CS 267 Applications of Parallel Computers

Lecture 11:

Sources of Parallelism and Locality (Part 2)

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Recap of last lecture

- Simulation models
- A model problem: sharks and fish
- Discrete event systems
- Particle systems
- Lumped systems (Ordinary Differential Equations, ODEs)

Outline

° Continuation of (ODEs)

° Partial Differential Equations (PDEs)

Ordinary Differential Equations ODEs

Solving ODEs

- Explicit methods to compute solution(t)
  - Ex: Euler's method
  - Simple algorithm: sparse matrix vector multiply
  - May need to take very small timesteps, especially if system is stiff (i.e. can change rapidly)
- Implicit methods to compute solution(t)
  - Ex: Backward Euler's Method
  - Larger timesteps, especially for stiff problems
  - More difficult algorithm: solve a sparse linear system
- Computing modes of vibration
  - Finding eigenvalues and eigenvectors
  - Ex: do resonant modes of building match earthquakes?
- All these reduce to sparse matrix problems
  - Explicit: sparse matrix-vector multiplication
  - Implicit: solve a sparse linear system
    - direct solvers (Gaussian elimination)
    - iterative solvers (use sparse matrix-vector multiplication)
  - Eigenvalue/vector algorithms may also be explicit or implicit

Solving ODEs - Details

- Assume ODE is x'(t) = f(x) = A*x, where A is a sparse matrix
  - Try to compute x(i*dt) = x[i] at i=0,1,2,…
  - Approximate x'(i*dt) by (x[i+1] - x[i])/dt
- Euler's method:
  - Approximate x'(t)=A*x by (x[i+1] - x[i])/dt = A*x[i] and solve for x[i+1]
  - x[i+1] = (I+dt*A)*x[i], i.e. sparse matrix-vector multiplication
- Backward Euler's method:
  - Approximate x'(t)=A*x by (x[i+1] - x[i])/dt = A*x[i+1] and solve for x[i+1]
  - (I - dt*A)*x[i+1] = x[i], i.e. we need to solve a sparse linear system of equations
- Modes of vibration
  - Seek solution of x''(t) = A*x of form x(t) = sin(f*t)*x0, x0 a constant vector
  - Plug in to get $-f^2$*x0 = A*x0, I.e. $-f^2$ is an eigenvalue and x0 is an eigenvector of A
  - Solution schemes reduce either to sparse-matrix multiplication, or solving sparse linear systems

Parallelism in Sparse Matrix-vector multiplication

° y = A*x, where A is sparse and n x n

° Questions

- which processors store
  - y[i], x[i], and A[i,j]
- which processors compute
  - y[i] = sum (from 1 to n) A[i,j] * x[j]
    = (row i of A) . x … a sparse dot product

° Partitioning

- Partition index set {1,…,n} = N1 u N2 u … u Np
- For all i in Nk, Processor k stores y[i], x[i], and row i of A
- For all i in Nk, Processor k computes y[i] = (row i of A) . x
  - "owner computes" rule: Processor k compute the y[i]s it owns

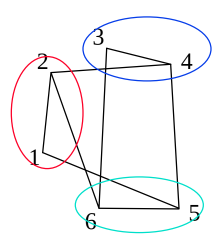
° Goals of partitioning

- balance load (how is load measured?)
- balance storage (how much does each processor store?)
- minimize communication (how much is communicated?)

Graph Partitioning and Sparse Matrices

° Relationship between matrix and graph

	1	2	3	4	5	6
1	1	1			1	
2	1	1		1		1
3			1	1		1
4		1	1	1	1	
5	1			1	1	1
6		1	1		1	1



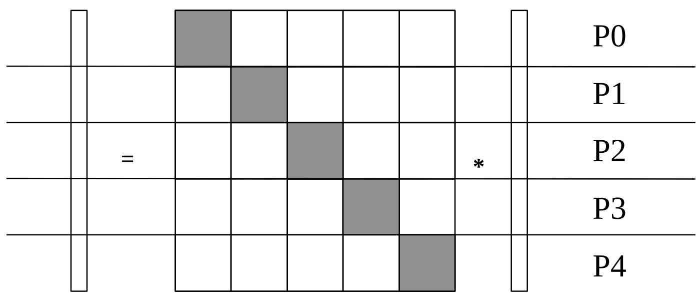
° A "good" partition of the graph has

- equal (weighted) number of nodes in each part (load and storage balance)
- minimum number of edges crossing between (minimize communication)

° Can reorder the rows/columns of the matrix by putting all the nodes in one partition together

More on Matrix Reordering via Graph Partitioning

° **"Ideal" matrix structure for parallelism: (nearly) block diagonal**
  • p (number of processors) blocks
  • few non-zeros outside these blocks, since these require communication



What about implicit methods and eigenproblems?

