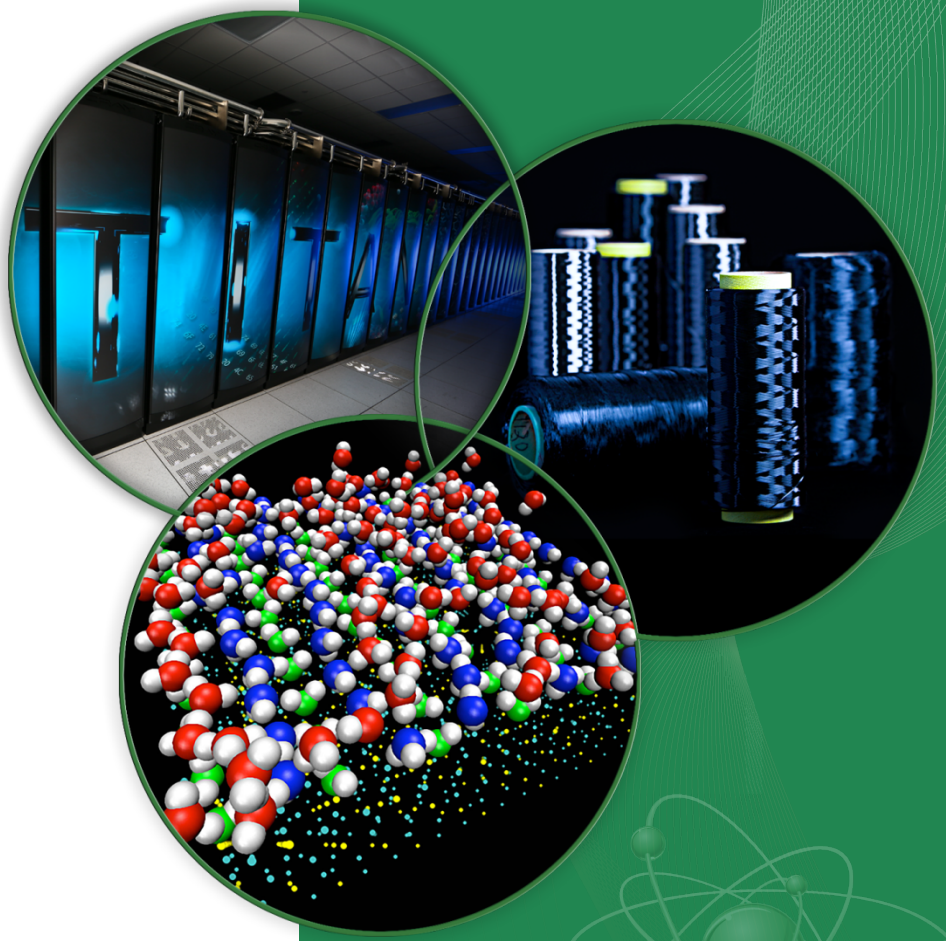
What is Parallelism?

