

A Particle in
Cell Corrected
Approach to
Direct Sum

Ben Lewis,
Bridget
Morales,
David
Marsico,
Jason
McKelvey,
Madie Wilkin

A Particle in Cell Corrected Approach to Direct Sum

Ben Lewis, Bridget Morales, David Marsico, Jason
McKelvey, and Madie Wilkin
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Co-advisers: Eric Wolf and Justin Droba

Michigan St. University

July 23, 2014

The N-Body Problem

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- Solar systems

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- Solar systems
- Interacting charges, gases and plasma

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- Solar systems
- Interacting charges, gases and plasma
- We want to solve the system of ODE's given by:

$$\frac{dx_i}{dt} = v_i \quad \frac{dv_i}{dt} = a_i = \frac{F_i(x_1, \dots, x_n)}{m_i}$$

for $i = 1, \dots, n$.

Traditional Solutions

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- Direct Sum
- Particle Mesh
- Particle-Particle Particle-Mesh

- The net force on particle i is:

$$F_i = \sum_{\substack{j=1 \\ j \neq i}}^n q_i E_{j,i}$$

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- $E_{j,i}$ is the electric field from particle j at the location of particle i and q_i is the charge
- To calculate the force on all of the particles, we must repeat this summation for each of the n particles
- The problem with direct sum is that it is $\mathcal{O}(N^2)$

Goal

- Find efficient ways to solve the n-body problem.

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Goal

- Find efficient ways to solve the n-body problem.
- Improve efficiency from $\mathcal{O}(n^2)$ to $\mathcal{O}(n) + \mathcal{O}(k^2)$ where $k \ll n$ and k is the number of particles per cell.

Table: Theoretical Time Comparison (3600 MHz computer)

$$E_{j,i} = \frac{q_j}{\epsilon_0} \mathcal{G}(x_j|x_i)$$

$$F_{j,i} = q_i * E_{j,i}$$

N	$\mathcal{O}(N^2)$	$\mathcal{O}(N)$
10	10^{-8} sec	10^{-9} sec
10^3	10^{-4} sec	10^{-7} sec
10^6	5 min	10^{-4} sec
10^9	8 yrs	.28 sec
10^{12}	10^6 yrs	4.6 min

We are working on it.

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- We made a Finite Difference Mesh based method, which is a variation of the Particle-Particle Particle-Mesh method, that improved efficiency from $\mathcal{O}(n^2)$ to approximately $\mathcal{O}(n)$

We are working on it.

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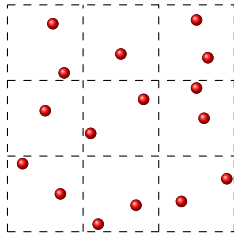
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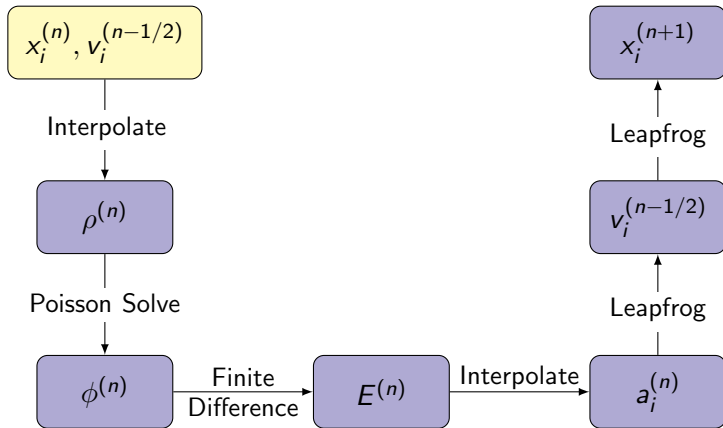
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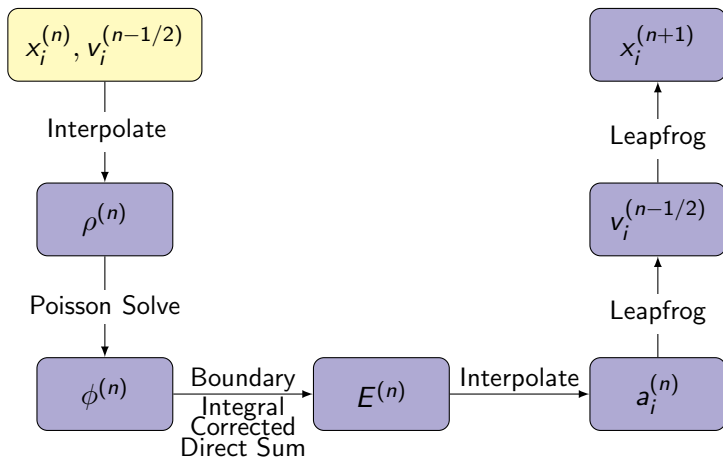
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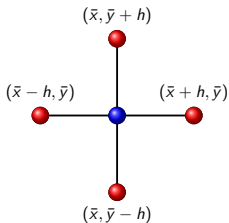
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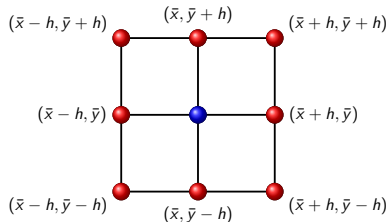
Using Finite Difference to Solve

