PARLab Parallel Boot Camp

Sources of Parallelism and Locality in Simulation

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Parallelism and Locality in Simulation

- Parallelism and data locality both critical to performance
  - Arguments must be in same place to perform an operation
  - Moving data most expensive operation
- Real world problems have parallelism and locality:
  - Many objects operate independently of others.
  - Objects often depend much more on nearby than distant objects.
  - Dependence on distant objects can often be simplified.
    - » Example of all three: particles moving under gravity
- Scientific models may introduce more parallelism:
  - When a continuous problem is discretized, time dependencies are generally limited to adjacent time steps.
    - » Helps limit dependence to nearby objects (eg collisions)
  - Far-field effects may be ignored or approximated in many cases.
- Many problems exhibit parallelism at multiple levels

Basic Kinds of Simulation

- Discrete Event Systems
  - "Game of Life", Manufacturing Systems, Finance, Circuits, Pacman …
- Particle Systems
  - Billiard balls, Galaxies, Atoms, Circuits, Pinball …
- Lumped Systems (Ordinary Differential Eqns – ODEs)
  - Structural Mechanics, Chemical kinetics, Circuits, Star Wars: The Force Unleashed
- Continuous Systems (Partial Differential Eqns – PDEs)
  - Heat, Elasticity, Electrostatics, Finance, Circuits, Medical Image Analysis, Terminator 3: Rise of the Machines
- A given phenomenon can be modeled at multiple levels
- Many simulations combine multiple techniques
- For more on simulation in games, see
  - www.cs.berkeley.edu/b-cam/Papers/Parker-2009-RTD

Example: Circuit Simulation

- Circuits are simulated at many different levels

Discrete Event

Lumped Systems

Continuous Systems

Level	Primitives	Examples
Instruction level	Instructions	SimOS, SPIM
Cycle level	Functional units	VIRAM-p
Register Transfer Level (RTL)	Register, counter, MUX	VHDL
Gate Level	Gate, flip-flop, memory cell	Thor
Switch level	Ideal transistor	Cosmos
Circuit level	Resistors, capacitors, etc.	Spice
Device level	Electrons, silicon	

Outline

- Discrete event systems
  - Time and space are discrete
- Particle systems
  - Important special case of lumped systems
- Lumped systems (ODEs)
  - Location/entities are discrete, time is continuous
- Continuous systems (PDEs)
  - Time and space are continuous

discrete ↕ continuous

- Identify common problems and solutions

Model Problem: Sharks and Fish

- Illustrates parallelization of these simulations
- Basic idea: sharks and fish living in an ocean
  - rules for movement (discrete and continuous)
  - breeding, eating, and death
  - forces in the ocean
  - forces between sea creatures
- 6 different versions
  - Different sets of rules, to illustrate different simulations
- Available in many languages
  - Matlab, pThreads, MPI, OpenMP, Split-C, Titanium, CMF, …
  - See bottom of www.cs.berkeley.edu/~demmel/cs267_Spr13/

– One or two will be used as lab assignments
  - See bottom of www.cs.berkeley.edu/~driscoll/cs267
  - Rest available for your own classes!

"7 Dwarfs" of High Performance Computing

- Phil Colella (LBL) identified 7 kernels of which most simulation and data-analysis programs are composed:

1. Dense Linear Algebra
   - Ex: Solve Ax=b or Ax = λx where A is a dense matrix
2. Sparse Linear Algebra
   - Ex: Solve Ax=b or Ax = λx where A is a sparse matrix (mostly zero)
3. Operations on Structured Grids
   - Ex: $A_{new}(i,j) = 4*A(i,j) - A(i-1,j) - A(i+1,j) - A(i,j-1) - A(i,j+1)$
4. Operations on Unstructured Grids
   - Ex: Similar, but list of neighbors varies from entry to entry
5. Spectral Methods
   - Ex: Fast Fourier Transform (FFT)
6. Particle Methods
   - Ex: Compute electrostatic forces on n particles, move them
7. Monte Carlo
   - Ex: Many independent simulations using different inputs

DISCRETE EVENT SYSTEMS

Discrete Event Systems

- Systems are represented as:
  - finite set of variables.
  - the set of all variable values at a given time is called the state.
  - each variable is updated by computing a transition function depending on the other variables.
- System may be:
  - synchronous: at each discrete timestep evaluate all transition functions; also called a state machine.
  - asynchronous: transition functions are evaluated only if the inputs change, based on an "event" from another part of the system; also called event driven simulation.
- Example: The "game of life:"
  - Space divided into cells, rules govern cell contents at each step
  - Also available as Sharks and Fish #3 (S&F 3)

Parallelism in Game of Life

- The simulation is synchronous
  - use two copies of the grid (old and new).
  - the value of each new grid cell depends only on 9 cells (itself plus 8 neighbors) in old grid.
  - simulation proceeds in timesteps-- each cell is updated at every step.
- Easy to parallelize by dividing physical domain: *Domain Decomposition*

P1	P2	P3
P4	P5	P6
P7	P8	P9

Repeat

compute locally to update local system

barrier()

