# 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

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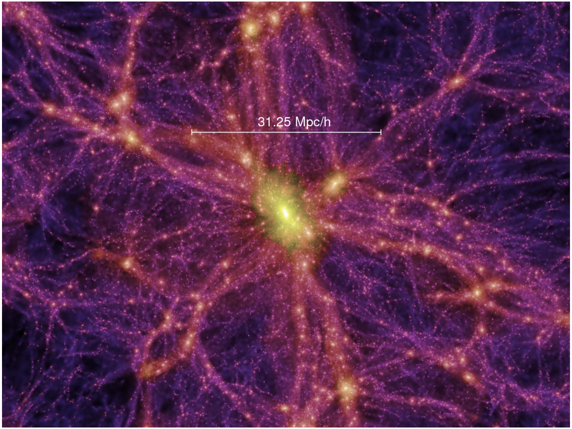
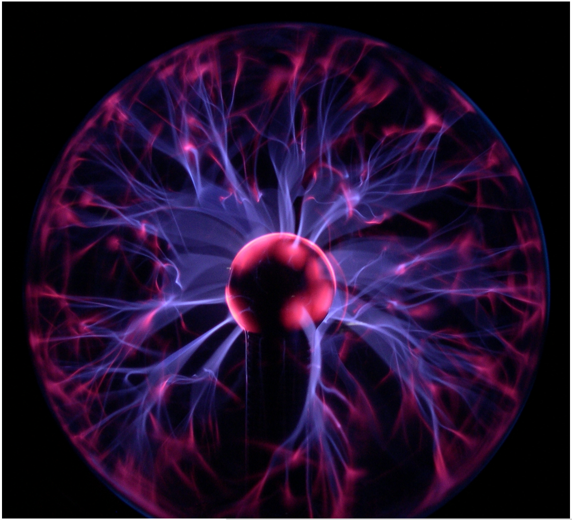
- Approximation methods devised

# The N body problem

## Applications



# The N body problem
## Applications



# The N body problem
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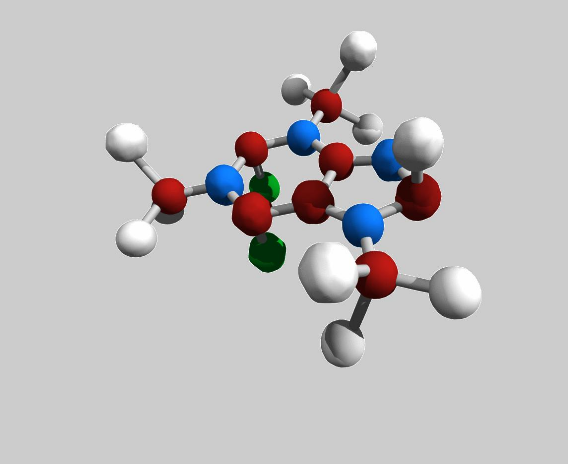

# The basic solution
## Algorithm

- 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

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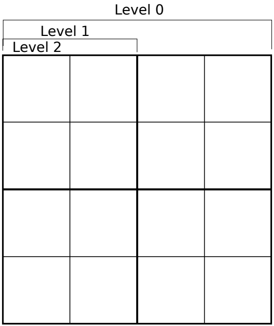
- The Mesh
- Multipole Expansions

# The Fast Multipole Algorithm

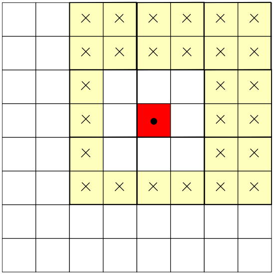
## The Mesh

### The Particle Mesh



# The Fast Multipole Algorithm
## The Mesh

Well separated cells



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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

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- Repeat the above for each level
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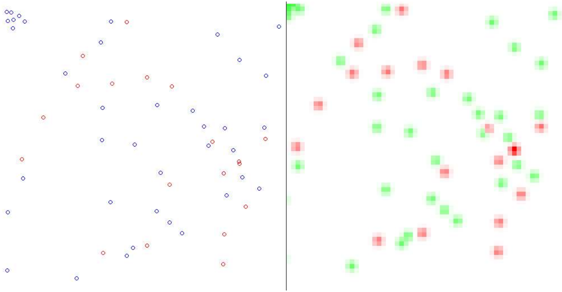
- Translate this to children nodes, repeat to the lowest mesh level.

