N-Body Simulation using Multipole Expansion

AST 245 Computational Astrophysics

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January 31, 2024

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Implementation

C++ based implementation using *`OpenMP`*, *`MathGL`* and *`Eigen3`*.

- Data.cc - Handle input data
- System.cc - Computes relevant const values and factors.
- Histogram.cc & Shell.cc - Histogram creation based on shells.
- Particle.cc - Stores relevant data about particle.
- Treecode.cc & Node.cc - Octree and multipole expansion.
- Types.h - Definition of relevant types.

Task 1: Direct Force Calculation

Hernquist Density

Density profile:

$$\rho(r) = \frac{M}{2\pi} \frac{a}{r} \frac{1}{(r+a)^3} \tag{1}$$

Cumulative Mass distribution:

$$M(r) = M \frac{r^2}{(r+a)^2} \tag{2}$$

Scale length:

$$a = \frac{r_{hm}}{1+\sqrt{2}} \tag{3}$$

Comparing Distributions

Logarithmic binning for B shells:

$$r_b = r_{\text{min}} \left(\frac{r_{\text{max}}}{r_{\text{min}}} \right)^{\frac{b}{B}}, \quad b \in \{0 \dots B\} \tag{4}$$

Bin density:

$$\rho_b = \frac{n_b M_b}{V_b} \tag{5}$$

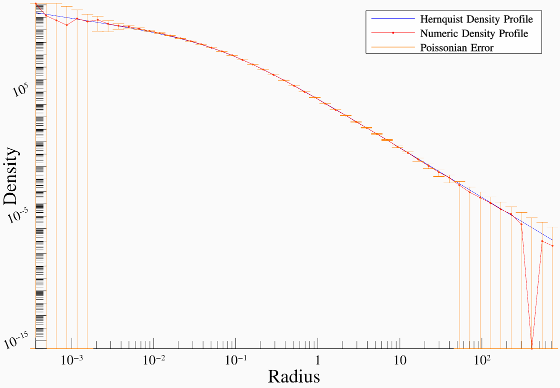
Expected number of particles and standard deviation:

$$\begin{aligned} \lambda &= \frac{N}{B} \\ \sigma &= \sqrt{\lambda} \end{aligned} \tag{6}$$

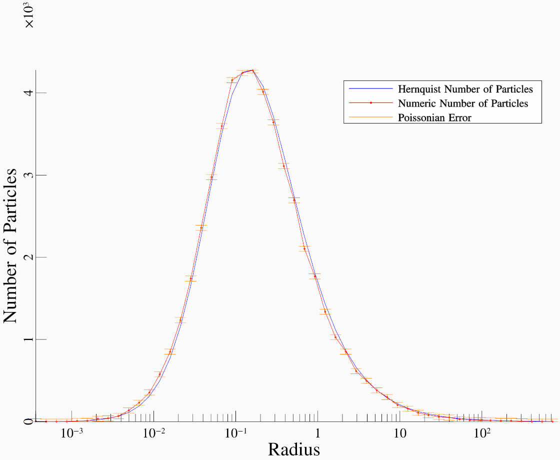
Resulting in Poisson density error:

$$\rho_b^{err} = \frac{\sigma M_b}{V_b} \tag{7}$$

Density Distribution



Particle Distribution



Dimensionless Quantities

- Gravitational constant $G = 1$
- Dimensionless Quantities:

$$\mathbf{r}' = \frac{\mathbf{r}}{R_0}, \quad m' = \frac{m}{M_0}, \quad t' = \frac{t}{T_0} \tag{8}$$

- Derived quantities for consistency:

$$\mathbf{v}' = \frac{\mathbf{v}}{V_0} = \mathbf{v}\frac{T_0}{R_0}, \quad \mathbf{a}' = \frac{\mathbf{a}}{A_0} = \mathbf{a}\frac{T_0^2}{R_0} \tag{9}$$

- Repercussions for setting $G = 1$

$$\begin{aligned} \mathbf{a}_i &= -G\sum_{j\neq i} m_j \frac{\mathbf{r}_i - \mathbf{r}_j}{\left|\mathbf{r}_i - \mathbf{r}_j\right|^3} \\ \Rightarrow \mathbf{a}_i' &= \underbrace{\left\{\frac{GM_0T_0^2}{R_0^3}\right\}}_{G'} \sum_{j\neq i} m_j' \frac{\mathbf{r}_i' - \mathbf{r}_j'}{\left|\mathbf{r}_i' - \mathbf{r}_j'\right|^3} \end{aligned} \tag{10}$$