° **Direct methods (Gaussian elimination)**
  • Called LU Decomposition, because we factor A = L*U
  • Future lectures will consider both dense and sparse cases
  • More complicated than sparse-matrix vector multiplication

° **Iterative solvers**
  • Will discuss several of these in future
    - Jacobi, Successive overrelaxiation (SOR) , Conjugate Gradients (CG), Multigrid,...
  • Most have sparse-matrix-vector multiplication in kernel

° **Eigenproblems**
  • Future lectures will discuss dense and sparse cases
  • Also depend on sparse-matrix-vector multiplication, direct methods

° **Graph partitioning**
  • Algorithms will be discussed in future lectures

Partial Differential Equations

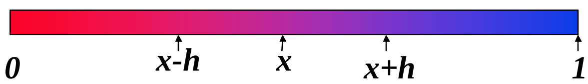
PDEs

Continuous Variables, Continuous Parameters

Examples of such systems include

- **Heat flow:** Temperature(position, time)
- **Diffusion:** Concentration(position, time)
- **Electrostatic or Gravitational Potential:** Potential(position)
- **Fluid flow:** Velocity,Pressure,Density(position,time)
- **Quantum mechanics:** Wave-function(position,time)
- **Elasticity:** Stress,Strain(position,time)

Example: Deriving the Heat Equation



Consider a simple problem

- **A bar of uniform material, insulated except at ends**
- **Let $u(x,t)$ be the temperature at position x at time t**
- **Heat travels from $x-h$ to $x+h$ at rate proportional to:**

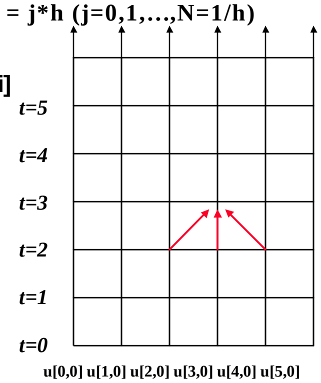
$$\frac{d\,u(x,t)}{dt} = C * \frac{(u(x-h,t)-u(x,t))/h - (u(x,t)- u(x+h,t))/h}{h}$$

- **As $h \to 0$, we get the heat equation:**

$$\frac{d\,u(x,t)}{dt} = C * \frac{d^2\,u(x,t)}{dx^2}$$

Explicit Solution of the Heat Equation

- **For simplicity, assume $C=1$**
- **Discretize both time and position**
- **Use finite differences with u[j,i] as the heat at**
  - time t= i*dt (i = 0,1,2,...) and position x = j*h (j=0,1,...,N=1/h)
  - initial conditions on u[j,0]
  - boundary conditions on u[0,i] and u[N,i]
- **At each timestep i = 0,1,2,...**




```
For j=0 to N
    u[j,i+1]= z*u[j-1,i]+ (1-2*z)*u[j,i]+
              z*u[j+1,i]
```

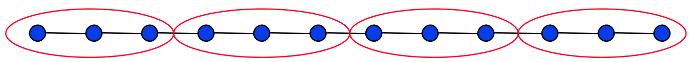
where $z = dt/h^2$

- **This corresponds to**
  - matrix vector multiply (what is matrix?)
  - nearest neighbors on grid

Parallelism in Explicit Method for PDEs

° **Partitioning the space (x) into p largest chunks**

- good load balance (assuming large number of points relative to p)
- minimized communication (only p chunks)



