CS 267 Sources of Parallelism and Locality in Simulation Lecture 6

James Demmel

www.cs.berkeley.edu/~demmel

Parallelism and Locality in Simulation

- Parallelism and data locality both critical to performance
  - Recall that moving data is the 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 variables depending on continuous parameters
  - aka Ordinary Differential Equations (ODEs),
  - Structural mechanics, Chemical kinetics, Circuits, Star Wars: The Force Unleashed
- Continuous variables depending on continuous parameters
  - aka Partial Differential Equations (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 more than one of these 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
  - Next lecture

- Identify common problems and solutions

discrete

continuous

A Model Problem: Sharks and Fish

- Illustration of parallel programming
  - Original version (discrete event only) proposed by Geoffrey Fox
  - Called WATOR
- 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 problems (S&F1 - S&F6)
  - Different sets of rules, to illustrate different phenomena
- Available in many languages (see class web page)
  - Matlab, pThreads, MPI, OpenMP, Split-C, Titanium, CMF, CMMD, pSather (not all problems in all languages)
- Some homework based on these

Sharks and Fish

- **S&F 1.** Fish alone move continuously subject to an external current and Newton's laws.
- **S&F 2.** Fish alone move continuously subject to gravitational attraction and Newton's laws.
- **S&F 3.** Fish alone play the "Game of Life" on a square grid.
- **S&F 4.** Fish alone move randomly on a square grid, with at most one fish per grid point.
- **S&F 5.** Sharks and Fish both move randomly on a square grid, with at most one fish or shark per grid point, including rules for fish attracting sharks, eating, breeding and dying.
- **S&F 6.** Like Sharks and Fish 5, but continuous, subject to Newton's laws.

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:"
  - Also known as Sharks and Fish #3:
  - Space divided into cells, rules govern cell contents at each step

Parallelism in Game of Life (S&F 3)

- The simulation is synchronous
  - use two copies of the grid (old and new), “ping-pong” between them
  - 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*