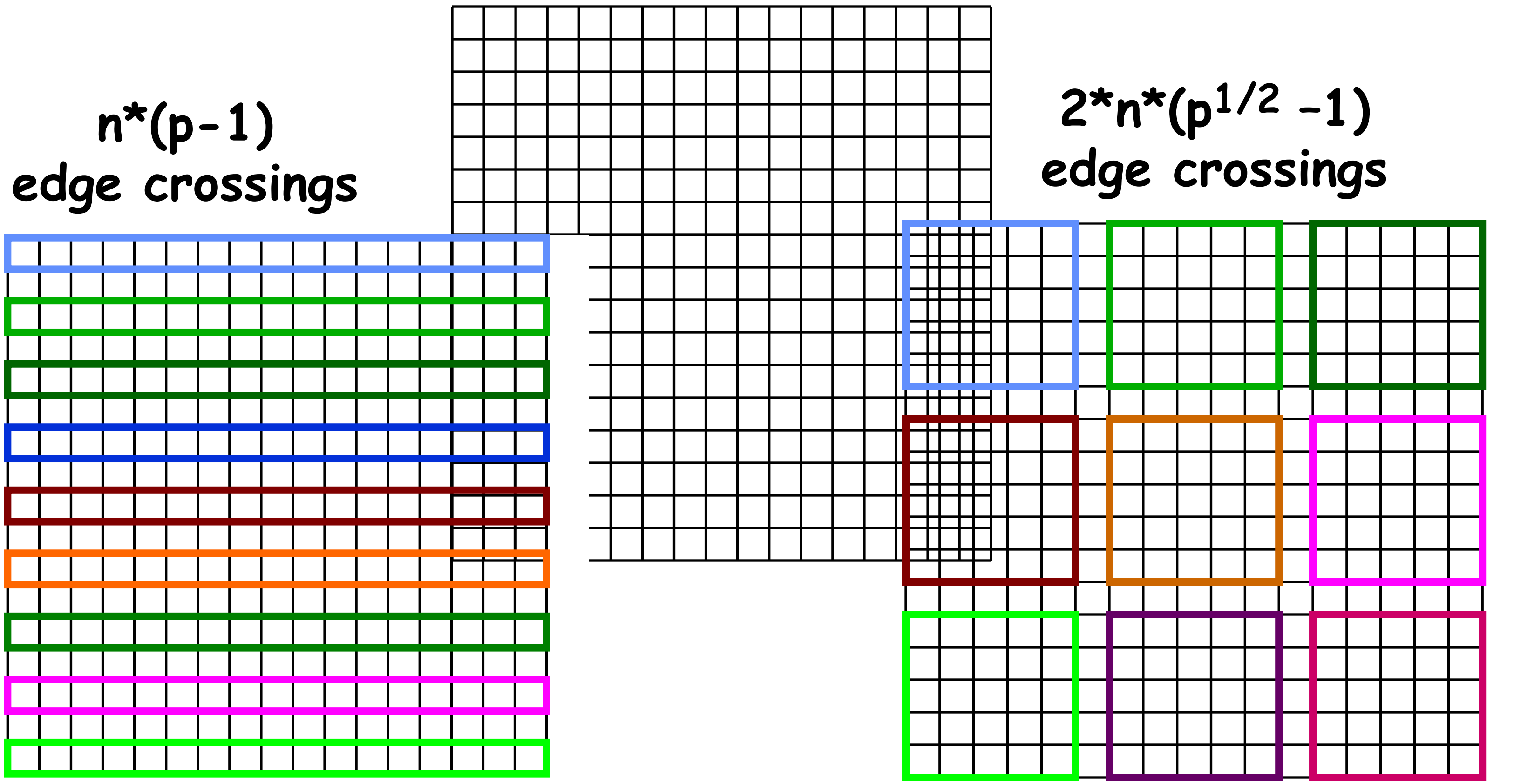
exchange state info with neighbors

until done simulating

- Locality is achieved by using large patches of the ocean
  - Only boundary values from neighboring patches are needed.
- How to pick shapes of domains?

Regular Meshes

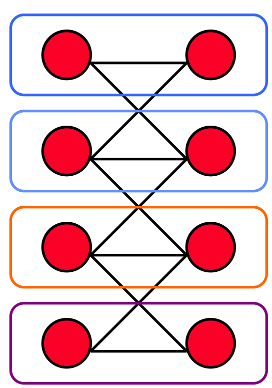
- Suppose graph is nxn mesh with connection NSEW neighbors
  - Which partition has less communication? (n=18, p=9)
- Minimizing communication on mesh ≡ minimizing "surface to volume ratio" of partition



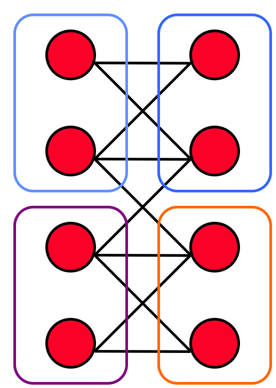
Synchronous Circuit Simulation

- Circuit is a **graph** made up of subcircuits connected by wires
  - Component simulations need to interact if they share a wire.
  - Data structure is (irregular) graph of subcircuits.
  - Parallel algorithm is timing-driven or **synchronous:**
    - » Evaluate all components at every timestep (determined by known circuit delay)
- **Graph partitioning** assigns subgraphs to processors
  - Determines parallelism and locality.
  - Goal 1 is to evenly distribute subgraphs to nodes (load balance).
  - Goal 2 is to minimize edge crossings (minimize communication).
  - Easy for meshes, NP-hard in general, so we will approximate (tools available!)

