AST245 Computational Astrophysics

Treecode-based: N-Body Simulation

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Preliminaries

- C++ based implementation using `OpenMP`, `MathGL` and `Eigen3`.
- `main.cpp` as center of application
- `particle.c/hpp` Holds Particle3D class with relevant members
- `data.c/hpp` reads in file
- `histogram.c/hpp` and `shell.c/hpp` handle histogram creation and binning
- `system.c/hpp` Global constants, factors and logic for direct summation.
- `treecode.c/hpp` Multipole expansion related class and methods

```
~/Projects/comp-astro-main/exercises/n-body/..
› cmake
› data
› docs
⌄ include
  │ data.hpp
  │ histogram.hpp
  │ node.hpp
  │ particle.hpp
  │ shell.hpp
  │ system.hpp
  │ treecode.hpp
  └ types.hpp
⌄ src
  │ data.cpp
  │ histogram.cpp
  │ main.cpp
  │ node.cpp
  │ particle.cpp
  │ shell.cpp
  │ system.cpp
  └ treecode.cpp
CMakeLists.txt
flake.lock
flake.nix
Makefile
README.md
```

Units and Dimension

From assumption $G = 1$ follows:
Dimensionless Quantities:

$$\mathbf{r}' = \frac{\mathbf{r}}{R_O}, \quad m' = \frac{m}{M_O}, \quad t' = \frac{t}{T_O} \tag{1}$$

Derived quantities for consistency:

$$\mathbf{v}' = \frac{\mathbf{v}}{V_O} = \mathbf{v}\frac{T_O}{R_O}, \quad \mathbf{a}' = \frac{\mathbf{a}}{A_O} = \mathbf{a}\frac{T_O^2}{R_O} \tag{2}$$

Repercussions for setting $G = 1$

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

Defining Units

Time scaling factor T_0:

$$\frac{GM_0 T_0^2}{R_0^3} = 1 \quad \Rightarrow \quad T_0 = \left(\frac{R_0^3}{GM_0}\right)^{1/2} \tag{4}$$

Where:

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

Force & Density Calculation

Analytic Hernquist

Density distribution:

$$\rho(r) = \frac{M}{2\pi} \frac{a}{r} \frac{1}{(r+a)^3} \tag{5}$$

Cumulative Mass distribution inside a radius:

$$M(r) = M \frac{r^2}{(r+a)^2} \tag{6}$$

Reformed Half-mass-radius equation, to get scale length

$$a = \frac{r_{1/2}}{1+\sqrt{2}} \tag{7}$$

Where:

- M - Total mass of the system
- a - Scale Length
- r - Particle position vector
- $r_{1/2}$ - Half-mass radius: calculated numerically

Numerical Density Approximation

Logarithmic binning via `Histogram` class into a `std::vector` of `Shell` classes.

$$i_{log} = |\mathbf{r}|_{min} \left(\frac{|\mathbf{r}|_{max}}{|\mathbf{r}|_{min}} \right)^{\frac{i_{lin}}{n}} \tag{8}$$

On histogram creation calculated for each shell:

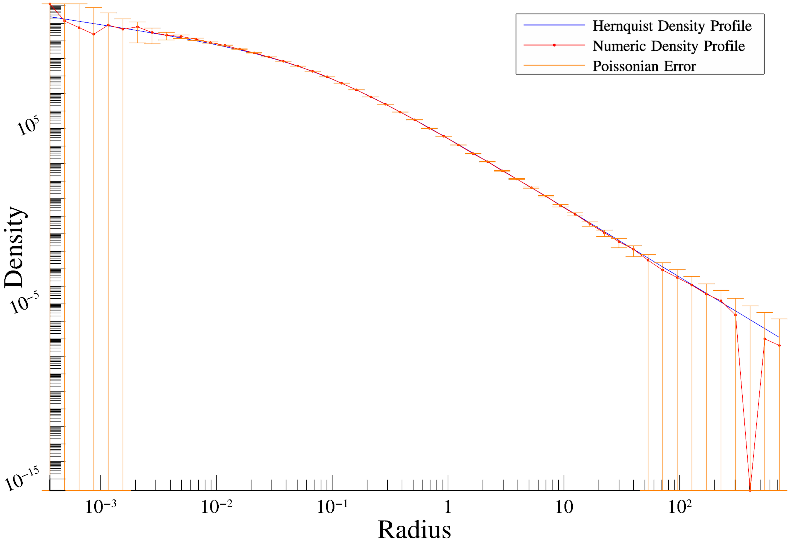
$$\rho_i = M_i / V_i \tag{9}$$

Poissonian density error with expected number of particles $\lambda = \frac{N}{B}$ and standard deviation $\sigma = \sqrt{\lambda}$:

$$\rho_{err} = \sigma \frac{m_p}{V_i} \tag{10}$$

Where:

- i - Shell index
- B - Number of bins in histogram
- N - Number of Particles
- m_p - Mass of a single particle


Hernquist Density Profile
Numeric Density Profile
Poissonian Error
Density
10^5
10^{-5}
10^{-15}
10^{-3}
10^{-2}
10^{-1}
1
10
10^2
Radius

Step 2: Analytic Force Reference

Assuming a Spherical System [1], substituting $M(r)$ from Eq. (6) and reducing:

$$F(r) = -\frac{GM(r)}{r^2} \Rightarrow F(r) = -\frac{M}{(r+a)^2} \tag{11}$$

Where:

- M - Total Mass of System
- r - Radius of shell
- a - Scale length of System

Step 2: Direct Force Calculation

Keeping in mind $G = 1$:

$$F_i = -Gm_i \sum_{j=1}^{N} \frac{m_j}{\left[\left(\mathbf{r}_i - \mathbf{r}_j\right)^2 + \varepsilon^2\right]^{3/2}} \left(\mathbf{r}_i - \mathbf{r}_j\right) \tag{12}$$

Softening equation (2.227) from *Galactic Dynamics*:

$$\varepsilon = -\frac{r_{max}^2 + \frac{3}{2}a^2}{(r_{max}^2 + a^2)^{3/2}} \tag{13}$$

or, as suggested, substituting a from above with:

$$d = \left[\frac{(4\pi/3)R_{hm}^3}{N}\right]^{1/3} \tag{14}$$

Where:

- i - Particle under consideration
- ε - Softening: accurate at $\approx 10^{-5}$
- r_{max} - Maximum radius
- d - Mean inter-particle separation
- a - Scale length
- $G = 1$

Step 2: Direct Force Calculation

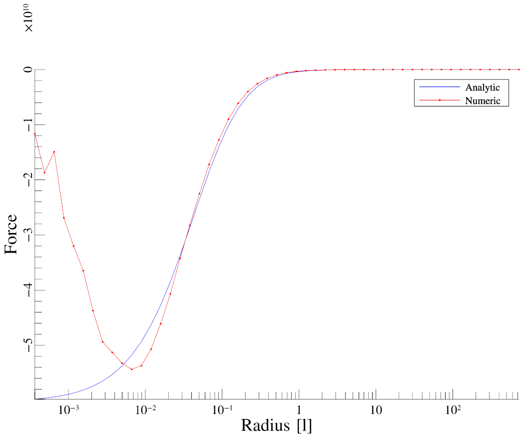
Vectors converted to scalars by **normalizing** the Force vector and **projecting** it on the center for numeric approximation and analytic comparison:

$$F^b_{avg} = \frac{1}{N_{Bin}} \sum_{i=0}^{N_{Bin}} \frac{\mathbf{r}_i \cdot \mathbf{F}_i}{|\mathbf{r}_i|} \tag{15}$$

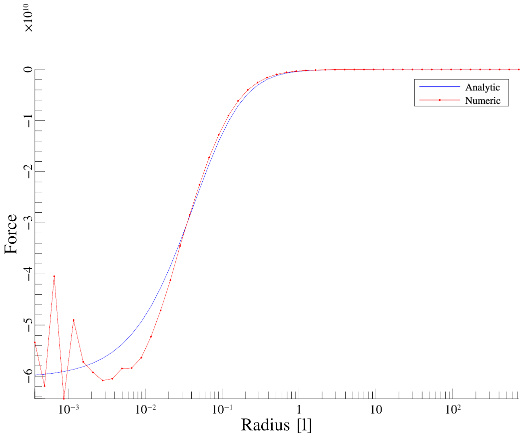
Where:

- N_{Bin} - Number of particles in a bin or shell
- $\mathbf{r}_i$ - Position vector of particle i
- $\mathbf{F}_i$ - Force Vector of particle i
- F^b_{avg} - Average force on bin b

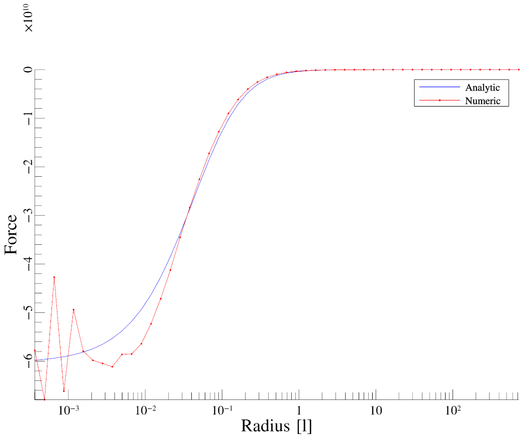
Softening $/= 1$, with a



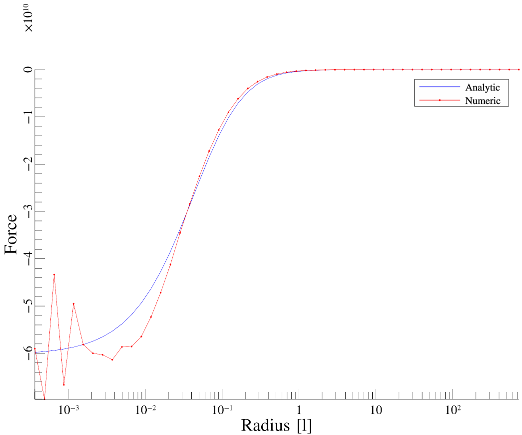
Softening /= 8, with *a*



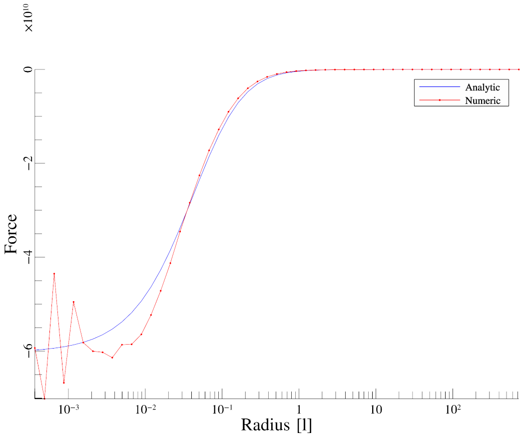
Softening $l = 16$, with a



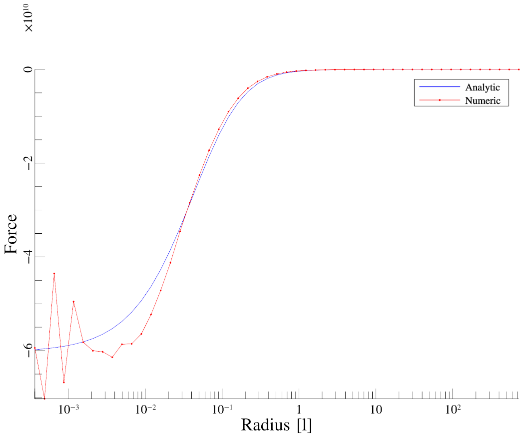
Softening $/= 32$, with a



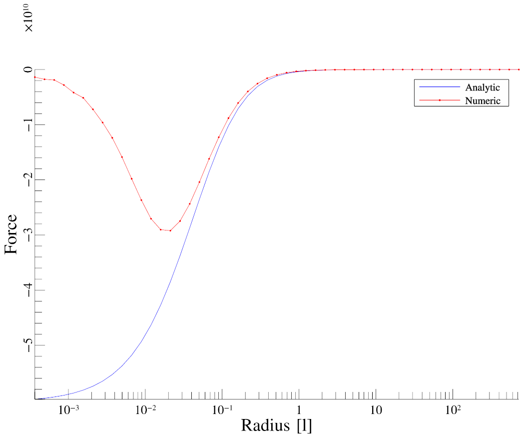
Softening $l = 64$, with a



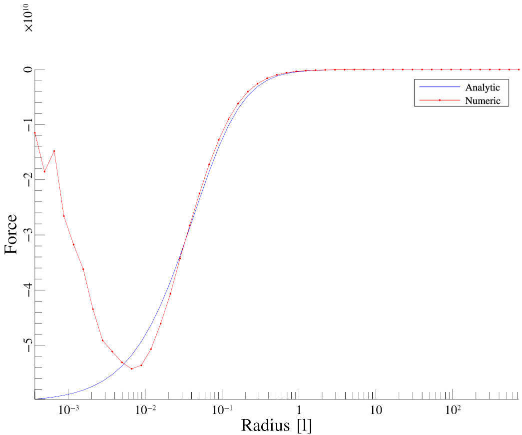
Softening $l = 128$, with a



