 4 & -1 & \ddots \\ \vdots & \vdots & \ddots & \ddots \end{pmatrix} \]
Finite Element Method

Remember the slides from the previous lecture


Main pluses/minuses of FEM vs FDM

- FEM can handle complex geometries
- FDM is easy to implement
Consider the 1-D Dirichlet problem:

\begin{equation}
    u''(x) = f(x), \quad \text{for } x \in (0, 1)
\end{equation}

and the Dirichlet boundary condition

\[ u(0) = u(1) = 0 \]

**Weak or Variational formulation:**

- Multiply (1) by smooth \( v \) and integrate over (0,1)

\[
    \int_0^1 f(x)v(x)dx = \int_0^1 u''(x)v(x)dx
\]

- Integrate by parts the above RHS

\[
    \int_0^1 u''(x)v(x)dx = u'(x)v(x)|_0^1 - \int_0^1 u'(x)v'(x)dx
\]

\[
    = -\int_0^1 u'(x)v'(x)dx \equiv -a(u, v)
\]

- Variational formulation: Find \( u \in H^1_0(0, 1) \) such that

\[
    \int_0^1 f(x)v(x)dx = -a(u, v) \text{ for } \forall v \in H^1_0(0, 1)
\]
Discretization (Galerkin FE problem):
- Replace $H^1_0(0, 1)$ with finite dimensional subspace $V$

Shown is a 4 dimensional space $V$ (basis in blue) and a linear combination (in red)

$$v_k(x) = \begin{cases} \frac{x-x_{k-1}}{x_k-x_{k-1}} & \text{if } x \in [x_{k-1}, x_k], \\
\frac{x_k+x_{k+1}-x}{x_{k+1}-x_k} & \text{if } x \in [x_k, x_{k+1}], \\
0 & \text{otherwise,} \end{cases}$$

What is the matrix form of the problem (Exercise)
Part II

Mesh Generation and Load Balancing

Part III

Tools for Numerical Solution of PDEs
Challenges:

- Software Complexity
- Data Distribution and Access
- Portability, Algorithms, and Data Redistribution

Read more in Chapter 21
There is software; to mention a few packages:

- **Overture**
  - OO framework for PDEs in complex moving geometry

- **PARASOL**
  - Parallel, sparse matrix solvers; in Fortran 90

- **SAMRAI**
  - OO framework for parallel AMR applications

- **HYPRE**
  - Large sparse linear solvers and preconditioners

- **PETSc**
  - Tools for numerical solution of PDEs

- **FFTW**
  - Parallel FFT routines

- **Diffpack**
  - OO framework for solving PDEs

- **Doug**
  - FEM for elliptic PDEs

- **POOMA**
  - OO framework for HP applications

- **UG**
  - PDEs on unstructured grids using multigrid

**PETSc**: Portable, Extensible Toolkit for Scientific computation

- for large-scale sparse systems
- facilitate extensibility
- provides interface to external packages, e.g. BlockSolve95, ESSL, Matlab, ParMeTis, PVODE, and SPAI.
- programed in C, usable from Fortran and C++
- uses MPI for all parallel communication
  - in a distributed-memory model
  - user do communication on level higher than MPI
- Computation and communication kernels: MPI, MPI-IO, BLAS, LAPACK
PETSc’s Main Numerical Components

Nonlinear Solvers
- Newton-based Methods
- Line Search
- Trust Region
- Other

Time Steppers
- Euler
- Backward Euler
- Pseudo Time Stepping
- Other

Krylov Subspace Methods
- GMRES
- CG
- CGS
- Bi-CG-STAB
- TFQMR
- Richardson
- Chebychev
- Other

Preconditioners
- Additive Schwarz
- Block Jacobi
- Jacobi
- ILU
- ICC
- LU
- (Sequential only)
- Others

Matrices
- Compressed Sparse Row (AIJ)
- Blocked Compressed Sparse Row (BAIJ)
- Block Diagonal (BDIAG)
- Dense
- Other

Vectors

Index Sets
- Indices
- Block Indices
- Stride
- Other

more info at: http://acts.nersc.gov/petsc/
Learning Goals

A brief overview of Numerical PDEs and related issues

- Mathematical modeling
- PDEs for describing changes in physical processes
- More specific discretization examples
  - Finite Differences (natural)
  - FEM
    - reinforce the idea and application of Petrov-Galerkin conditions
- Issues related to mesh generation and load balancing and importance in HPC
  - Adaptive methods
- Software