Go to Infinity in Real

Lattice Sum With Multipole Expansions

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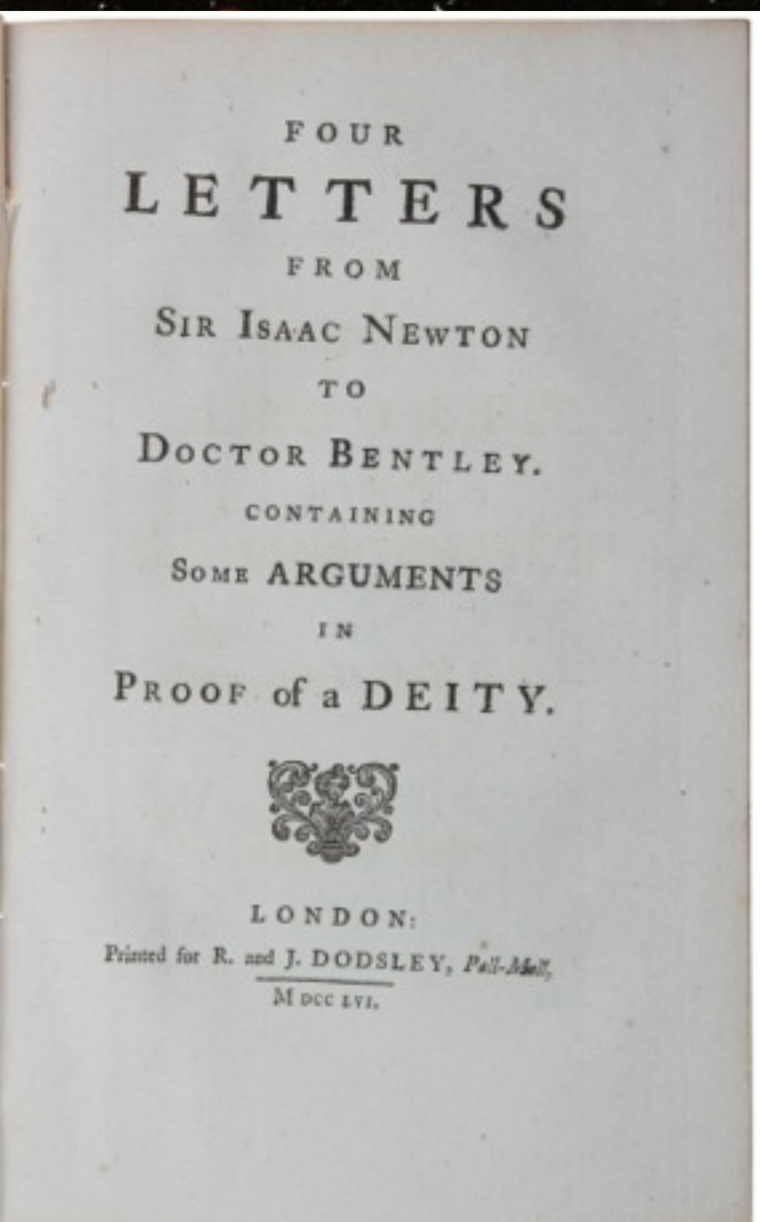
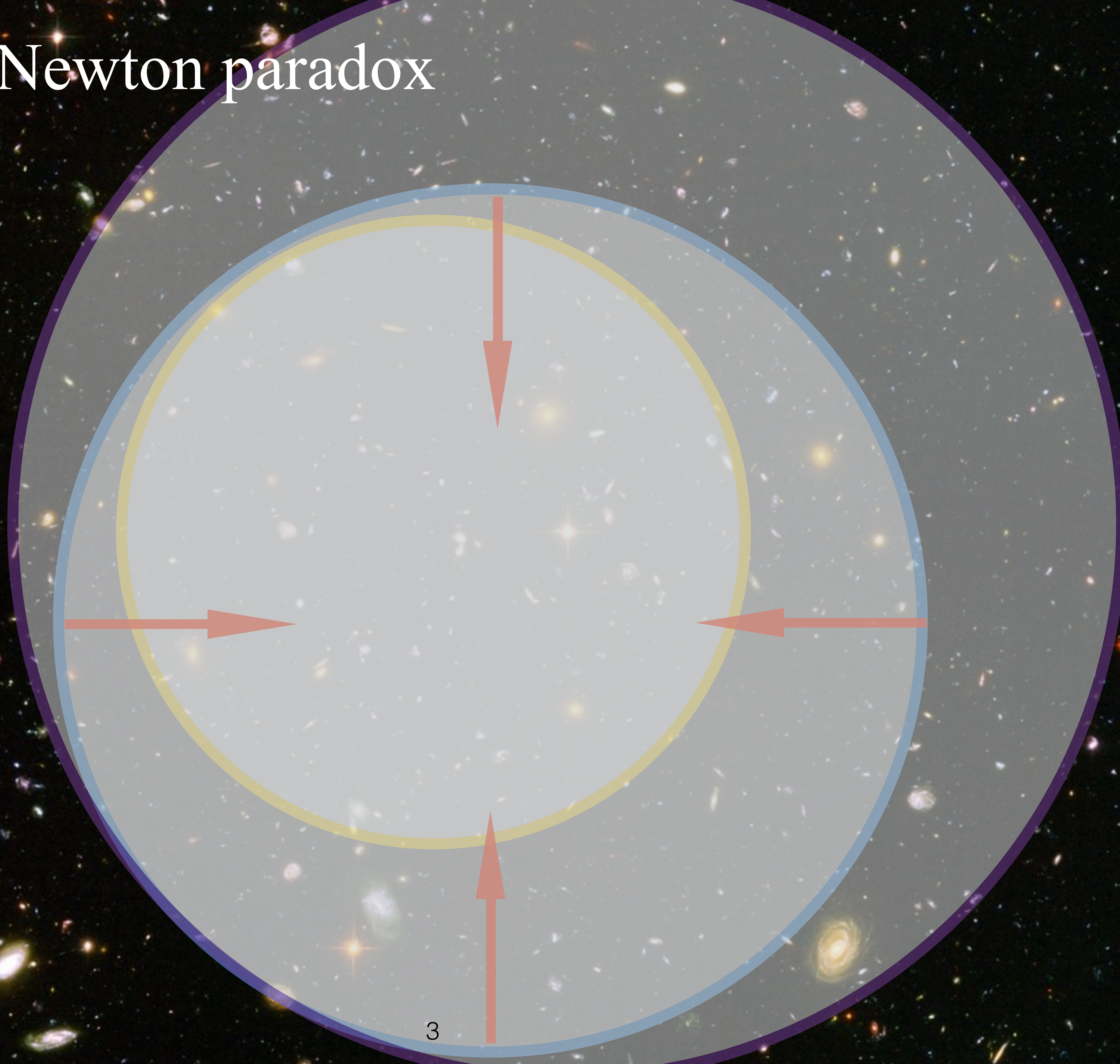
Pittsburgh in the news