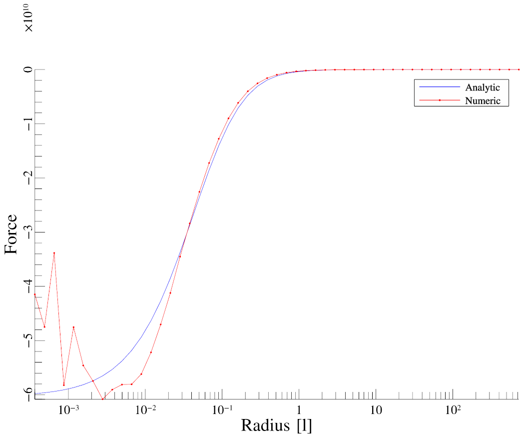
Softening $l = 1$, with d



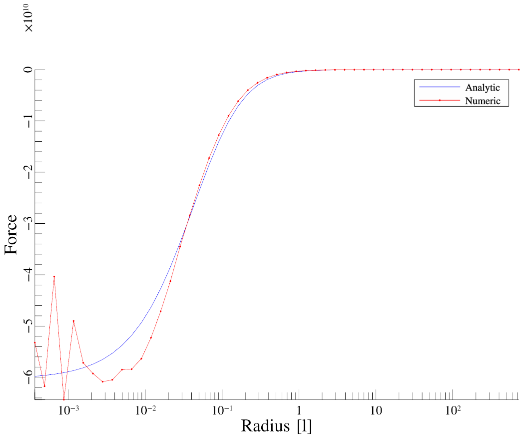
Softening /= 8, with d



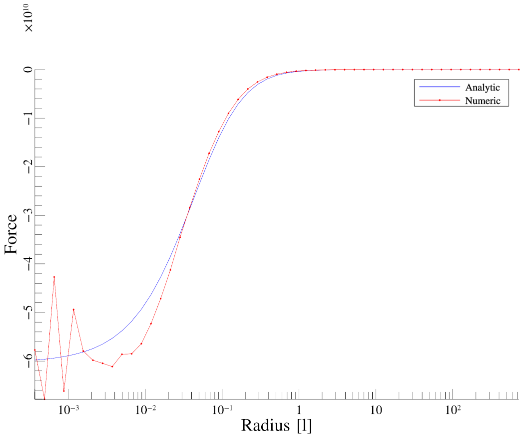
Softening $l = 32$, with d



Softening $l = 64$, with d



Softening $l = 128$, with d



Relaxation Timescale

$$v_c = \sqrt{GM(R_{hm})/R_{hm}} \tag{16}$$

$$t_{cross} = \frac{R_{hm}}{v_c} \tag{17}$$

$$t_{relax} = \frac{N}{8 \ln N} t_{cross} \tag{18}$$

Using:

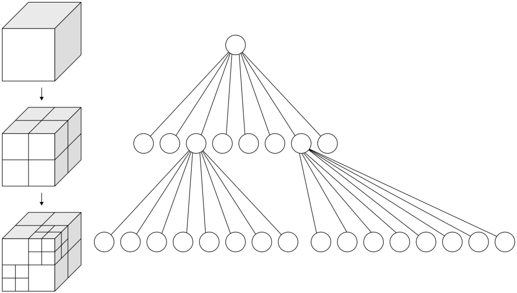
- $G = 4.300\,917\,270\,6 \times 10^{-3}\,\mathrm{pc}\,\mathrm{M}_{\odot}^{-1}\,(\mathrm{km/s})^2$
- $m = 92.4259\,\mathrm{M}_{\odot}$