Robert D. French

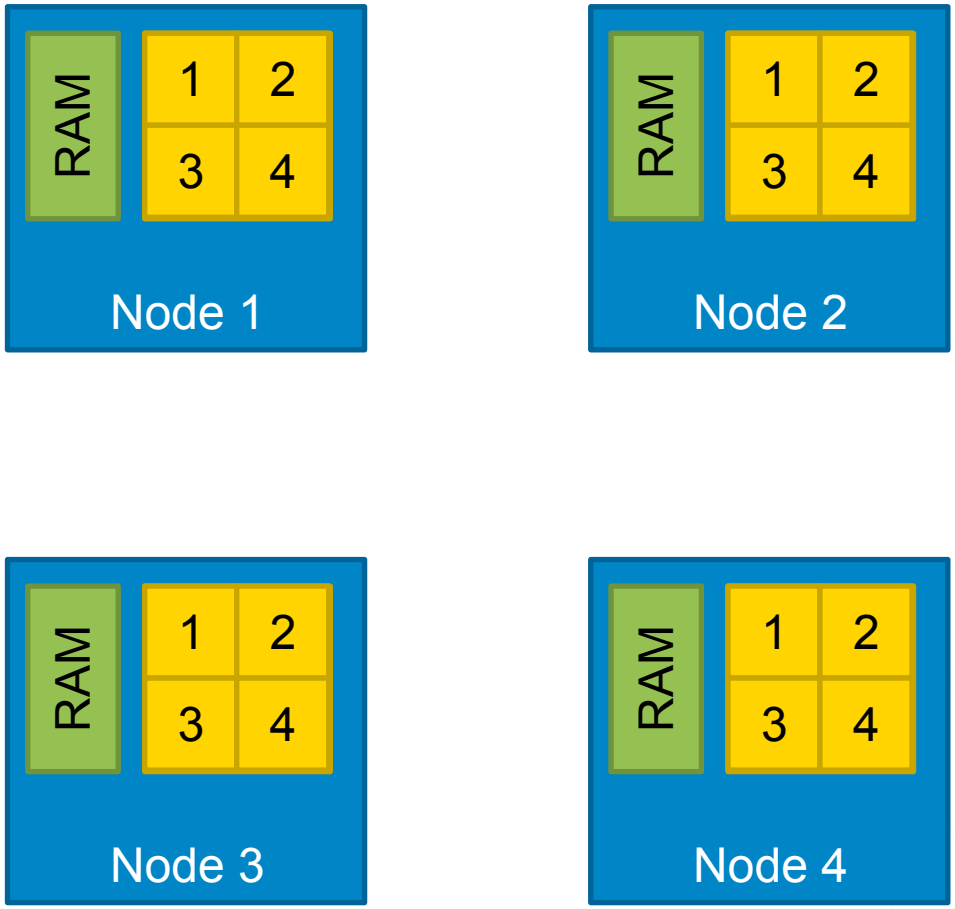
NCCS User Assistance



What is Parallelism

- Using multiple computers (or cores) to work on a single problem

What is Parallelism



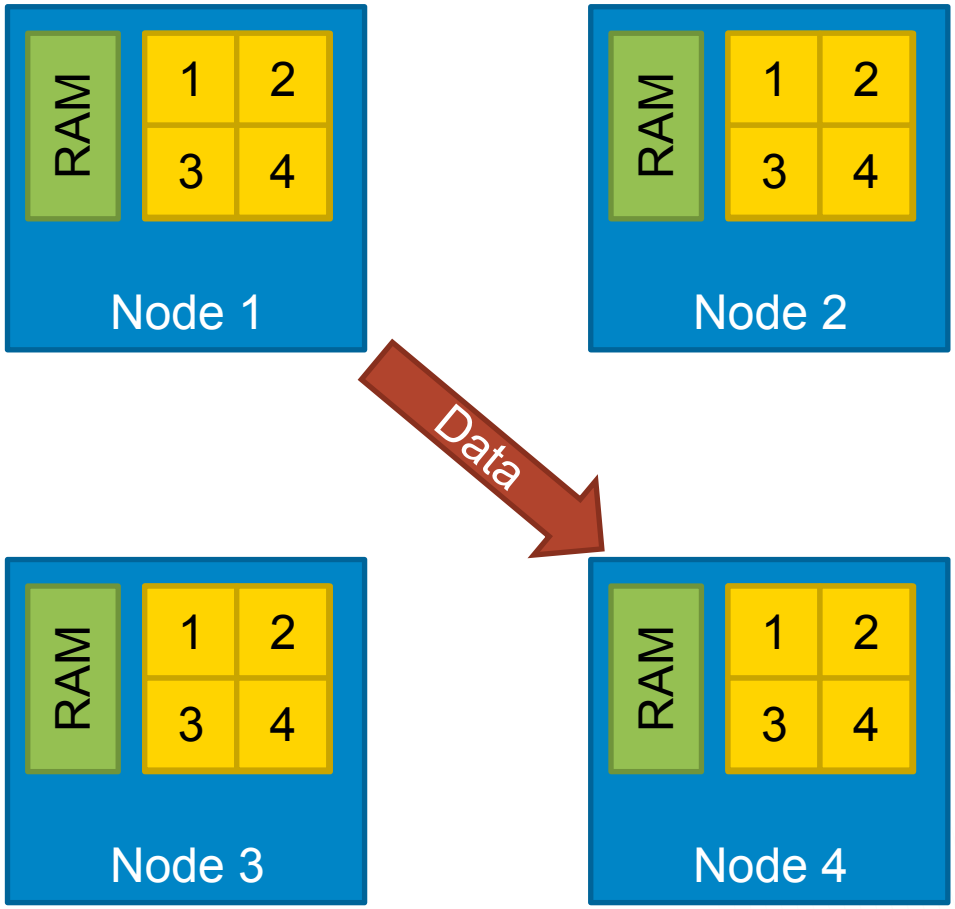
What is Parallelism

- Using multiple computers (or cores) to work on a single problem
- What kinds of problems actually need more than one computer?

What is Parallelism

- Using multiple computers (or cores) to work on a single problem
- What kinds of problems actually need more than one computer?
- What does it mean for computers to collaborate on the same problem?

What is Parallelism?



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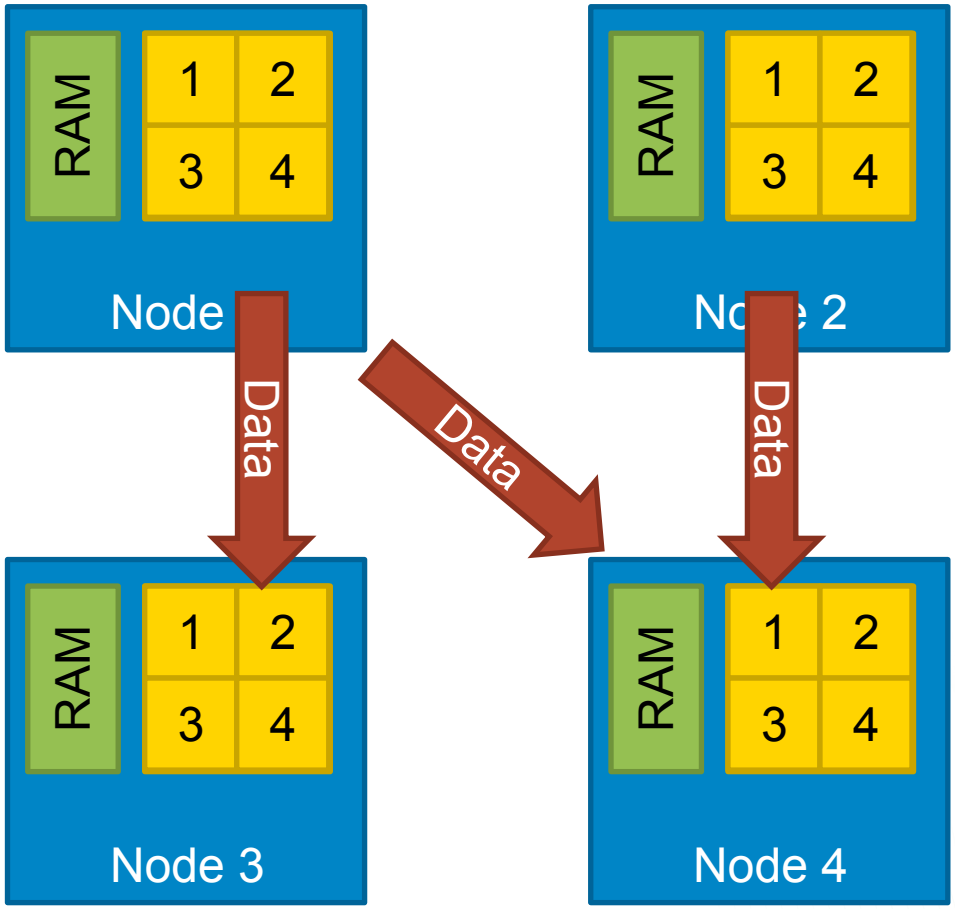