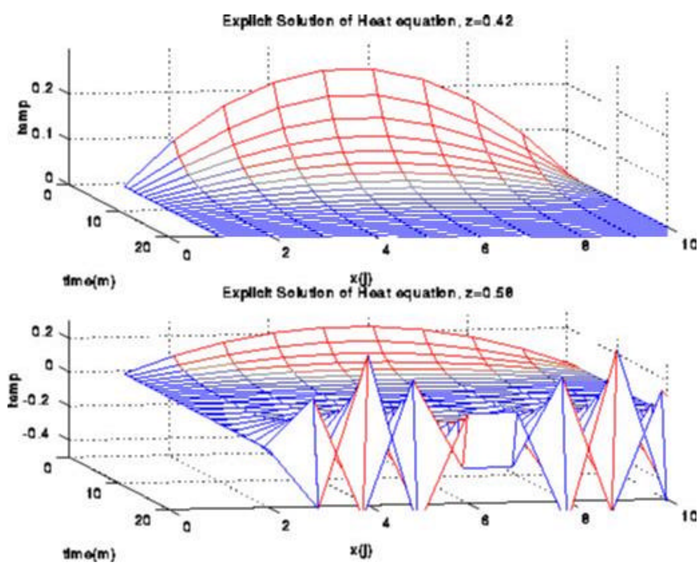
° **Generalizes to**

- multiple dimensions
- arbitrary graphs (= sparse matrices)

° **Problem with explicit approach**

- numerical instability
- solution blows up eventually if $z = dt/h^2 > .5$
- need to make the timesteps very small when h is small: $dt < .5*h^2$

Instability in solving the heat equation explicitly



Implicit Solution

° As with many (stiff) ODEs, need an implicit method

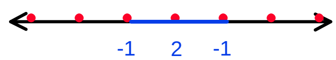
° This turns into solving the following equation

(I + (z/2)*T) * u[:,i+1]= (I - (z/2)*T) *u[:,i]

° Here I is the identity matrix and T is:

$$T = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

Graph and "stencil"



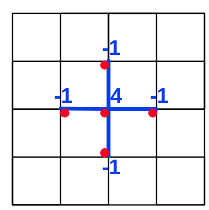
° I.e., essentially solving Poisson's equation in 1D

2D Implicit Method

° Similar to the 1D case, but the matrix T is now

$$T = \left(\begin{array}{ccc|ccc|ccc} 4 & -1 & & -1 & & & & & \\ -1 & 4 & -1 & & -1 & & & & \\ & -1 & 4 & & & -1 & & & \\ \hline -1 & & & 4 & -1 & & -1 & & \\ & -1 & & -1 & 4 & -1 & & -1 & \\ & & -1 & & -1 & 4 & & & -1 \\ \hline & & & -1 & & & 4 & -1 & \\ & & & & -1 & & -1 & 4 & -1 \\ & & & & & -1 & & -1 & 4 \end{array}\right)$$

Graph and "stencil"



° Multiplying by this matrix (as in the explicit case) is simply nearest neighbor computation on 2D grid

° To solve this system, there are several techniques

Algorithms for 2D Poisson Equation with N unknowns

Algorithm	Serial	PRAM	Memory	#Procs
Dense LU	N^3	N	N^2	N^2
Band LU	N^2	N	$N^{3/2}$	N
Jacobi	N^2	N	N	N
Explicit Inv.	N^2	log N	N^2	N^2
Conj.Grad.	$N^{3/2}$	$N^{1/2}$ *log N	N	N
RB SOR	$N^{3/2}$	$N^{1/2}$	N	N
Sparse LU	$N^{3/2}$	$N^{1/2}$	N*log N	N
FFT	N*log N	log N	N	N
Multigrid	N	$\log^2 N$	N	N
Lower bound	N	log N	N	

PRAM is an idealized parallel model with zero cost communication

(see next slide for explanation)

Short explanations of algorithms on previous slide

- Sorted in two orders (roughly):
  - from slowest to fastest on sequential machines
  - from most general (works on any matrix) to most specialized (works on matrices "like" T)
- Dense LU: Gaussian elimination; works on any N-by-N matrix
- Band LU: exploit fact that T is nonzero only on sqrt(N) diagonals nearest main diagonal, so faster
- Jacobi: essentially does matrix-vector multiply by T in inner loop of iterative algorithm
- Explicit Inverse: assume we want to solve many systems with T, so we can precompute and store inv(T) "for free", and just multiply by it
  - It's still expensive!
- Conjugate Gradients: uses matrix-vector multiplication, like Jacobi, but exploits mathematical properies of T that Jacobi does not
- Red-Black SOR (Successive Overrelaxation): Variation of Jacobi that exploits yet different mathematical properties of T
  - Used in Multigrid
- Sparse LU: Gaussian elimination exploiting particular zero structure of T
- FFT (Fast Fourier Transform): works only on matrices *very* like T
- Multigrid: also works on matrices like T, that come from elliptic PDEs
- Lower Bound: serial (time to print answer); parallel (time to combine N inputs)
- Details in class notes and www.cs.berkeley.edu/~demmel/ma221

