CS 267
Sources of Parallelism and Locality in Simulation – Part 2

James Demmel
www.cs.berkeley.edu/~demmel/cs267_Spr14

Recap of Last Lecture

- 4 kinds of simulations
  - Discrete Event Systems
  - Particle Systems
  - Ordinary Differential Equations (ODEs)
  - Partial Differential Equations (PDEs) (today)
- Common problems:
  - Load balancing
    - May be due to lack of parallelism or poor work distribution
    - Statically, divide grid (or graph) into blocks
    - Dynamically, if load changes significantly during run
  - Locality
    - Partition into large chunks with low surface-to-volume ratio
      - To minimize communication
    - Distributed particles according to location, but use irregular spatial decomposition (e.g., quad tree) for load balance
  - Constant tension between these two
    - Particle-Mesh method: can't balance particles (moving), balance mesh (fixed) and keep particles near mesh points without communication

Partial Differential Equations
PDEs

Continuous Variables, Continuous Parameters

Examples of such systems include

- **Elliptic problems (steady state, global space dependence)**
  - **Electrostatic or Gravitational Potential: Potential(position)**
- **Hyperbolic problems (time dependent, local space dependence):**
  - **Sound waves: Pressure(position,time)**
- **Parabolic problems (time dependent, global space dependence)**
  - **Heat flow: Temperature(position, time)**
  - **Diffusion: Concentration(position, time)**

Global vs Local Dependence

- **Global means either a lot of communication, or tiny time steps**
- **Local arises from finite wave speeds: limits communication**

Many problems combine features of above

- **Fluid flow: Velocity,Pressure,Density(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 $h \rightarrow 0$, we get the heat equation:

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

Details of the Explicit Method for Heat

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

- Discretize time and space using explicit approach (forward Euler) to approximate time derivative:

$$u(x,t+\delta) - u(x,t))/\delta = C\ [\ (u(x-h,t)-u(x,t))/h - (u(x,t)- u(x+h,t))/h\ ]\ /\ h$$
$$= C\ [u(x-h,t) - 2*u(x,t) + u(x+h,t)]/h^2$$

Solve for $u(x,t+\delta)$:

$$u(x,t+\delta) = u(x,t)+ C*\delta\ /h^2\ *(u(x-h,t) - 2*u(x,t) + u(x+h,t))$$

- Let z = C*δ /h^2, simplify:

$$u(x,t+\delta) = z^*\ u(x-h,t) + (1-2z)*u(x,t) + z*u(x+h,t)$$

- Change variable x to j*h, t to i*δ, and u(x,t) to u[j,i]

u[j,i+1]= z*u[j-1,i]+ (1-2*z)*u[j,i]+ z*u[j+1,i]

Explicit Solution of the Heat Equation

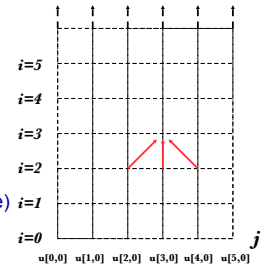
- Use "finite differences" with u[j,i] as the temperature at
  - **time t= i*δ (i = 0,1,2,…) and position x = j*h (j=0,1,…,N=1/h)**
  - **initial conditions on u[j,0]**
  - **boundary conditions on u[0,i] and u[N,i]**
- At each timestep i = 0,1,2,...

For j=1 to N-1

u[j,i+1]= z*u[j-1,i]+ (1-2*z)*u[j,i] + z*u[j+1,i]

where z =C*δ/h^2

- This corresponds to
  - Matrix-vector-multiply by T (next slide)
  - Combine nearest neighbors on grid



Matrix View of Explicit Method for Heat

- u[j,i+1]= z*u[j-1,i]+ (1-2*z)*u[j,i] + z*u[j+1,i], same as:
- u[:, i+1] = T * u[:, i] where T is tridiagonal:

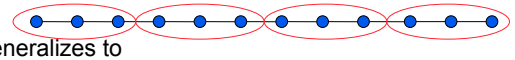
$$T = \begin{pmatrix} 1-2z & z & & & \\ z & 1-2z & z & & \\ & z & 1-2z & z & \\ & & z & 1-2z & z \\ & & & z & 1-2z \end{pmatrix} = I - z*L, \quad L = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

Graph and "3 point stencil"

- L called Laplacian (in 1D)
- For a 2D mesh (5 point stencil) the Laplacian is pentadiagonal
  - More on the matrix/grid views later