Defining Units

- Time scaling factor T_0:

$$\frac{GM_0T_0^2}{R_0^3} = 1 \quad \Rightarrow \quad T_0 = \left(\frac{R_0^3}{GM_0}\right)^{1/2} \tag{11}$$

- $T_0 \simeq 14.91 Myr$
- $M_0 = 1M_\odot$.
- $R_0 = 1pc$.
- $V_0 \simeq 0.065\frac{km}{s} \simeq 0.067\frac{pc}{Myr}$
- $A_0 \simeq 0.004\frac{pc}{Myr^2}$

Data from file assumed as $M_\odot$, pc and $\frac{km}{s}$

Step 2: Introducing Softening

- Analytic Force

$$\mathsf{F}(r) = -\frac{GM(r)}{r^2} \Rightarrow \mathsf{F}(r) = -\frac{M}{(r+a)^2} \tag{12}$$

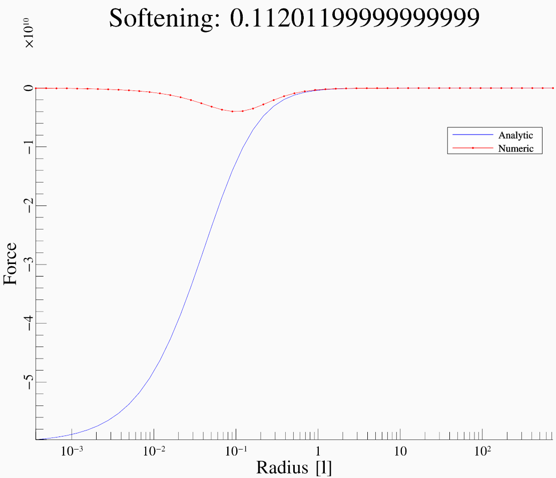
- Direct Force calculation with softening parameter ε:

$$\mathsf{F}_i = -Gm_i \sum_{j=1}^{N} m_j \frac{\mathbf{r}_i - \mathbf{r}_j}{\left(\left|\mathbf{r}_i - \mathbf{r}_j\right|^2 + \varepsilon^2\right)^{3/2}} \tag{13}$$

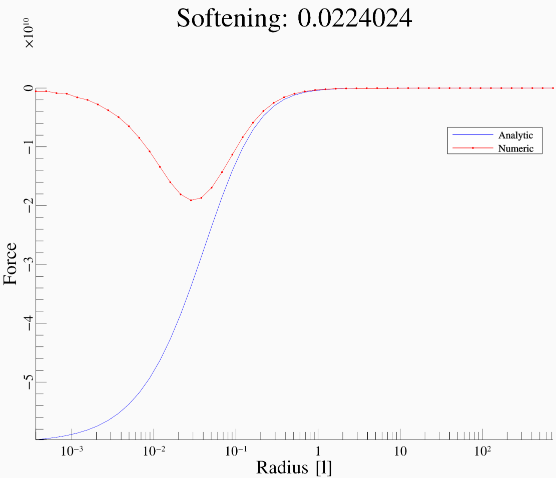
- Mean Interparticle Seperation:

$$\varepsilon = \left(\frac{V_{hm}}{N_{hm}}\right)^{1/3} = 0.0112012 \tag{14}$$

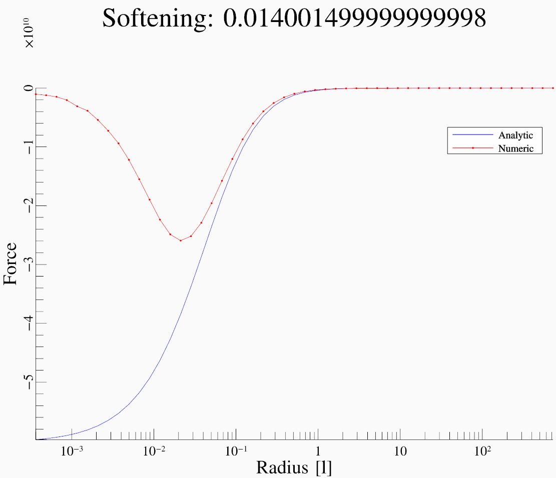
Softening \= 0.1



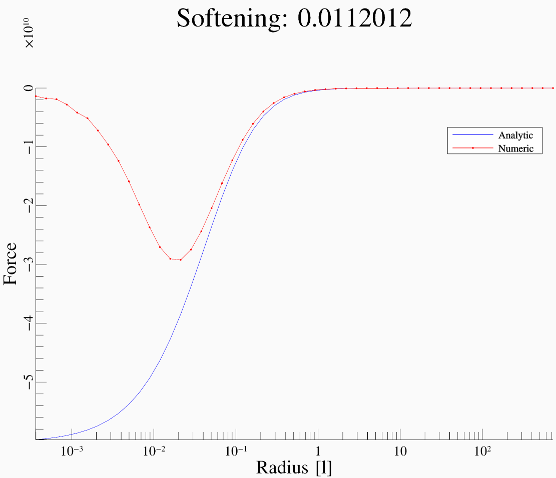
Softening \= 0.5



Softening \= 0.8

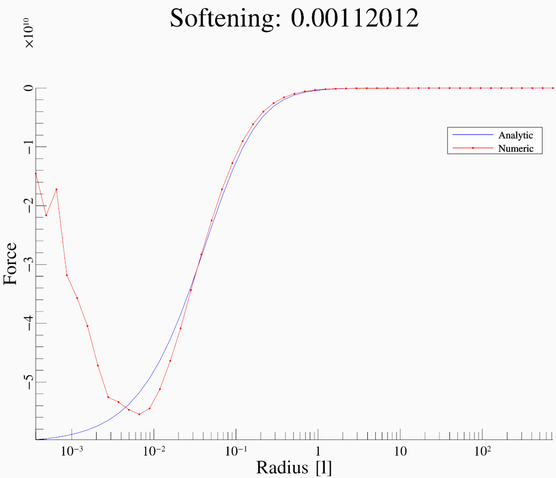


Softening \= 1

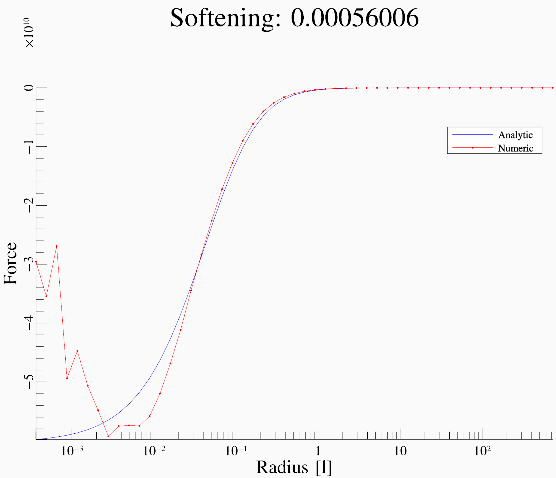


Softening: 0.0112012
$\times 10^{10}$
0
−1
−2
−3
−4
−5
Force
Analytic
Numeric
10^{-3}
10^{-2}
10^{-1}
1
10
10^{2}
Radius [l]