better →

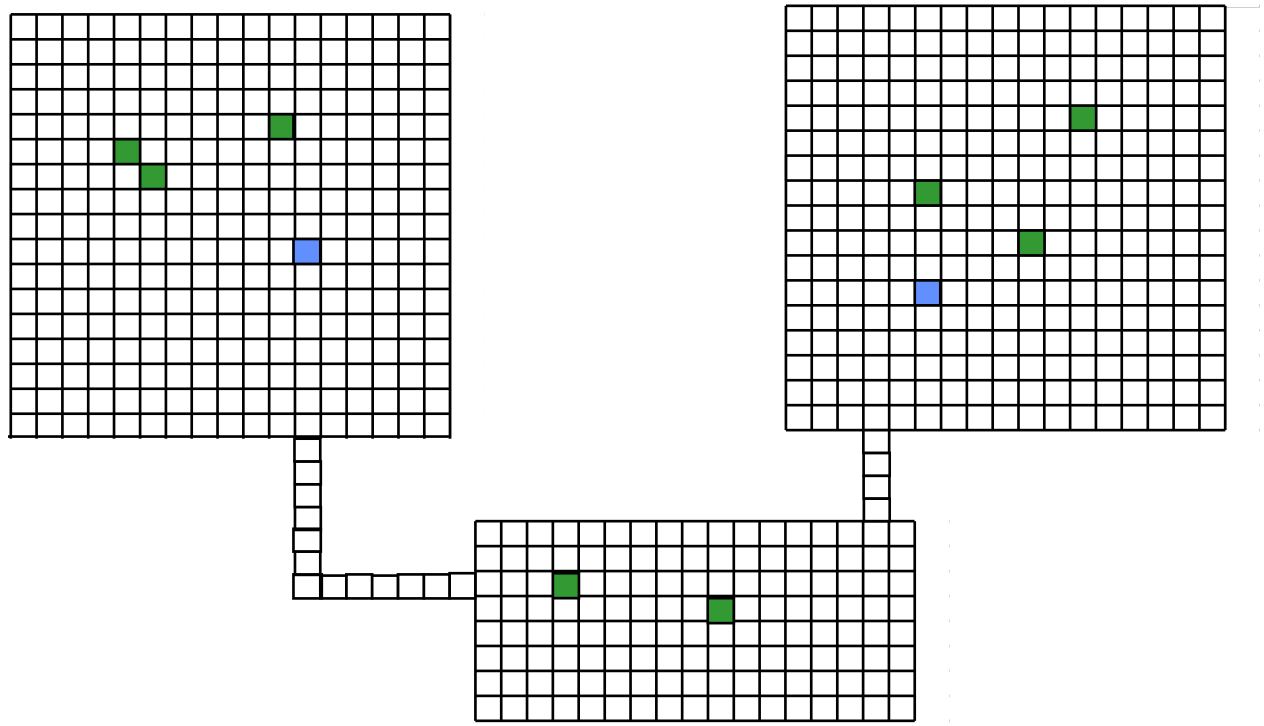


#edge crossings = 6



#edge crossings = 10

Sharks & Fish in Loosely Connected Ponds



- Parallelization: each processor gets a set of ponds with roughly equal total area
  - work is proportional to area, not number of creatures
- One pond can affect another (through streams) but infrequently
- Synchronous simulation communicates more than necessary

Asynchronous Simulation

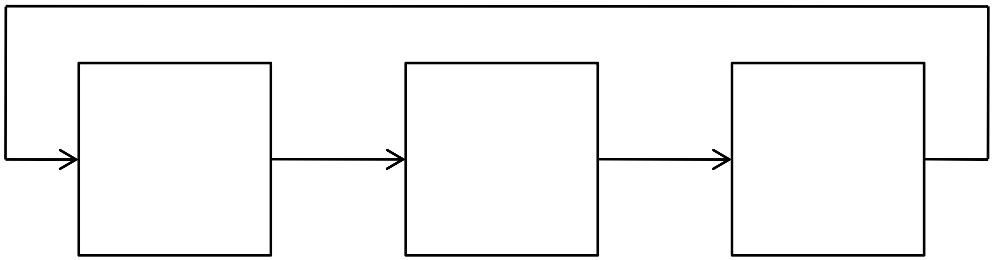
- Synchronous simulations may waste time:
  - Simulates even when the inputs do not change.
- Asynchronous (event-driven) simulations update only when an event arrives from another component:
  - No global time steps, but individual events contain time stamps.
  - Example: Game of life in loosely connected ponds (don't simulate empty ponds).
  - Example: Circuit simulation with delays (events are gates changing).
  - Example: Traffic simulation (events are cars changing lanes, etc.).
- Asynchronous is more efficient, but harder to parallelize
  - With message passing, events are naturally implemented as messages, but how do you know when to execute a "receive"?

Scheduling Asynchronous Circuit Simulation

- Conservative:
  - Only simulate up to (and including) the minimum time stamp of inputs.
  - Need deadlock detection if there are cycles in graph
    - » Example on next slide
  - Example: Pthor circuit simulator in Splash1 from Stanford.
- Speculative (or Optimistic):
  - Assume no new inputs will arrive and keep simulating.
  - May need to backup if assumption wrong, using timestamps
  - Example: Timewarp [D. Jefferson], Parswec [Wen,Yelick].
- Optimizing load balance and locality is difficult:
  - Locality means putting tightly coupled subcircuit on one processor.
  - Since "active" part of circuit likely to be in a tightly coupled subcircuit, this may be bad for load balance.

Deadlock in Conservative Asynchronous Circuit Simulation

- Example: Sharks & Fish 3, with 3 processors simulating 3 ponds connected by streams along which fish can move



- Suppose all ponds simulated up to time t_0, but no fish move, so no messages sent from one proc to another
  - So no processor can simulate past time t_0
- Fix: After waiting for an incoming message for a while, send out an "Are you stuck too?" message
  - If you ever receive such a message, pass it on
  - If you receive such a message that you sent, you have a deadlock cycle, so just take a step with latest input
- Can be a serial bottleneck

Summary of Discrete Event Simulations

- Model of the world is discrete
  - Both time and space
- Approaches
  - Decompose domain, i.e., set of objects
  - Run each component ahead using
    - » Synchronous: communicate at end of each timestep
    - » Asynchronous: communicate on-demand
      - Conservative scheduling – wait for inputs
        - –need deadlock detection
      - Speculative scheduling – assume no inputs
        - –roll back if necessary

PARTICLE SYSTEMS

Particle Systems

- A particle system has
  - a finite number of particles
  - moving in space according to Newton's Laws (i.e. $F = ma$)
  - time is continuous
- Examples
  - stars in space with laws of gravity
  - electron beam in semiconductor manufacturing
  - atoms in a molecule with electrostatic forces
  - neutrons in a fission reactor
  - cars on a freeway with Newton's laws plus model of driver and engine
  - flying objects in a video game …
- Reminder: many simulations combine techniques such as particle simulations with some discrete events (eg Sharks and Fish)

Forces in Particle Systems

- Force on each particle can be subdivided

force = external_force + nearby_force + far_field_force

- External force
  - ocean current to sharks and fish world (S&F 1)
  - externally imposed electric field in electron beam
- Nearby force
  - sharks attracted to eat nearby fish (S&F 5)
  - balls on a billiard table bounce off of each other
  - Van der Waals forces in fluid ($1/r^6$) … how Gecko feet work?
- Far-field force
  - fish attract other fish by gravity-like ($1/r^2$) force (S&F 2)
  - gravity, electrostatics, radiosity in graphics
  - forces governed by elliptic PDE