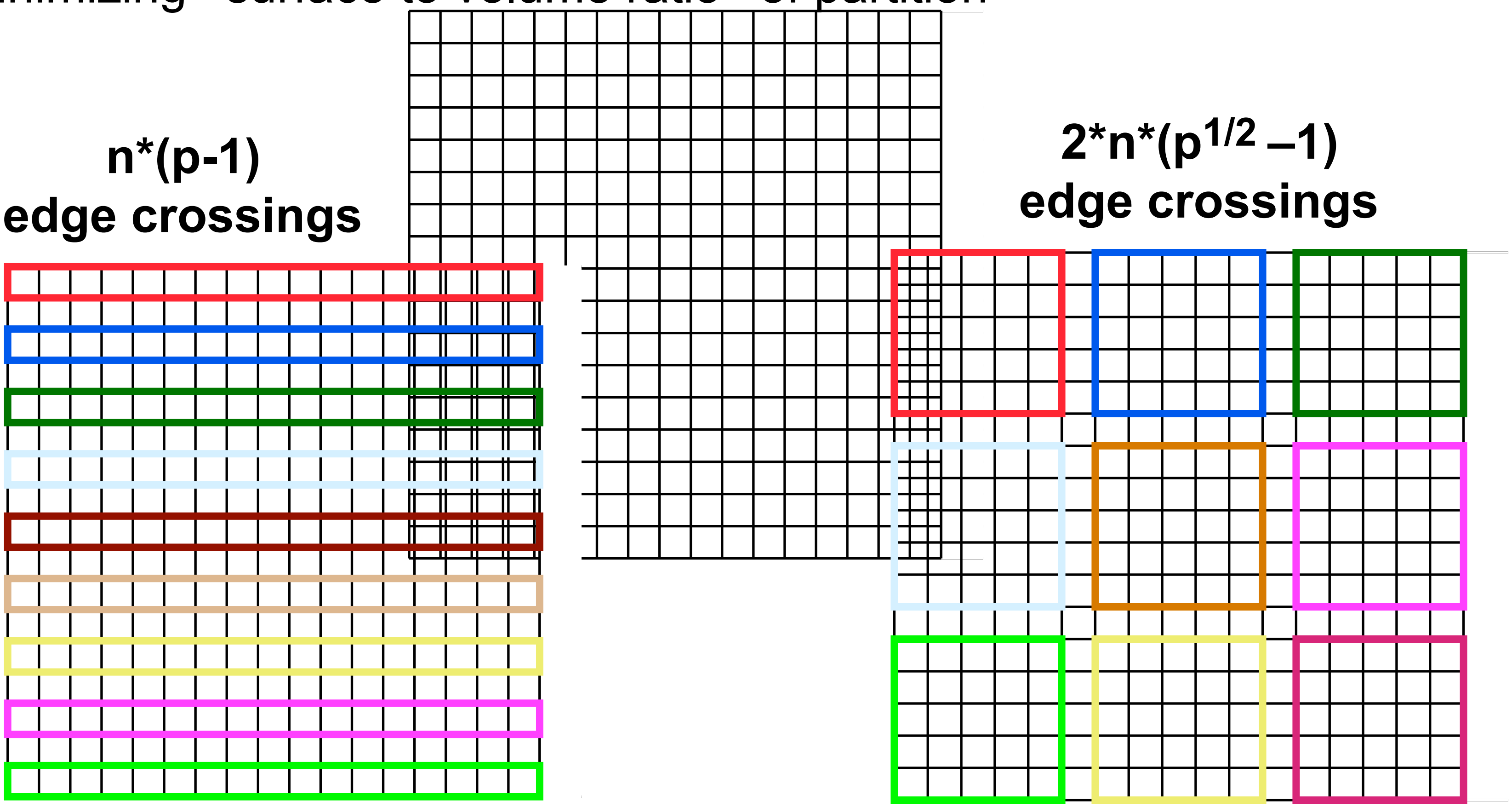
P1	P2	P3
P4	P5	P6
P7	P8	P9

```
Repeat
    compute locally to update local system
    barrier()
    exchange state info with neighbors
    finish updates
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 (e.g. Game of Life)

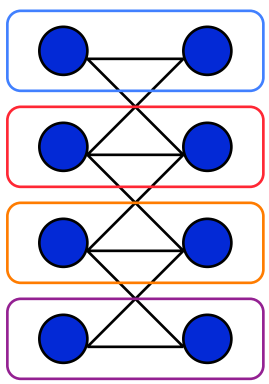
- Suppose graph is nxn mesh with connection NSEW neighbors
- Which partition has less communication? (n=18, p=9)
- Minimizing communication on mesh ≡ minimizing “surface to volume ratio” of partition



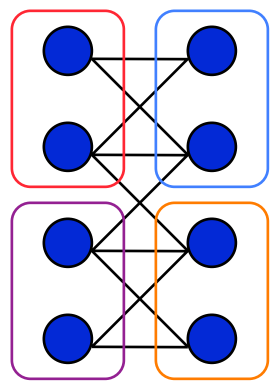
Synchronous Circuit Simulation

- 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 (future lecture)

better →

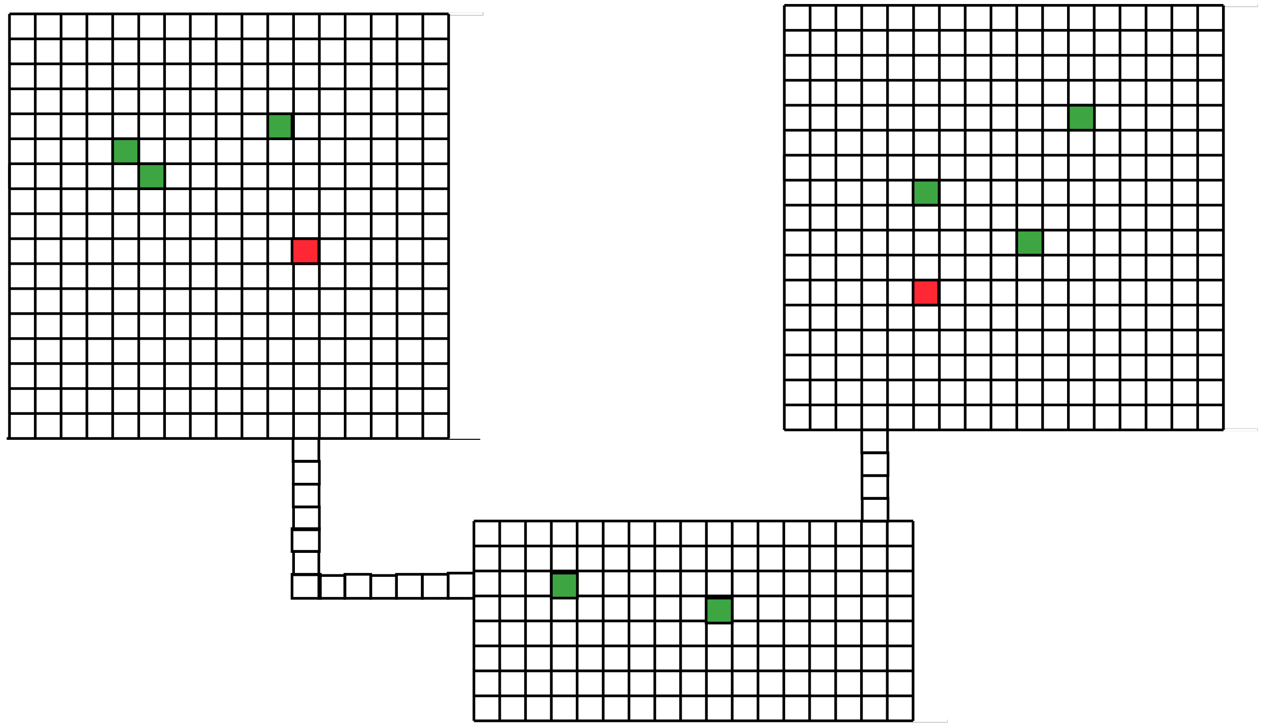


edge crossings = 6



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

Asynchronous Simulation

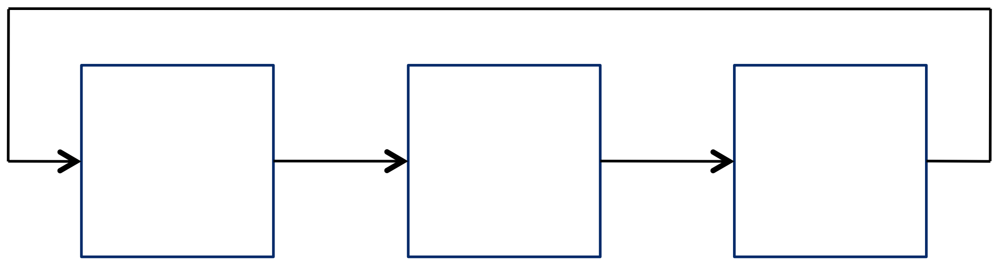
- Synchronous simulations may waste time:
  - Simulates even when the inputs do not change
- Asynchronous (event-driven) simulations update only when an event arrives from another component:
  - No global time steps, but individual events contain time stamp.
  - Example: Game of life in loosely connected 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
  - On distributed memory, events are naturally implemented as messages between processors (eg using MPI), 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

Summary of Lecture so far

- Parallelism and Locality arise naturally in simulation
  - So far: Discrete Event Simulation (time and space discrete)
  - Next: Particle Systems, Lumped variables (ODEs), Continuous variables (PDEs)
- Discrete Event Simulation
  - Game of Life, Digital Circuits, Pacman, …
  - Finite set of variables, values at a given time called state
  - Each variable updated by transition function depending on others
  - Assign work to processors (*domain decomposition)*
    - Goals*:* balance load and minimize communication
    - Represent problem by graph
      - Nodes are states, edges are dependencies
      - Partition graph (NP hard, so approximate)
  - Synchronous: update all values at each discrete timestep
  - Asynchronous: update a value only if inputs change, when an "event" occurs; also called event driven simulation
    - Conservative vs Speculative approaches

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 and positions are 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
  - balls in a pinball game
- Reminder: many simulations combine techniques such as particle simulations with some discrete events (Ex Sharks and Fish)

Forces in Particle Systems

- Force on each particle can be subdivided

$$\text{force} = \text{external\_force} + \text{nearby\_force} + \text{far\_field\_force}$$

- External force
  - ocean current in 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: integrate using Euler's method with varying step size
%   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)),1);
    end
```