Bentley-Newton paradox

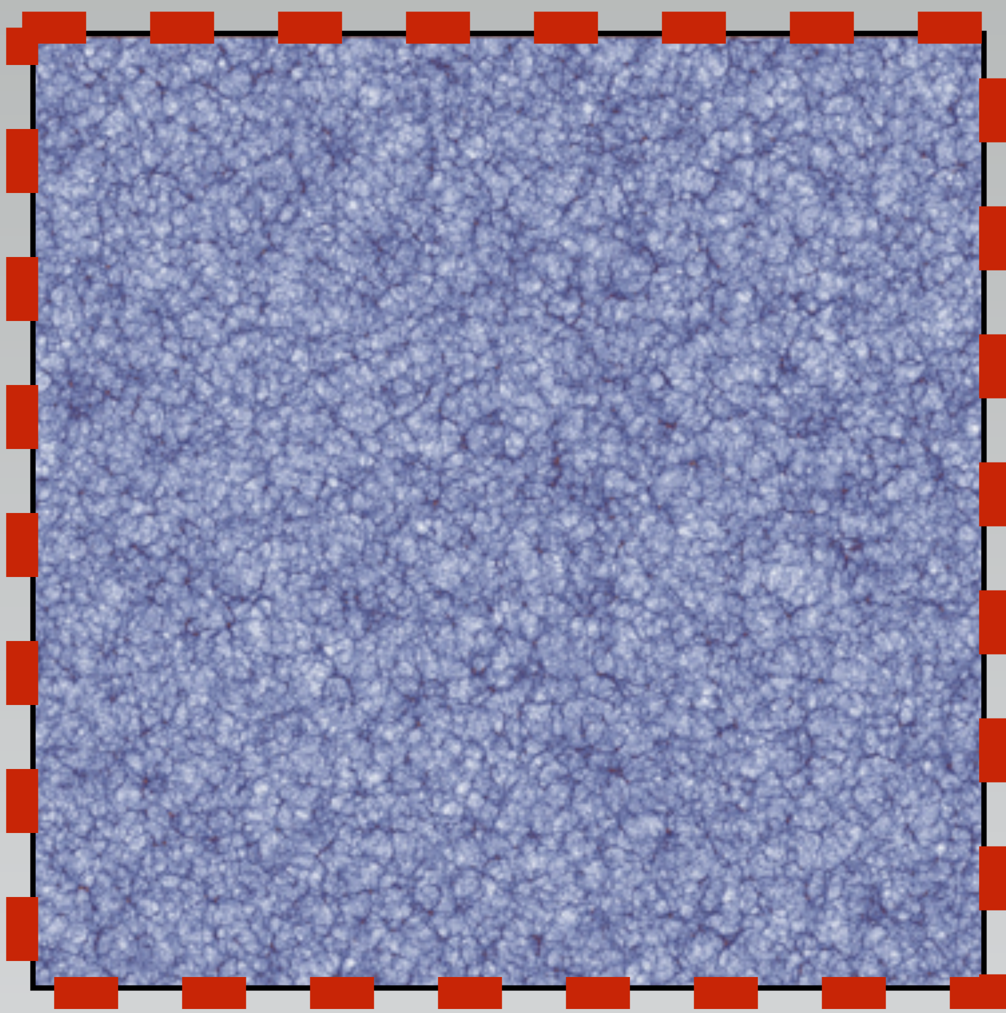

FOUR
LETTERS
FROM
SIR ISAAC NEWTON
TO
DOCTOR BENTLEY.
CONTAINING
SOME ARGUMENTS
IN
PROOF of a DEITY.

LONDON:
Printed for R. and J. DODSLEY, Pall-Mall,
M DCC LVI.

