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_Spr12/

– One or two will be used as lab assignments
  - See bottom of www.cs.berkeley.edu/~knight/cs267/resources.html
  - 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 $Ax = \lambda x$ where A is a dense matrix
2. Sparse Linear Algebra
   - Ex: Solve $Ax=b$ or $Ax = \lambda x$ 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()

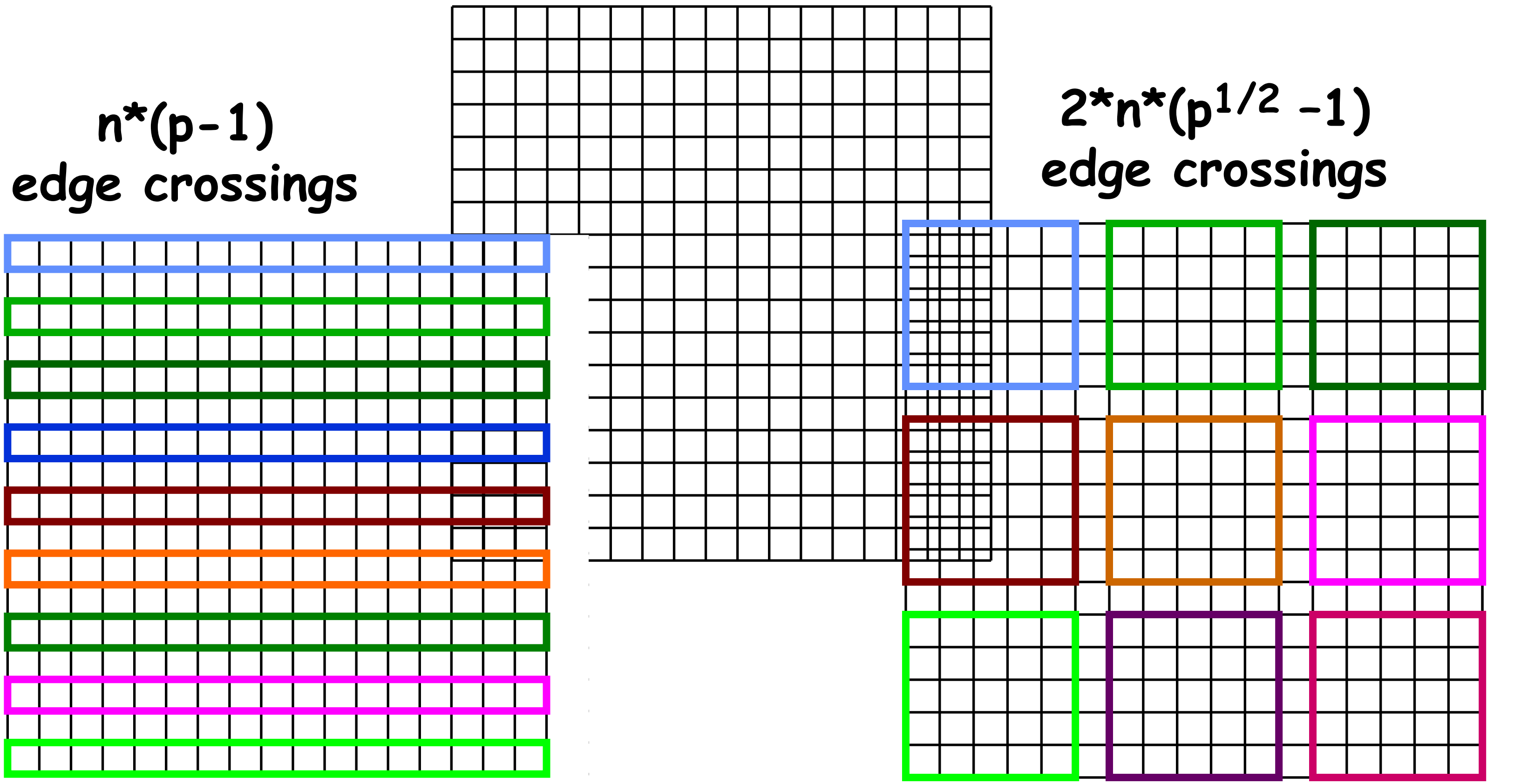
    exchange state info with neighbors

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

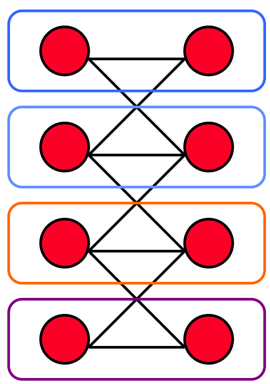