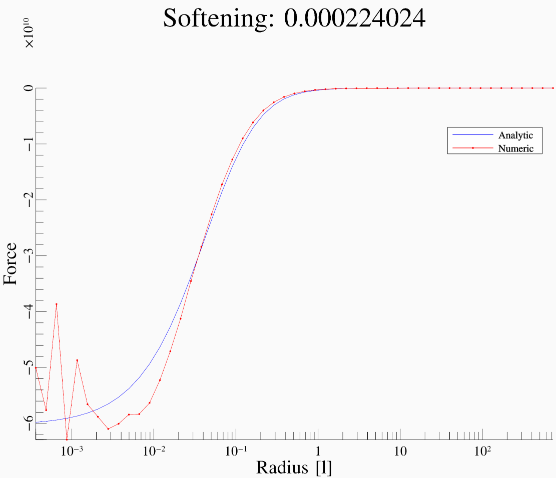
Softening \= 10



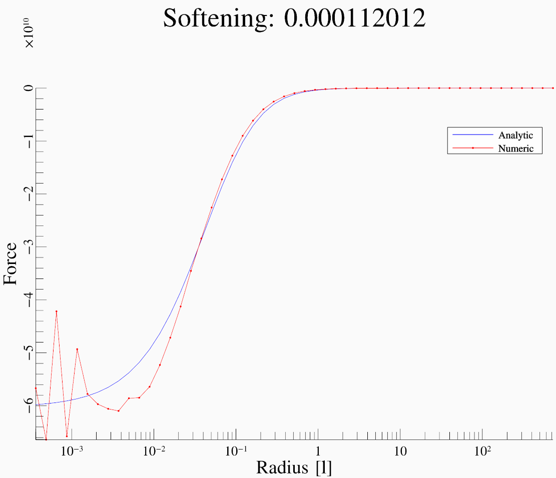
Softening \= 20



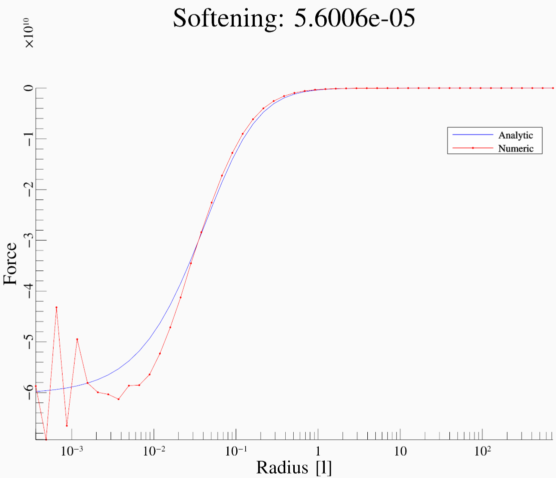
Softening \= 50



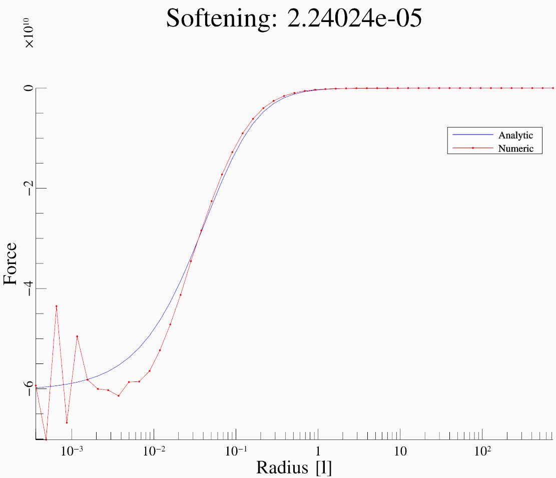
Softening \= 100



Softening \= 200



Softening \= 500



Relaxation

- Circular Velocity:

$$v_c = \sqrt{GM(R_{hm})/R_{hm}} = 225.959 \frac{pc}{Myr} \tag{15}$$

- Crossing time:

$$t_{cross} = \frac{R_{hm}}{v_c} = 898.319yr \tag{16}$$

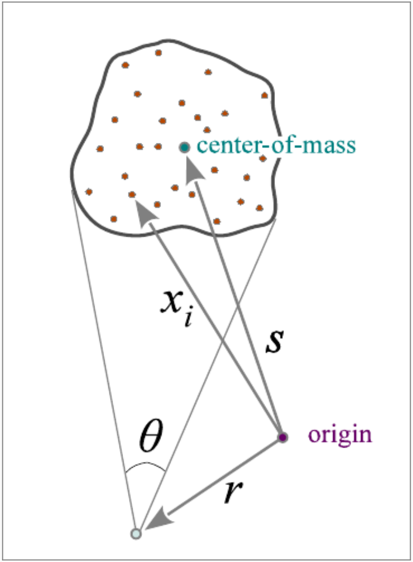
- Relaxation time:

$$t_{relax} = \frac{N}{8 \ln N} t_{cross} = 0.519Myr \tag{17}$$

Task 2: Multipole Expansion (tree-code)

Multipole Expansion

- r is sufficiently far away
- Seen under small opening angle θ
- Orders of multipole corrections