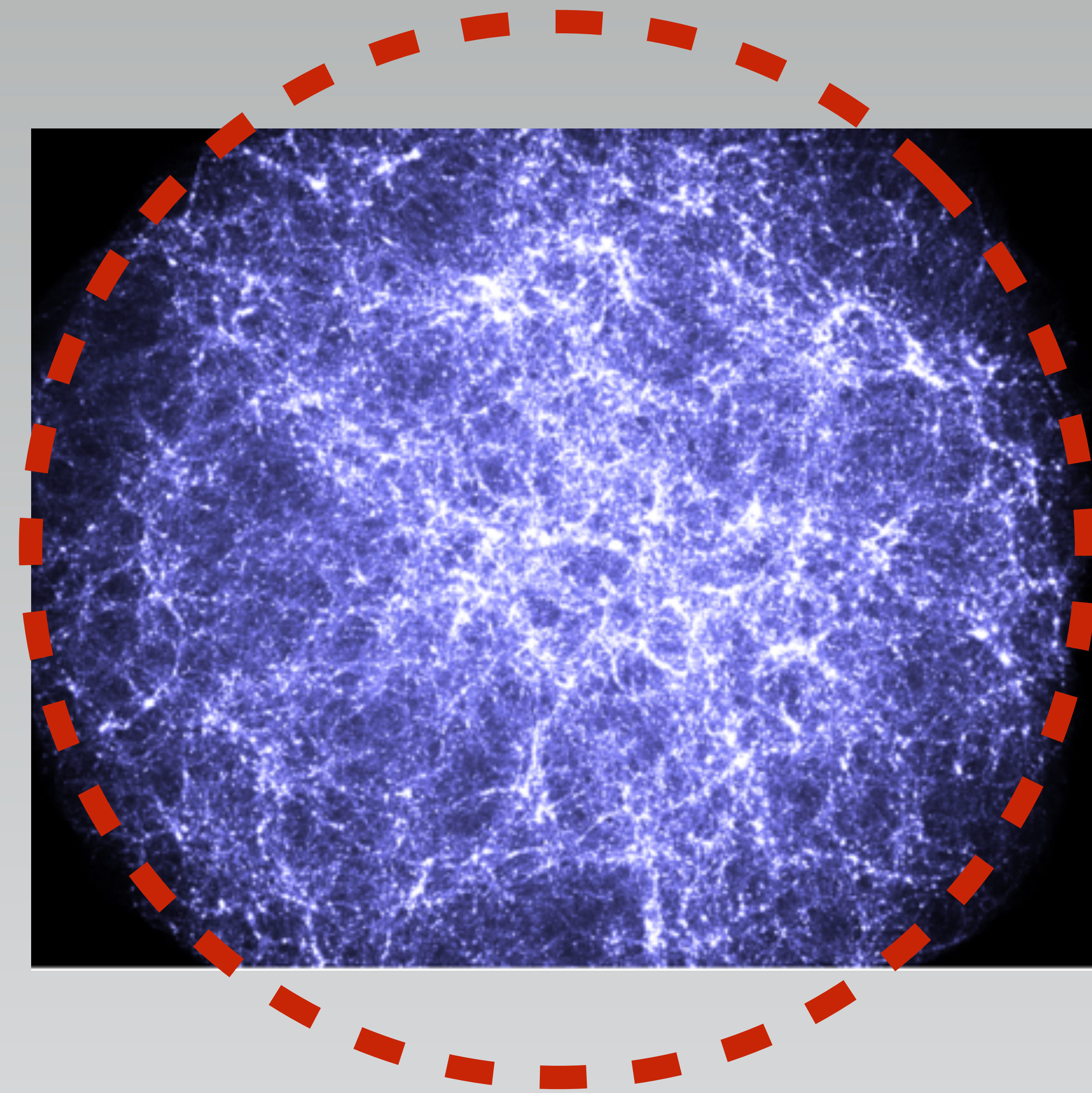
Bentley-Newton paradox



Spot the difference



Millennium-XXL
Angulo+2012



Hamada+2009

Hubble ultra deep field

Universe in computers

Who started it? “Gang of Four”

"Gang of Four" Receives $500,000 Gruber Cosmology Prize for Reconstructing How the Universe Grew

June 1, 2011, New York, NY –Four astronomers who found a way to recreate the growth of the universe are the recipients of the 2011 Cosmology Prize of The Peter and Patricia Gruber Foundation. Marc Davis, a professor in the Departments of Astronomy and Physics at the University of California at Berkeley; George