Lecture 4: Locality and parallelism in simulation I

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Logistics

Distributed memory machines

- Each node has local memory
  - ... and no direct access to memory on other nodes
- Nodes communicate via network interface
- Example: our cluster!
- Or almost any other current multi-node machine

Message-passing programming model

- Collection of named processes
- Data is *partitioned*
- Communication by send/receive of explicit message
- Lingua franca: MPI (Message Passing Interface)

Message passing dot product: v1

Processor 1:

1. Partial sum s1
2. Send s1 to P2
3. Receive s2 from P2
4. s = s1 + s2

Processor 2:

1. Partial sum s2
2. Send s2 to P1
3. Receive s1 from P1
4. s = s1 + s2

What could go wrong? Think of phones vs letters...

Message passing dot product: v1

Processor 1:

1. Partial sum s1
2. Send s1 to P2
3. Receive s2 from P2
4. s = s1 + s2

Processor 2:

1. Partial sum s2
2. Receive s1 from P1
3. Send s2 to P1
4. s = s1 + s2

Better, but what if more than two processors?

MPI: the de facto standard

- Pro: *Portability*
- Con: least-common-denominator for mid 80s

The “assembly language” (or C?) of parallelism...
but, alas, assembly language can be high performance.

The story so far

- Even *serial* performance is a complicated function of the underlying architecture and memory system. We need to understand these effects in order to design data structures and algorithms that are fast on modern machines. Good serial performance is the basis for good parallel performance.
- *Parallel* performance is additionally complicated by communication and synchronization overheads, and by how much parallel work is available. If a small fraction of the work is completely serial, Amdahl's law bounds the speedup, independent of the number of processors.
- We have discussed serial architecture and some of the basics of parallel machine models and programming models.
- Now we want to describe how to think about the shape of parallel algorithms for some scientific applications.

Reminder: what do we want?

- High-level: solve big problems fast
- Start with good *serial* performance
- Given p processors, could then ask for
  - Good *speedup*: p^{-1} times serial time
  - Good *scaled speedup*: p times the work in same time
- Easiest to get good speedup from cruddy serial code!

Parallelism and locality

- Real world exhibits *parallelism* and *locality*
  - Particles, people, etc function independently
  - Nearby objects interact more strongly than distant ones
  - Can often simplify dependence on distant objects
- Can get more parallelism / locality through model
  - Limited range of dependency between adjacent time steps
  - Can neglect or approximate far-field effects
- Often get parallism at multiple levels
  - Hierarchical circuit simulation
  - Interacting models for climate
  - Parallelizing individual experiments in MC or optimization

Basic styles of simulation

- Discrete event systems (continuous or discrete time)
  - Game of life, logic-level circuit simulation
  - Network simulation
- Particle systems (our homework)
  - Billiards, electrons, galaxies, ...
  - Ants, cars, ...?
- Lumped parameter models (ODEs)
  - Circuits (SPICE), structures, chemical kinetics
- Distributed parameter models (PDEs / integral equations)
  - Heat, elasticity, electrostatics, ...

Often more than one type of simulation appropriate.
Sometimes more than one at a time!

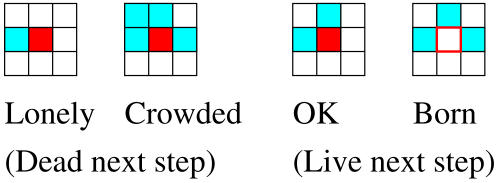
Discrete events

Basic setup:

- Finite set of variables, updated via transition function
- *Synchronous* case: finite state machine
- *Asynchronous* case: event-driven simulation
- Synchronous example: Game of Life

Nice starting point — no discretization concerns!

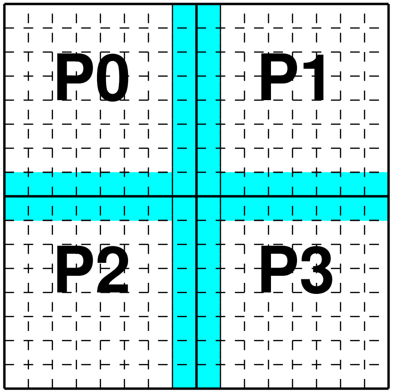
Game of Life



Game of Life (John Conway):

1. Live cell dies with < 2 live neighbors
2. Live cell dies with > 3 live neighbors
3. Live cell lives with 2–3 live neighbors
4. Dead cell becomes live with exactly 3 live neighbors

Game of Life



Easy to parallelize by *domain decomposition*.

- Update work involves *volume* of subdomains
- Communication per step on *surface* (cyan)

Game of Life: Pioneers and Settlers

What if pattern is “dilute”?

- Few or no live cells at surface at each step
- Think of live cell at a surface as an “event”
- Only communicate events!
  - This is *asynchronous*
  - Harder with message passing — when do you receive?

Asynchronous Game of Life

How do we manage events?

- Could be *speculative* — assume no communication across boundary for many steps, back up if needed
- Or *conservative* — wait whenever communication possible
  - possible $\not\equiv$ guaranteed!
  - Deadlock: everyone waits for everyone else to send data
  - Can get around this with NULL messages

How do we manage load balance?