Crossing Timescale: 898.302 *yr*
Relaxation Timescale: 0.520 *Myr*

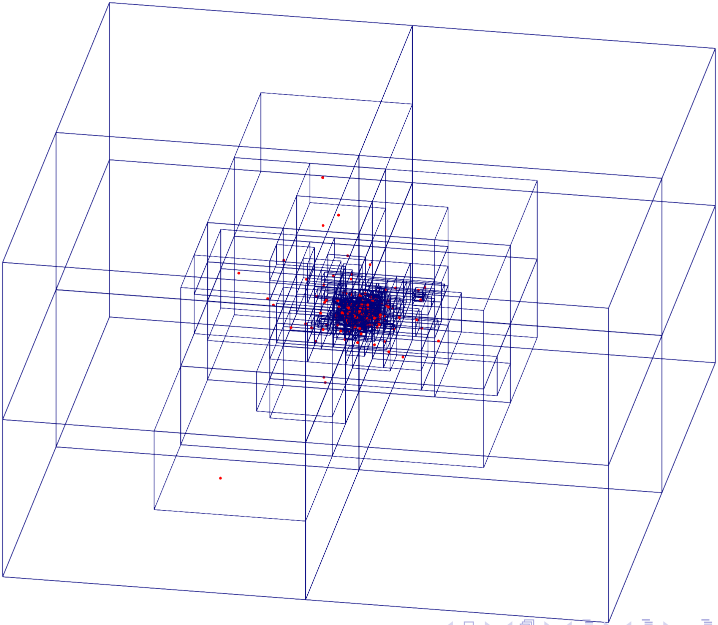
Tree-Code - Multipole Expansion

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

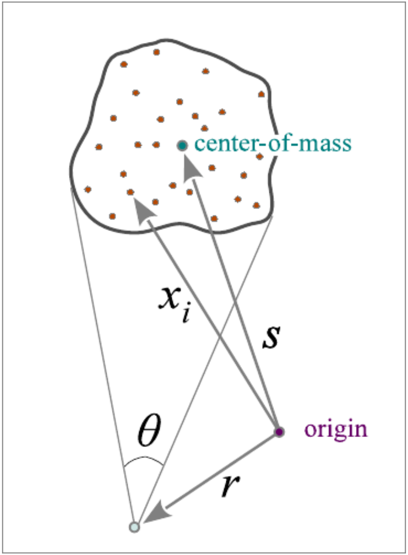


Octree



Multipole Expansion

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



Multipole Moments

- Monopole

$$M = \sum_i m_i \tag{19}$$

- Center of Mass

$$\mathbf{s} = \frac{1}{M} \sum_i m_i \mathbf{x_i} \tag{20}$$

- Quadrupole, Tensor calculation ($\mathbf{Q} \in \mathbb{R}^{3\times3}$)

$$\mathbf{Q}_{ij} = \sum_k m_k \left[3\left(\mathbf{s} - \mathbf{x}_k\right)_i \left(\mathbf{s} - \mathbf{x}_k\right)_j - \delta_{ij} \left(\mathbf{s} - \mathbf{x}_k\right)^2 \right] \tag{21}$$

Gravitational Potential & Force

- Potential:

$$\Phi(\mathbf{r_i}) = -G\left[\frac{M}{|\mathbf{y}|} + \frac{1}{2}\frac{\mathbf{y}^T\mathbf{Q}\mathbf{y}}{|\mathbf{y}|^5}\right], \quad \mathbf{y} = \mathbf{r}_i - \mathbf{s} \tag{22}$$

- Monopole Force:

$$\mathbf{F}_M(\mathbf{r}_i) = -G\frac{m_i M}{|\mathbf{y}|^3}\mathbf{y} \tag{23}$$

- Quadrupole Force:

$$\mathbf{F}_Q(\mathbf{r}_i) = G\left[\frac{\mathbf{Q}\mathbf{y}}{|\mathbf{y}|^4} - \frac{5}{2}\frac{\mathbf{y}^T\mathbf{Q}\mathbf{y}}{|\mathbf{y}|^4}\mathbf{y}\right] \tag{24}$$

- Total Force:

$$\mathbf{F}(\mathbf{r}_i) = \mathbf{F}_M + \mathbf{F}_Q \tag{25}$$

When to apply the expansion?