Efstathiou, the director of the Kavli Institute for Cosmology in Cambridge; Carlos Frenk, the director of the Institute for Computational Cosmology at Durham University; and Simon White, a director of the Max Planck Institute for Astrophysics in Garching, Germany, will share the $500,000 award.

Marc Davis

George Efstathiou

Carlos Frenk

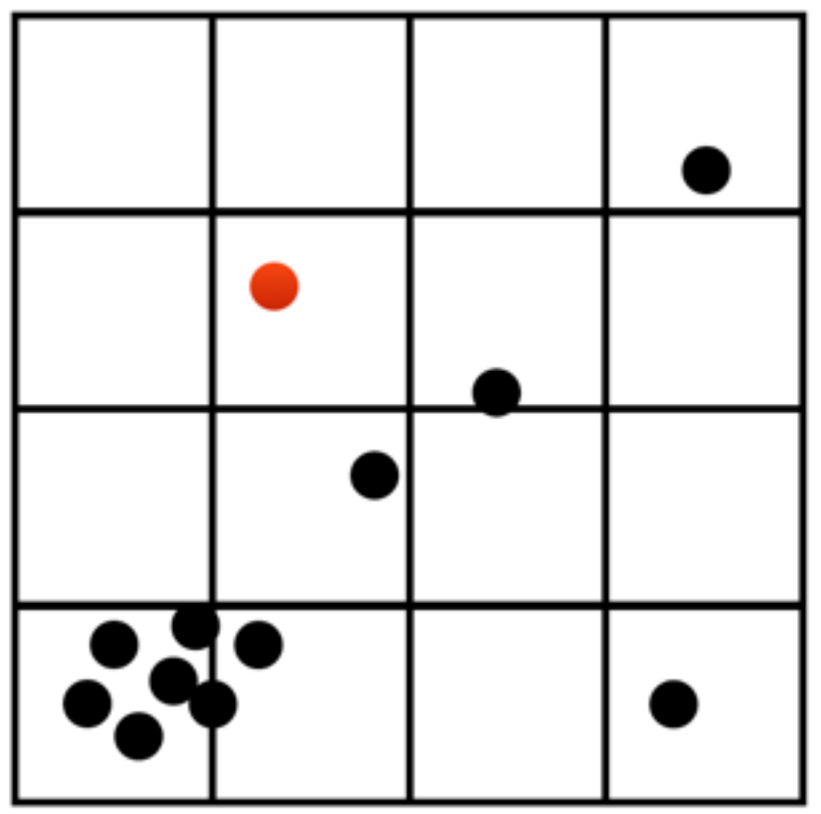
Simon White

Solving Poisson's equation in Fourier space

In *theory*: $\nabla^2\Phi(\mathbf{r}) = 4\pi G\rho(\mathbf{r}) \xrightarrow{\exp(-i\mathbf{k}\cdot\mathbf{r})} -k^2\hat{\Phi}(\mathbf{k}) = 4\pi G\hat{\rho}(\mathbf{k})$