- No need to simulate quiescent parts of the game!
- Maybe dynamically assign smaller blocks to processors?

Particle simulation

Particles move via Newton ($F = ma$), with

- External forces: ambient gravity, currents, etc.
- Local forces: collisions, Van der Waals ($1/r^6$), etc.
- Far-field forces: gravity and electrostatics ($1/r^2$), etc.
  - Simple approximations often apply (Saint-Venant)

A forced example

Example force:

$$f_i = \sum_j G m_i m_j \frac{(x_j - x_i)}{r_{ij}^3} \left(1 - \left(\frac{a}{r_{ij}}\right)^4\right), \qquad r_{ij} = \|x_i - x_j\|$$

- Long-range attractive force (r^{-2})
- Short-range repulsive force (r^{-6})
- Go from attraction to repulsion at radius a

A simple serial simulation

In MATLAB, we can write

```
npts = 100;
t = linspace(0, tfinal, npts);
[tout, xyv] = ode113(@fnbody, ...
                    t, [x; v], [], m, g);
xout = xyv(:,1:length(x))';
```

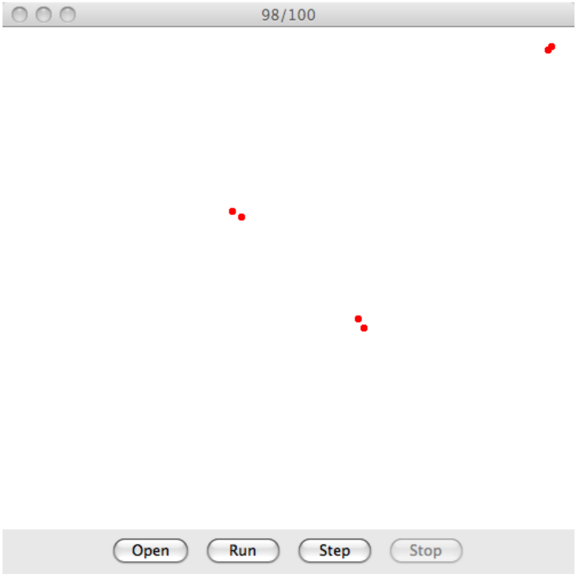
... but I can't call `ode113` in C in parallel (or can I?)

A simple serial simulation

Maybe a fixed step leapfrog will do?

```
npts = 100;
steps_per_pt = 10;
dt = tfinal/(steps_per_pt*(npts-1));
xout = zeros(2*n, npts);
xout(:,1) = x;
for i = 1:npts-1
  for ii = 1:steps_per_pt
    x = x + v*dt;
    a = fnbody(x, m, g);
    v = v + a*dt;
  end
  xout(:,i+1) = x;
end
```

Plotting particles



Pondering particles

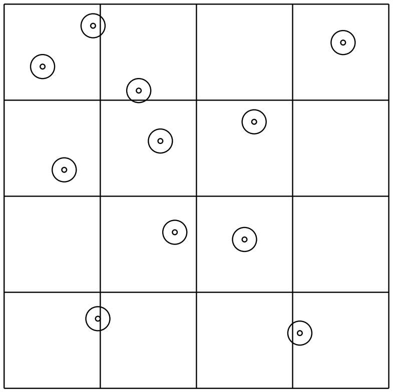
- Where do particles “live” (esp. in distributed memory)?
  - Decompose in space? By particle number?
  - What about clumping?
- How are long-range force computations organized?
- How are short-range force computations organized?
- How is force computation load balanced?
- What are the boundary conditions?
- How are potential singularities handled?
- What integrator is used? What step control?

External forces

Simplest case: no particle interactions.

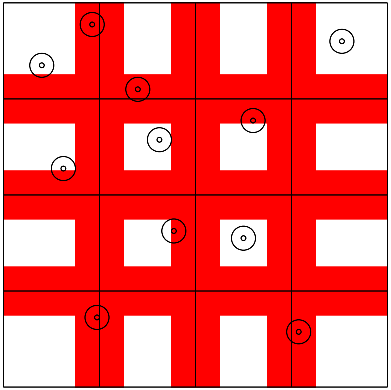
- Embarrassingly parallel (like Monte Carlo)!
- Could just split particles evenly across processors
- Is it that easy?
  - Maybe some trajectories need short time steps?
  - Even with MC, load balance may not be entirely trivial.