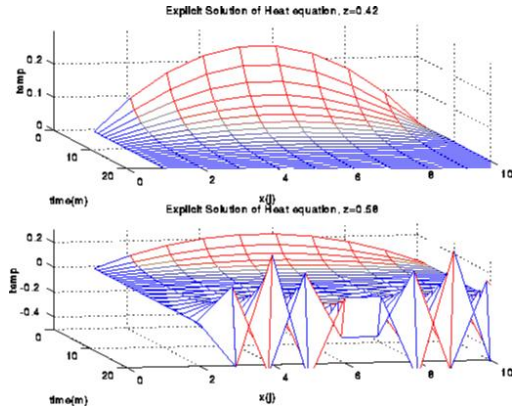
Parallelism in Explicit Method for PDEs

- Sparse matrix vector multiply, via Graph Partitioning
- Partitioning the space (x) into p chunks
  - good load balance (assuming large number of points relative to p)
  - minimize communication (least dependence on data outside chunk)



- Generalizes to
  - multiple dimensions.
  - arbitrary graphs (= arbitrary sparse matrices).
- Explicit approach often used for hyperbolic equations
  - Finite wave speed, so only depend on nearest chunks
- Problem with explicit approach for heat (parabolic):
  - numerical instability.
  - solution blows up eventually if $z = C\delta/h^2 > .5$
  - need to make the time step δ very small when h is small: $\delta < .5*h^2/C$

Instability in Solving the Heat Equation Explicitly



Implicit Solution of the Heat Equation

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

- Discretize time and space using implicit approach (Backward Euler) to approximate time derivative:

$(u(x,t+\delta) - u(x,t))/dt = C*(u(x-h,t+\delta) - 2*u(x,t+\delta) + u(x+h, t+\delta))/h^2$

$u(x,t) = u(x,t+\delta) - C*\delta/h^2 *(u(x-h,t+\delta) - 2*u(x,t+\delta) + u(x+h,t+\delta))$

- Let $z = C*\delta/h^2$ and change variable t to i*δ, x to j*h and u(x,t) to u[j,i]

$(I + z*L)* u[:, i+1] = u[:,i]$

- Where I is identity and L is Laplacian as before

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

Implicit Solution of the Heat Equation

- The previous slide derived Backward Euler
  - **(I + z *L)* u[:, i+1] = u[:,i]**
- But the Trapezoidal Rule has better numerical properties:

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

- Again **I** is the identity matrix and **L** is:

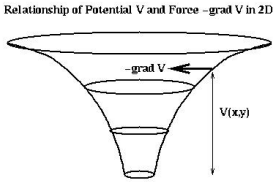
$$\mathbf{L} = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

Graph and "stencil"

- Other problems (elliptic instead of parabolic) yield Poisson's equation (Lx = b in 1D)

Relation of Poisson to Gravity, Electrostatics

- Poisson equation arises in many problems
- E.g., force on particle at (x,y,z) due to particle at 0 is
  -(x,y,z)/r^3, where r = 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 working this out!)



$$\frac{d^2V}{dx^2} + \frac{d^2V}{dy^2} + \frac{d^2V}{dz^2} = 0$$

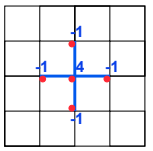
2D Implicit Method

- Similar to the 1D case, but the matrix L is now

$L =$

4	-1		-1											
-1	4	-1		-1										
	-1	4			-1									
-1			4	-1		-1								
	-1		-1	4	-1		-1							
		-1		-1	4			-1						
			-1			4	-1							
				-1		-1	4	-1						
					-1		-1	4						

Graph and "5 point stencil"



3D case is analogous
(7 point 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 (3D) Poisson Equation (N vars)

Algorithm	Serial	PRAM	Memory	#Procs
• Dense LU	N^3	N	N^2	N^2
• Band LU	N^2 ($N^{7/3}$)	N	$N^{3/2}$ ($N^{5/3}$)	N($N^{4/3}$)
• Jacobi	N^2 ($N^{5/3}$)	N ($N^{2/3}$)	N	N
• Explicit Inv.	N^2	log N	N^2	N^2
• Conj.Gradients	$N^{3/2}$ ($N^{4/3}$)	$N^{1/2}$ (1/3) *log N	N	N
• Red/Black SOR	$N^{3/2}$ ($N^{4/3}$)	$N^{1/2}$ ($N^{4/3}$)	N	N
• Sparse LU	$N^{3/2}$ (N^2)	$N^{1/2}$ ($N^{2/3}$)	N*log N ($N^{4/3}$)	N($N^{4/3}$)
• FFT	N*log N	log N	N	N
• Multigrid	N	$\log^2$ N	N	N
• Lower bound	N	log N	N	

All entries in "Big-Oh" sense (constants omitted)
PRAM is an idealized parallel model with zero cost communication
References: James Demmel, Applied Numerical Linear Algebra, SIAM, 1997.
Decision tree to help choose algorithms:
www.netlib.org/linalg/html_templates/Templates.html

Overview of Algorithms

- 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: Exploits the fact that T is nonzero only on sqrt(N) diagonals nearest main diagonal.
- 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 (but still expensive).
- Conjugate Gradient: Uses matrix-vector multiplication, like Jacobi, but exploits mathematical properties of T that Jacobi does not.
- Red-Black SOR (successive over-relaxation): Variation of Jacobi that exploits yet different mathematical properties of T. Used in multigrid schemes.
- 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.