- Opening angle:

$$\theta \approx \frac{c}{|\mathbf{y}|} \tag{26}$$

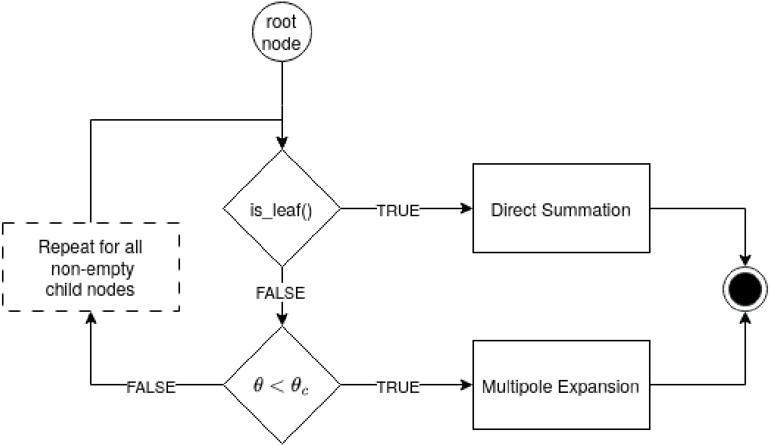
- Tolerance Angle $\theta_c \in [0.5, 1]$
- In the limit $\theta_c \to 0$ direct summation force.

Where:

- c - Length of cube side
- $\mathbf{y}$ - Vector: particle position to center of mass

Tree Walk

- Depth-First traversal



Integration with Direct Summation

$T = 5 \times t_{cross}$ in dimensionless calculation with $\Delta t = \eta t_{cross}$.

Iteration on each particle with `OpenMP` and on each particle **Leapfrog** integration in *kick-drift-kick* form:

- $v_{n+1/2} = r_0 + a_0 \frac{\Delta t}{2}$
- $r_{n+1} = r_0 + v_{n+1/2} \Delta t$
- $a_{n+1} = df(\Delta t)$
- $v_{n+1} = v_{n+1/2} + a_{n+1} \frac{\Delta t}{2}$

Where:

- $\eta = [0.1, 0.01]$
- $t_{cross} \approx 6e^{-6}$
- $df(\Delta t)$ - Direct force summation

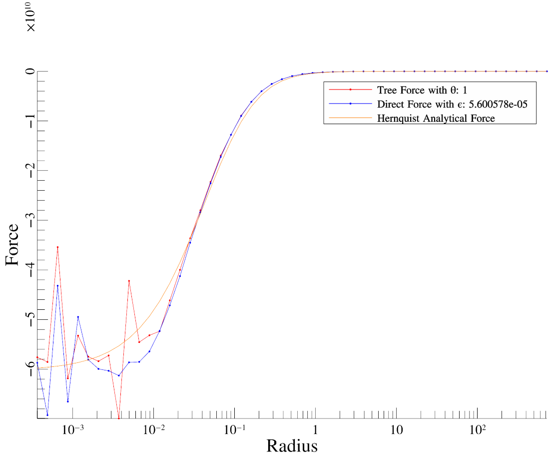
SHOW GIFS

Force Comparison - Accuracy

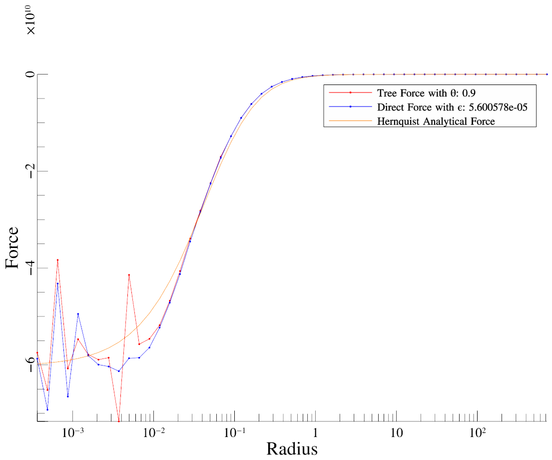
Assumption: Direct Force summation considered most accurate.

$\lim_{\theta_c \to 0}$ leads to Direct Summation, often considered in the range of $[0.5, 1.0]$.