- Suppose graph is nxn mesh with connection NSEW neighbors
  - Which partition has less communication? (n=18, p=9)
- Minimizing communication on mesh ≡ minimizing "surface to volume ratio" of partition



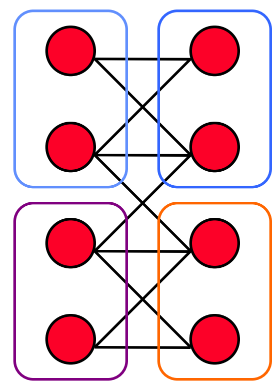
Synchronous Circuit Simulation

- 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 →

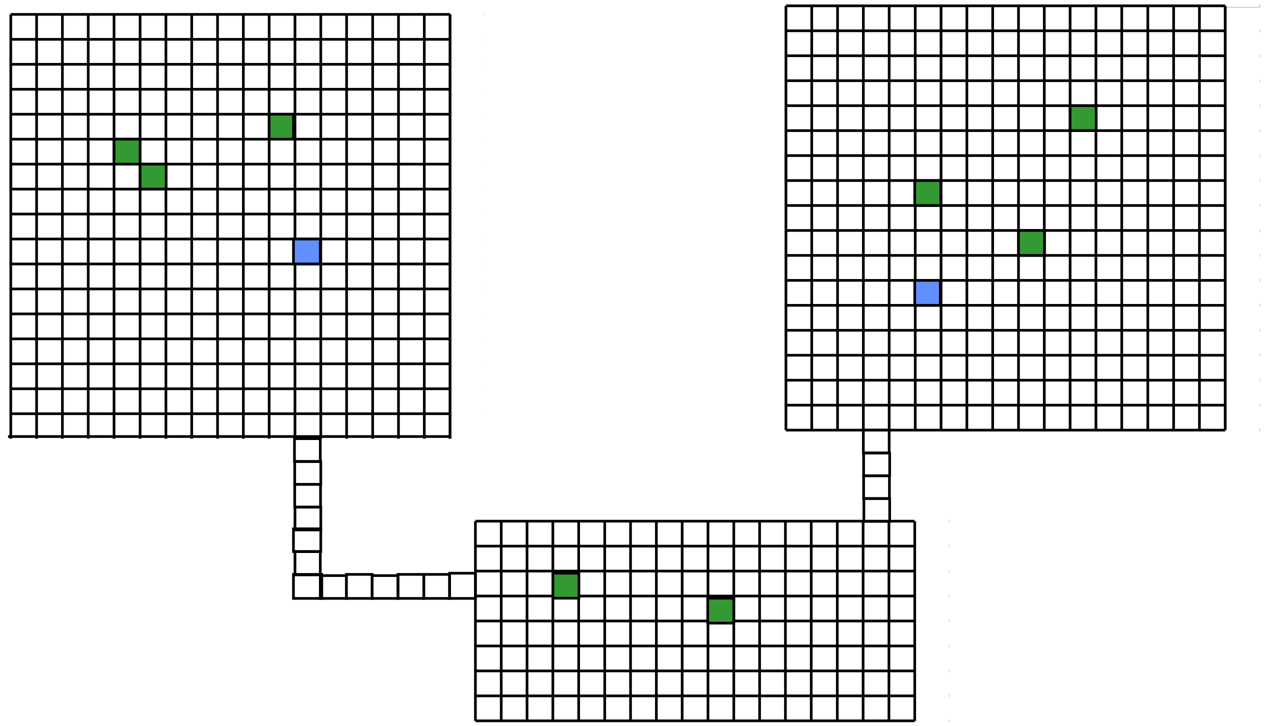


#edge crossings = 6



#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

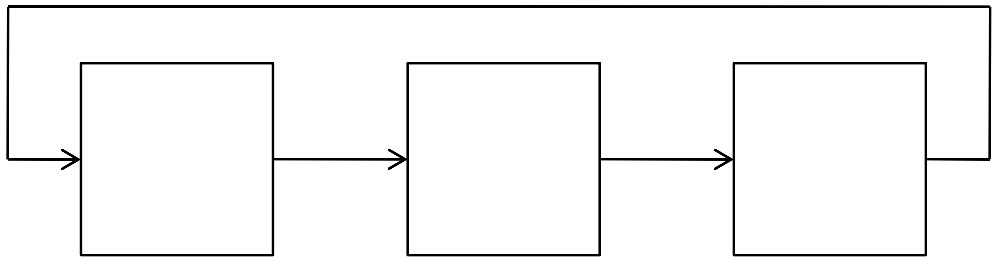
- Synchronous simulations may waste time:
  - Simulates even when the inputs do not change.
- Asynchronous (event-driven) simulations update only when an event arrives from another component:
  - No global time steps, but individual events contain time stamps.
  - Example: Game of life in loosely connected 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
```

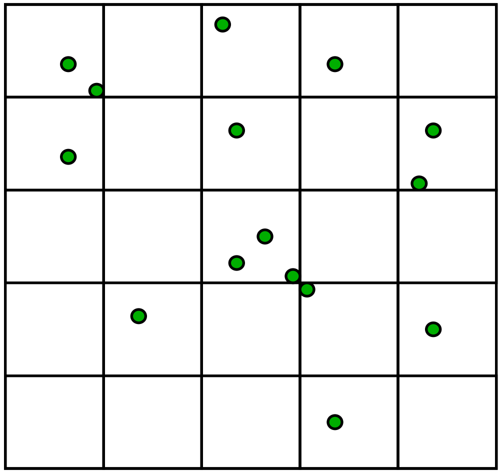
Parallelism in External Forces

- 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

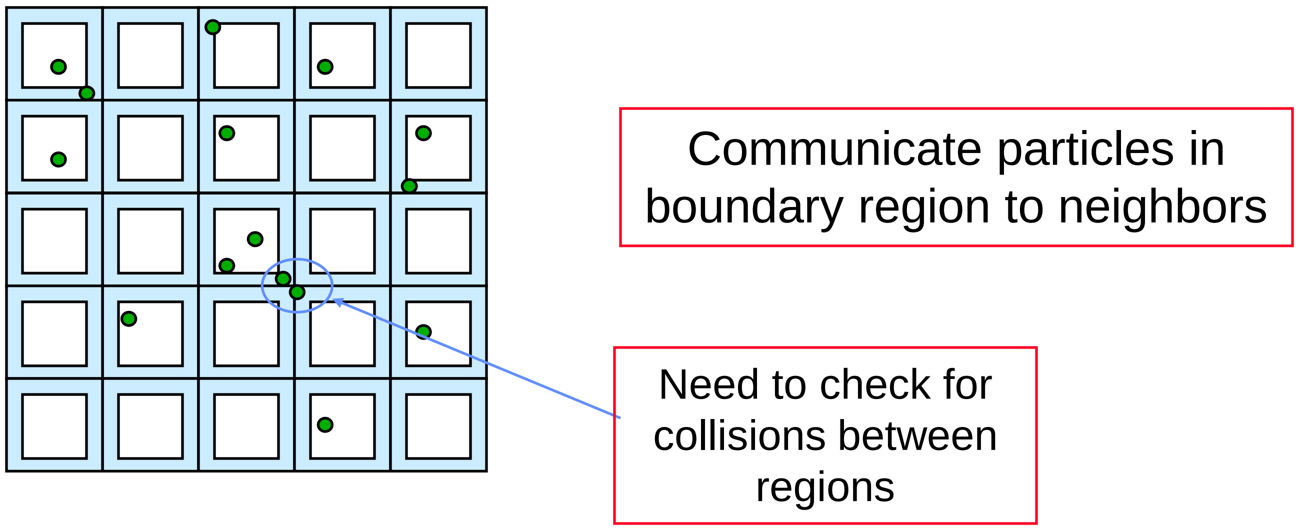
Parallelism in Nearby Forces

- 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.



