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

Wednesday April 04, 2012

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)

Outline

- **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)

Mathematical Modeling:

Real world   Model

Navier-Stokes equations:

$\longleftrightarrow$

$$
\begin{aligned}
\nabla \cdot u &= 0 \\
\frac{\partial u}{\partial t} &= -(u \cdot \nabla) u - \frac{1}{\rho} \nabla p + \nu \nabla^2 u + f \\
B.C. &, \quad etc.
\end{aligned}
$$

Mathematical Modeling

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

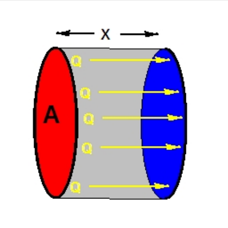
- Partial Differential Equations

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 : amount of heat
k : material conductivity
T : temperature
A : area of cross-section



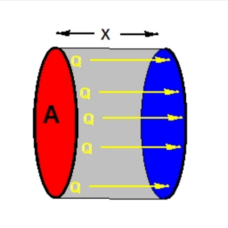
Heat Transfer

The Law of Heat Conduction

$$\frac{\triangle Q}{\triangle t} = k\ A\ \frac{\triangle T}{\triangle x}$$

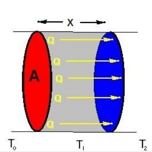
Change of heat is proportional to the gradient of the temperature and the area A of the cross-section.

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 $t + \triangle t$

$$T_1(t + \triangle t) = ?$$

Heat Transfer

$$
\begin{aligned}
T_1(t + \triangle t) \approx \quad & T_1(t) \\
+ \quad & k \triangle t \frac{(T_2(t) - T_1(t))}{(\triangle x)^2} \\
+ \quad & k \triangle t \frac{(T_0(t) - T_1(t))}{(\triangle x)^2} \\
= \quad & T_1(t) + k \triangle t \frac{T_2(t) - 2T_1(t) + T_0(t)}{(\triangle x)^2}
\end{aligned}
$$

Take $lim_{\triangle x, \triangle t \rightarrow 0}$

$$
\Rightarrow \qquad \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} \qquad (\mathit{Exercise})
$$

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

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

Known as the Heat equation

Other Important PDEs

- Poisson equation (elliptic)

$$\triangle u = f$$

- Heat equation (parabolic)

$$\frac{\partial T}{\partial t} = k \triangle T + f$$

- Wave equation (hyperbolic)

$$\frac{1}{\nu^2}\frac{\partial^2 u}{\partial t^2} = \triangle u + f$$

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 discontinuoities) 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

A Finite Difference Method Example

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 $u(x), u(x+h), u(x-h)$

$$u(x+h) = u(x) + h\frac{du}{dx}(x) + \frac{h^2}{2}\frac{d^2 u}{dx^2}(x) + \frac{h^3}{3!}\frac{d^3 u}{dx^3}(x) + \mathcal{O}(h^4)$$
$$u(x-h) = u(x) - h\frac{du}{dx}(x) + \frac{h^2}{2}\frac{d^2 u}{dx^2}(x) - \frac{h^3}{3!}\frac{d^3 u}{dx^3}(x) + \mathcal{O}(h^4)$$

$$\Rightarrow \frac{d^2 u}{dx^2}(x) = \frac{1}{h^2}(u(x+h) + u(x-h) - 2u(x)) + \mathcal{O}(h^2)$$

A Finite Difference Method Example

Similarly in 2-D

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

$$u(x+h, y) = u(x, y) + h\frac{\partial u}{\partial x}(x, y) + \frac{h^2}{2}\frac{\partial^2 u}{\partial x^2}(x, y) + \frac{h^3}{3!}\frac{\partial^3 u}{\partial x^3}(x, y) + \mathcal{O}(h^4)$$

$$u(x-h, y) = u(x, y) - h\frac{\partial u}{\partial x}(x, y) + \frac{h^2}{2}\frac{\partial^2 u}{\partial x^2}(x, y) - \frac{h^3}{3!}\frac{\partial^3 u}{\partial x^3}(x, y) + \mathcal{O}(h^4)$$

$$u(x, y+h) = u(x, y) + h\frac{\partial u}{\partial y}(x, y) + \frac{h^2}{2}\frac{\partial^2 u}{\partial y^2}(x, y) + \frac{h^3}{3!}\frac{\partial^3 u}{\partial y^3}(x, y) + \mathcal{O}(h^4)$$

$$u(x, y-h) = u(x, y) - h\frac{\partial u}{\partial y}(x, y) + \frac{h^2}{2}\frac{\partial^2 u}{\partial y^2}(x, y) - \frac{h^3}{3!}\frac{\partial^3 u}{\partial y^3}(x, y) + \mathcal{O}(h^4)$$

$$\Rightarrow \Delta u(x, y) = \frac{1}{h^2}\left(u(x+h, y) + u(x-h, y) + u(x, y+h) + u(x, y-h) - 4u(x)\right) + \mathcal{O}(h^2)$$