In *practice*:

$$\{x_i, y_i, z_i\} \xrightarrow{\text{gridding}} \rho(\mathbf{r}) \xrightarrow{\text{FFT}} \hat{\rho}(\mathbf{k}) \xrightarrow{-\frac{1}{k^2}} \hat{\Phi}(\mathbf{k}) \xrightarrow{\text{IFFT}} \Phi(\mathbf{r}) \xrightarrow{\text{FD}} \mathbf{F}(\mathbf{r})$$



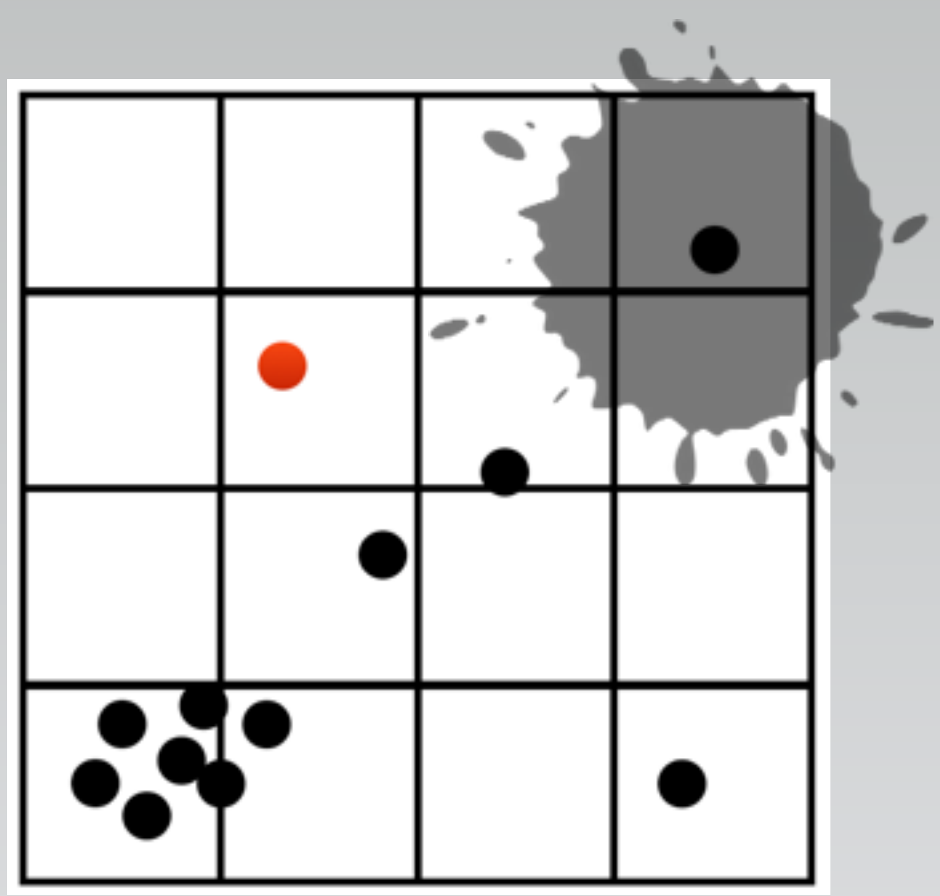
- Perturbations are calculated in Fourier space;
- PM is much faster than pure direct summation;
- Also faster than BH tree (1986);
- Inaccuracies in short range compensated by P3M;
- Somebody else has already written FFT(fully tested)
- Periodic boundary condition done right for free.

Solving Poisson's equation in Fourier space

$$\{x_i, y_i, z_i\} \xrightarrow{\text{gridding}} \rho(\mathbf{r}) \xrightarrow{\text{FFT}} \hat{\rho}(\mathbf{k}) \xrightarrow{-\frac{1}{k^2}} \hat{\Phi}(\mathbf{k}) \xrightarrow{\text{IFFT}} \Phi(\mathbf{r}) \xrightarrow{\text{FD}} \mathbf{F}(\mathbf{r})$$

real-space solvers

loss of translational symmetry



- Mass assignment (NGP, CIC, TSC, QPM…);
- Force anisotropy: W = W(x)W(y)W(z);
- Finite difference operator;
- Match the accuracies in real- and Fourier- forces;
- Density field is always under-sampled: ***aliasing***.