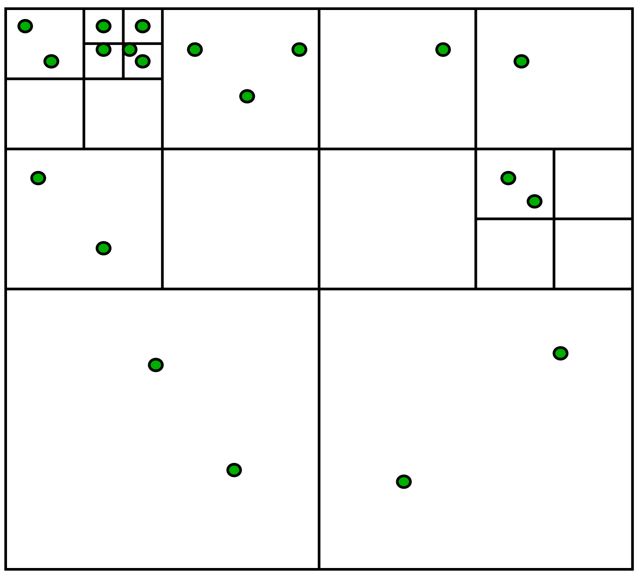
Parallelism in Nearby Forces

- 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

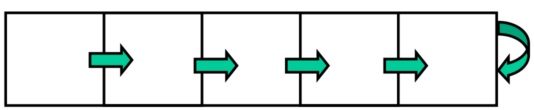
- Challenge 2: load imbalance, if particles cluster:
  - galaxies, electrons hitting a device wall.
- To reduce load imbalance, divide space unevenly.
  - Each region contains roughly equal number of particles.
  - **Quad-tree** in 2D, **Oct-tree** in 3D.



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.



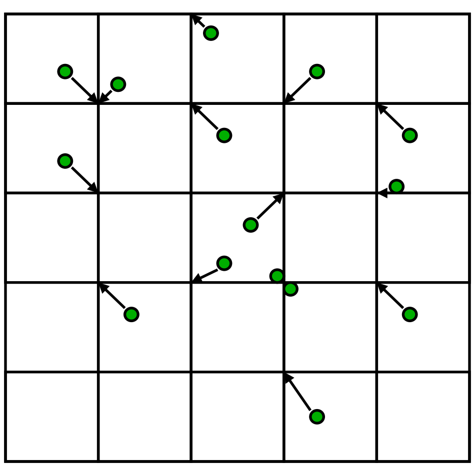
Implement by rotating particle sets.