Example S&F 1: Fish in an External Current

```
%   fishp = array of initial fish positions (stored as complex numbers)
%   fishv = array of initial fish velocities (stored as complex numbers)
%   fishm = array of masses of fish
%   tfinal = final time for simulation (0 = initial time)
%   Algorithm: update position [velocity] using velocity [acceleration]
%      at each time step
%   Initialize time step, iteration count, and array of times
    dt = .01;   t = 0;
% loop over time steps
    while t < tfinal,
       t = t + dt;
       fishp = fishp + dt*fishv;
       accel = current(fishp)./fishm;      % current depends on position
       fishv = fishv + dt*accel;
%      update time step (small enough to be accurate, but not too small)
       dt = min( .1*max(abs(fishv))/max(abs(accel)), .01);
    end
```

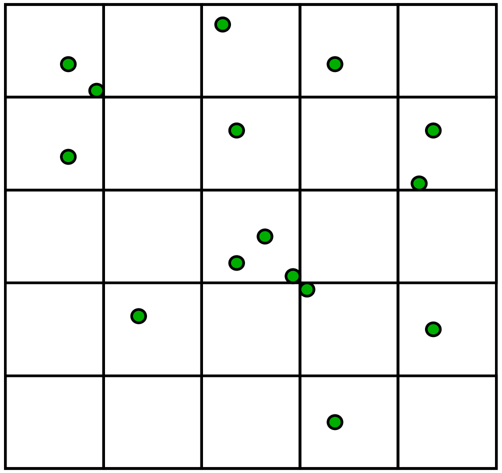
Parallelism in External Forces

- These are the simplest
- The force on each particle is independent
- Called "embarrassingly parallel"
  - Corresponds to "map reduce" pattern

- Evenly distribute particles on processors
  - Any distribution works
  - Locality is not an issue, no communication
- For each particle on processor, apply the external force
  - May need to "reduce" (eg compute maximum) to compute time step, other data

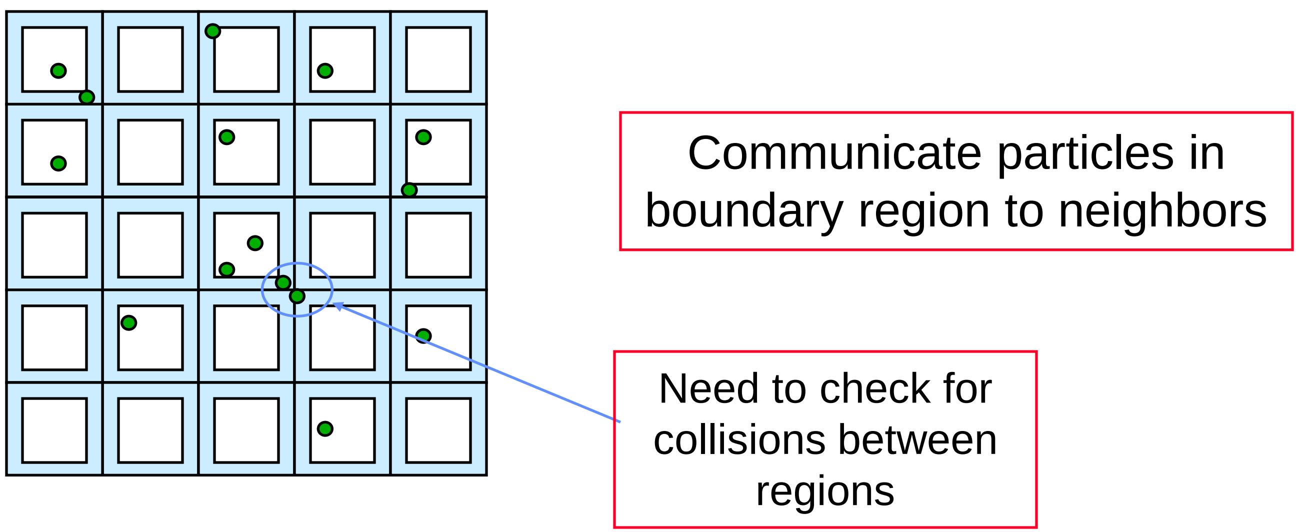
Parallelism in Nearby Forces

- Nearby forces require interaction and therefore communication.
- Force may depend on other nearby particles:
  - Example: collisions.
  - simplest algorithm is $O(n^2)$: look at all pairs to see if they collide.
- Usual parallel model is **domain decomposition** of physical region in which particles are located
  - $O(n/p)$ particles per processor if evenly distributed.



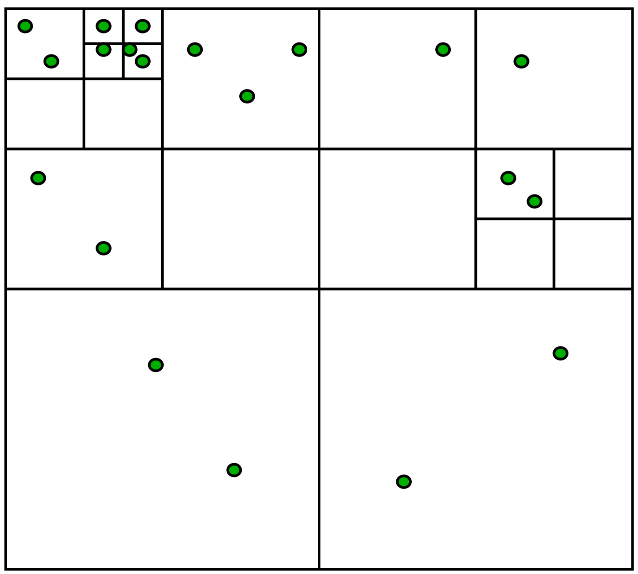
Parallelism in Nearby Forces

- Challenge 1: interactions of particles near processor boundary:
  - need to communicate particles near boundary to neighboring processors.
  - **Low surface to volume ratio** means low communication.
    - » Use squares, not slabs



Parallelism in Nearby Forces

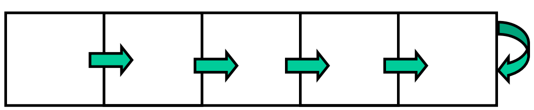
- Challenge 2: load imbalance, if particles cluster:
  - galaxies, electrons hitting a device wall.
- To reduce load imbalance, divide space unevenly.
  - Each region contains roughly equal number of particles.
  - **Quad-tree** in 2D, **Oct-tree** in 3D.