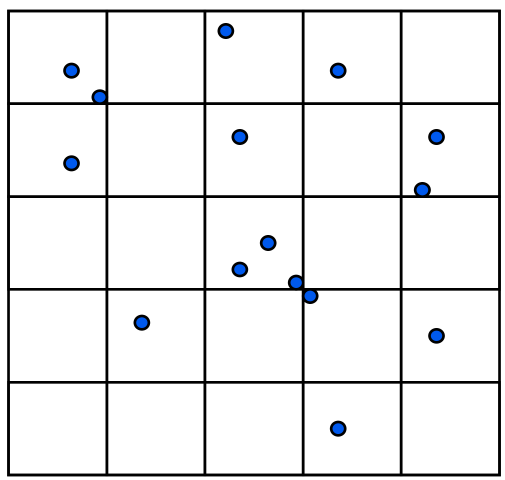
Parallelism in External Forces

- These are the simplest
- The force on each particle is independent
- Called “embarrassingly parallel”
  - Sometimes called “map reduce” by analogy

- Evenly distribute particles on processors
  - Any distribution works
  - Locality is not an issue
- For each particle on processor, apply the external force
  - Also called “map”
  - May need to “reduce” (eg compute maximum) to compute time step, other data

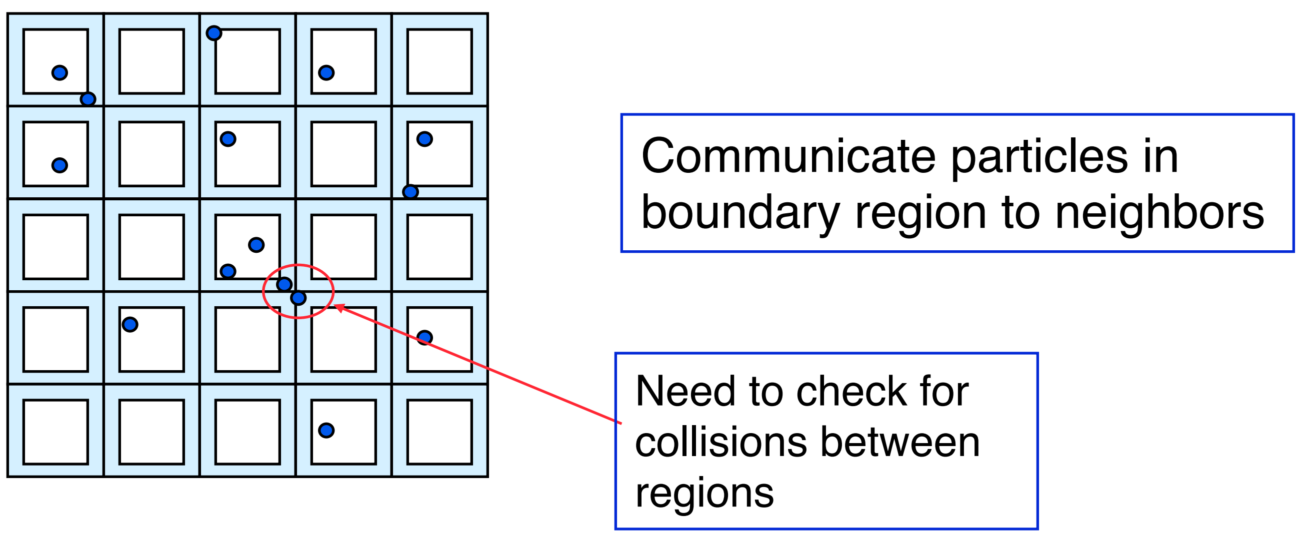
Parallelism in Nearby Forces

- 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.



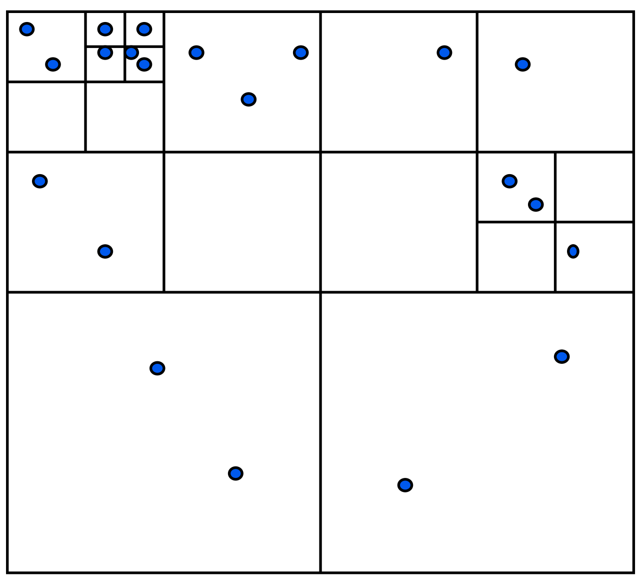
Parallelism in Nearby Forces

- Challenge 1: interactions of particles near processor boundary:
  - need to communicate particles near boundary to neighboring processors.
    - Region near boundary called "ghost zone" or "halo"
  - Low surface to volume ratio means low communication.
    - Use squares, not slabs, to minimize ghost zone sizes



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.

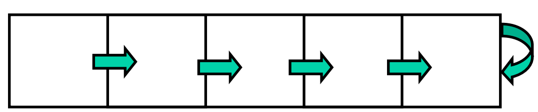


Example: each square contains at most 3 particles

- May need to rebalance as particles move, hopefully seldom

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 reduce communication
- Use more clever algorithms to beat $O(n^2)$.

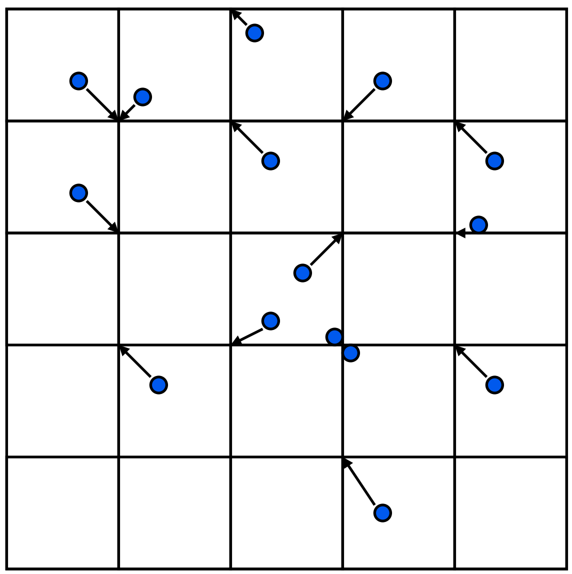
Far-field Forces: Particle-Mesh Methods

- Based on approximation:
  - Superimpose a regular mesh.
  - “Move” particles to nearest grid point.
- Exploit fact that the far-field force satisfies a PDE that is easy to solve on a regular mesh:
  - FFT, multigrid (described in future lectures)
  - Cost drops to O(n log n) or O(n) instead of O(n^2)
- Accuracy depends on the fineness of the grid is and the uniformity of the particle distribution.