Multipole Moments

- Monopol

$$M = \sum_i m_i \tag{18}$$

- Center of Mass

$$\mathsf{s} = \frac{1}{M} \sum_i m_i \mathsf{x_i} \tag{19}$$

- Quadrupol ($\mathsf{Q} \in \mathbb{R}^{3\times 3}$)

$$\mathsf{Q}_{ij} = \sum_k m_k \left[3 \left(\mathsf{s} - \mathsf{x}_k \right)_i \left(\mathsf{s} - \mathsf{x}_k \right)_j - \delta_{ij} \left(\mathsf{s} - \mathsf{x}_k \right)^2 \right] \tag{20}$$

Gravitational Potential & Force

- Potential:

$$\Phi(\mathbf{r_i}) = -G\left(\frac{M}{|\mathbf{y}|} + \frac{1}{2}\frac{\mathbf{y}^T\mathbf{Q}\mathbf{y}}{|\mathbf{y}|^5}\right), \quad \mathbf{y} = \mathbf{r}_i - \mathbf{s} \tag{21}$$

- Monopole Force:

$$\mathbf{F}_M(\mathbf{r}_i) = -G\frac{m_i M}{|\mathbf{y}|^3}\mathbf{y} \tag{22}$$

- Quadrupole Force:

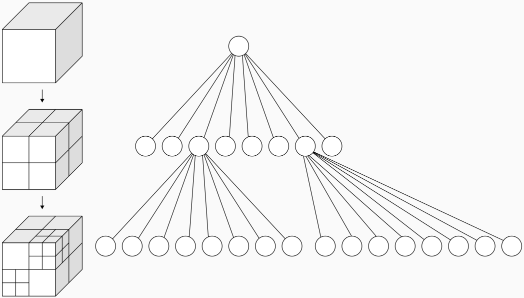
$$\mathbf{F}_Q(\mathbf{r}_i) = G\left(\frac{\mathbf{Q}\mathbf{y}}{|\mathbf{y}|^4} - \frac{5}{2}\frac{\mathbf{y}^T\mathbf{Q}\mathbf{y}}{|\mathbf{y}|^4}\mathbf{y}\right) \tag{23}$$

- Total Force:

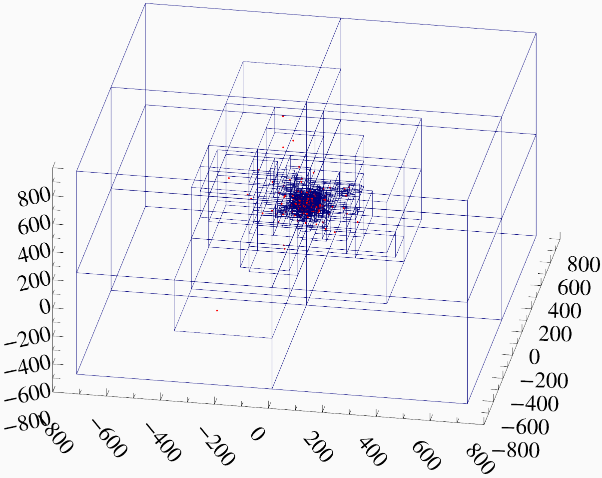
$$\mathbf{F}(\mathbf{r}_i) = \mathbf{F}_M + \mathbf{F}_Q \tag{24}$$

Hierarchical Grouping

- Octree
- Axis-aligned cubes
- Every particle is a leaf node
- Empty cubes not stored
- Children have $c' = \frac{1}{2}c$ side length



Octree



800
600
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−200
−400
−600
−800
−800
−600
−400
−200
0
200
400
600
800
800
600
400
200
0
−200
−400
−600
−800

When to apply the expansion?