A Finite Difference Method Example

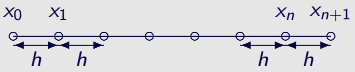
Consider the 1-D equation:

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

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 approxmation 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 $u_0 = u_{n+1} = 0$,

(slide used material from Julien Langou's presentation)

we obtain a linear system of the form

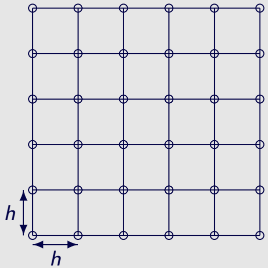
$$Ax = b$$

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

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

A Finite Difference Method Example

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



Consider the 2-D Poisson equation:

$$\Delta u = f$$

and the Dirichlet boundary condition

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

$$A = \frac{1}{h^2}\begin{pmatrix} B & -I & & & & \\ -I & B & -1 & & & \\ & -I & B & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -I & B & -I \\ & & & & -I & B \end{pmatrix} \quad \text{where} \quad B = \begin{pmatrix} 4 & -1 & & & & \\ -1 & 4 & -1 & & & \\ & -1 & 4 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 4 & -1 \\ & & & & -1 & 4 \end{pmatrix}$$

(slide used material from Julien Langou's presentation)

Finite Element Method

- Remember the slides from lecture 2
  - http://www.cs.utk.edu/~dongarra/WEB-PAGES/SPRING-2010/Lect02-2010.pdf

Main pluses/minuses of FEM *vs* FDM

- FEM can handle complex geometries
- FDM is easy to implement

A Finite Element Method Example

Consider the 1-D Dirichlet problem:

$$(1) \qquad u''(x) = f(x), \quad \text{for } x \in (0,1)$$

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

$$\begin{aligned}\int_0^1 u''(x)v(x)dx &= u'(x)v(x)|_0^1 - \int_0^1 u'(x)v'(x)dx \\ &= -\int_0^1 u'(x)v'(x)dx \equiv -a(u,v)\end{aligned}$$

- Variational formulation: Find $u \in H_0^1(0,1)$ such that

$$\int_0^1 f(x)v(x)dx = -a(u,v) \text{ for } \forall v \in H_0^1(0,1)$$

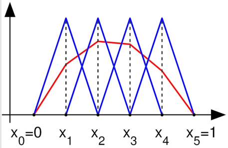
A Finite Element Method Example

Discretization (Galerkin FE problem):

- Replace $H_0^1(0,1)$ with finite dimensional subspace V

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

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



What is the matrix form of the problem (Exercise)

Part II

Mesh Generation and Load Balancing

slides at: http://www.cs.utk.edu/~dongarra/WEB-PAGES/SPRING-2010/Lect09-p2.pdf

Part III

Tools for Numerical Solution of PDEs

Parallel PDE Computations

Challenges:

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

Read more in Chapter 21

Software for PDEs

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

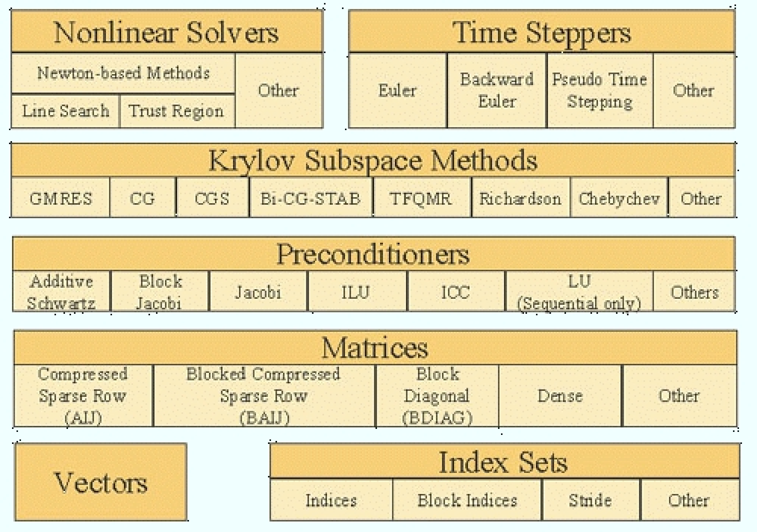
See also: http://www.mgnet.org/ http://www.nhse.org/ http://www.netlib.org/

PETSc

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



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