1) Particles are moved to nearby mesh points (scatter)

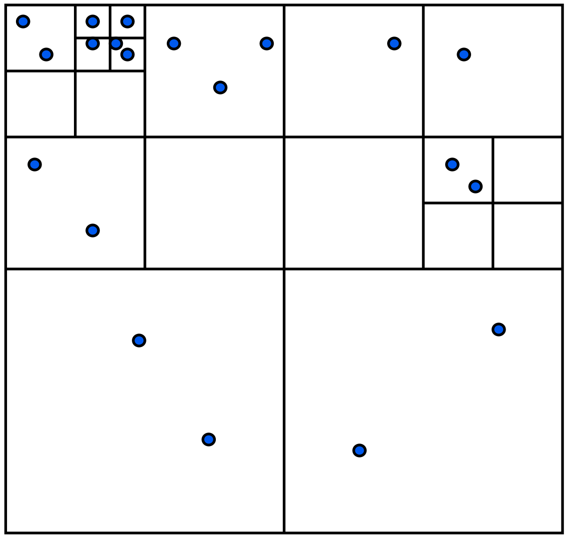
2) Solve mesh problem

3) Forces are interpolated at particles from mesh points (gather)



Far-field forces: Tree Decomposition

- Based on approximation.
  - Forces from group of far-away particles “simplified” -- resembles a single large particle.
  - Use tree; each node contains an approximation of descendants.
- Also O(n log n) or O(n) instead of O(n^2).
- Several Algorithms
  - Barnes-Hut.
  - Fast multipole method (FMM) of Greengard/Rohklin.
  - Anderson’s method.
- Discussed in later lecture.



Summary of Particle Methods

- Model contains discrete entities, namely, particles
- Time is continuous – must be discretized to solve

- Simulation follows particles through timesteps
  - Force = external _force + nearby_force + far_field_force
  - All-pairs algorithm is simple, but inefficient, $O(n^2)$
  - Particle-mesh methods approximates by moving particles to a regular mesh, where it is easier to compute forces
  - Tree-based algorithms approximate by treating set of particles as a group, when far away

- May think of this as a special case of a "lumped" system

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.
    - wires are edges.
    - 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

  $\left.\right\}$ all at times 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 CE at Berkeley looks at this section of 880, among others

Gaming Example

Star Wars – The Force Unleashed …

www.cs.berkeley.edu/b-cam/Papers/Parker-2009-RTD

Solving ODEs

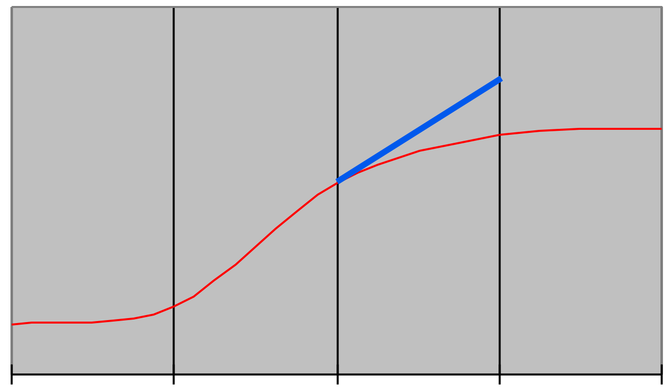
- In these examples, and most others, the matrices are sparse:
  - i.e., most array elements are 0.
  - neither store nor compute on these 0's.
  - Sparse because each component only depends on a few others

- 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: Explicit Methods

- Assume ODE is x'(t) = f(x) = A*x(t), where A is a sparse matrix
  - Compute x(i*dt) = x[i]
    at i=0,1,2,…
  - ODE gives x' (i*dt) = slope
    x[i+1]=x[i] + dt*slope

Use slope at x[i]

