The Fast Multipole Algorithm vs. The Particle Mesh Ewald Method

Joshua Nelson

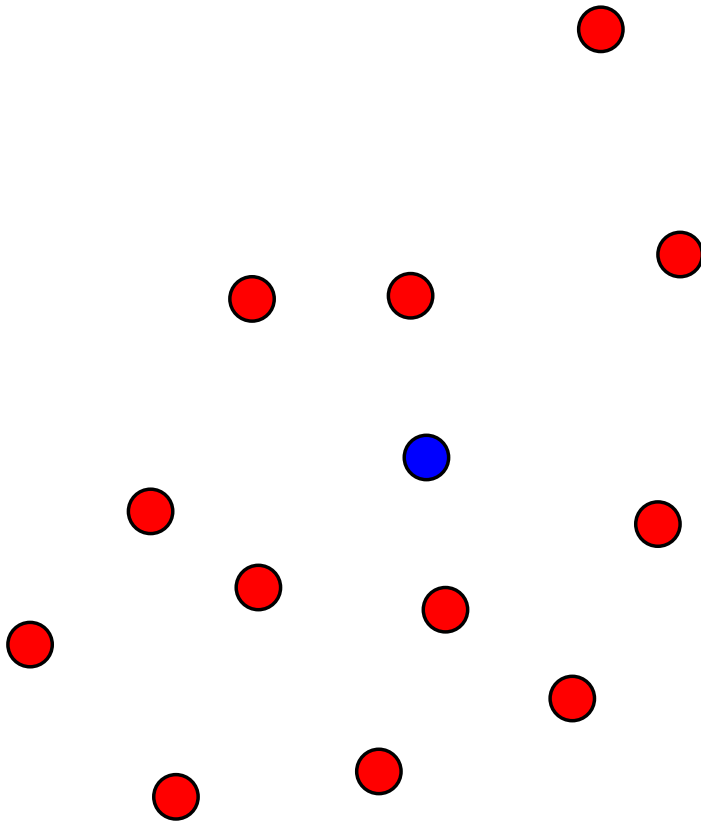
COMP3006 Research Project

August 15, 2012

The N-body problem

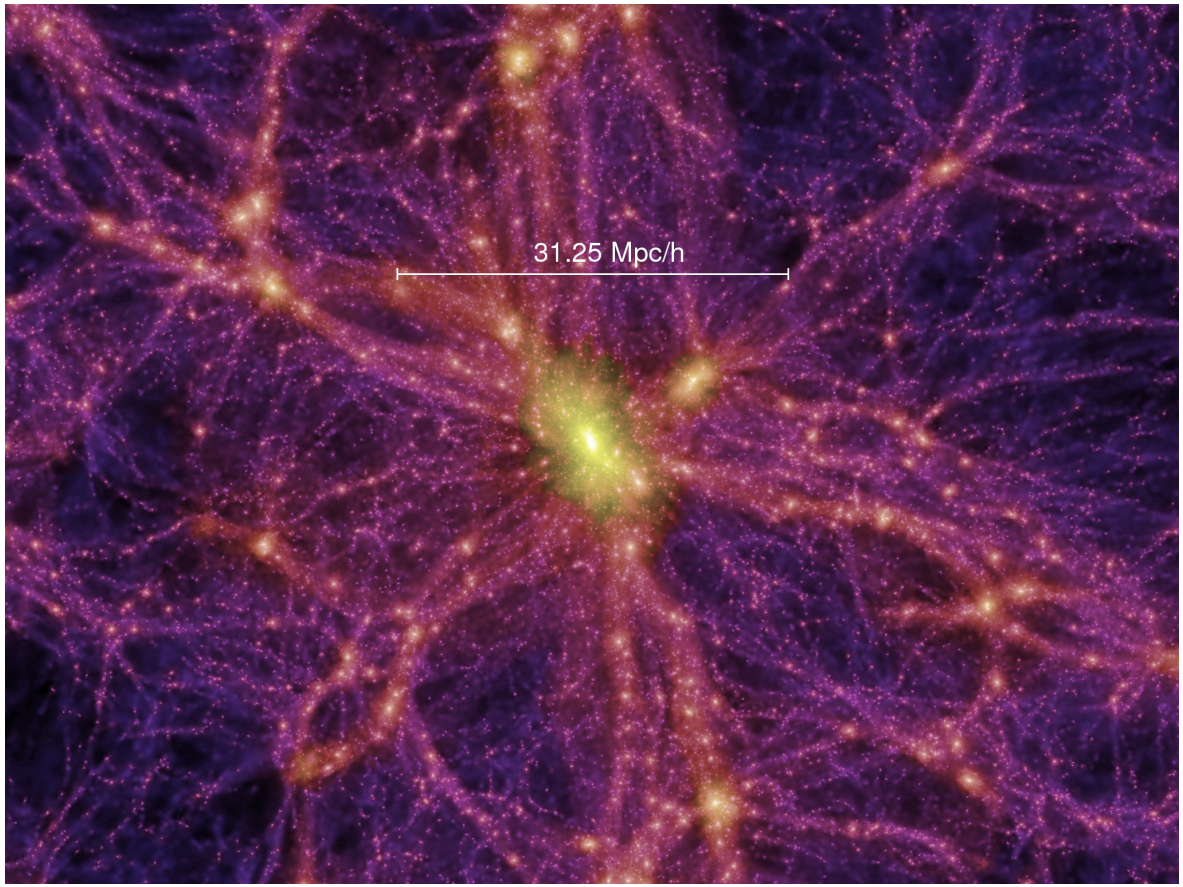
- The problem
  - N bodies in space - calculate some interaction between them