Example: each square contains at most 3 particles

Parallelism in Far-Field Forces

- Far-field forces involve all-to-all interaction and therefore communication.
- Force depends on all other particles:
  - Examples: gravity, protein folding
  - Simplest algorithm is $O(n^2)$ as in S&F 2, 4, 5.
  - Just decomposing space does not help since every particle needs to "visit" every other particle.



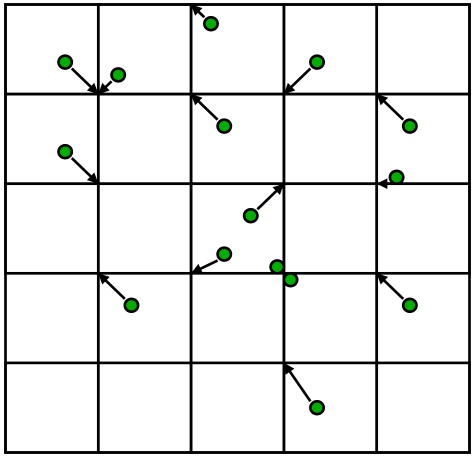
Implement by rotating particle sets.

- Keeps processors busy
- All processors eventually see all particles

- Use more clever algorithms to communicate less
- Use even more clever algorithms to beat $O(n^2)$.

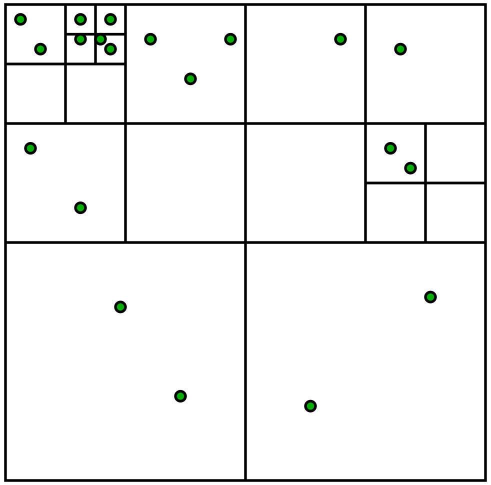
Far-field Forces: O(n log n) or O(n), not O(n²)

- Based on approximation:
  - Settle for the answer to just 3 digits, or just 15 digits …
- Two approaches
  - "Particle-Mesh"
    - » Approximate by particles on a regular mesh
    - » Exploit structure of mesh to solve for forces fast (FFT)
  - "Tree codes" (Barnes-Hut, Fast-Multipole-Method)
    - » Approximate clusters of nearby particles by single "metaparticles"
    - » Only need to sum over (many fewer) metaparticles



: Particle-Mesh

Tree code:



LUMPED SYSTEMS - ODES

System of Lumped Variables

- Many systems are approximated by
  - System of "lumped" variables.
  - Each depends on continuous parameter (usually time).
- Example -- circuit:
  - approximate as graph.
    - » edges are wires
    - » nodes are connections between 2 or more wires.
    - » each edge has resistor, capacitor, inductor or voltage source.
  - system is "lumped" because we are not computing the voltage/current at every point in space along a wire, just endpoints.
  - Variables related by Ohm's Law, Kirchoff's Laws, etc.
- Forms a system of ordinary differential equations (ODEs)
  - Differentiated with respect to time
  - Variant: ODEs with some constraints
    - » Also called DAEs, Differential Algebraic Equations

Circuit Example

- State of the system is represented by
  - $v_n(t)$ node voltages
  - $i_b(t)$ branch currents
  - $v_b(t)$ branch voltages

  } all at time t
- Equations include
  - Kirchoff's current
  - Kirchoff's voltage
  - Ohm's law
  - Capacitance
  - Inductance

$$\begin{pmatrix} 0 & A & 0 \\ A' & 0 & -I \\ 0 & R & -I \\ 0 & -I & C*d/dt \\ 0 & L*d/dt & I \end{pmatrix} * \begin{pmatrix} v_n \\ i_b \\ v_b \end{pmatrix} = \begin{pmatrix} 0 \\ S \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

- A is sparse matrix, representing connections in circuit
  - One column per branch (edge), one row per node (vertex) with +1 and -1 in each column at rows indicating end points
- Write as single large system of ODEs or DAEs

Structural Analysis Example

- Another example is structural analysis in civil engineering:
  - Variables are displacement of points in a building.
  - Newton's and Hook's (spring) laws apply.
  - Static modeling: exert force and determine displacement.
  - Dynamic modeling: apply continuous force (earthquake).
  - Eigenvalue problem: do the resonant modes of the building match an earthquake

OpenSees project in CEE at Berkeley looks at this section of 880, among others

Gaming Example

Star Wars – The Force Unleashed…

graphics.cs.berkeley.edu/papers/Parker-RTD-2009-08/

Solving ODEs

- In these examples, and most others, the matrices are sparse:
  - i.e., most array elements are 0.
  - neither store nor compute on these 0's.
  - Sparse because each component only depends on a few others

- Given a set of ODEs, two kinds of questions are:
  - Compute the values of the variables at some time t
    - » Explicit methods
    - » Implicit methods
  - Compute modes of vibration
    - » Eigenvalue problems