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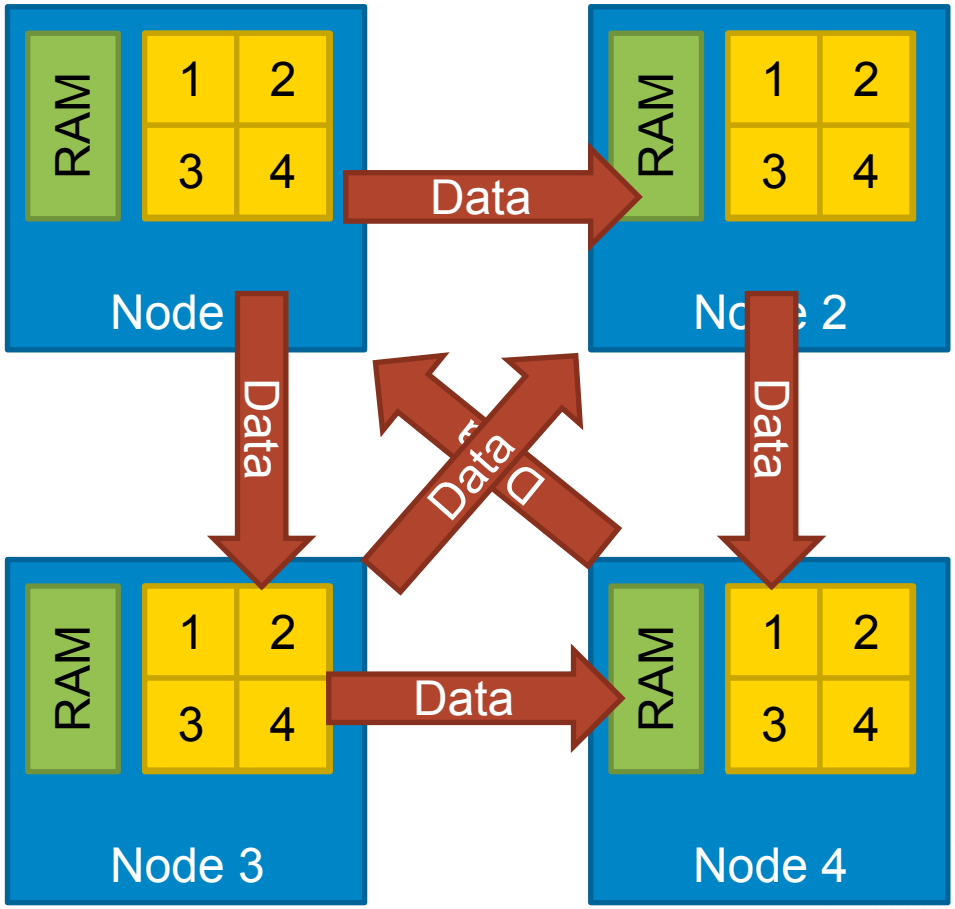

Smoothed Particle Hydrodynamics

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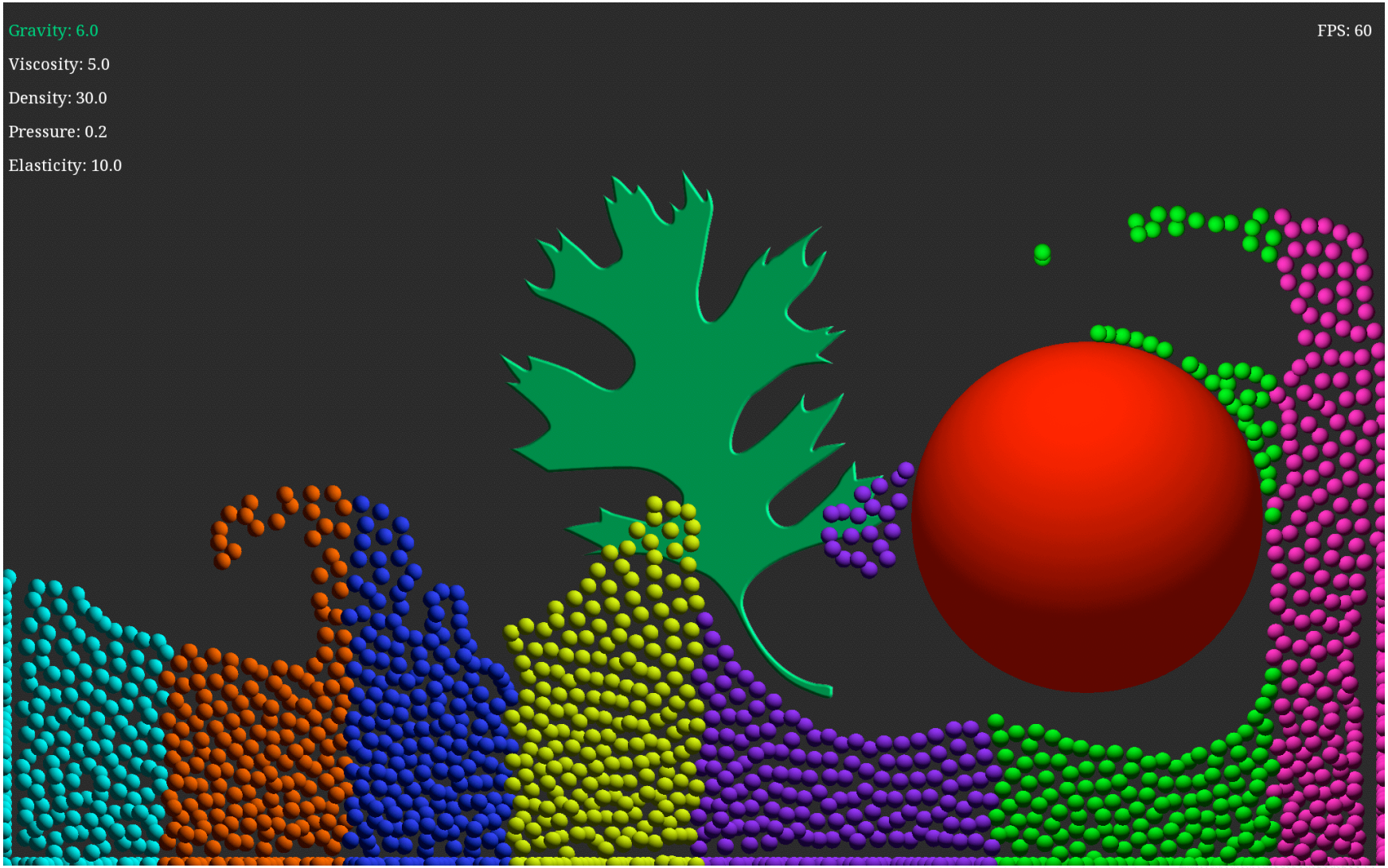
Smoothed Particle Hydrodynamics

- Understanding the motion of liquids
- Can answer the question:

“What does it look like when water sloshes around?”

Smoothed Particle Hydrodynamics



Smoothed Particle Hydrodynamics

- How the simulation works (*The Algorithm*)
  1. Calculate the force between each pair of particles
  2. Total force on each particle determines its *acceleration*
  3. Update particle *position*
  4. Proceed to next *time step*
- Real easy, right?

