The Fast Multipole Algorithm vs. the Particle Mesh Ewald Method

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COMP3006 - Research Project

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The N body problem

Statement of the problem

Given N bodies that all interact with each other in some way, how do we efficiently calculate the effect each body has on every other body?

The N body problem

History

- First formally specified by Isaac Newton

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- No exact formula solution

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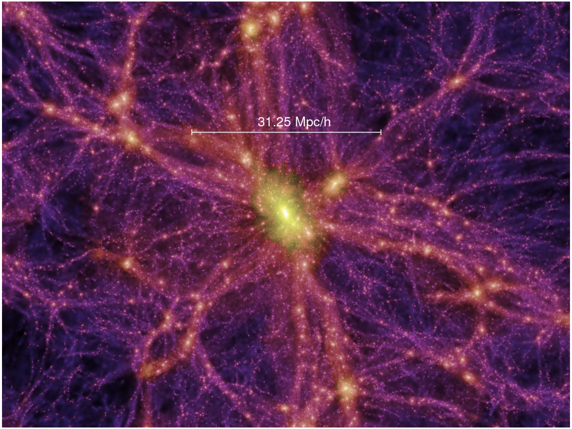
History

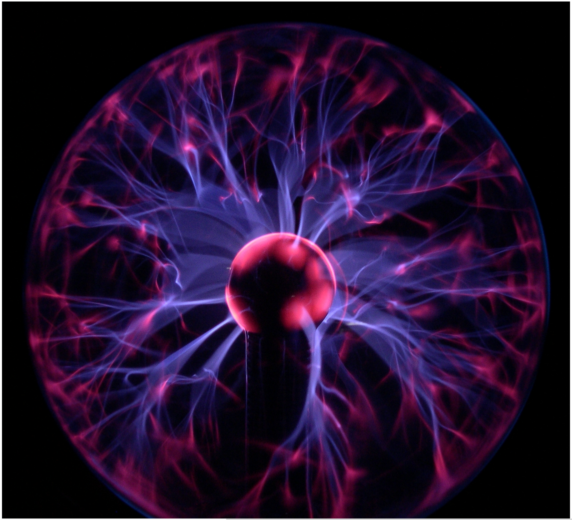
- First formally specified by Isaac Newton
- No exact formula solution
- Approximation methods devised

The N body problem
Applications



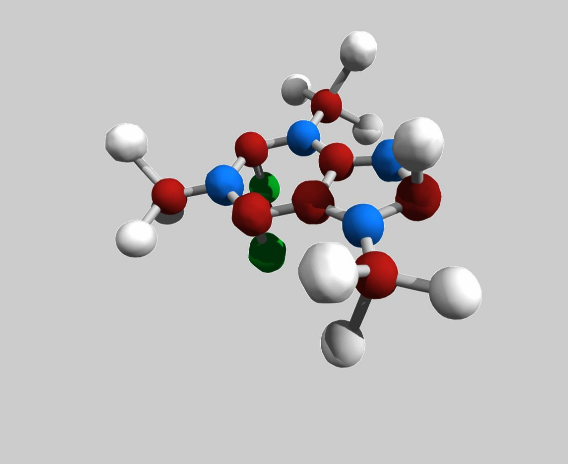
The N body problem

Applications



The N body problem

Applications



The basic solution
Algorithm

- Say that a particle at position r_i with charge q_i gives a potential Q at a particle r_j with charge q_j according to the formula

$$Q = \frac{q_i * q_j}{|r_i - r_j|}$$

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- Order $O(n^2)$ complexity.

The Fast Multipole Algorithm

Key components to the Fast Multipole Algorithm

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- The Mesh

The Fast Multipole Algorithm

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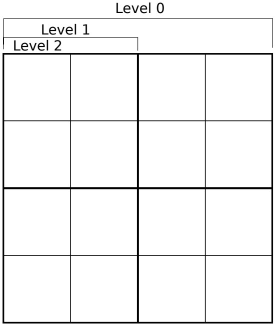
- The Mesh
- Multipole Expansions

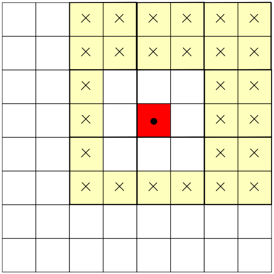
The Fast Multipole Algorithm

The Mesh

The Particle Mesh



Well separated cells



The Fast Multipole Algorithm

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The Fast Multipole Algorithm

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- Multipole Expansions: A series, centered on a particular cell, which can approximate the potential from the cell's particles near that cell
- Local Expansions: A series, centered on a particular cell, formed from a Multipole Expansion, which approximates the potential from within the cell at some distance away from that cell.

The Fast Multipole Algorithm

Aglorithm

- Form Multipole Expansions at the lowest mesh level

The Fast Multipole Algorithm

Aglorithm

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- Translate them to their parent's cells, combining the four children by summing them to form the parent's Multipole Expansion

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- Repeat the above for each level

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Aglorithm

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- Repeat the above for each level
- At the highest level, from the Multipole Expansion, form a Local Expansion.
- Translate this to children nodes, repeat to the lowest mesh level.

Basic structure of the Particle Mesh Ewald Method

- Interpolate particles to a grid

Particle Mesh Ewald Method

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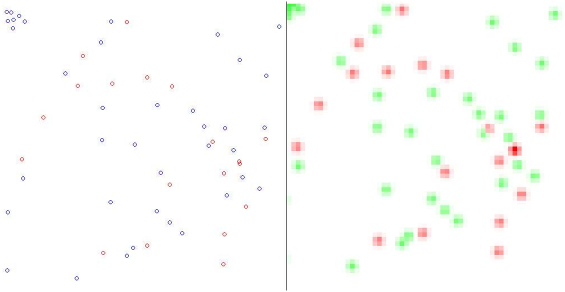

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Characteristics of the Particle Mesh Ewald Method

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