Relation of Poisson's equation to Gravity, Electrostatics

° Force on particle at (x,y,z) due to particle at 0 is

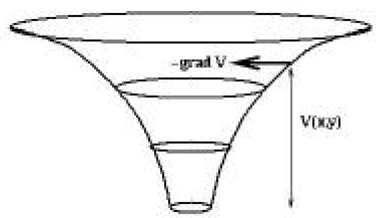
  -(x,y,z)/r^3, where $r = \mathrm{sqrt}(x^2+y^2+z^2)$

° Force is also gradient of potential V = -1/r

  = -(d/dx V, d/dy V, d/dz V) = -grad V

° V satisfies Poisson's equation (try it!)

Relationship of Potential V and Force -grad V in 2D

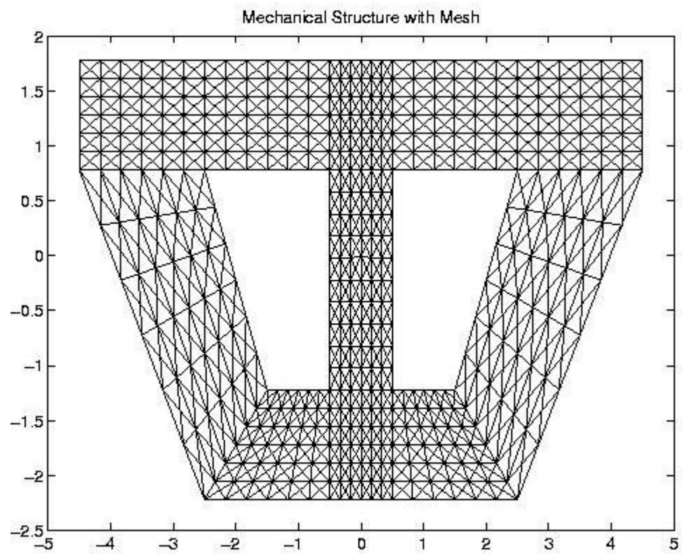


Comments on practical meshes

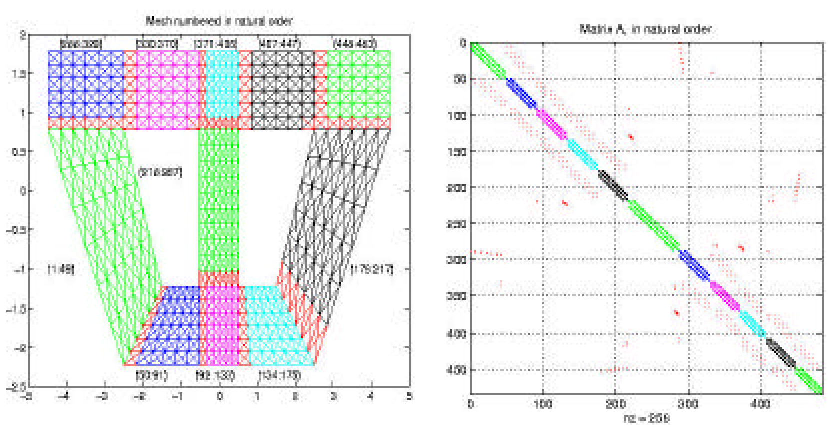
° Regular 1D, 2D, 3D meshes
  - Important as building blocks for more complicated meshes

° Practical meshes are often irregular
  - Composite meshes, consisting of multiple "bent" regular meshes joined at edges
  - Unstructured meshes, with arbitrary mesh points and connectivities
  - Adaptive meshes, which change resolution during solution process to put computational effort where needed