- Keeps processors busy
- All processors eventually see all particles

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

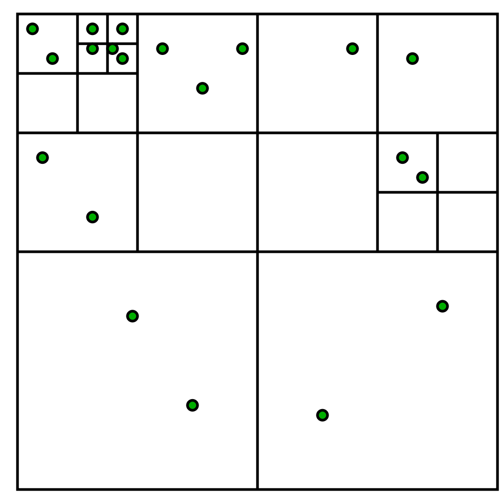
Far-field Forces: $O(n \log n)$ or $O(n)$, not $O(n^2)$

- 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

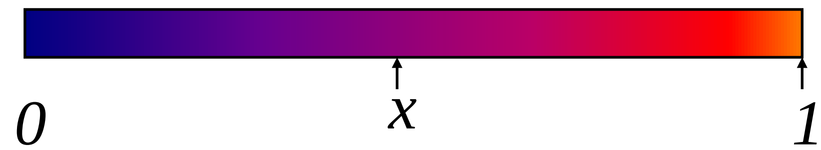
- Global means either a lot of communication, or tiny time steps
- Local arises from finite wave speeds: limits communication

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

- Solve sparse linear system again

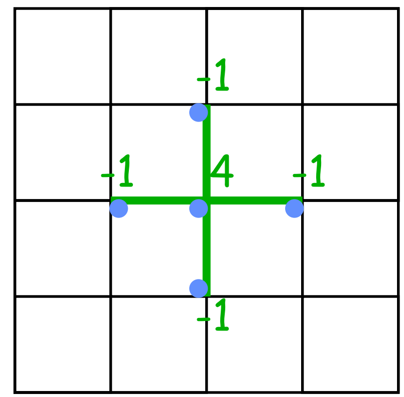
$$L = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}$$

2D Implicit Method

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

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

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.

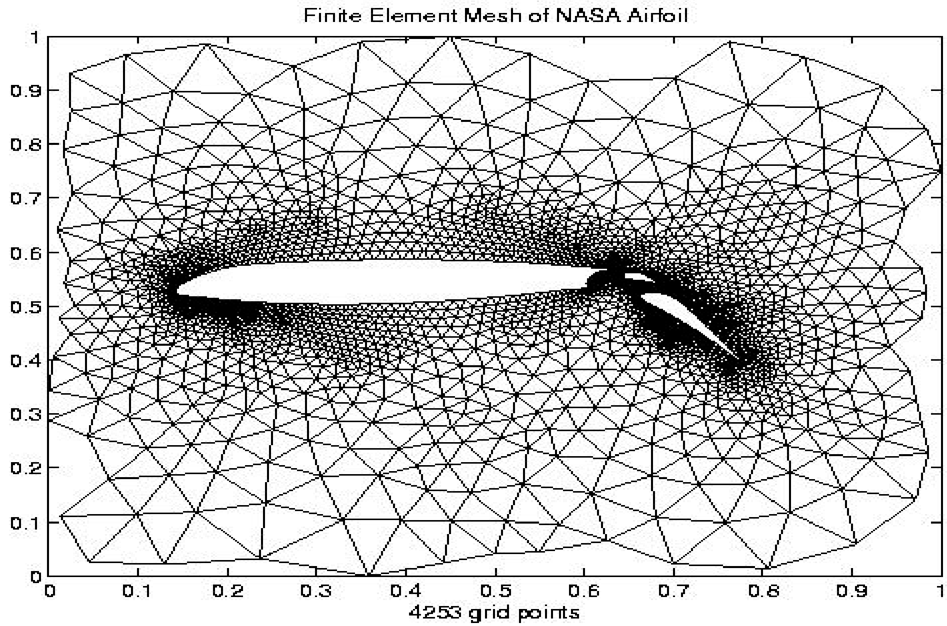
For more information: take Ma221 this semester!

