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

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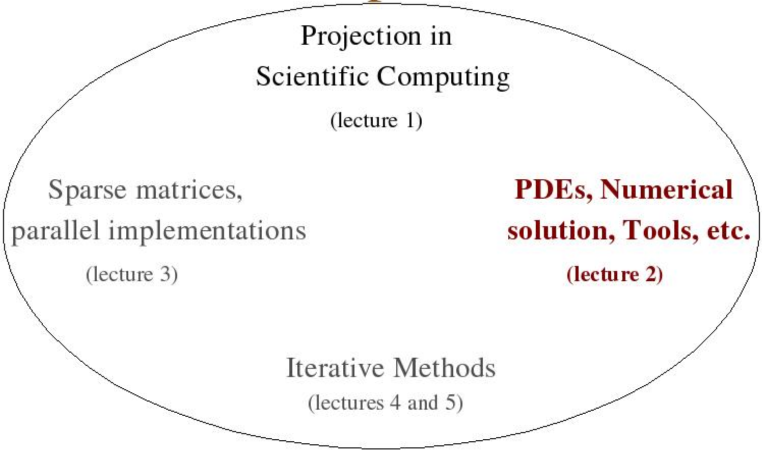
Topics


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)

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

$\longleftrightarrow$

Navier-Stokes equations:

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

Mathematical Modeling

We are interested in models that are

- Dynamic
  i.e. account for changes in time
- Heterogeneous
  i.e. account for heterogeneous systems

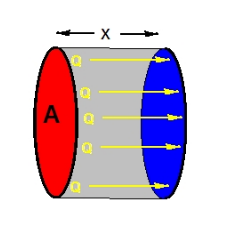
Typically represented with

- Partial Differential Equations

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



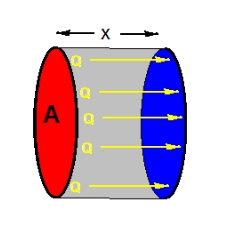
Heat Transfer

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.

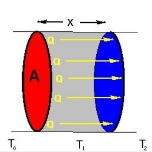
Q : amount of heat
k : material conductivity
T : temperature
A : area of cross-section



Heat Transfer

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 $t + \triangle t$

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

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

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

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

Heat Transfer

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

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

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

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

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

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

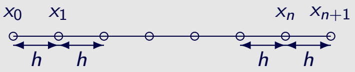
Consider the 1-D equation:

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

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

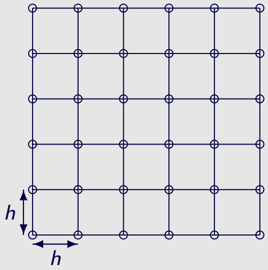
Consider the 2-D Poisson equation:

$$\Delta u = f$$

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



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

(slide used material from Julien Langou's presentation)

Finite Element Method

- Remember the slides from the previous lecture
  - http://www.cs.utk.edu/~dongarra/WEB-PAGES/SPRING-2013/Lect10-2013.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

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

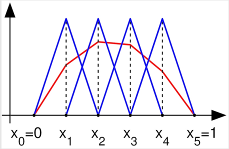
A Finite Element Method Example

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-2013/Lect12-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

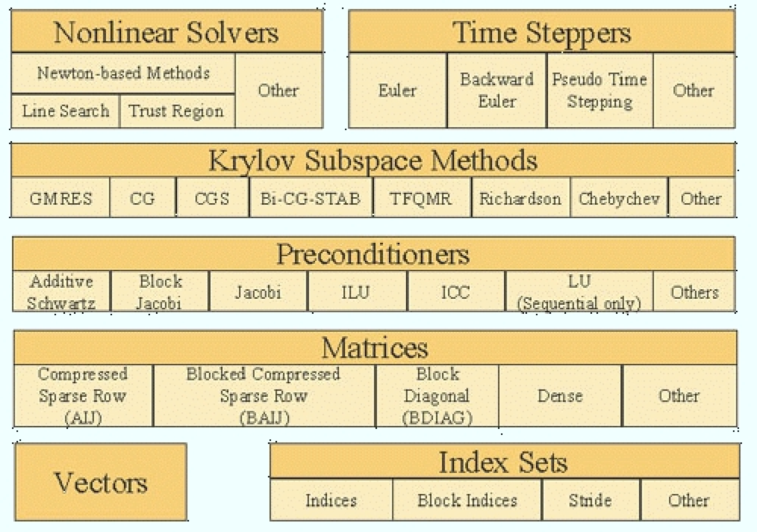
See also: http://www.mgnet.org/ http://www.nhse.org/ http://www.netlib.org/

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