Vary the mesh size; perturb the mesh locations…

- Jing 2004; Cui 2008; Sefusatti 2017; Hand 2017…

From exact to approximate gravity solvers

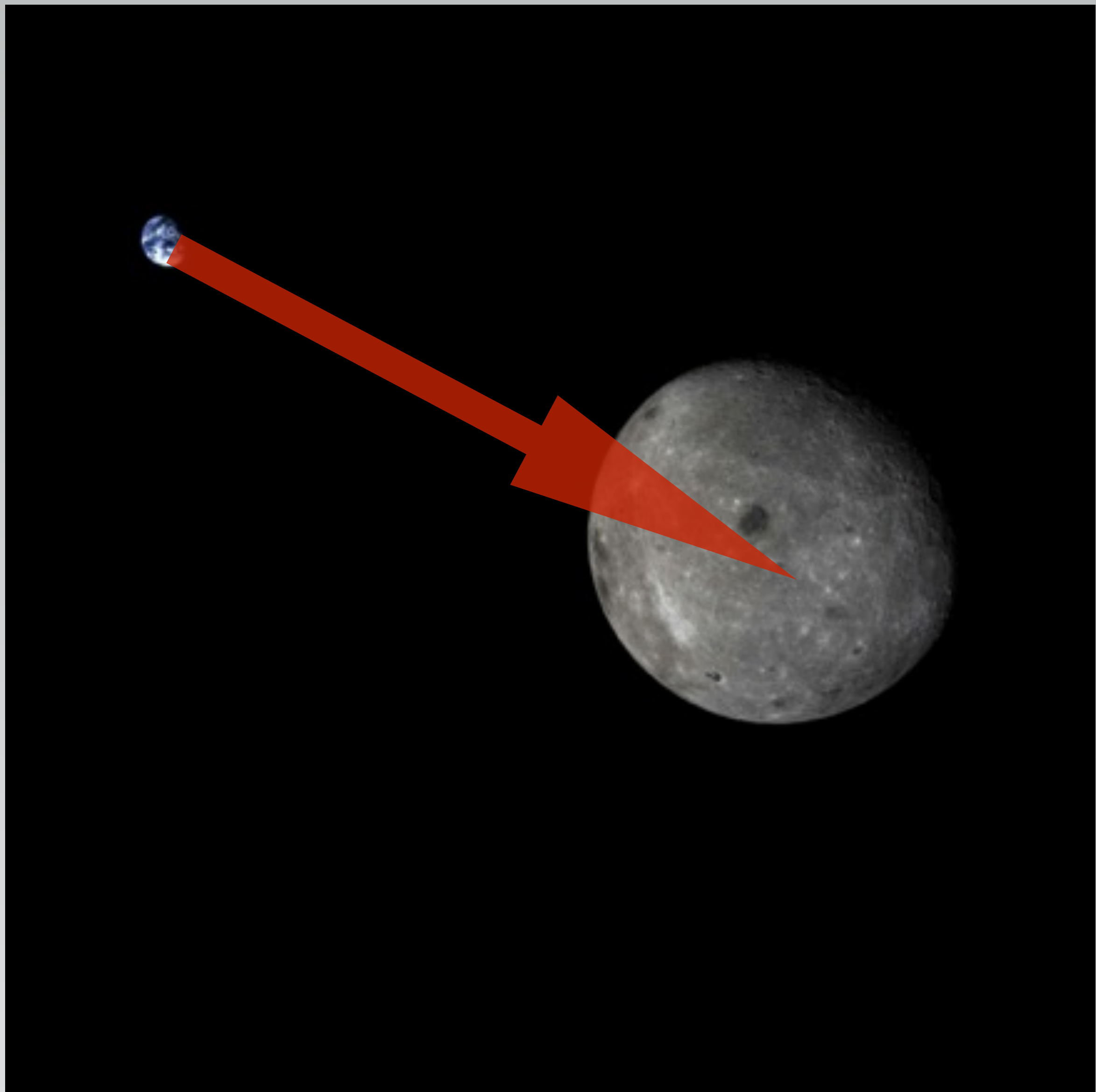
$$\mathcal{O}(N^2) \xrightarrow{\text{sources}} \mathcal{O}(N\log(N)) \xrightarrow{\text{sinks}} \mathcal{O}(N)$$

direct summation | BH tree | FMM

Key idea of FMM:

Approximate the force from a group of particles onto another group of particles with a single operation.