Smoothed Particle Hydrodynamics

- Say we have One Million Particles

Smoothed Particle Hydrodynamics

- Say we have One Million Particles
- That's one trillion force pairs to calculate.
- *That's a lot of work for one computer*
- This is why we need parallelism

Threads

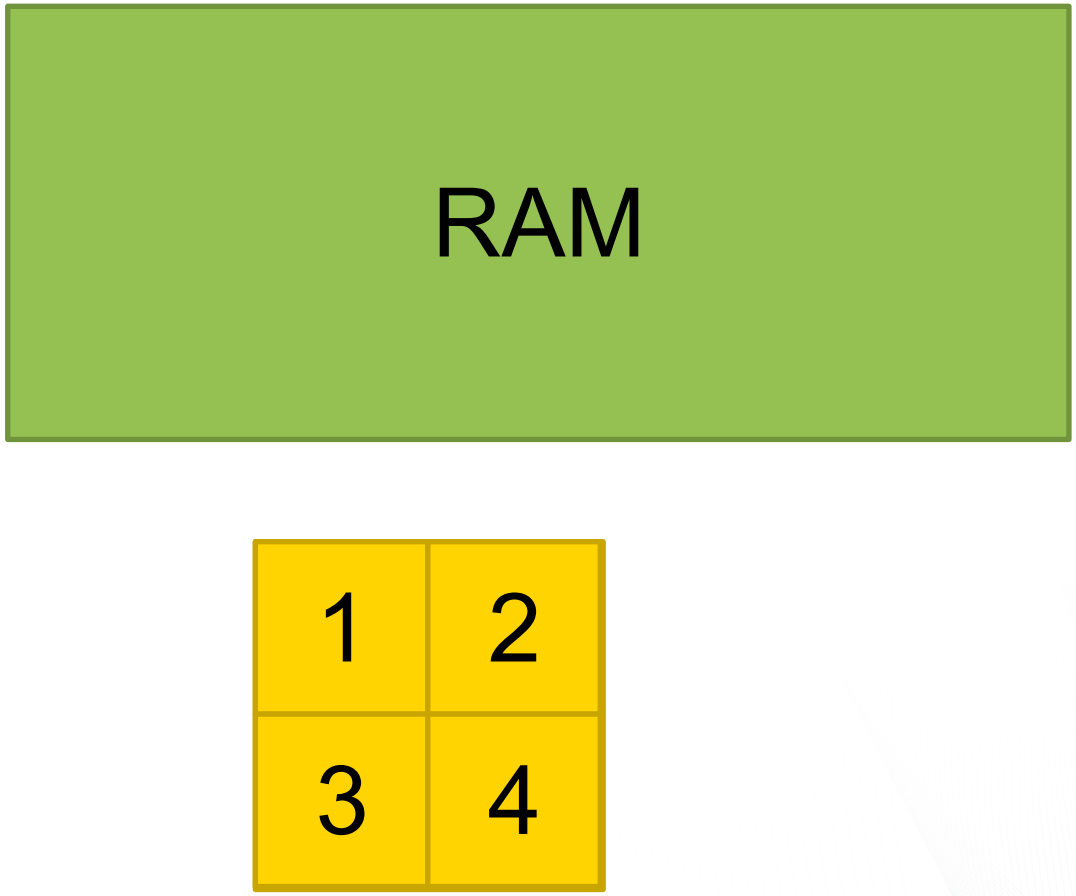
Threads

- Sometimes called “Shared Memory Parallelism”
- Parallelism using multi-core processors
- Can be used to divide work within a program
- Each thread can handle a subset of the force pair calculations

Threads

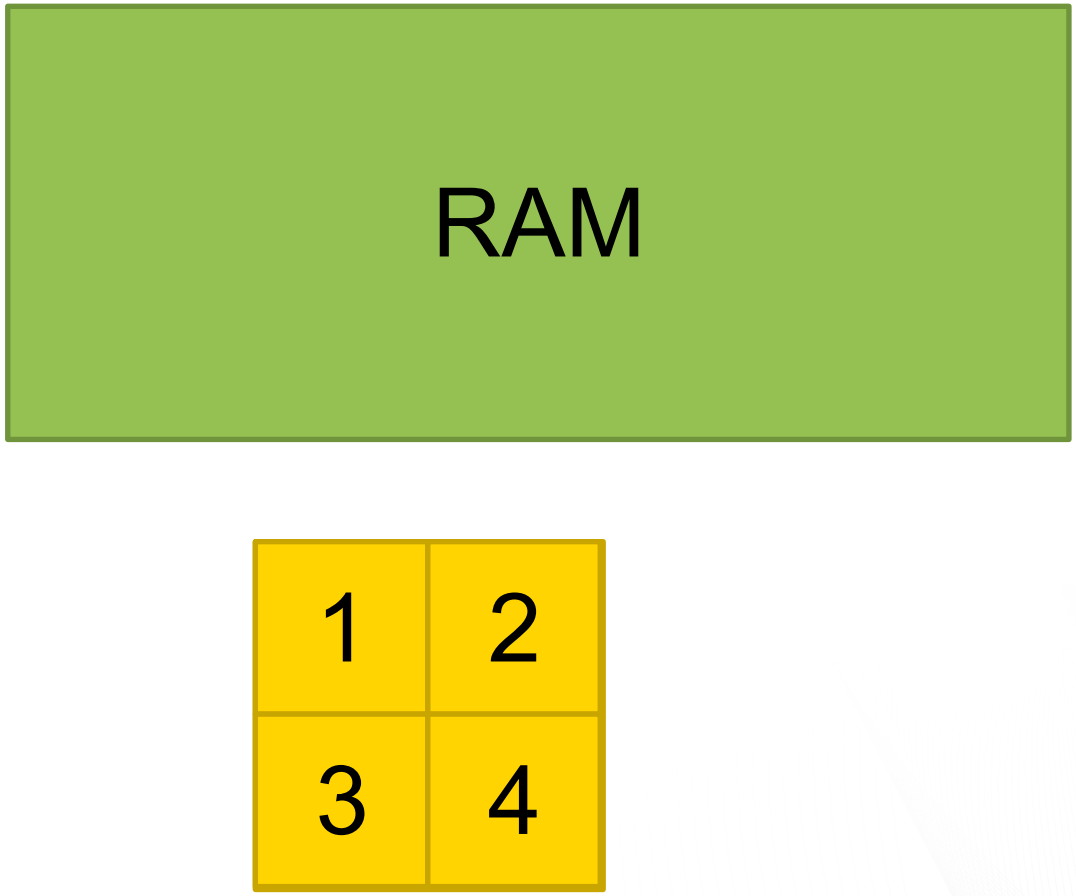
- In our SPH example, more cores means less work for each core
- A quad-core CPU can work about 4x than a single core CPU
- We need *threads* to manage this workload