Mflop/s Versus Run Time in Practice

- Problem: Iterative solver for a convection-diffusion problem; run on a 1024-CPU NCUBE-2.
- Reference: Shadid and Tuminaro, SIAM Parallel Processing Conference, March 1991.

Solver	Flops	CPU Time(s)	Mflop/s
Jacobi	3.82×10^{12}	2124	1800
Gauss-Seidel	1.21×10^{12}	885	1365
Multigrid	2.13×10^{9}	7	318

- Which solver would you select?

Summary of Approaches to Solving PDEs

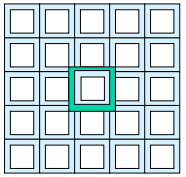
- As with ODEs, either explicit or implicit approaches are possible
  - Explicit, sparse matrix-vector multiplication
  - Implicit, sparse matrix solve at each step
    - Direct solvers are hard (more on this later)
    - Iterative solves turn into sparse matrix-vector multiplication
      - Graph partitioning
- Graph and sparse matrix correspondence:
  - Sparse matrix-vector multiplication is nearest neighbor "averaging" on the underlying mesh
- Not all nearest neighbor computations have the same efficiency
  - Depends on the mesh structure (nonzero structure) and the number of Flops per point.

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

Parallelism in Regular meshes

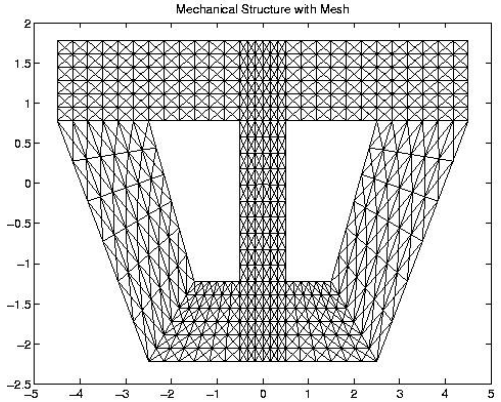
- Computing a Stencil on a regular mesh
  - need to communicate mesh points near boundary to neighboring processors.
    - Often done with ghost regions
  - Surface-to-volume ratio keeps communication down, but
    - Still may be problematic in practice



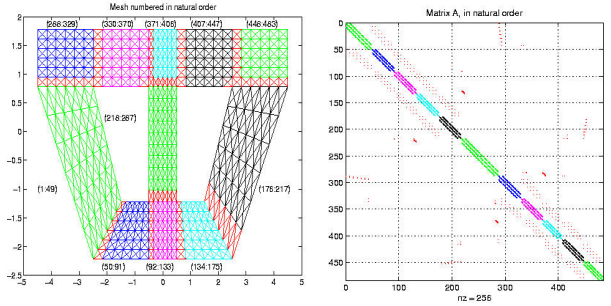
Implemented using "ghost" regions.

Adds memory overhead

Composite mesh from a mechanical structure

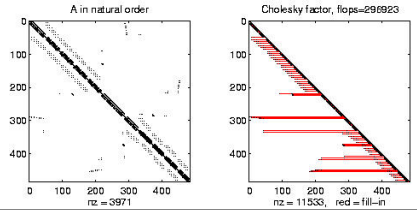


Converting the mesh to a matrix

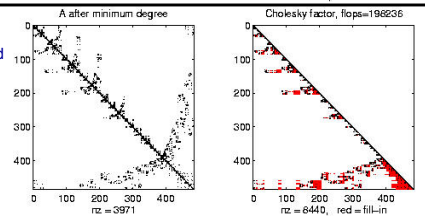


Example of Matrix Reordering Application

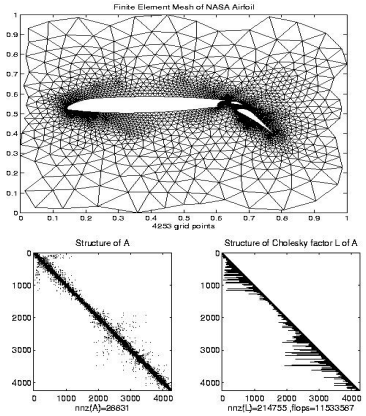
When performing Gaussian Elimination Zeros can be filled ☹