***Jargon*: multipole-to-local (M2L), cell-cell interaction…**



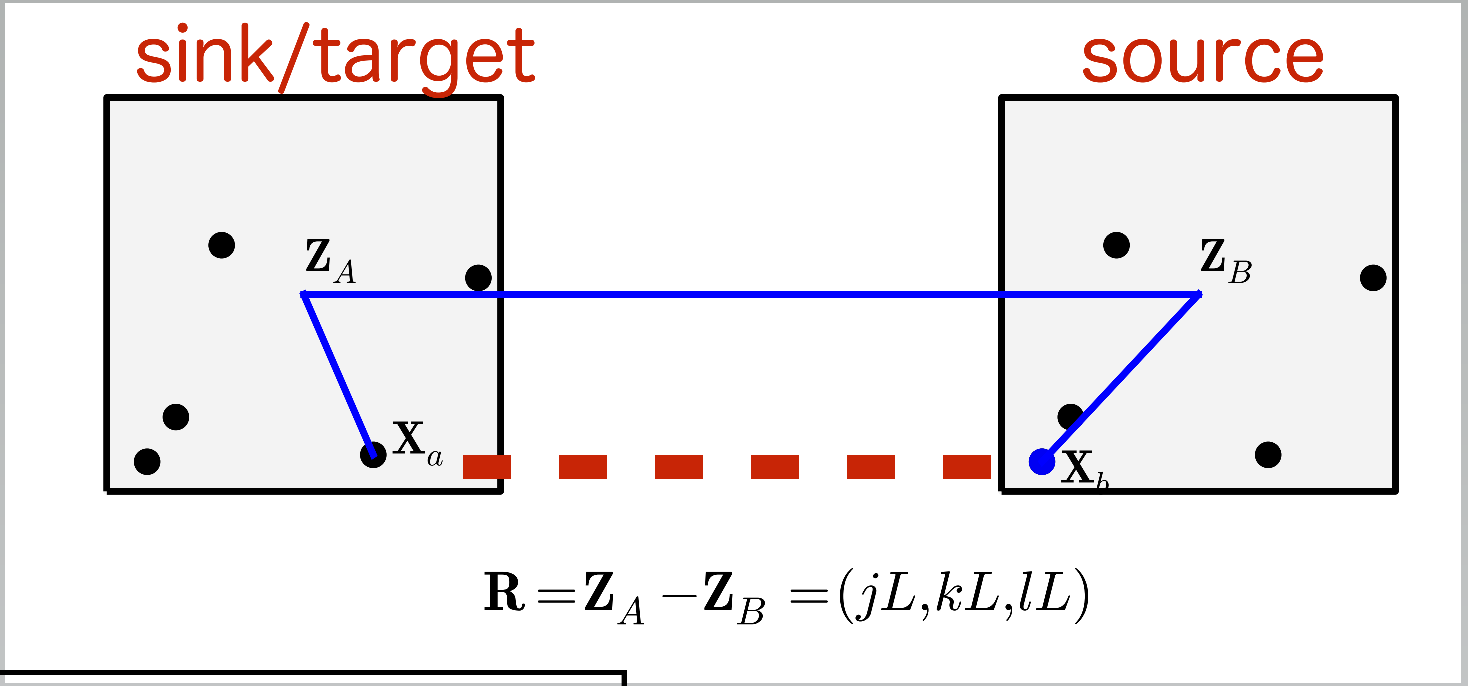
FMM Taylor expand 1/r on both sides

pre-80s: Maxwell; Kellog

80s: Greengard, Rokhlin;