Threads



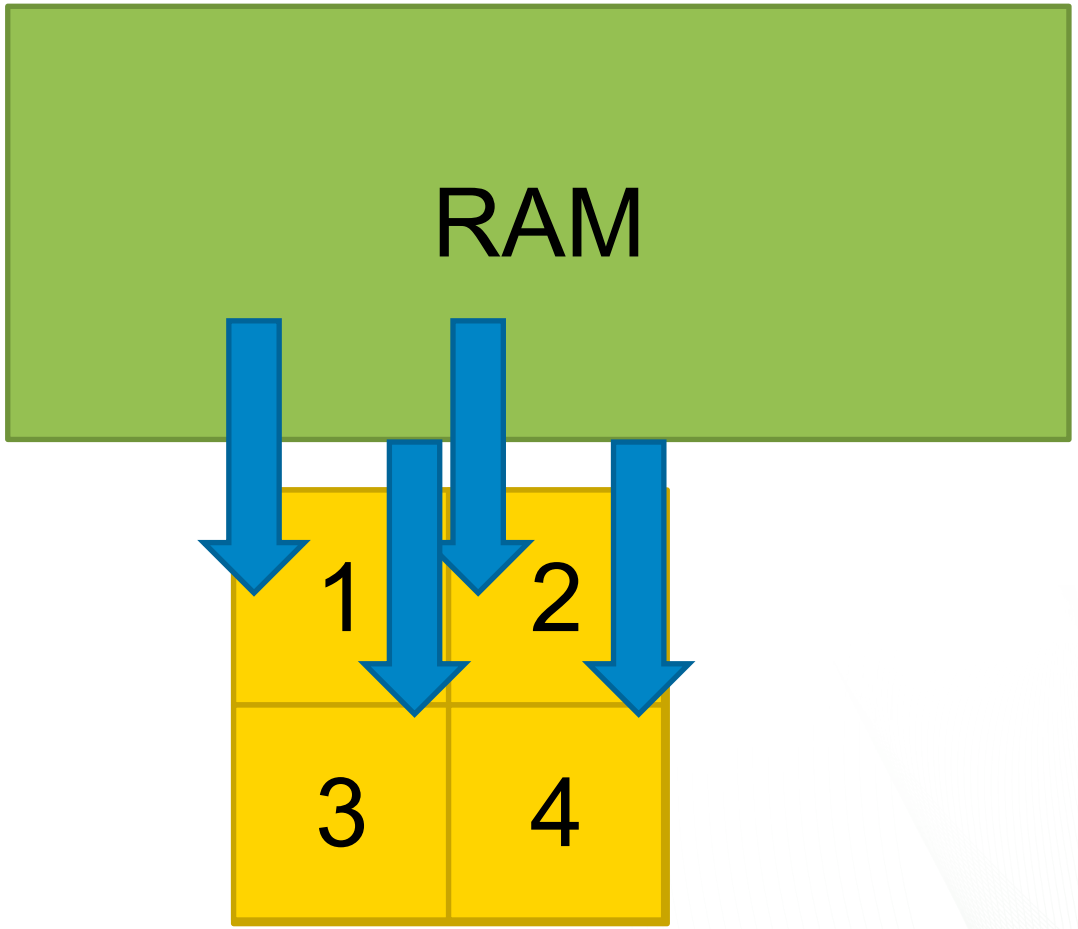
Threads

The particle information stays in RAM



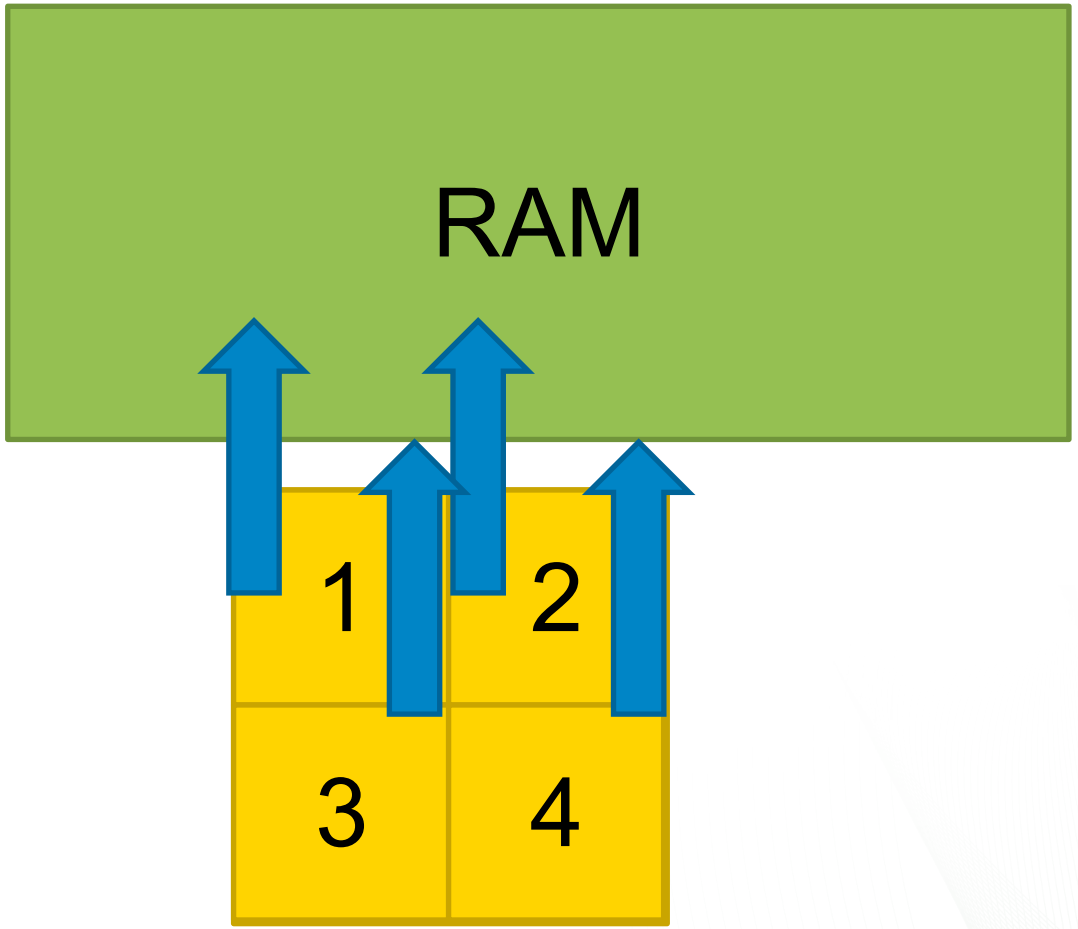
Threads

Particle Info moves to CPUs for Force Calculation



Threads

CPUs send updated positions back to RAM



Threads

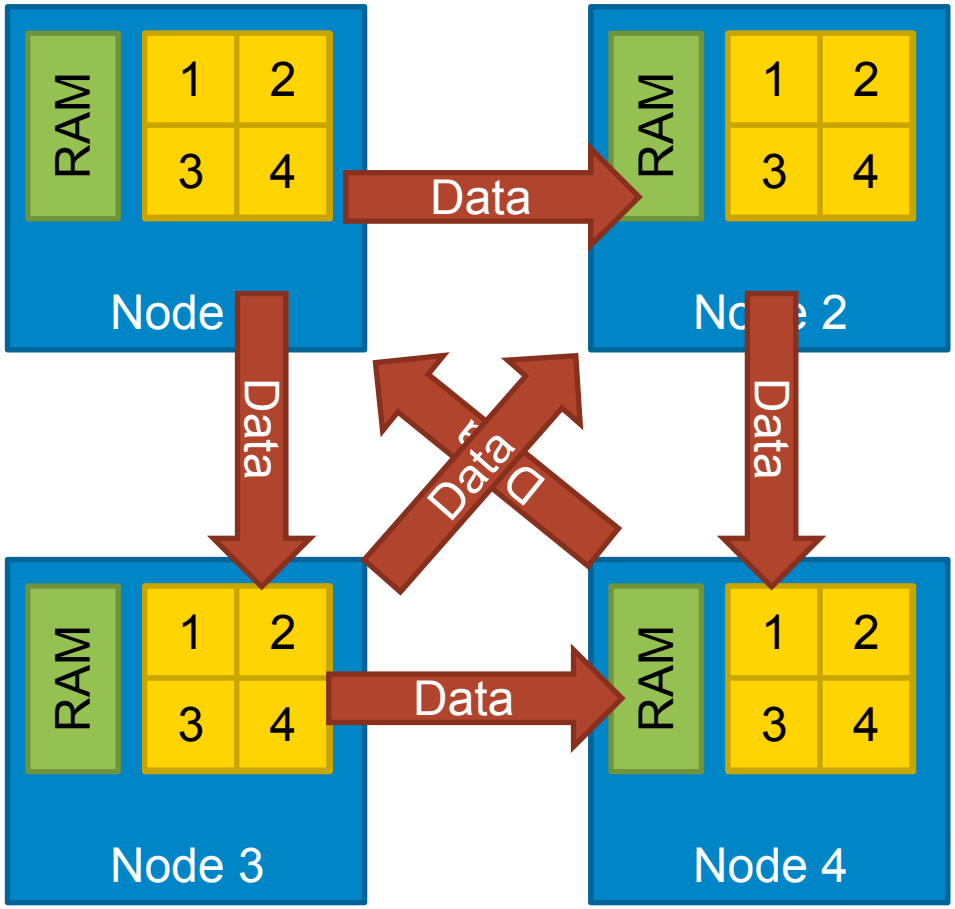
- Even still, 1 Trillion Force Pairs is a lot of work for 4 CPUs
- Is there any way to leverage the CPUs on other computers?

Ranks

Ranks

- Sometimes called “Distributed Memory Parallelism”
- Parallelism *between* nodes
- Makes use of multiple computers (Ranks)on a shared network
- Ranks communicate by *passing data* from one computer to another