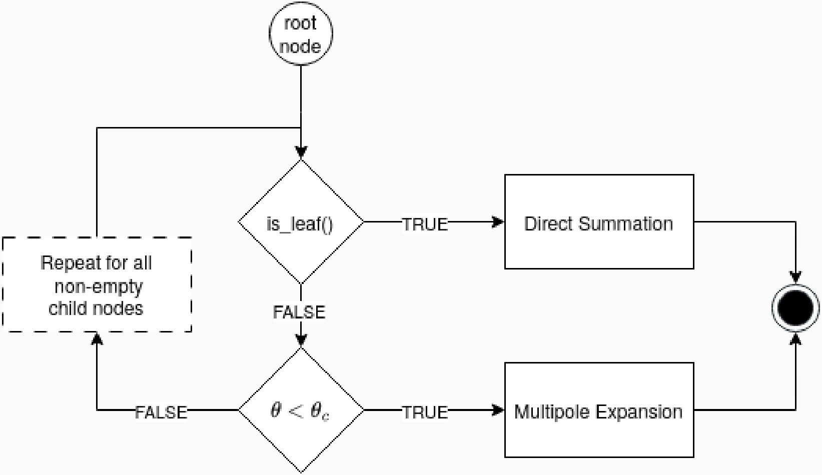
- Opening angle:

$$\theta \simeq \frac{c}{|\mathbf{y}|} \tag{25}$$

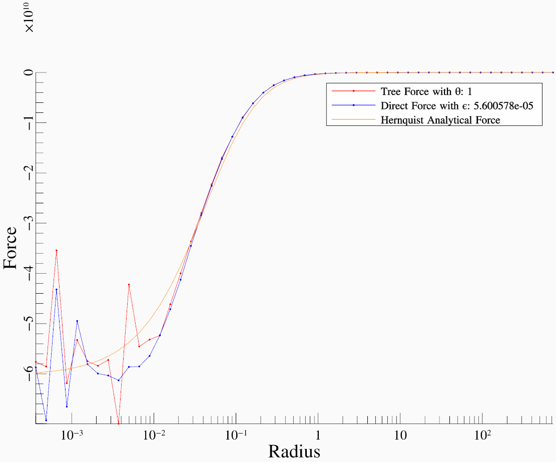
- Tolerance Angle θ_c
- In the limit $\theta_c \to 0$ direct summation force.

