Computational Requirements of Scientific Applications

Goals of lecture

- Understand computational requirements of scientific applications.
- Introduce the notions of regular and irregular problems.

Computational Science Applications

Simulation of physical phenomena

- fluid flow over aircraft (Boeing 777 designed by simulation)
- fatigue fracture in aircraft bodies
- bone growth
- evolution of galaxies

Two main approaches

- continuous methods: fields and partial differential equations (pde's) (eg. Navier-Stokes equations, Maxwell's equations, elasiticity equations..)
- discrete methods: particles and forces between them (eg. Gravitational/Coulomb forces)

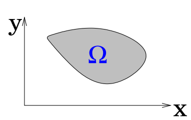
We will focus on pde's in this lecture.

Modeling physical phenomena using pde's

PDE : $L u = f$

eg: $\left(\frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} \right) u = 0$

Domain: Ω



Boundary conditions: on $\delta\Omega$ $\quad u(x,y) = x + y \mid (x,y) \text{ on } \delta\Omega$

General technique: find an approximate solution that is a linear combination of known functions

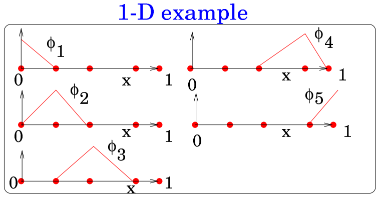
$$u^*(x,y) = \sum_i c_i \, \Phi_i(x,y)$$

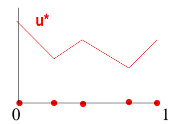
Question: How do we choose the known functions?
How do we find the best choice of c's, given the functions?

Choice of known functions:

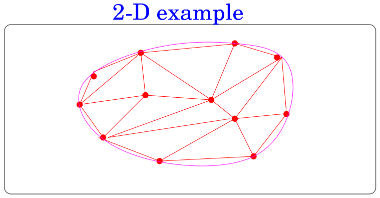
- periodic boundary conditions: can use sines and cosines
- finite element method : generate a mesh that discretizes the domain
  use low degree piecewise polynomials on mesh

1-D example





2-D example

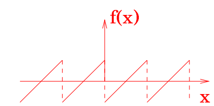


Mesh generation

Finding the best choices of the coefficients:

Analogy with Fourier series:

$$f(x) = a_0 + \sum_i a_i \cos(ix) + \sum_i b_i \sin(ix)$$



How do you find 'best' choices for a's and b's?

$$\int_{-\pi}^{+\pi} f(x)\cos(kx)\,dx = \int_{-\pi}^{+\pi} \left(a_0 + \sum_i a_i \cos(ix) + \sum_i b_i \sin(ix)\right)\cos(kx)\,dx$$

$$= \int_{-\pi}^{+\pi} a_k \cos(kx)\cos(kx)\,dx$$

$$= a_k \pi$$

Key idea:
- residual $f(x) - a_0 + \sum_i a_i \cos(ix) + \sum_i b_i \sin(ix)$
- weight residual by known function and integrate to find corresponding coefficient

Weighted Residual Technique:

Residual: $(L u^* - f) = (L(\sum_i^N c_i \phi_i) - f)$

Weighted Residual $= (L(\sum_i^N c_i \phi_i) - f) \quad \phi_k$

Equation for k^{th} unknown: $\int_\Omega \phi_k * (L(\sum_i^N c_i \phi_i) - f)\, dV = 0 \quad \Rightarrow$

If the differential equation is linear:

$$c_1 \int_\Omega \phi_k * L\phi_1 \, dV + \ldots + c_N \int_\Omega \phi_k * L\phi_N \, dV = \int_\Omega \phi_k \, f \, dV$$

$k = 1,2,\ldots N$

This system can be written as

$K c = b$ where

$$K(i,j) = \int_\Omega \phi_i * L\phi_j \, dV \qquad b(i) = \int_\Omega \phi_i \, f \, dV$$

Key insight: Calculus problem of solving pde is converted to linear algebra problem of solving K c = b where K is sparse

Jacobi: a (slow) iterative solver

Example:

```
4x + 2y = 8
3x + 4y = 11
```

Iterative system:

$$x_{n+1} = (8 - 2y_n)/4$$
$$y_{n+1} = (11 - 3x_n)/4$$

n	1	2	3	4	5	6	7	8	
x	0	2	0.625	1.375	0.8594	1.1406	0.9473	1.0527	...
y	0	2.75	1.250	2.281	1.7188	2.1055	1.8945	2.0396	...