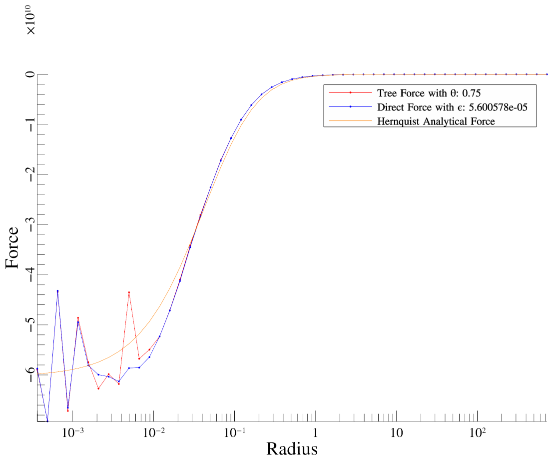
Force Comparison I



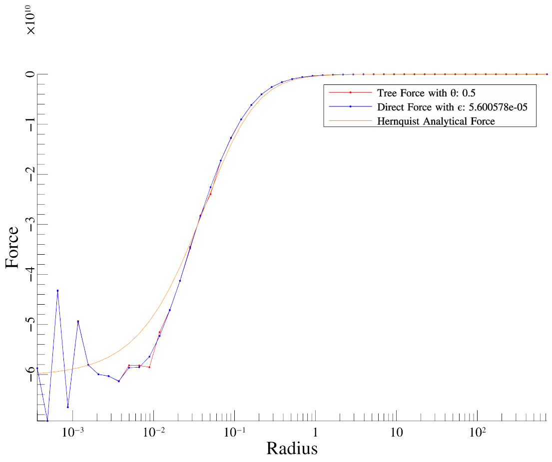
Force Comparison II



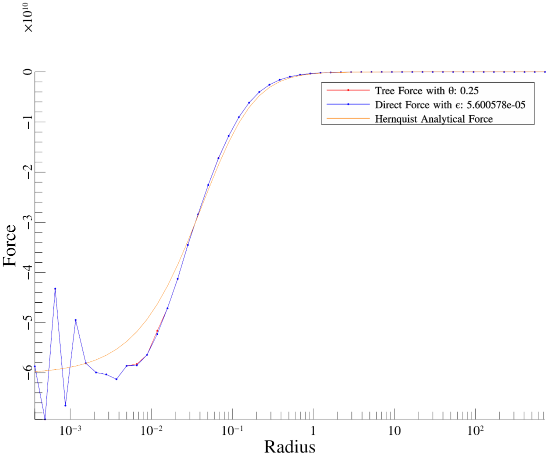
Force Comparison III



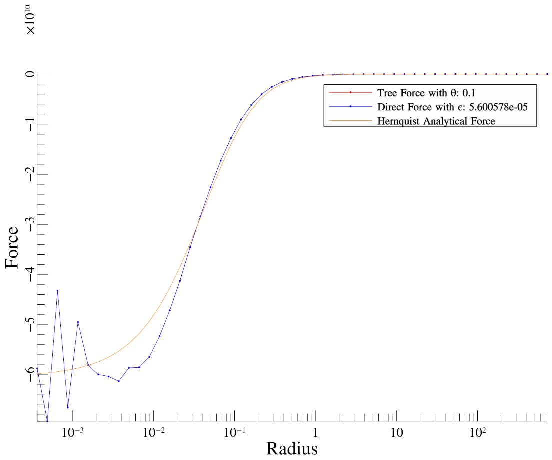
Force Comparison IV



Force Comparison V



Force Comparison VI



Computational Cost Comparison

Direct Force Computation:

- $\mathcal{O}(N^2)$ - Comparison of each particle with every other, parallelizable
- $\frac{N^2}{2}$ - Comparison of each particle only with unvisited particles, not parallelizable

Tree Force Computation:

$$N_{nodes} = \frac{4\pi}{\theta_c^3} \ln \frac{R}{d} \propto \frac{\ln N}{\theta_c^3}. \tag{27}$$

Expected $\mathcal{O}(N \log N)$ observed values near $\approx \frac{N^2}{100}$

Discussion

Questions?

Source Code:
`https://github.com/arminveres/comp-astro-hs23`

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