## Basic structure of the Particle Mesh Ewald Method

- Interpolate particles to a grid



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- Calculate in real space directly for near particles, and use interpolated grid values for the long range potential.

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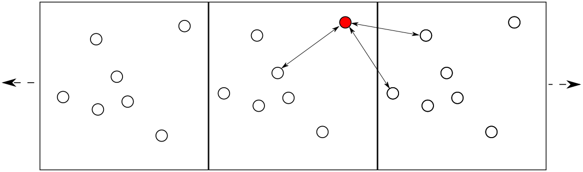
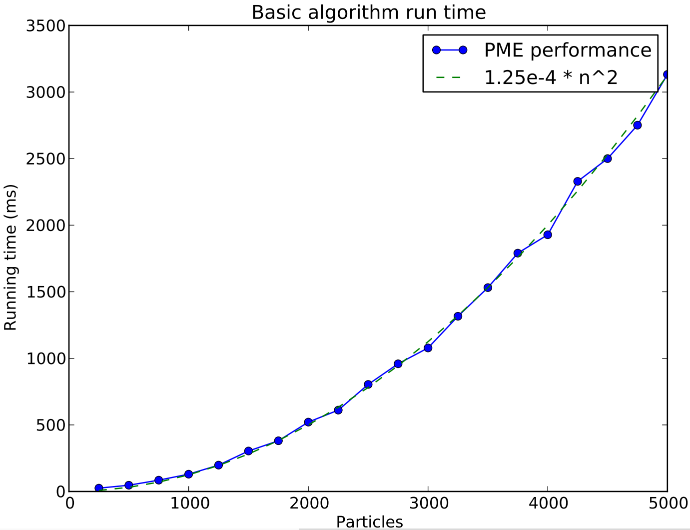
- Complexity of $O(n\log(n))$
- Fourier transformation technique leads to Periodic Boundary Conditions



# Results
## Basic Algorithm



# Results
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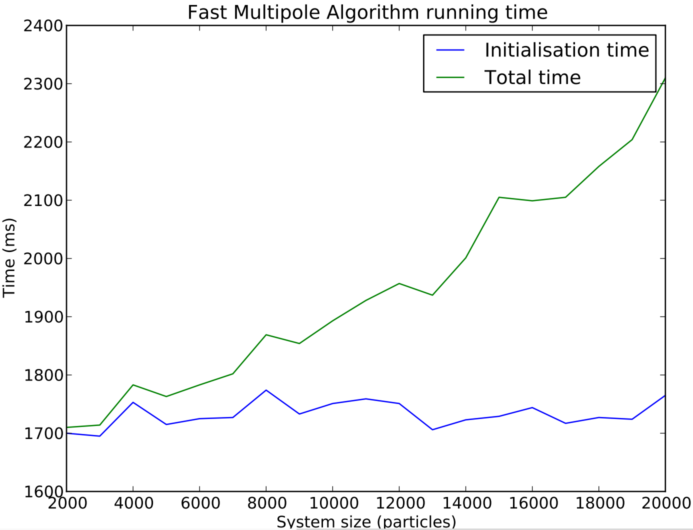
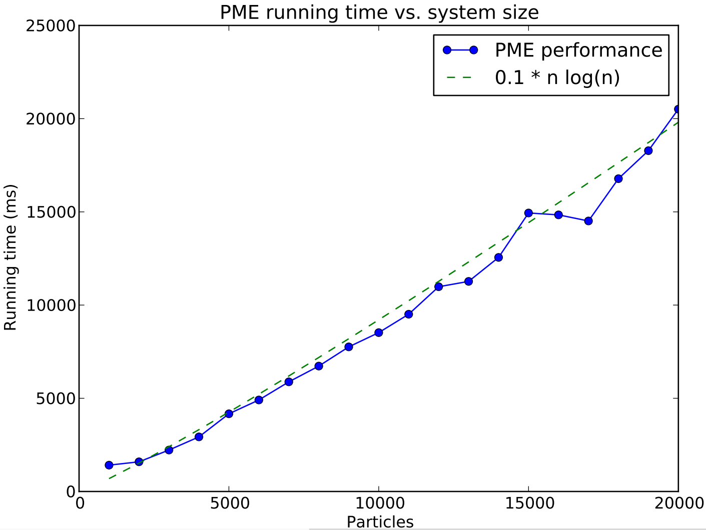