Algorithms and Motifs

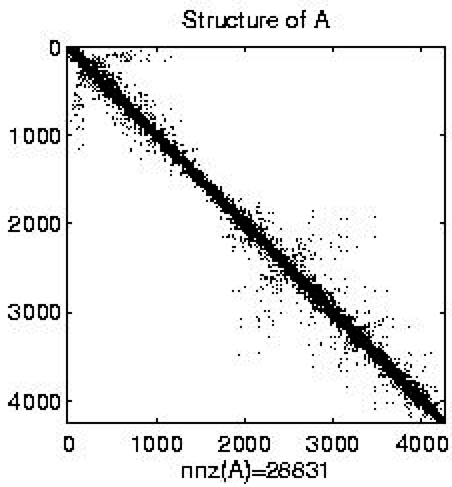
Algorithm	Motifs
• Dense LU	Dense linear algebra
• Band LU	Dense linear algebra
• Jacobi	(Un)structured meshes, Sparse Linear Algebra
• Explicit Inv.	Dense linear algebra
• Conj.Gradients	(Un)structured meshes, Sparse Linear Algebra
• Red/Black SOR	(Un)structured meshes, Sparse Linear Algebra
• Sparse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

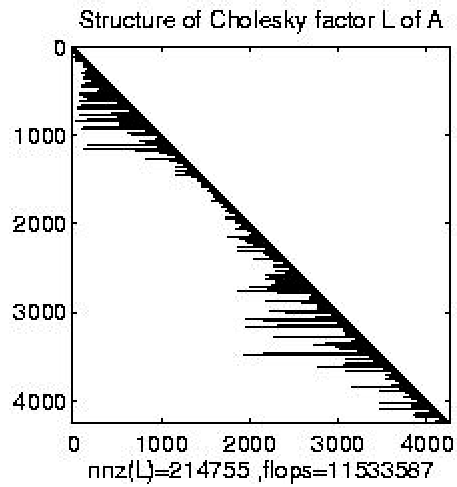
Irregular mesh: NASA Airfoil in 2D