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Five-Point Stencil

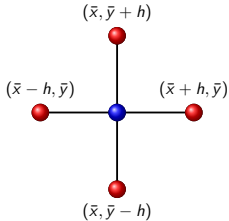


Nine-Point Stencil

Using Finite Difference to Solve

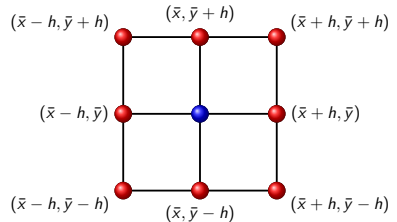
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■ $\nabla^2 \phi = \partial_{xx} \phi + \partial_{yy} \phi$

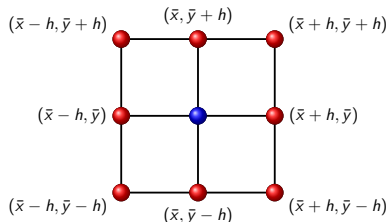
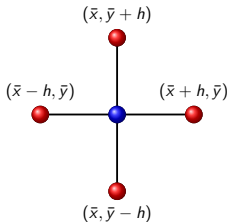


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Five-Point Stencil

- $\nabla^2 \phi = \partial_{xx} \phi + \partial_{yy} \phi$

- $\nabla^2 \phi =$

$$\frac{\phi^{j+1,k} - 2\phi^{j,k} + \phi^{j-1,k}}{(\Delta x)^2} + \frac{\phi^{j,k+1} - 2\phi^{j,k} + \phi^{j,k-1}}{(\Delta y)^2} + \mathcal{O}(\Delta x^2 + \Delta y^2)$$

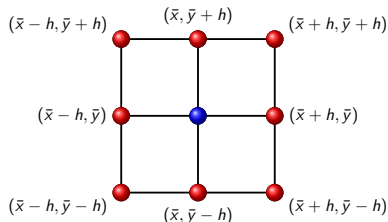
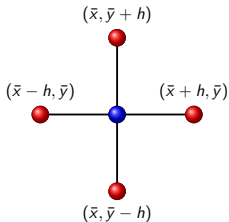
where j is the index for x and k is the index for y

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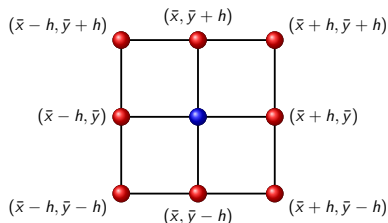
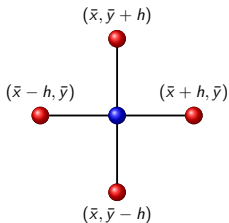
- $A\vec{\phi} = \vec{\rho}$

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where j is the index for x and k is the index for y

- $A\vec{\phi} = \vec{\rho}$

- $E_y(x, y) = \frac{\phi(x, y+h) - \phi(x, y-h)}{2h},$

- $E_x(x, y) = \frac{\phi(x+h, y) - \phi(x-h, y)}{2h}$

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- Acceleration is used to find the velocity at $t = n + .5$