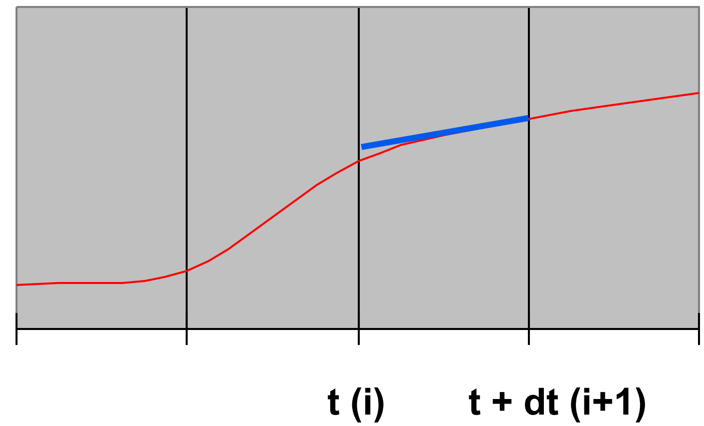


- Explicit methods, e.g., (Forward) Euler's method.
  - Approximate x'(t)=A*x(t) by (x[i+1] - x[i])/dt = A*x[i].
  - x[i+1] = x[i]+dt*A*x[i], i.e. sparse matrix-vector multiplication.
- Tradeoffs:
  - Simple algorithm: sparse matrix vector multiply.
  - Stability problems: May need to take very small time steps, especially if system is stiff (i.e. A has some large entries, so x can change rapidly).

Solving ODEs: Implicit Methods

- Assume ODE is $x'(t) = f(x) = A*x(t)$, where A is a sparse matrix
  - Compute $x(i*dt) = x[i]$
    at $i=0,1,2,\ldots$
  - ODE gives $x'((i+1)*dt) = \text{slope}$
    $x[i+1]=x[i] + dt*\text{slope}$

Use slope at x[i+1]



- Implicit method, e.g., Backward Euler solve:
  - Approximate $x'(t)=A*x(t)$ by $(x[i+1] - x[i])/dt = A*x[i+1]$.
  - $(I - dt*A)*x[i+1] = x[i]$, i.e. we need to solve a sparse linear system of equations.
- Trade-offs:
  - Larger timestep possible: especially for stiff problems
  - More difficult algorithm: need to solve a sparse linear system of equations at each step

Solving ODEs: Eigensolvers

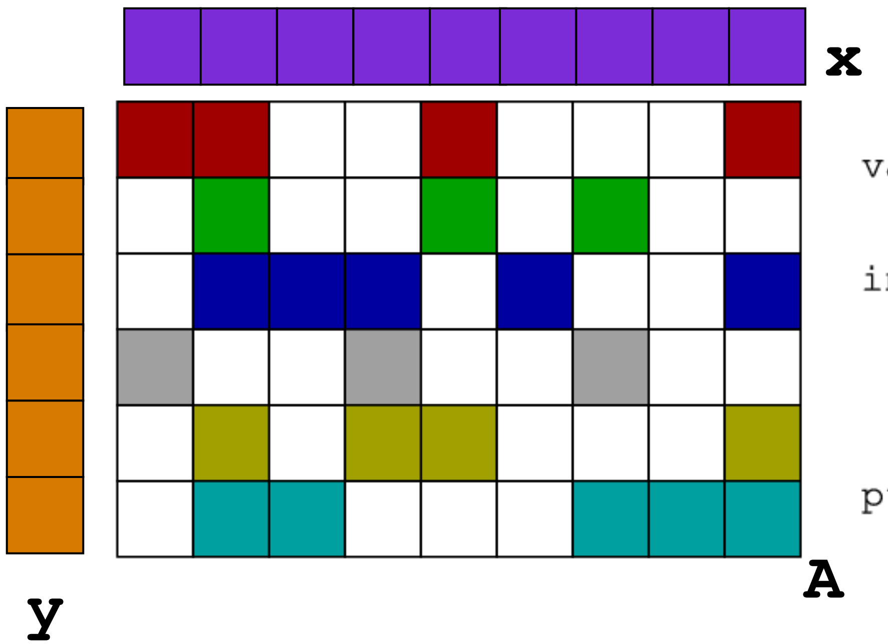
- Computing modes of vibration: finding eigenvalues and eigenvectors.
  - Seek solution of $d^2x(t)/dt^2 = A*x(t)$ of form $x(t) = \sin(\omega*t) * x_0$, where x_0 is a constant vector
    - ω called the frequency of vibration
    - x_0 sometimes called a "mode shape"
  - Plug in to get $-\omega^2 *x_0 = A*x_0$, so that $-\omega^2$ is an eigenvalue and x_0 is an eigenvector of A.
  - Solution schemes reduce either to sparse-matrix multiplications, or solving sparse linear systems.