Tree Walk

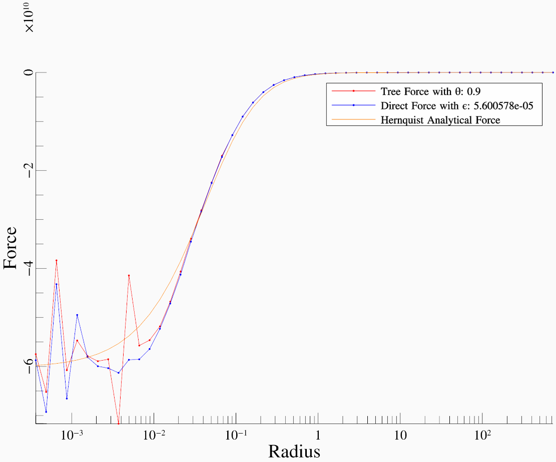
- Depth-First traversal



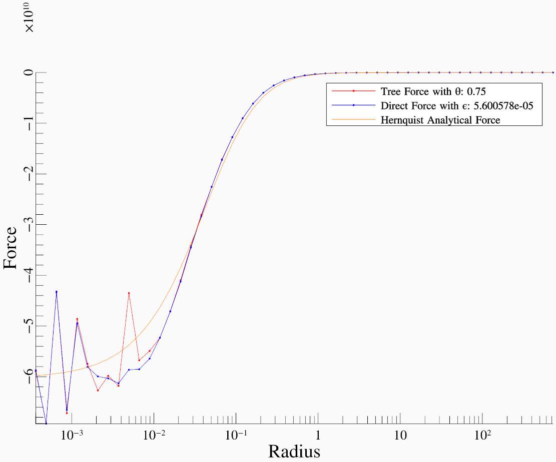
Force Comparison $\theta_c = 1.0$



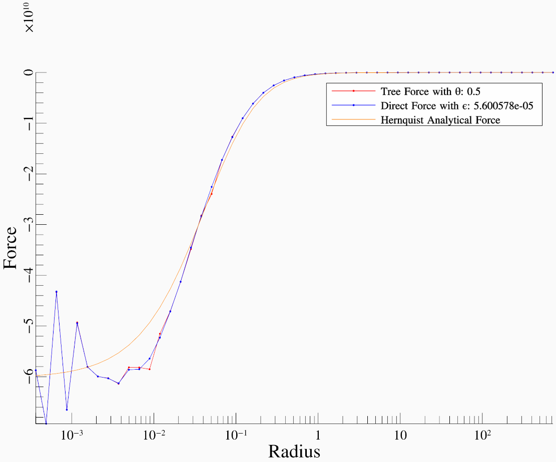
Force Comparison $\theta_c = 0.9$



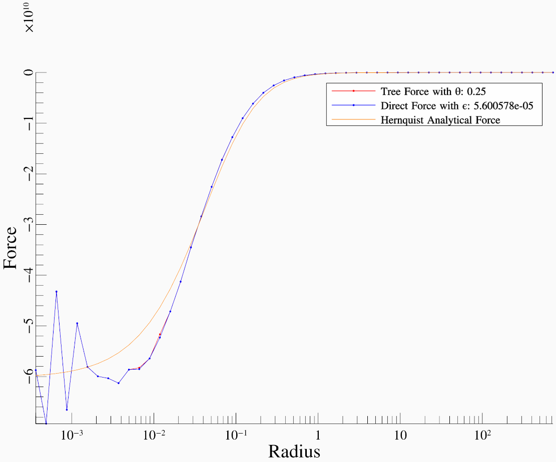
Force Comparison $\theta_c = 0.75$



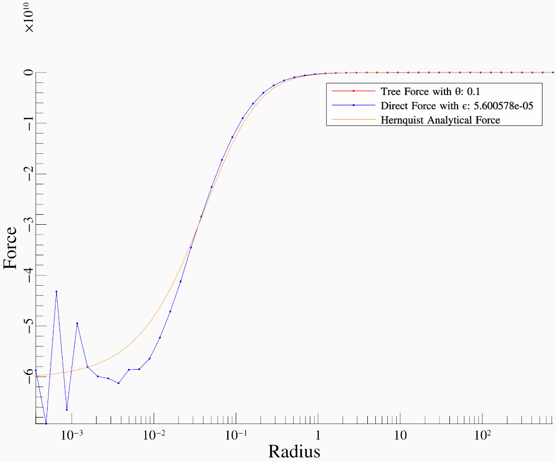
Force Comparison $\theta_c = 0.5$



Force Comparison $\theta_c = 0.25$



Force Comparison $\theta_c = 0.1$



Computational Cost

Expected Complexity

- Tree-code: $\mathcal{O}(N \log N) = 2.4 \cdot 10^5$
- Direct Sum: $\mathcal{O}(N^2) = 2.5 \cdot 10^9$

Actually (Average interaction per particle):

Tolerance Angle (θ_c)	1.0	0.9	0.75	0.5	0.25	0.1
Multipole Exp	502	542	675	1782	5229	5637
Direct Sum	87	94	128	542	3852	20161

Integration with Direct Summation

- $T = 3t_{cross}$ in dimensionless calculation with $\Delta t = \eta t_{cross}$.
- $\eta = [0.1, 0.01]$
- $t_{cross} \approx 6 \cdot 10^{-6}$
- Softening Divisors = $[1, 100, 250]$

Iteration on each particle with *OpenMP* and Leapfrog integration:

- $f(\mathbf{r}) = \ddot{\mathbf{r}} = \mathbf{a}$ given by equation (13)
- $\mathbf{v}_{n+\frac{1}{2}} = \mathbf{v}_n + f(\mathbf{r}_n)\frac{\Delta t}{2}$
- $\mathbf{r}_{n+1} = \mathbf{r}_n + \mathbf{v}_{n+\frac{1}{2}}\Delta t$
- $\mathbf{v}_{n+1} = \mathbf{v}_{n+\frac{1}{2}} + f(\mathbf{r}_{n+1})\frac{\Delta t}{2}$

Time Integration (Force)

SHOW GIFS

Magnitude of Relaxation

- Kinetic Energy:

$$E_{kin} = \frac{1}{2} \sum_{i=0}^{N} m_i \mathbf{v}^2 \tag{26}$$

- Potential Energy:

$$E_{pot} = -G \sum_{i=0}^{N} \sum_{j=i+1}^{N} \frac{m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|} \tag{27}$$