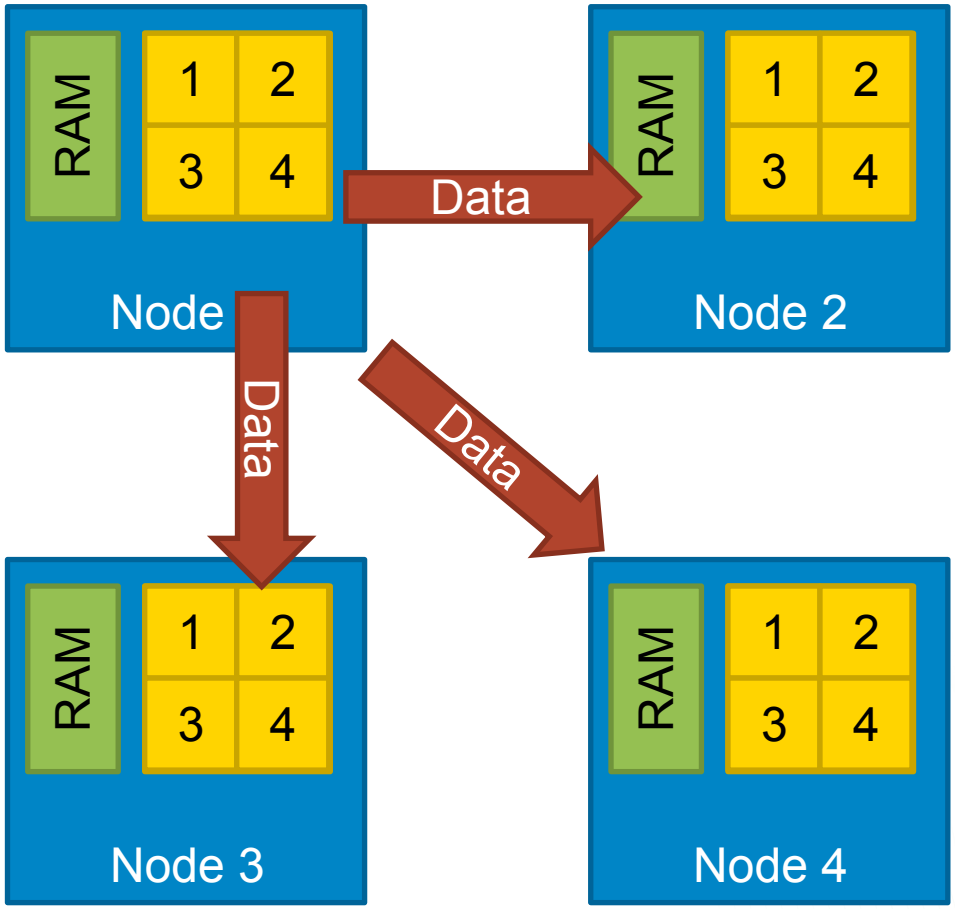
Ranks



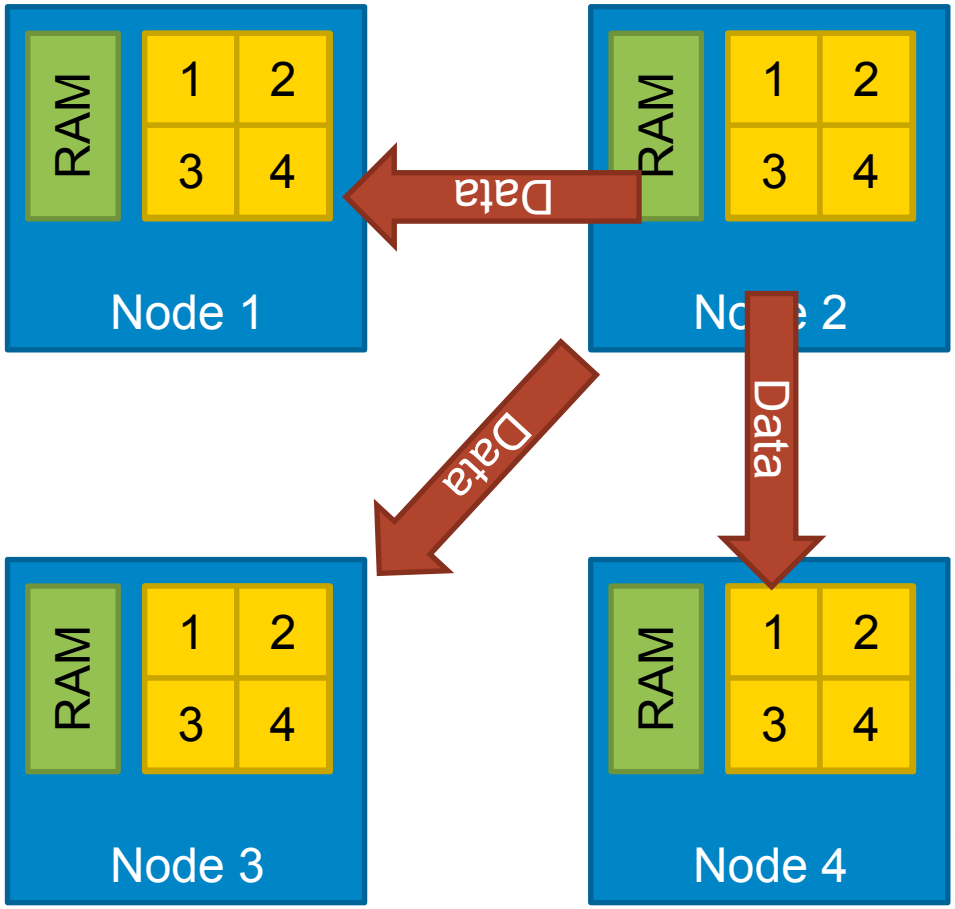
Ranks

- For SPH, this means sending particle information between ranks
- Each rank is responsible for computing the forces of one set of particles
- Once the positions are updated, this information must be shared with *every other rank*