Matrix view of Jacobi Iteration

Iterative method for solving linear systems Ax = b

Jacobi method: $M * X_{k+1} = (M - A) * X_k + b$ (M is DIAGONAL(A))

```
while (not converged) do

   do j = 1..N
     Y[i] = b[i]
     do i = 1..N
       Y[i] = Y[i] - A[i,j]*X[j]

   do i = 1..N
     X[i] = Y[i]/A[i,i]  + X[i]

   check convergence
```

Matrix-vector product

vector operations

Inner product of vectors

Matrix-vector product: $O(N^2)$ work

vector operations: O(N) work

Most of the time is spent in matrix-vector product.

Lesson for software systems people: optimize MVM

Solving system of linear algebraic equations:

- K c = b
- Orders of magnitude for realistic problems
  - large (~ 10 million unknowns) (roughly equal to number of mesh points)
  - sparse (~ 100 non-zero entries per row) (roughly equal to connectivity of a point)
  - same K, many b's in some problems
- Algorithms:
  - iterative methods (Jacobi,conjugate gradient, GMRES)

    start with an initial approximation to solution
    and keep refining it till you get close enough

  - factorization methods (LU,Cholesky,QR)

    factorize K into LU where L is lower triangular and U is upper triangular

    LUc = b

    Solve for c by solving two triangular systems

Tangential Discussion

- Calculus problem $Lu = f \Rightarrow$ linear algebra problem $Kc = b$.
- In some problems, we need to solve for multiple variables at each mesh point (temperature, pressure, velocity etc.)
  => solve many linear equations with same K, different b's.
- This is viewed as matrix equation $KC = B$ where C and B are matrices.
- Algorithms for solving single system can be used to solve multiple systems as well.
- Key computation in iterative methods: matrix-matrix multiplication (MMM) rather than matrix-vector multiplication (MVM).
- Non-linear pde's lead to non-linear algebraic systems which are solved iteratively (Newton's method etc.).
  Key computation: MMM or MVM.

Reality check:

- Jacobi is a very old method of solving linear systems iteratively.
- More modern methods: conjugate gradient (CG), GMRES, etc. converge faster in most cases.
- However, the structure of these algorithms is similar: MVM is the key operation.
- Major area of research in numerical analysis: speeding up iterative algorithms further by *preconditioning*.

Computational Requirements

Let us estimate storage and time requirements.

- Assume 10^6 mesh points (rows/columns of A)
- Assume iterative solver needs 100 iterations to converge
- Assume simulation runs for 1000 time steps.

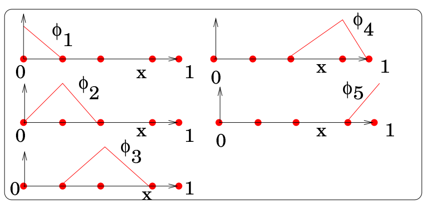
One MVM requires roughly 10^{12} flops

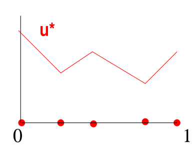
=>

Overall simulation requires 10^{17} flops and 10^{12} bytes of storage!

Can we do better?

1-D case





$$K(i,j) = \int_{\Omega} \phi_i * L(\phi_j)\, d\Omega$$

Structure of the K matrix for any pde: K[i,j] is 0 if ϕ_i and ϕ_j do not overlap!

For our example, K is

$$\begin{bmatrix} x & x & 0 & 0 & 0 \\ x & x & x & 0 & 0 \\ 0 & x & x & x & 0 \\ 0 & 0 & x & x & x \\ 0 & 0 & 0 & x & x \end{bmatrix}$$

Half the entries are zero!
In 2-D and 3-D, an even larger percentage of matrix is zero!

Typical 3-D numbers: 10^6 rows but only 100-500 non-zeros per row!