Solving ODEs

- Suppose ODE is $x'(t) = A \cdot x(t)$, where A is a sparse matrix
  - Discretize: only compute $x(i \cdot dt) = x[i]$ at $i=0,1,2,\ldots$
  - ODE gives $x'(t)$ = slope at t, and so $x[i+1] \approx x[i] + dt \cdot slope$
- Explicit methods (ex: Forward Euler)
  - Use slope at $t = i \cdot dt$, so slope $= A \cdot x[i]$.
  - $x[i+1] = x[i] + dt \cdot A \cdot x[i]$, i.e. **sparse matrix-vector multiplication**.
- Implicit methods (ex: Backward Euler)
  - Use slope at $t = (i+1) \cdot dt$, so slope $= A \cdot x[i+1]$.
  - Solve $x[i+1] = x[i] + dt \cdot A \cdot x[i+1]$ for $x[i+1] = (I - dt \cdot A)^{-1} \cdot x[i]$, i.e. **solve a sparse linear system of equations** for $x[i+1]$
- Tradeoffs:
  - Explicit: simple algorithm but may need tiny time steps dt for stability
  - Implicit: more expensive algorithm, but can take larger time steps dt
- Modes of vibration – eigenvalues of A
  - Algorithms also either multiply $A \cdot x$ or solve $y = (I - d \cdot A) \cdot x$ for x

CONTINUOUS SYSTEMS - PDES

Continuous Systems - PDEs

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

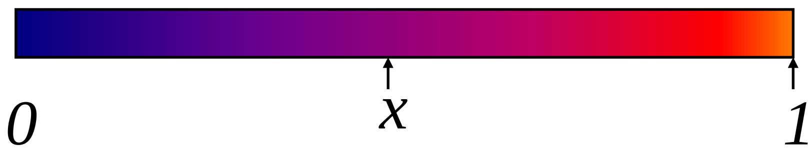
- Global means either a lot of communication, or tiny time steps
- Local arises from finite wave speeds: limits communication

Many problems combine features of above

- Fluid flow: Velocity,Pressure,Density(position,time)
- Elasticity: Stress,Strain(position,time)

Implicit Solution of the 1D Heat Equation

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



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

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

- Let $z = C \cdot \delta/h^2$ and discretize variable x to $j \cdot h$, t to $i \cdot \delta$, and u(x,t) to u[j,i]; solve for u at next time step:

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

- I is identity and

  L is Laplacian

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

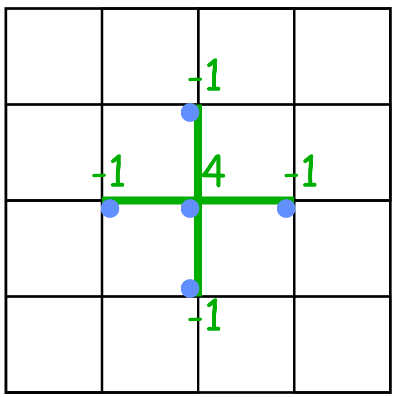
- Solve sparse linear system again

2D Implicit Method

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

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

Graph and "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 mesh.
- To solve this system, there are several techniques.

Algorithms for Solving Ax=b (N vars)

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.Gradients	$N^{3/2}$	$N^{1/2} * \log N$	N	N
• Red/Black 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	

All entries in "Big-Oh" sense (constants omitted)

PRAM is an idealized parallel model with zero cost communication

Reference: James Demmel, Applied Numerical Linear Algebra, SIAM, 1997.

Algorithms for 2D (3D) Poisson Equation ($N = n^2$ (n^3) 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	$N^{3/2}$ ($N^{4/3}$)	$N^{1/2}$ ($N^{1/3}$)	N	N
• Sparse LU	$N^{3/2}$ (N^2)	$N^{1/2}$	N*log N($N^{4/3}$)	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 ∞ procs, zero cost communication

Reference: J.D. , Applied Numerical Linear Algebra, SIAM, 1997.

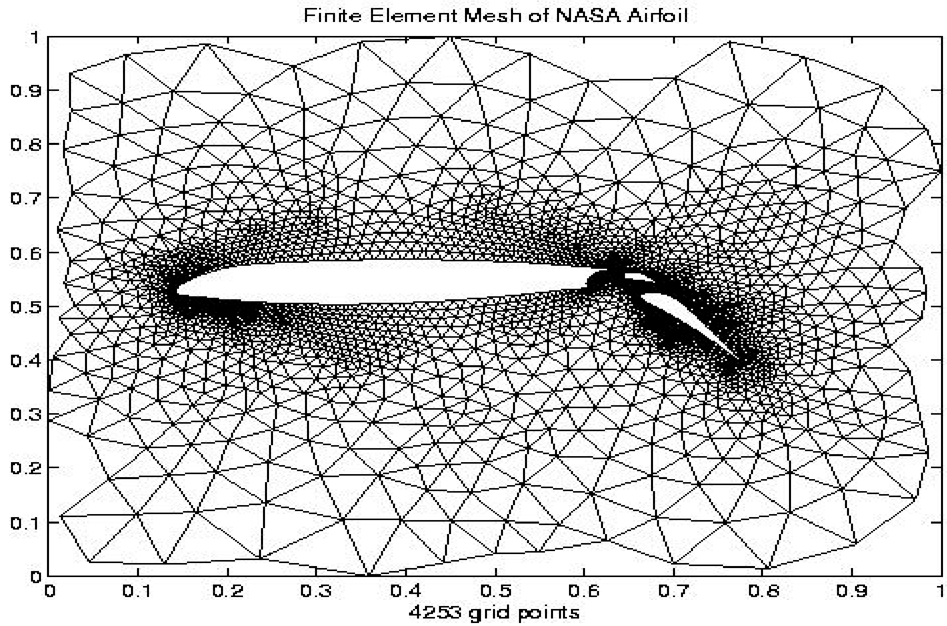
For more information: take Ma221 this semester!