Local forces



- Simplest all-pairs check is $O(n^2)$ (expensive)
- Or only check close pairs (via binning, quadtrees?)
- Communication required for pairs checked
- Usual model: domain decomposition

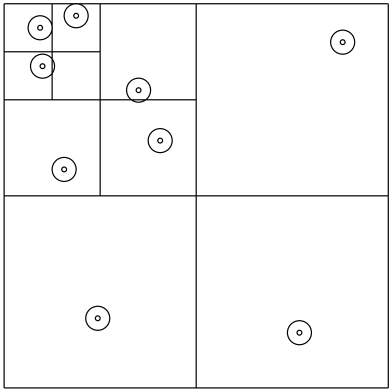
Local forces: Communication



Minimize communication:

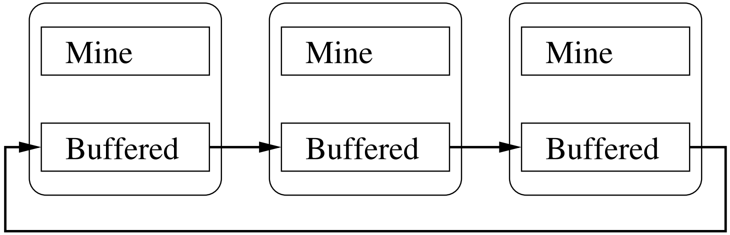
- Send particles that might affect a neighbor “soon”
- Trade extra computation against communication
- Want low surface area-to-volume ratios on domains

Local forces: Load balance



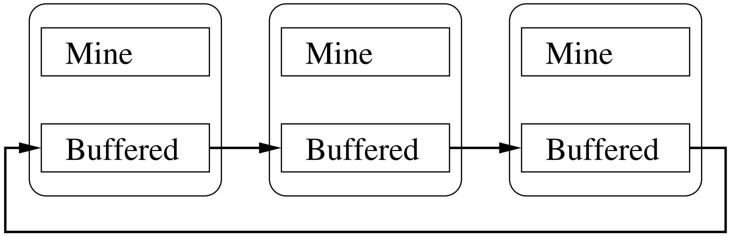
- Are particles evenly distributed?
- Do particles remain evenly distributed?
- Can divide space unevenly (e.g. quadtree/octtree)

Far-field forces



- Every particle affects every other particle
- All-to-all communication required
  - Overlap communication with computation
  - Poor memory scaling if everyone keeps everything!
- Idea: pass particles in a round-robin manner

Passing particles for far-field forces



```
copy local particles to current buf
for phase = 1:p
  send current buf to rank+1 (mod p)
  recv next buf from rank-1 (mod p)
  interact local particles with current buf
  swap current buf with next buf
end
```

Passing particles for far-field forces

Suppose $n = N/p$ particles in buffer. At each phase

$$t_{\text{comm}} \approx \alpha + \beta n$$
$$t_{\text{comp}} \approx \gamma n^2$$

So we can mask communication with computation if

$$n \geq \frac{1}{2\gamma}\left(\beta + \sqrt{\beta^2 + 4\alpha\gamma}\right) > \frac{\beta}{\gamma}$$

More efficient serial code
$\implies$ larger n needed to mask communication!
$\implies$ worse speed-up as p gets larger (fixed N)
but scaled speed-up (n fixed) remains unchanged.

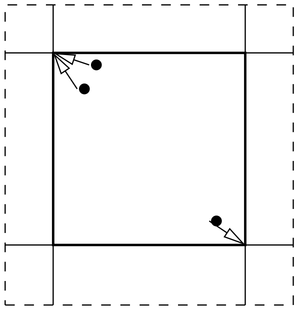
This analysis neglects overhead term in LogP.

Far-field forces: particle-mesh methods

Consider r^{-2} electrostatic potential interaction

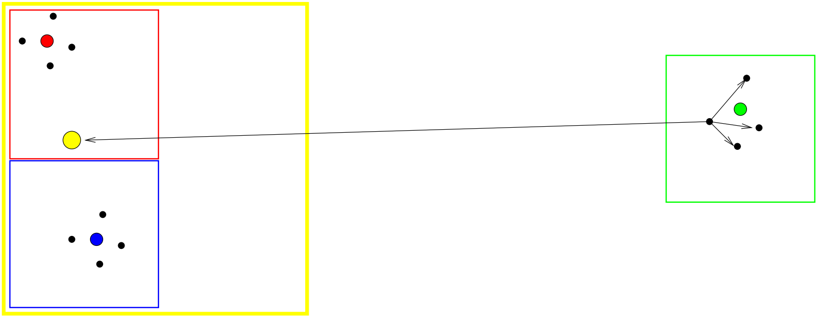
- Enough charges looks like a continuum!
- Poisson equation maps charge distribution to potential
- Use fast Poisson solvers for regular grids (FFT, multigrid)
- Approximation depends on mesh and particle density
- Can clean up leading part of approximation error

Far-field forces: particle-mesh methods



- Map particles to mesh points (multiple strategies)
- Solve potential PDE on mesh
- Interpolate potential to particles
- Add correction term – acts like local force

Far-field forces: tree methods



- Distance simplifies things
  - Andromeda looks like a point mass from here?
- Build a tree, approximating descendants at each node
- Several variants: Barnes-Hut, FMM, Anderson’s method
- More on this later in the semester

Summary of particle example

- Model: Continuous motion of particles
  - Could be electrons, cars, whatever...
- Step through discretized time
- Local interactions
  - Relatively cheap
  - Load balance a pain
- All-pairs interactions
  - Obvious algorithm is expensive ($O(n^2)$)
  - Particle-mesh and tree-based algorithms help

An important special case of lumped/ODE models.