Summary of ODE Methods

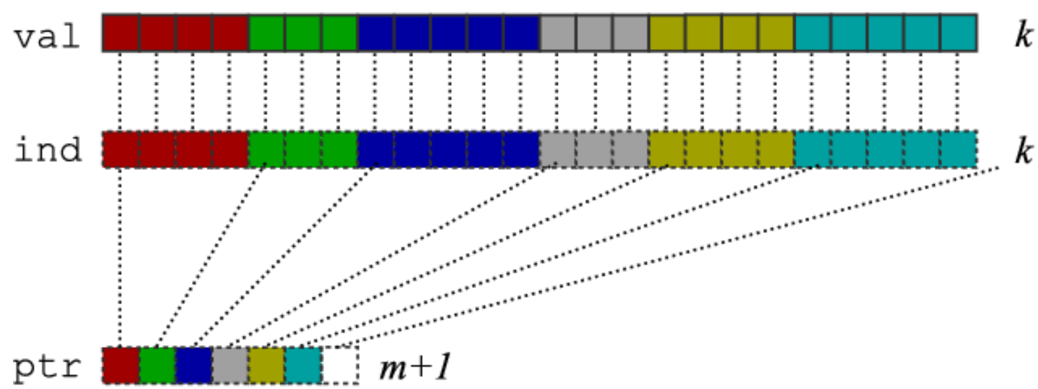
- Explicit methods for ODEs need sparse-matrix-vector mult.
- Implicit methods for ODEs need to solve linear systems
- Direct methods (Gaussian elimination)
  - Called LU Decomposition, because we factor A = L*U.
  - Future lectures will consider both dense and sparse cases.
  - More complicated than sparse-matrix vector multiplication.
- Iterative solvers
  - Will discuss several of these in future.
    - Jacobi, Successive over-relaxation (SOR) , Conjugate Gradient (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.

SpMV in Compressed Sparse Row (CSR) Format

SpMV: y = y + A*x, only store, do arithmetic, on nonzero entries
CSR format is simplest one of many possible data structures for A



Representation of **A**

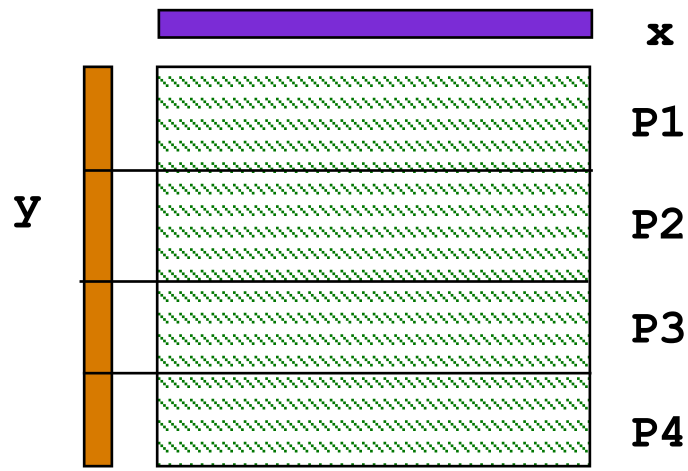


Matrix-vector multiply kernel: $y(i) \leftarrow y(i) + A(i,j) \cdot x(j)$

```
for each row i
  for k=ptr[i] to ptr[i+1]-1 do
       y[i] = y[i] + val[k]*x[ind[k]]
```