Algorithms and Motifs

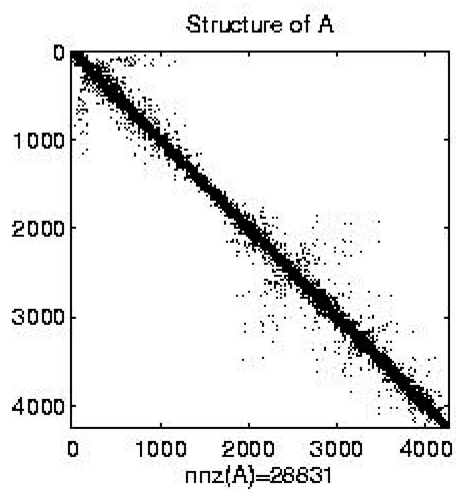
Algorithm	Motifs
Dense LU	Dense linear algebra
Band LU	Dense linear algebra
Jacobi	(Un)structured meshes, Sparse Linear Algebra
Explicit Inv.	Dense linear algebra
Conj.Gradients	(Un)structured meshes, Sparse Linear Algebra
Red/Black SOR	(Un)structured meshes, Sparse Linear Algebra
Sparse LU	Sparse Linear Algebra
FFT	Spectral
Multigrid	(Un)structured meshes, Sparse Linear Algebra

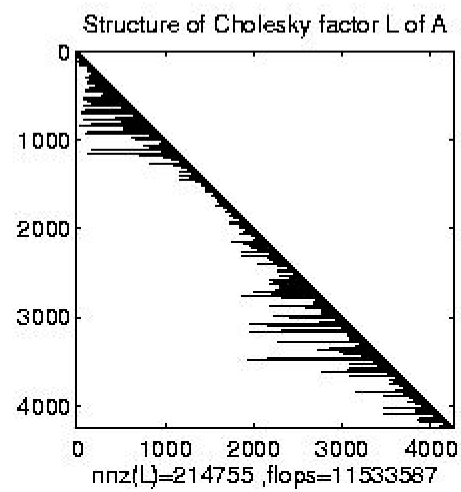
Irregular mesh: NASA Airfoil in 2D

Mesh of airfoil



Pattern of sparse matrix A

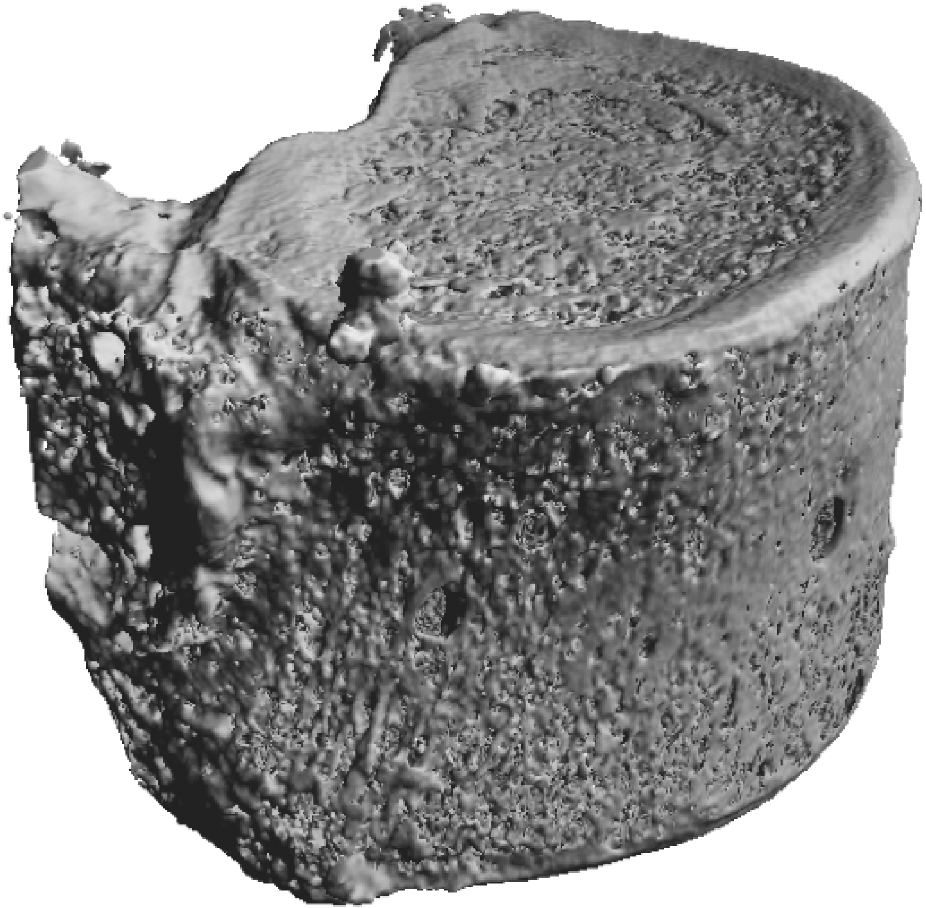




Pattern of A after LU

Source of Irregular Mesh: Finite Element Model of Vertebra

Study failure modes of trabecular Bone under stress



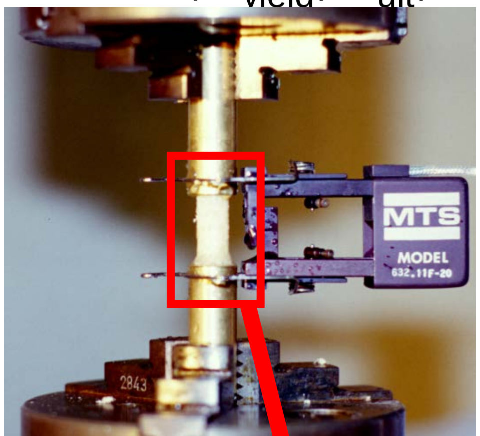
Source: M. Adams, H. Bayraktar, T. Keaveny, P. Papadopoulos, A. Gupta

Methods: μFE modeling (Gordon Bell Prize, 2004)