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- Acceleration is used to find the velocity at $t = n + .5$
- That velocity is then used to find the position of each particle at $t = n + 1$

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- This is the leapfrog algorithm

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- That velocity is then used to find the position of each particle at $t = n + 1$
- This is the leapfrog algorithm
- $v_{1/2} = v_0 + a_0 \cdot \frac{dt}{2}$
- $v_{n+1/2} = v_{n-1/2} + a_n \cdot dt$
- $x_n = x_{n-1} + v_{n-1/2} \cdot dt$

Deriving Green's Identity

$$\phi(x) = \sum_{i=1}^N G(x_i - x_0) - \int_{\partial V} (G(x - x_0) \nabla \phi - \phi \nabla G(x - x_0)) \cdot \vec{n} ds$$

Deriving Green's Identity

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$$\int_V \nabla \cdot \vec{F} dv = \int_{\partial V} \vec{F} \cdot \vec{n} ds$$

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$$\int_V \nabla \cdot \vec{F} dv = \int_{\partial V} \vec{F} \cdot \vec{n} ds$$

Let $\vec{F} = \theta \gamma$ where θ is a scalar function, $\gamma = \nabla \psi$ is a vector function.

$$\int_V (\theta \nabla^2 \psi + \nabla \theta \cdot \nabla \psi) dV = \int_{\partial V} (\theta \nabla \psi \cdot \vec{n}) ds$$

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$$\int_V (\theta \nabla^2 \psi + \nabla \theta \cdot \nabla \psi) dV = \int_{\partial V} (\theta \nabla \psi \cdot \vec{n}) ds$$

If we let $\theta = G(x - x_0)$ and $\psi = \phi$, then we can solve for the potential $\phi(x)$

- We can use the fact that

$$\rho = \sum_{i=1}^N \delta(x - x_i)$$

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- We can solve for ϕ to obtain:

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- $\phi_{x,j} = \sum_{\substack{i=1 \\ i \neq j}}^N \frac{-1}{2\pi} \ln(\|x_i - x_j\|_2) + \oint_{\partial \Omega} (\phi \nabla G - G \nabla \phi) \cdot \vec{n} ds$

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- New equation because Potential Theory tells us it is the same

$$\phi_{x,j} = \sum_{\substack{i=1 \\ i \neq j}}^N \frac{-1}{2\pi} \ln(\|x_i - x_j\|_2) + \oint_{\partial \Omega} \sigma_s(y) G(x_j - y) ds(y)$$

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- σ is like a surface charge

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- We use direct sum to calculate the field due to local particles

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- In order to evaluate the boundary integral, we solve using numerical quadrature.

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- We end up with a matrix that we have to invert to obtain the surface charge.

- We use direct sum to calculate the field due to local particles
- In order to evaluate the boundary integral, we solve using numerical quadrature.
- We end up with a matrix that we have to invert to obtain the surface charge.
- Then, instead of doing this everywhere which would be $\mathcal{O}(n^2)$, we make this a subcell method which gives $\mathcal{O}(n) + \mathcal{O}(k^2)$.

Solving for Sigma

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$$\blacksquare \int_{s_1}^{s_2} \sigma G ds$$

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- $\int_{s_1}^{s_2} \sigma G ds$

- We take a limit to the boundary with respect to variable x and get the integral equation

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- $\int_{s_1}^{s_2} \sigma G ds$
- We take a limit to the boundary with respect to variable x and get the integral equation
- We turn the integral into discrete approximations that we can solve

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- The integral becomes four sums

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- We turn the integral into discrete approximations that we can solve
- The integral becomes four sums
- We use integral mean value theorem and trapezoid rule to end up with the Green's matrix
- $\sum_{i=1}^{4k} \int_{s_1}^{s_2} \sigma G ds$

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- The integral becomes four sums
- We use integral mean value theorem and trapezoid rule to end up with the Green's matrix
- $\sum_{i=1}^{4k} \int_{s_1}^{s_2} \sigma G ds$
- Then we end up with a system of equations in which we need to perform a Green's matrix inversion