N-body diagram



Why is this useful?

The millenium run



Plasma physics simulation

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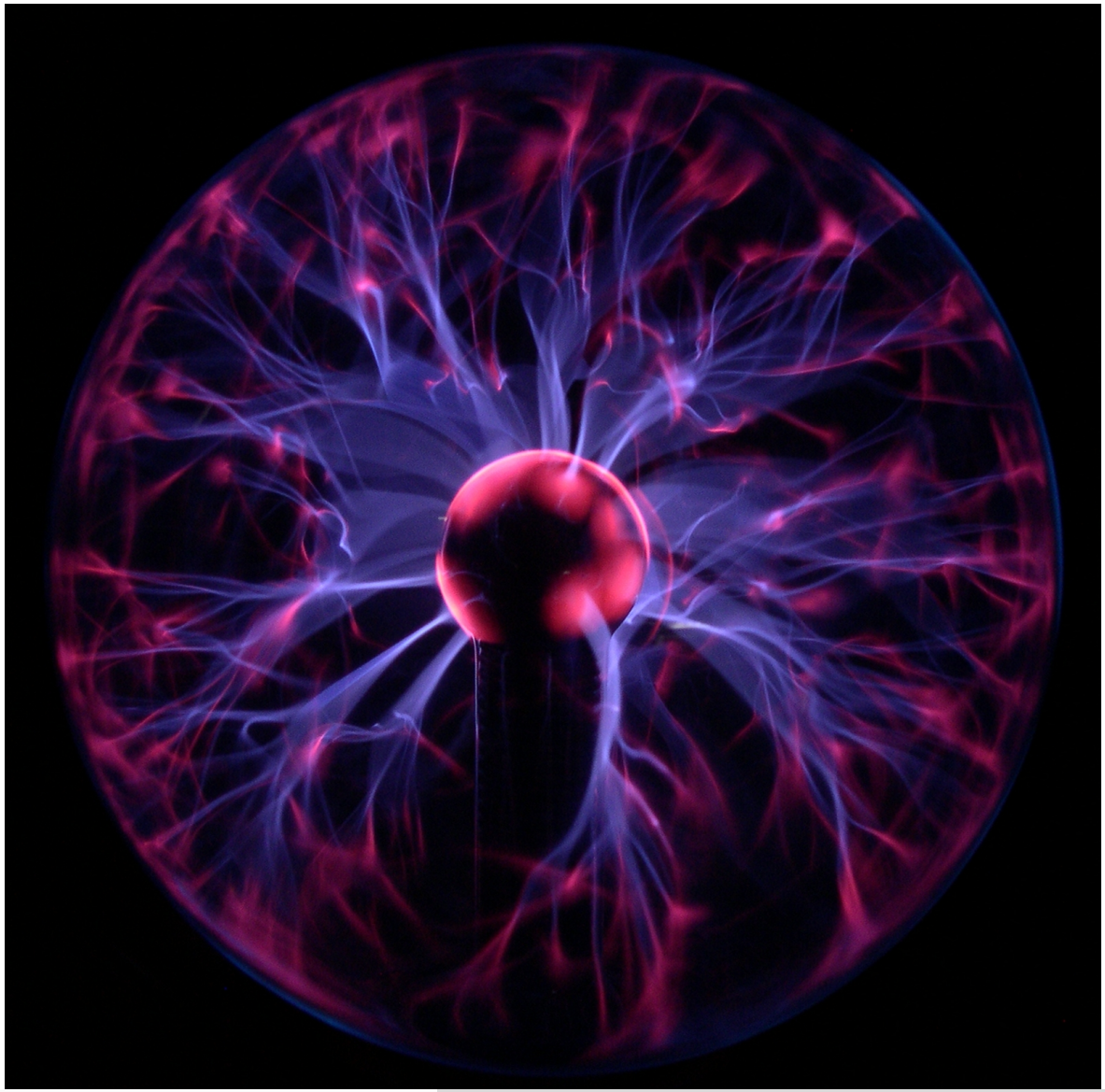
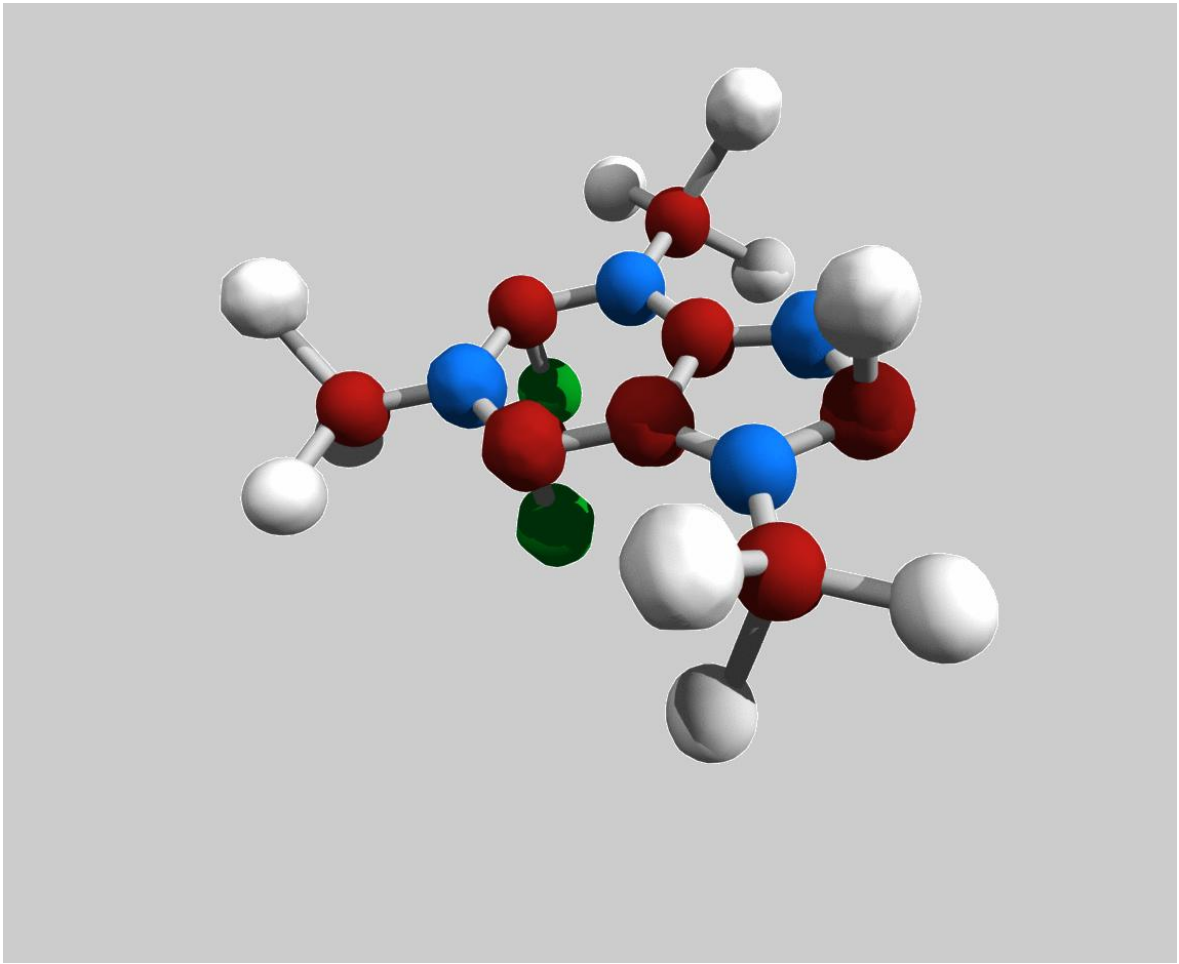
Motivation