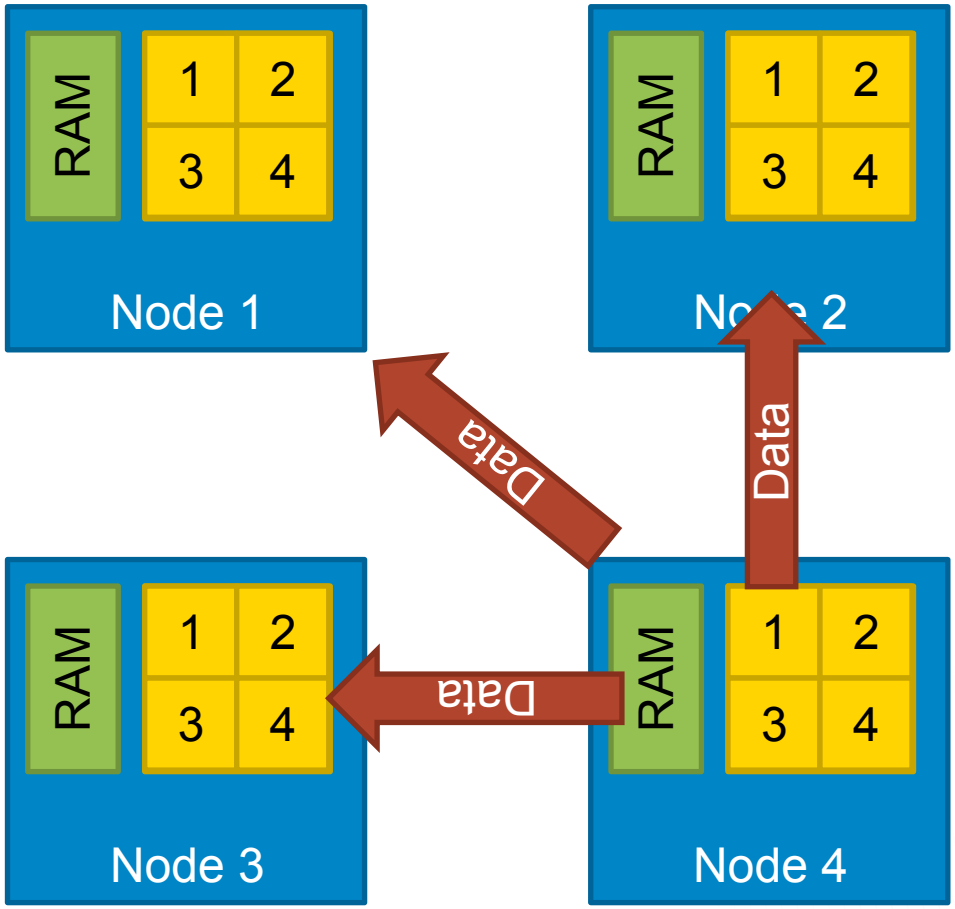
Ranks



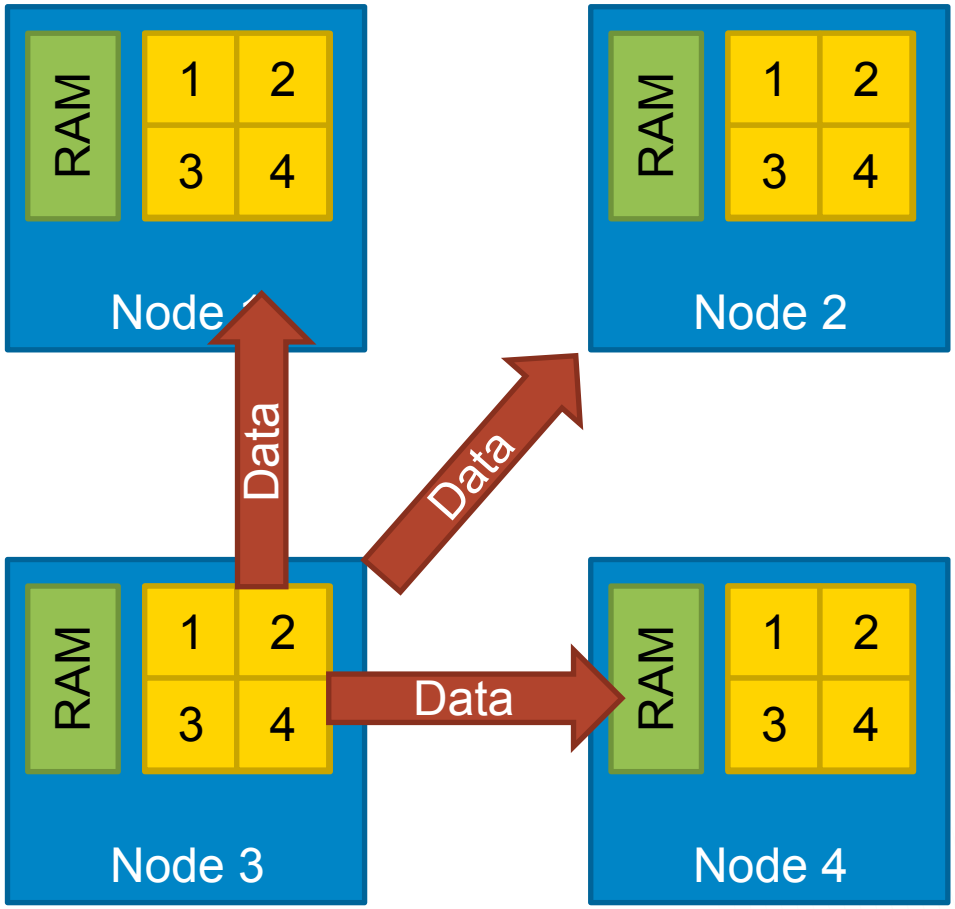
Ranks



Ranks



Ranks



Ranks

- Once every rank knows what every other rank has done, we can move to the next timestep

Quick Recap

Quick Recap

- We are simulating a liquid using 1 million particles
- We need to calculate the forces between *each pair* of particles
  - 1 million X 1 million = 1 trillion force pairs

Quick Recap

- Each of 4 *ranks* is responsible for 250,000 particles
  - That's 250 billion force pair calculations
- Each node has a quad-core CPU
- This means each rank can use 4 threads
  - That's 250 billion / 4 = 62.5 billion force pairs per core

Quick Recap

- Let's guesstimate that each force pair calculation requires 100 flops
  - A "flops" is a Floating Point Operation Per Second, or just an add or a multiply – basic arithmetic.
- So that's 100 basic arithmetic "moves" to calculate each force pair
- A top-dollar 3Ghz CPU can give us ~ 20 Gigaflops, or 20 billion arithmetic moves per second
- That's about 200 Million Force-pairs per core per second

Quick Recap

- I apologize for all the math, here's what I'm getting at:
  - At 200 Million force pairs per second, it will take each core more than 5 minutes to finish its 62.5 Billion force pairs