Mesh of airfoil



Pattern of sparse matrix A

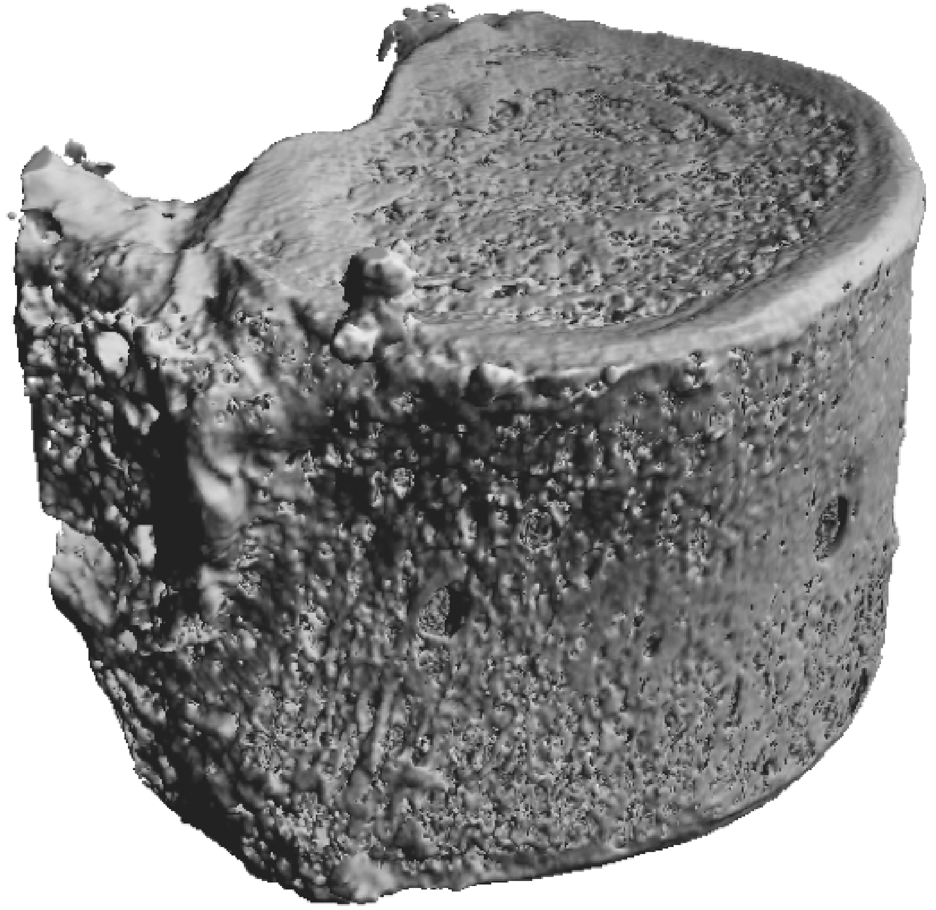




Pattern of A after LU

Source of Irregular Mesh: Finite Element Model of Vertebra

Study failure modes of trabecular Bone under stress



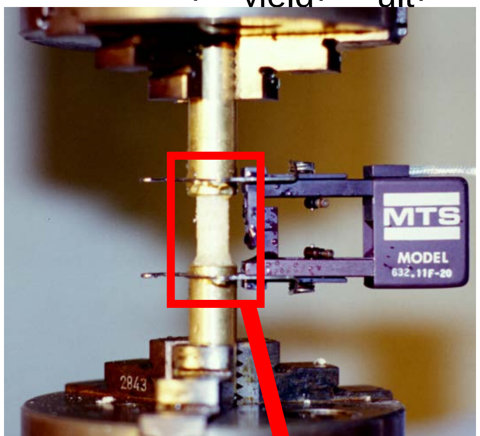
Source: M. Adams, H. Bayraktar, T. Keaveny, P. Papadopoulos, A. Gupta

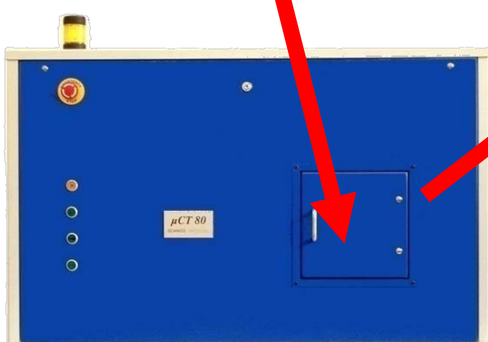
Methods: μFE modeling (Gordon Bell Prize, 2004)

Mechanical Testing

Source: Mark Adams, PPPL

E, ε_{yield}, σ_{ult}, etc.