Matrix can be reordered to reduce this fill
But it's not the same ordering as for parallelism



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



Irregular mesh: Tapered Tube (multigrid)

Example of Prometheus meshes

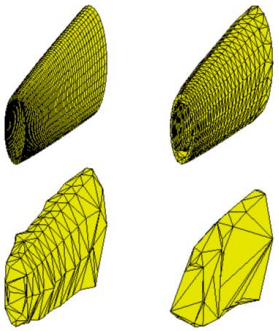


Figure 6 Sample input grid and coarse grids

Source of Unstructured Finite Element Mesh: Vertebra

Study failure modes of trabecular Bone under stress

Source: M. Adams, H. Bayraktar, T. Keaveny, P. Papadopoulos, A. Gupta

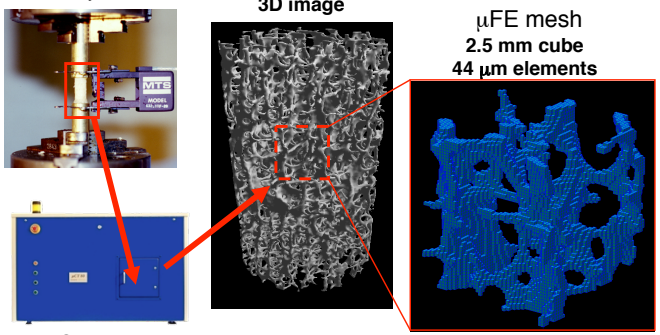
Methods: μFE modeling (Gordon Bell Prize, 2004)

Mechanical Testing
E, ε_{yield}, σ_{ult}, etc.

Source: Mark Adams, PPPL

3D image

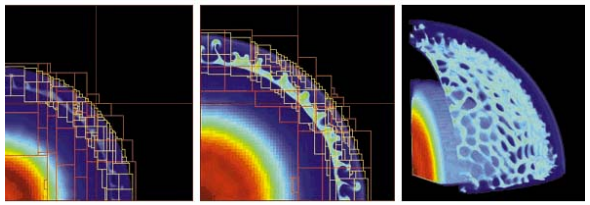
μFE mesh
2.5 mm cube
44 μm elements



Micro-Computed Tomography
μCT @ 22 μm resolution

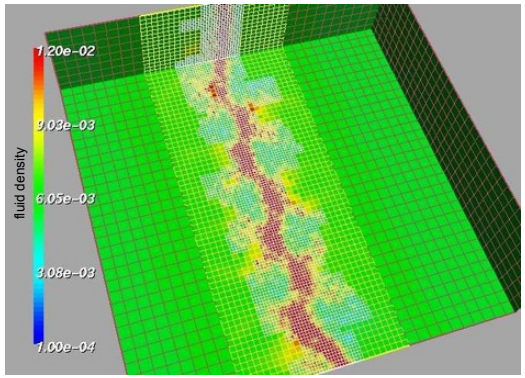
Up to 537M unknowns

Adaptive Mesh Refinement (AMR)



- Adaptive mesh around an explosion
  - Refinement done by estimating errors; refine mesh if too large
- Parallelism
  - Mostly between "patches," assigned to processors for load balance
  - May exploit parallelism within a patch
- Projects:
  - Titanium (http://www.cs.berkeley.edu/projects/titanium)
  - Chombo (P. Colella, LBL), KeLP (S. Baden, UCSD), J. Bell, LBL

Adaptive Mesh



Shock waves in gas dynamics using AMR (Adaptive Mesh Refinement)
See: http://www.llnl.gov/CASC/SAMRAI/

Challenges of Irregular Meshes

- How to generate them in the first place
  - Start from geometric description of object
  - Triangle, a 2D mesh partitioner by Jonathan Shewchuk
  - 3D harder!
- 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
- How to design direct solvers
  - SuperLU, parallel sparse Gaussian elimination
- These are challenges to do sequentially, more so in parallel

Summary – sources of parallelism and locality

- Current attempts to categorize main "kernels" dominating simulation codes
- "Seven Dwarfs" (P. Colella)
  - Structured grids
    - including locally structured grids, as in AMR
  - Unstructured grids
  - Spectral methods (Fast Fourier Transform)
  - Dense Linear Algebra
  - Sparse Linear Algebra
    - Both explicit (SpMV) and implicit (solving)
  - Particle Methods
  - Monte Carlo/Embarrassing Parallelism/Map Reduce (easy!)

What do commercial and CSE applications have in common?

Motif/Dwarf: Common Computational Methods
(Red Hot → Blue Cool)