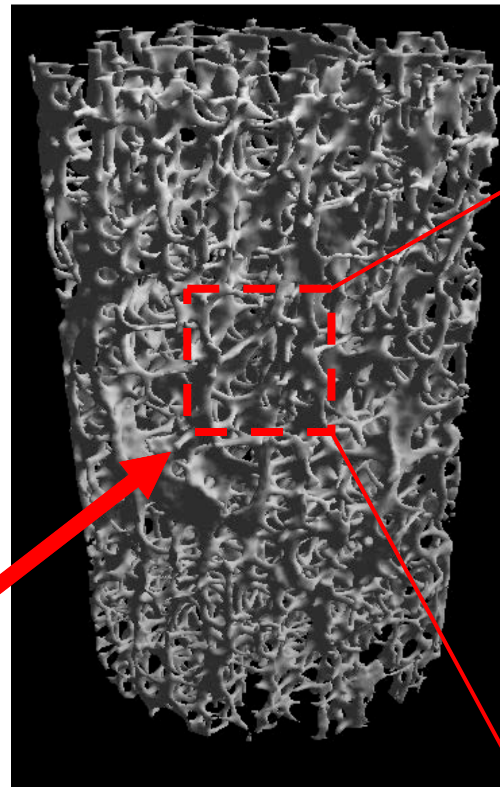
Mechanical Testing

Source: Mark Adams, PPPL

E, ε_{yield}, σ_{ult}, etc.



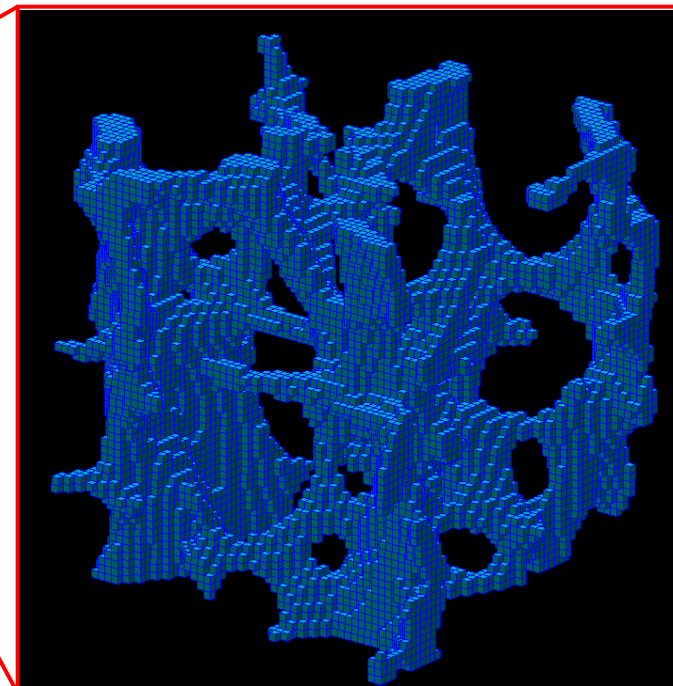
3D image



μFE mesh

2.5 mm cube

44 μm elements

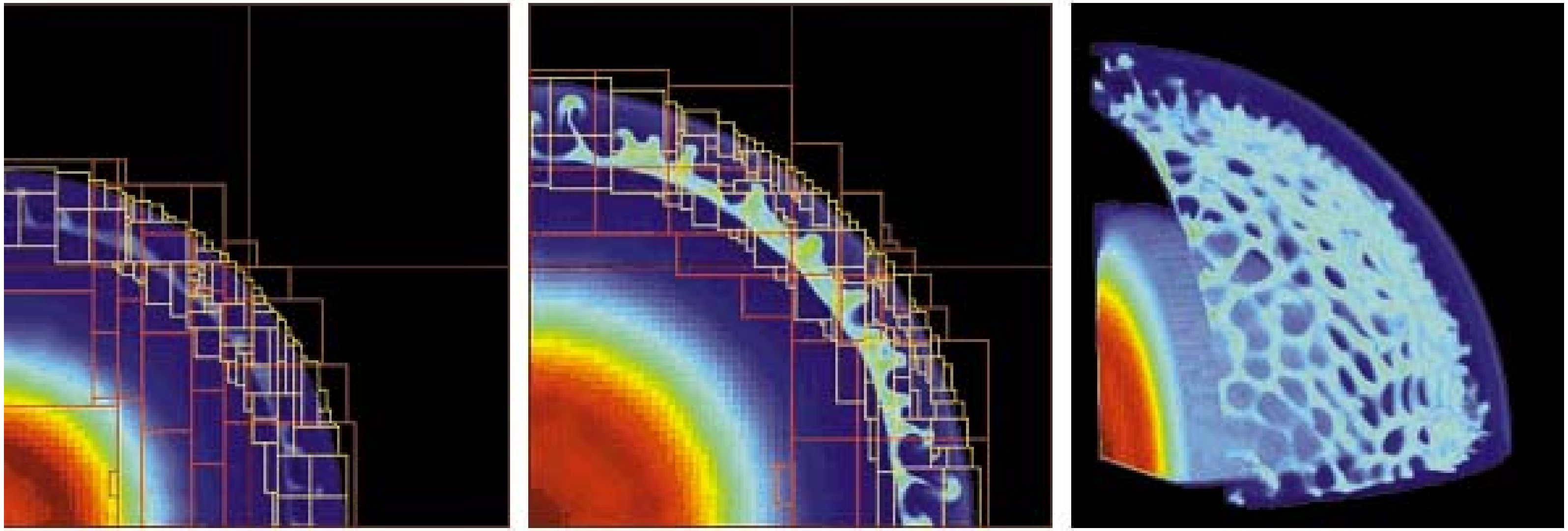


Micro-Computed Tomography

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://titanium.cs.berkeley.edu)
    - Chombo (P. Colella, LBL), KeLP (S. Baden, UCSD), J. Bell, LBL

Summary: Some Common Problems

- Find parallelism and locality

- Load Balancing
  - Statically - Graph partitioning
    - » Discrete systems
    - » Sparse matrix vector multiplication
  - Dynamically – if load changes significantly during job
- Linear algebra
  - Solving linear systems (sparse and dense)
  - Eigenvalue problems will use similar techniques
  - Sometimes formulated as structured/unstructured meshes
- Fast Particle Methods
  - $O(n \log n)$ instead of $O(n^2)$