  - That's only for 1 timestep
  - If we need to simulate 10,000 timesteps, it will take more than a month

Accelerators

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Accelerators

- Normal CPUs are designed to do lots of different things:
  - PowerPoint
  - Email
  - Netflix
  - Etc…

Accelerators

- Graphics Processors (GPUs) are designed to be really awesome at just one thing:
  - Video Games

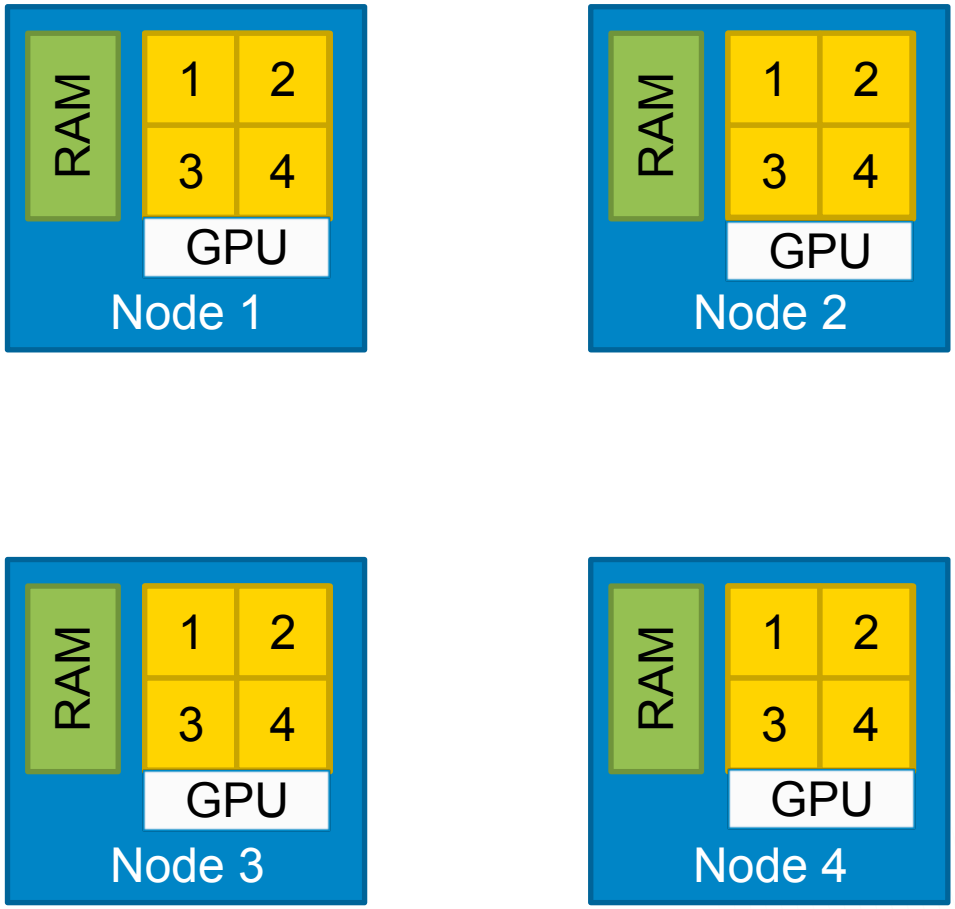
Accelerators

- Animating video games requires *tons and tons* of low-level arithmetic
  - Rotating landscapes, specular lighting, etc all make heavy use of trig functions
- Scientific simulations also require *tons and tons* of low-level arithmetic
  - Linear Algebra, Linear Algebra, Linear Algebra…

Accelerators

- Because GPUs were designed for video games, they offer heaping truckloads of *flops*
- The GPUs in Titan offer more than 1 Teraflop each
  - That's 1 Trillion arithmetic moves per second
- Let's put one of these in each of our 4 compute nodes

Accelerators



Accelerators

- Offloading the force-pair calculations to the GPU makes each node about 10x faster
- This means roughly 30s per timestep for 1 million particles
- Down to 3 days for a 10,000 timestep simulation.

Questions?

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