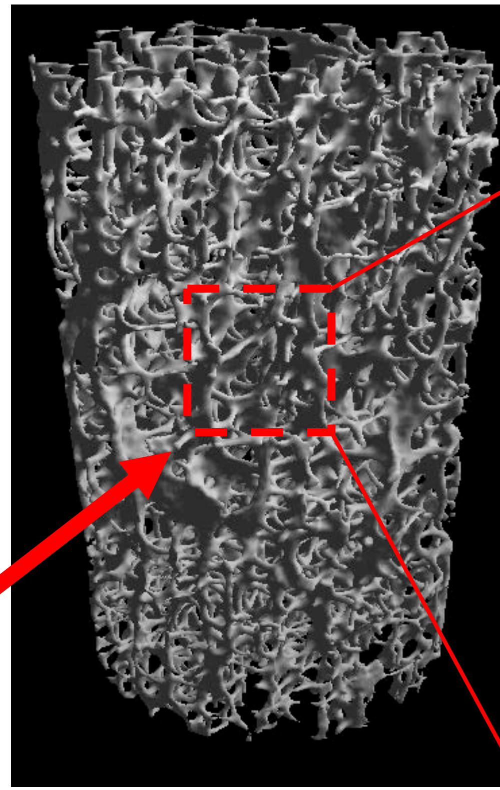




Micro-Computed Tomography

μCT @ 22 μm resolution

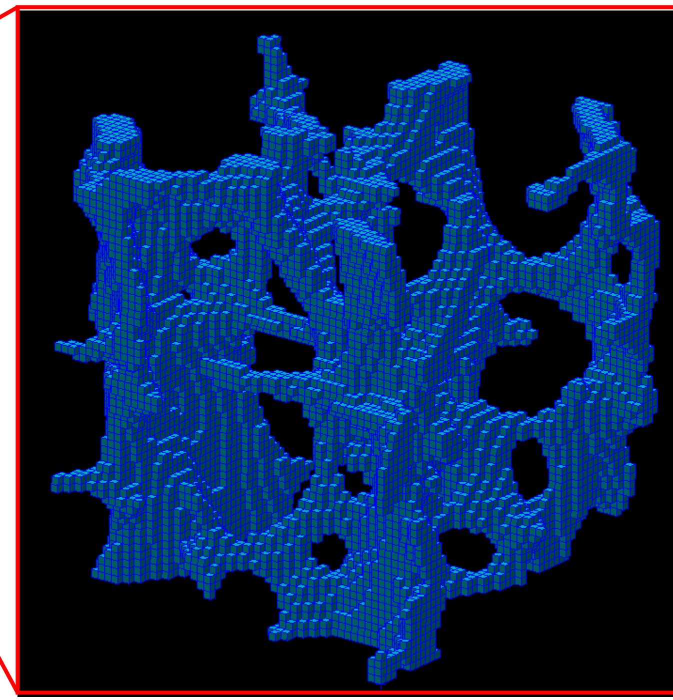
3D image



μFE mesh

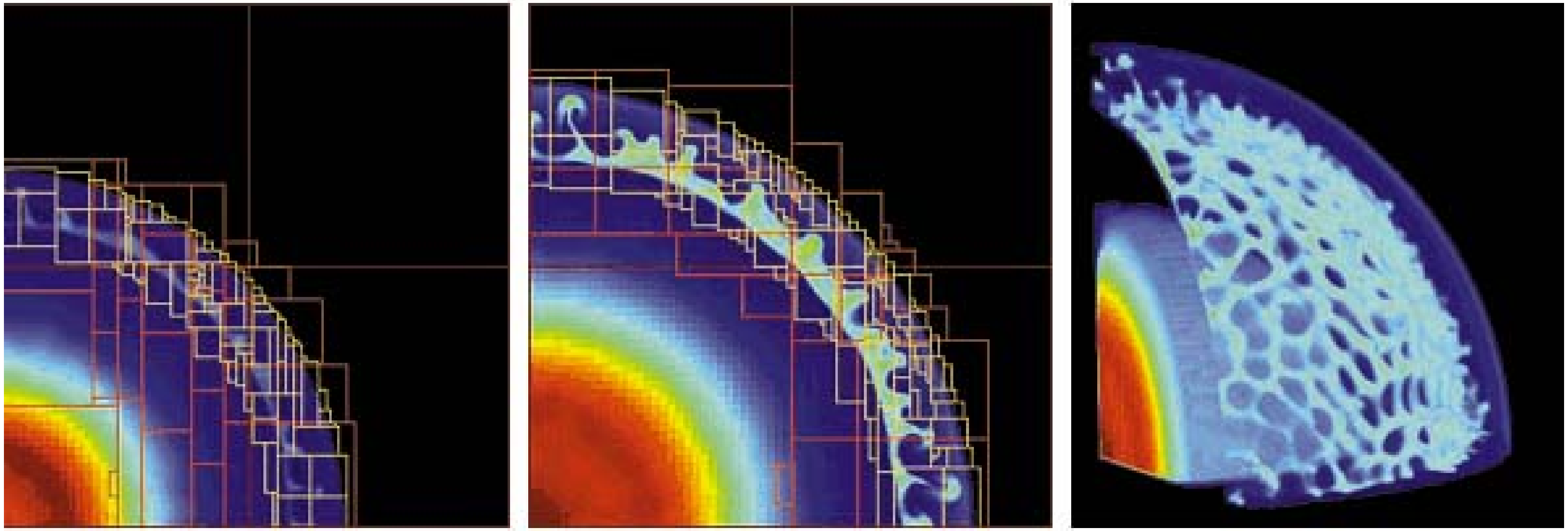
2.5 mm cube

44 μm elements



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
  - Dynamically – if load changes significantly during job
  - Statically - Graph partitioning
    - » Discrete systems
    - » Sparse matrix vector multiplication
- 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 $O(n^2)$