Parallel Sparse Matrix-vector multiplication

- y = A*x, where A is a sparse n x n matrix

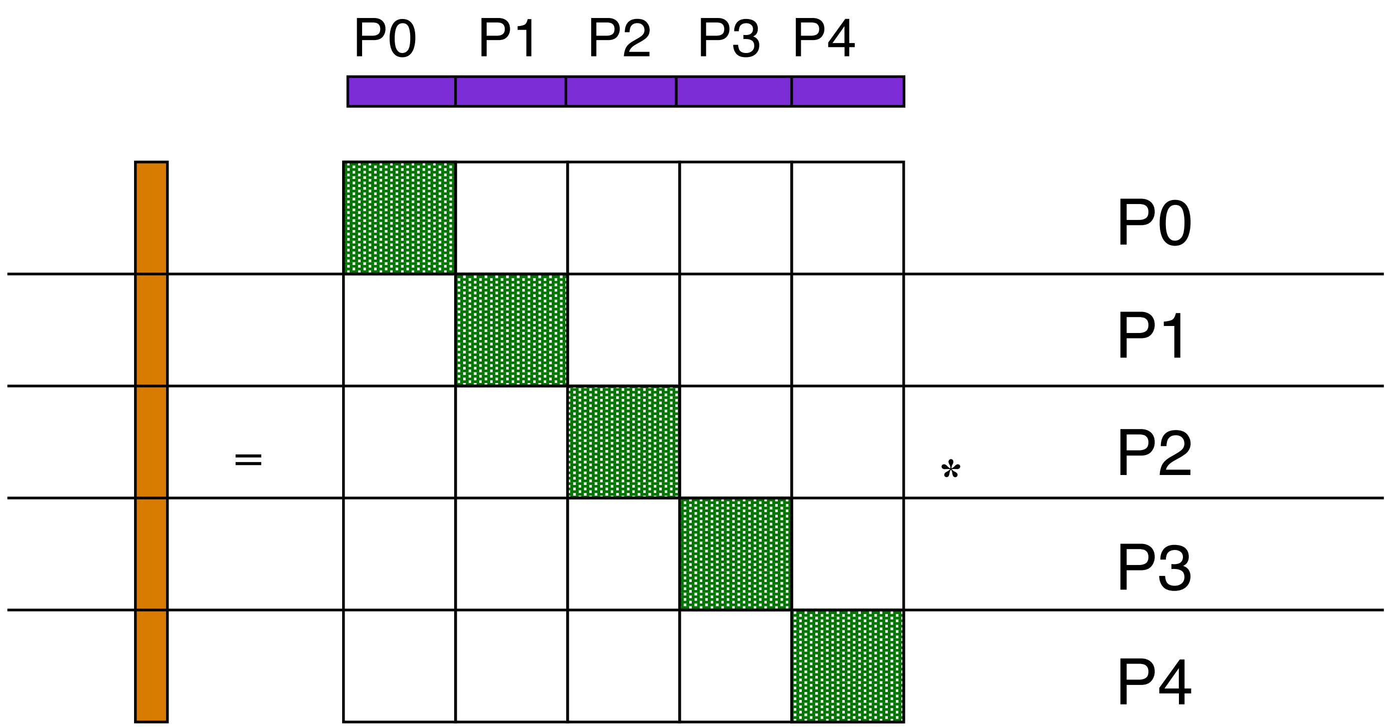


- Questions
  - which processors store
    - y[i], x[i], and A[i,j]
  - which processors compute
    - y[i] = sum (from 1 to n) A[i,j] * x[j]
      = (row i of A) * x … a sparse dot product
- Partitioning
  - Partition index set {1,…,n} = N1 ∪ N2 ∪ … ∪ Np.
  - For all i in Nk, Processor k stores y[i], 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 computes the y[i]s it owns.

May require communication

Matrix Reordering via Graph Partitioning

- "Ideal" matrix structure for parallelism: block diagonal
  - p (number of processors) blocks, can all be computed locally.
  - If no non-zeros outside these blocks, no communication needed
- Can we reorder the rows/columns to get close to this?
  - Most nonzeros in diagonal blocks, few outside



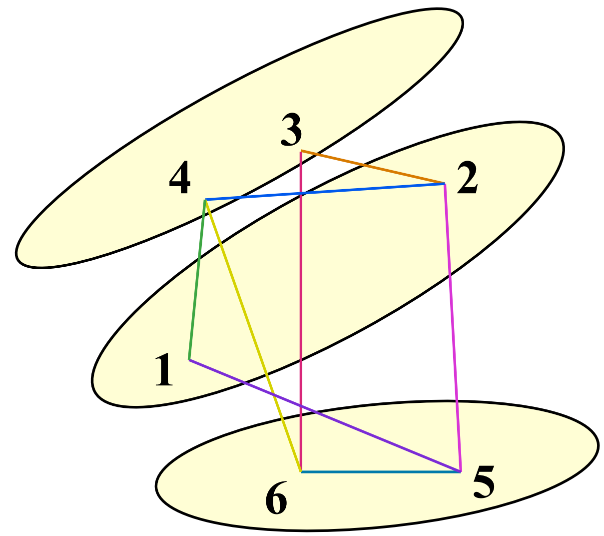
Goals of Reordering

- Performance goals
  - balance load (how is load measured?).
    - Approx equal number of nonzeros (not necessarily rows)
  - balance storage (how much does each processor store?).
    - Approx equal number of nonzeros
  - minimize communication (how much is communicated?).
    - Minimize nonzeros outside diagonal blocks
    - Related optimization criterion is to move nonzeros near diagonal
  - improve register and cache re-use
    - Group nonzeros in small vertical blocks so source (x) elements loaded into cache or registers may be reused (temporal locality)
    - Group nonzeros in small horizontal blocks so nearby source (x) elements in the cache may be used (spatial locality)
- Other algorithms reorder rows/columns for other reasons
  - Reduce # nonzeros in matrix after Gaussian elimination
  - Improve numerical stability

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



- Edges in the graph are nonzero in the matrix: here the matrix is symmetric (edges are unordered) and weights are equal (1)
- If divided over 3 procs, there are 14 nonzeros outside the diagonal blocks, which represent the 7 (bidirectional) edges

Summary: Common Problems

- Load Balancing
  - Statically - Graph partitioning
    - Discrete event simulation
    - 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
- Fast Particle Methods
  - $O(n \log n)$ instead of $O(n^2)$

What do commercial and CSE applications have in common?

Motif/Dwarf: Common Computational Methods

(Red Hot → Blue Cool)