Matrix is sparse.

Exploiting sparsity

Store sparse matrices in special formats to avoid storing zeros

=> storage costs are reduced!

Avoid computing with zeros when working with sparse matrices.

=> MFlops needs are reduced!

Question: How do we represent sparse matrices and how do we compute with them?

Three Sparse Matrix Representations

A

	1	2	3	4
1	a		b	
2		c		d
3	e		f	
4			g	h

CRS

A.val	a	b	c	d	e	f	g	h
A.column	1	3	2	4	1	3	3	4

A.rowptr

Indexed access to a row

CCS

A.val	a	e	c	b	f	g	d	h
A.row	1	3	2	1	3	4	2	4

A.colptr

Indexed access to a column

Co-ordinate Storage

A.val	a	h	c	b	e	f	g	d
A.row	1	4	2	1	3	3	4	2
A.column	1	4	2	3	1	3	3	4

Indexed access to neither rows nor columns

MVM for CRS

```
for I = 1 to N do
    for JJ = A.rowptr(I) to A.rowptr(I+1) -1 do
        Y(I) = Y(I) + A.val(JJ)*X(A.column(JJ))
    od
od
```

MVM for Co-ordinate storage

```
for P = 1 to NZ do
    Y(A.row(P)) = Y(A.row(P)) + A.val(P)*X(A.column(P))
od
```

Sparse matrix computations introduce subscripts with indirection.

Computational Requirements with sparse matrices

- Assume 10^6 mesh points (rows/columns of A).
- Assume roughly 100 non-zeros per row.
- Assume iterative solver needs 100 iterations to converge.
- Assume simulation runs for 1000 time steps.

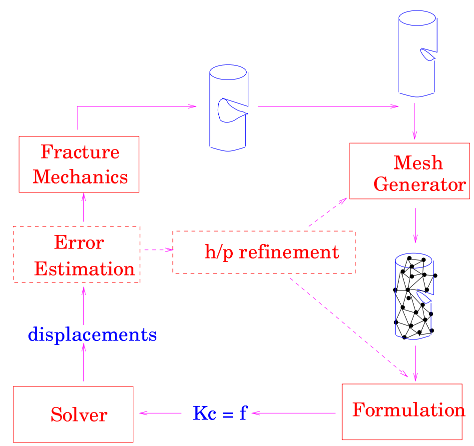
One MVM requires roughly 10^8 flops

=>

Overall simulation requires 10^{13} flops and 10^8 bytes of storage!

This is roughly 100 seconds on a 100 Gflop supercomputer.
Doable!

Flow-chart of Adaptive Finite-element Simulation of Fracture



Time-consuming Portions of Simulation

- Mesh generation: Takes many hours to produce meshes of sizes of interest to applications people (10^6 to 10^7 elements). From CS perspective, this is a problem that involves building, traversing, and modifying large graphs. Example of what compiler people call *irregular codes*.

- Solving linear systems $Ax = b$: Takes many hours to solve large systems. Matrix A can be dense or sparse. Manipulations of dense matrices are called *regular codes*. Manipulations of sparse matrices are somewhere in between regular and irregular.

Characteristics of regular problems: dense array codes in which loop bounds and array subscripts are affine functions of loop variables and loop constants.

Summary

- Computational science applications: solving pde's or pushing particles
- PDE's are solved using approximate techniques such as finite-element method
- Time-consuming part: mesh generation and solving large linear algebraic systems
- Mesh generation: graph manipulation. Example of irregular problem
- Solving linear systems: matrix may be dense or sparse. Dense matrix manipulations are examples of regular problems. Sparse matrix manipulations are examples of irregular problems.

- Two approachs to solving linear systems: iterative methods and direct (factorization) methods
- Factorization methods
  - Cholesky factorization
  - LU factorization with pivoting
  - QR factorization
- Key operations in iterative methods:
  Basic Linear Algebra Subroutines (BLAS)
  - Level-1 BLAS: inner-product of vectors, saxpy
  - Level-2 BLAS: matrix-vector product, triangular-solve
  - Level-3 BLAS: matrix-matrix product, triangular-solve with multiple right-hand-sides
- Exploiting sparsity complicates code.