# Results
## Particle Mesh Ewald Algorithm





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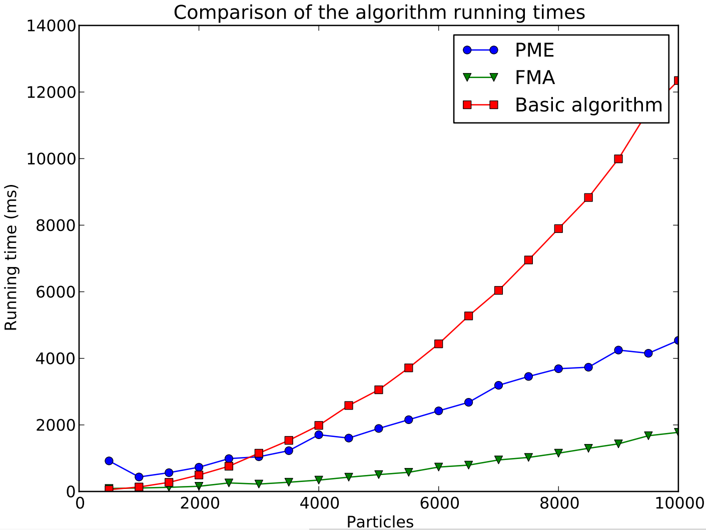

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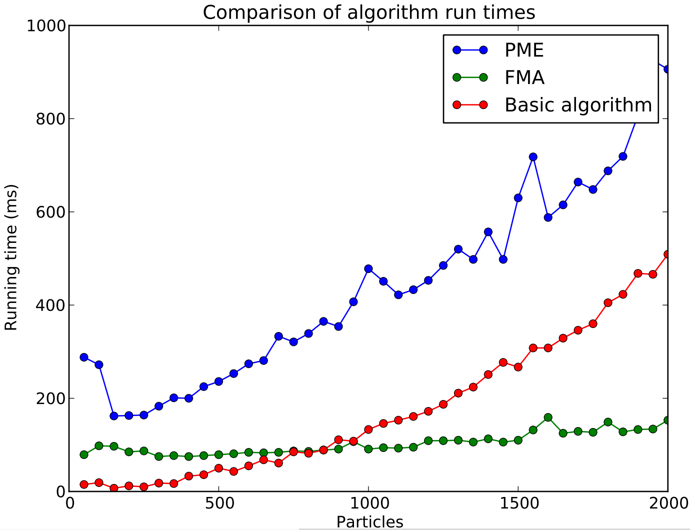

# Conclusion
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- Particle Mesh Ewald has desriable features and more potential for paralellisation and optimisation
- The Basic solution is not feasible for very large system sizes

# Conclusion

## Contributions





- Created fucntional implementations of the Basic, Particle Mesh Ewald, and Fast Multipole algorithms in Java.

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- Complexity analysis of algorithms, crossover points found.

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- Well documented and coded with readability in mind
- Actualization of often abstractly defined algorithms
- Complexity analysis of algorithms, crossover points found.
- Bridged the gap between mathematicians, computer scientists, and computational chemists.