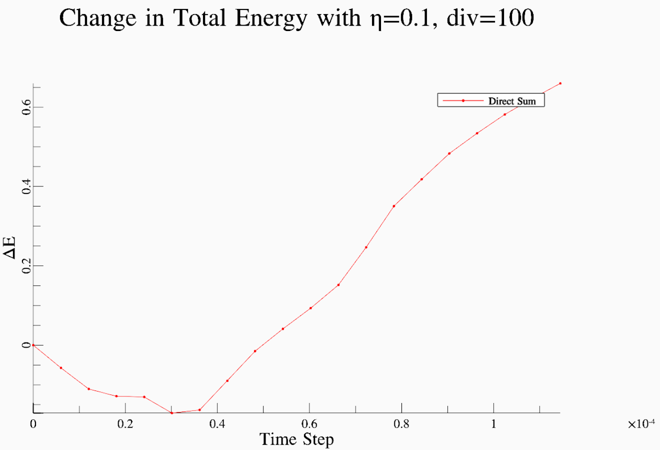
- Total Energy:

$$E_{tot} = E_{kin} + E_{pot} \tag{28}$$

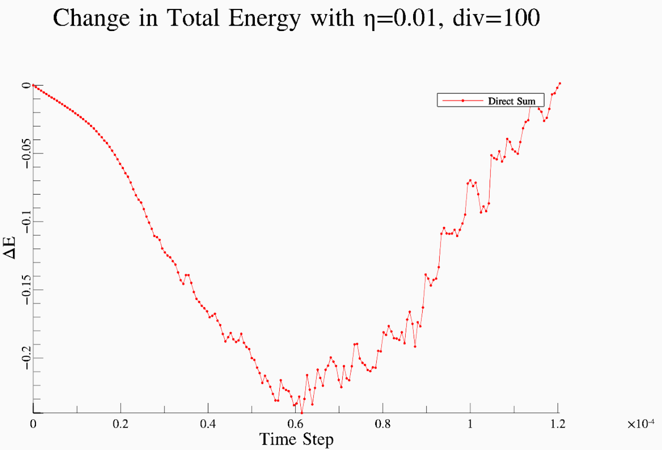
- Normalized change of Energy:

$$\Delta E_n = \frac{E_{tot}(t_0) - E_{tot}(t_n)}{|E_{tot}(t_0)|} \tag{29}$$

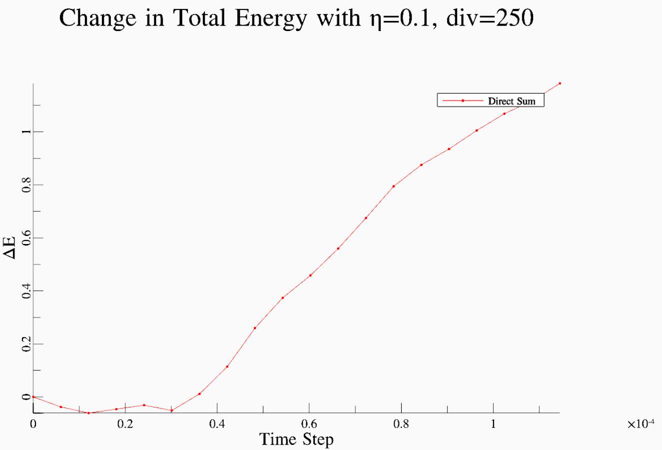
Numerical Relaxation



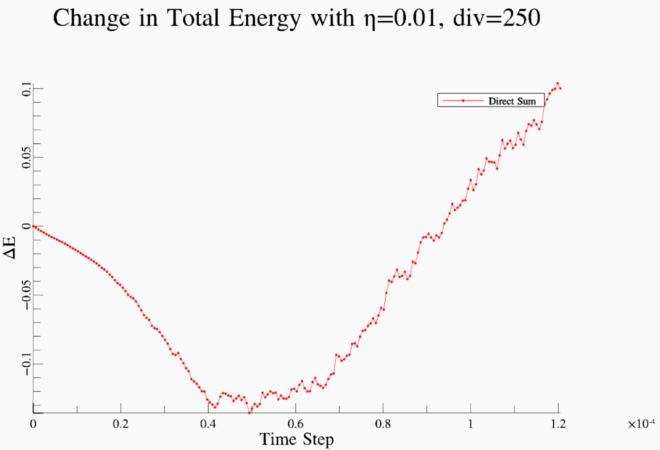
Numerical Relaxation



Numerical Relaxation



Numerical Relaxation



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