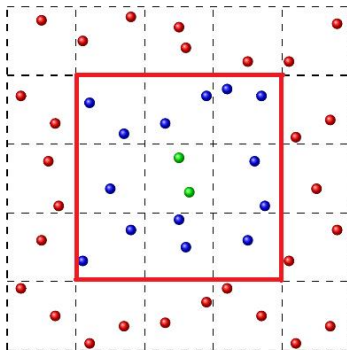
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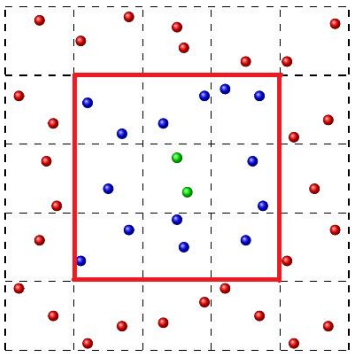
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Electric Fields we need several things

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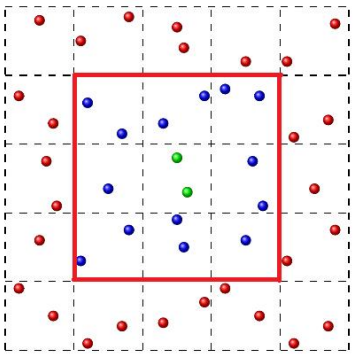
- List of all particles inside the cell



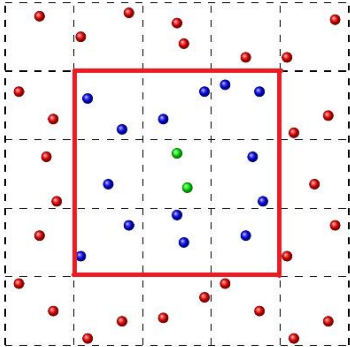
- List of all particles in boundary cells



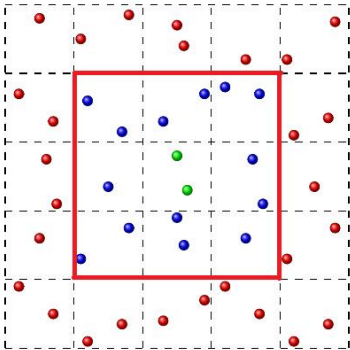
- Potential at all 12 border points per cell



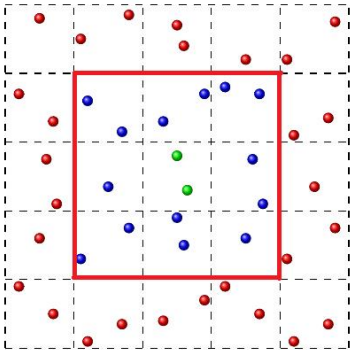
- Something to take the above and calculate the electric field



- For loop over all cells



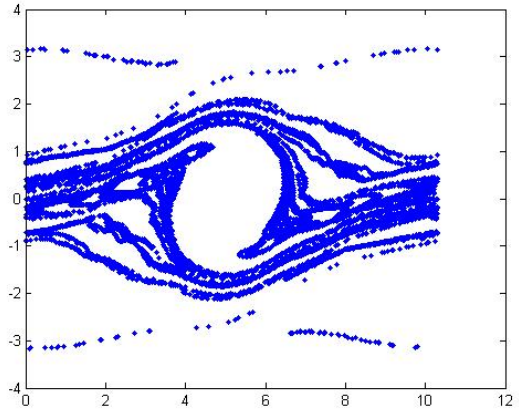
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If we can get this done, then it's a matter of increasing customizability

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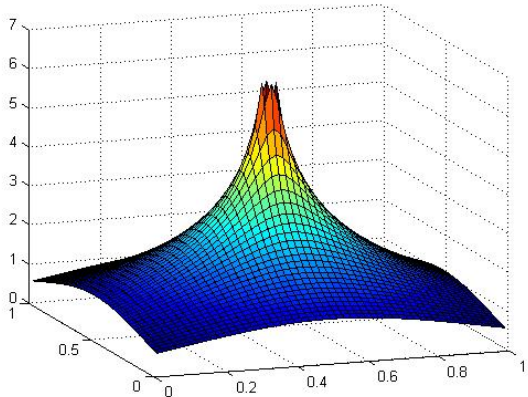
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Figure: Uncorrected



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Figure: Point charge at the center