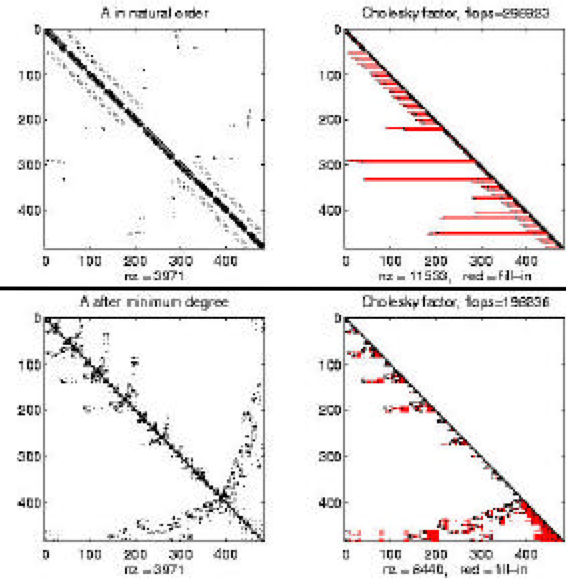
Composite mesh from a mechanical structure



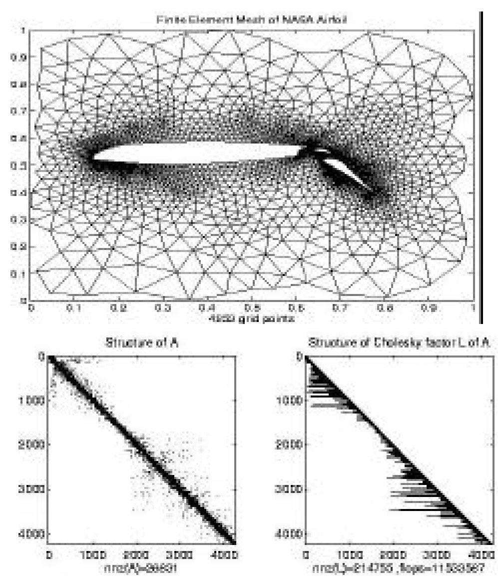
Converting the mesh to a matrix



Effects of Ordering Rows and Columns on Gaussian Elimination



Irregular mesh: NASA Airfoil in 2D (direct solution)



Irregular mesh: Tapered Tube (multigrid)

Example of Prometheus meshes

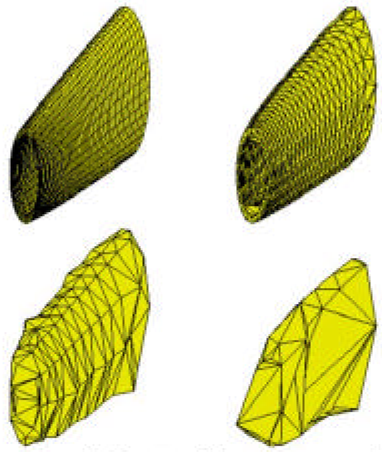
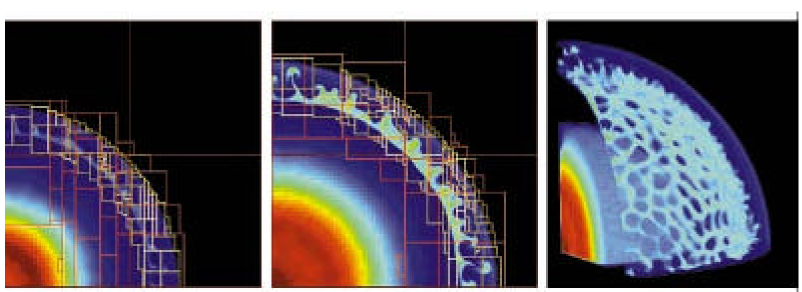


Figure 6 Sample input grid and coarse grids

Adaptive Mesh Refinement (AMR)



° Adaptive mesh around an explosion
° John Bell and Phil Colella at LBL (see class web page for URL)
° Goal of Titanium is to make these algorithms easier to implement in parallel

Challenges of irregular meshes (and a few solutions)

- How to generate them in the first place
  - Triangle, a 2D mesh partitioner by Jonathan Shewchuk
- How to partition them
  - ParMetis, a parallel graph partitioner
- How to design iterative solvers
  - PETSc, a Portable Extensible Toolkit for Scientific Computing
  - Prometheus, a multigrid solver for finite element problems on irregular meshes
  - Titanium, a language to implement Adaptive Mesh Refinement
- How to design direct solvers
  - SuperLU, parallel sparse Gaussian elimination
- These are challenges to do sequentially, the more so in parallel