Alternative solutions

My project



Molecular dynamics



The basic solution

- The naïve solution
  - Calculate interactions between every pair of bodies

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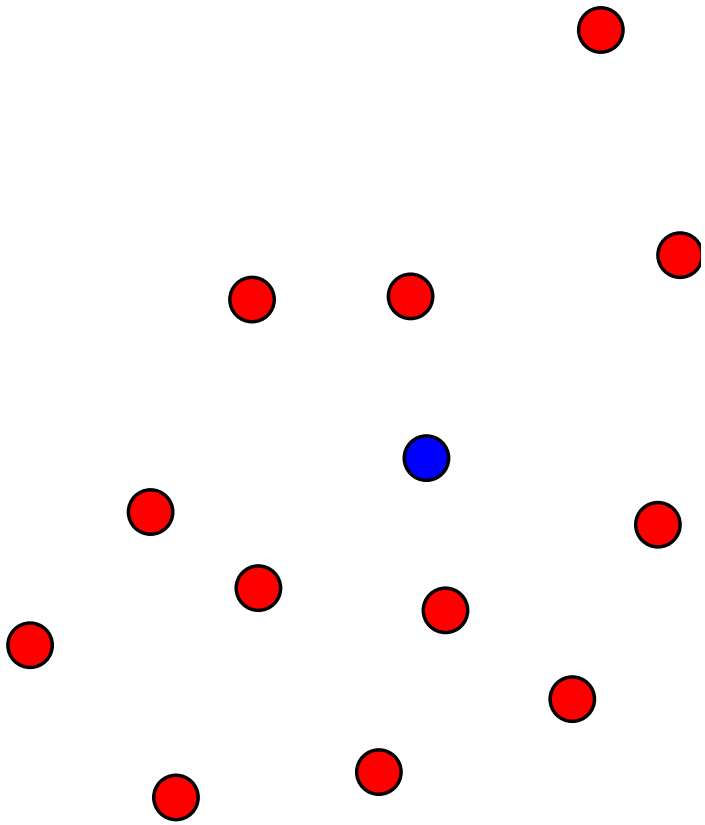
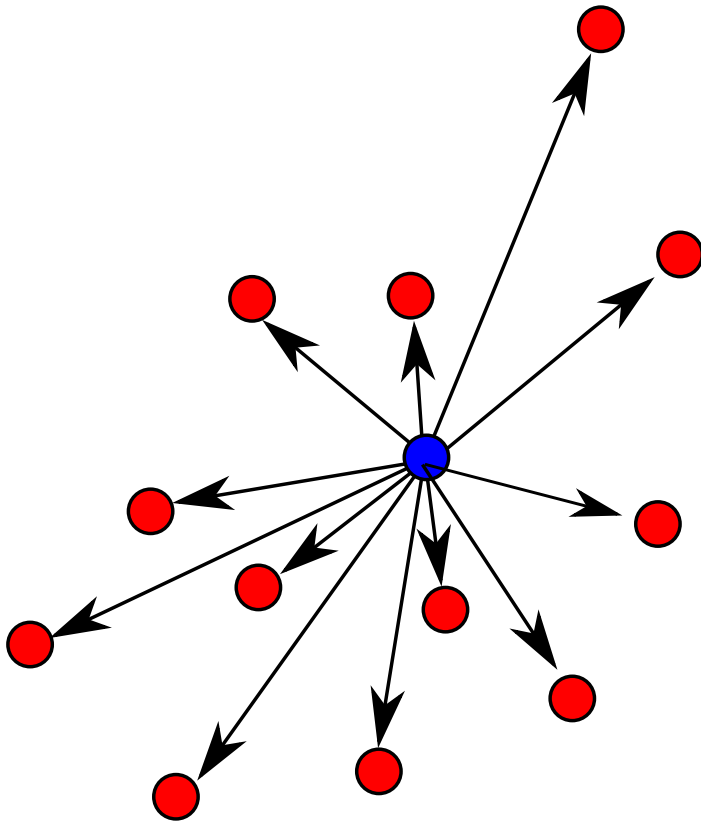
  - Calculate interactions between every pair of bodies
  - $O(n^2)$ complexity for N bodies.

N-body diagram



N-body diagram



Alternative solutions

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- Can this be done faster?

Alternative solutions

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- Can this be done faster?
  - The fast multipole method

Alternative solutions

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- Can this be done faster?
  - The fast multipole method
  - The particle mesh ewald method

The fast multipole method

- Form a grid and group particles in the grid

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The particle mesh ewald method

- We take the potential function, and apply a fast fourier transform over a discrete mesh, then interpolate

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- Turns out to be $O(n\log n)$

Comparing

- Which is more commonly used?

Comparing

- Which is more commonly used?
- Particle Mesh Ewald Method, $O(n\log n)$...

The scope

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My project

- Compare these two algorithms

The scope

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- Attempt to improve the algorithms and their implementations

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- Compare these two algorithms
- Attempt to improve the algorithms and their implementations
- Determine the point at which each algorithm is preferable