F. Zhao(赵峰)

90s—now: Warren, Dehnen, Stadel…



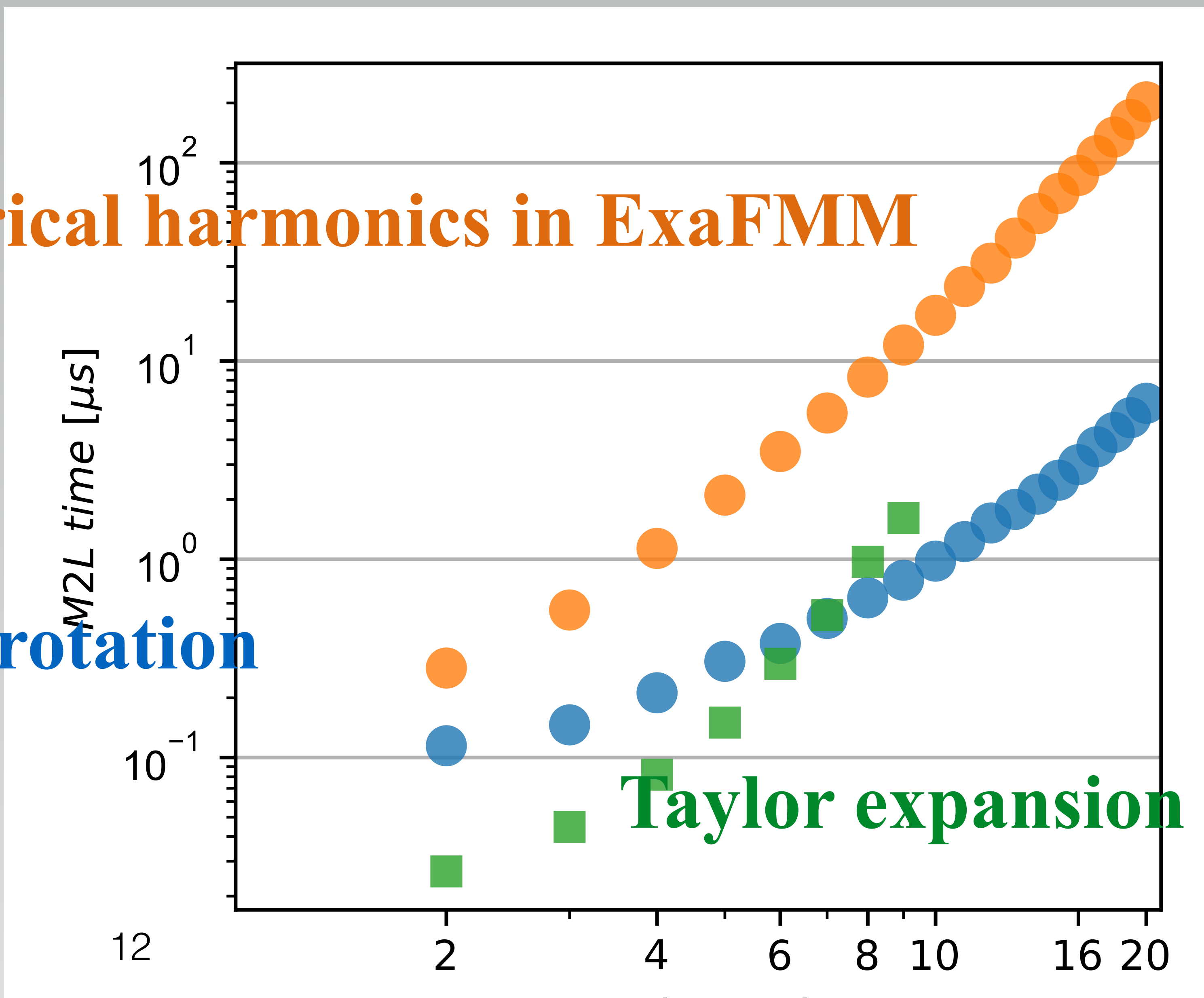
$$\Phi(\mathbf{X}_a - \mathbf{X}_b) = \Phi(\mathbf{r}_a - \mathbf{r}_b + \mathbf{R})$$
$$= \sum_{|\mathbf{n}|=0}^{\infty} \frac{1}{\mathbf{n}!}\mathbf{r}_a^{\mathbf{n}} \sum_{\mathbf{m}=0}^{p-|\mathbf{n}|} \frac{1}{\mathbf{m}!}(-\mathbf{r}_b)^{\mathbf{m}} \nabla^{\mathbf{n}+\mathbf{m}}\Phi(\mathbf{R})$$
$$\approx \sum_{|\mathbf{n}|=0}^{p} \frac{1}{\mathbf{n}!}\mathbf{r}_a^{\mathbf{n}} \sum_{\mathbf{m}=0}^{p-|\mathbf{n}|} \frac{1}{\mathbf{m}!}(-\mathbf{r}_b)^{\mathbf{m}} \nabla^{\mathbf{n}+\mathbf{m}}\Phi(\mathbf{R})$$

momentum-conserving, $\text{error} \sim \dfrac{(r_a + r_b)^p}{(R - r_a - r_b)^p}$

Taylor expansion is faster than SH at small *p*

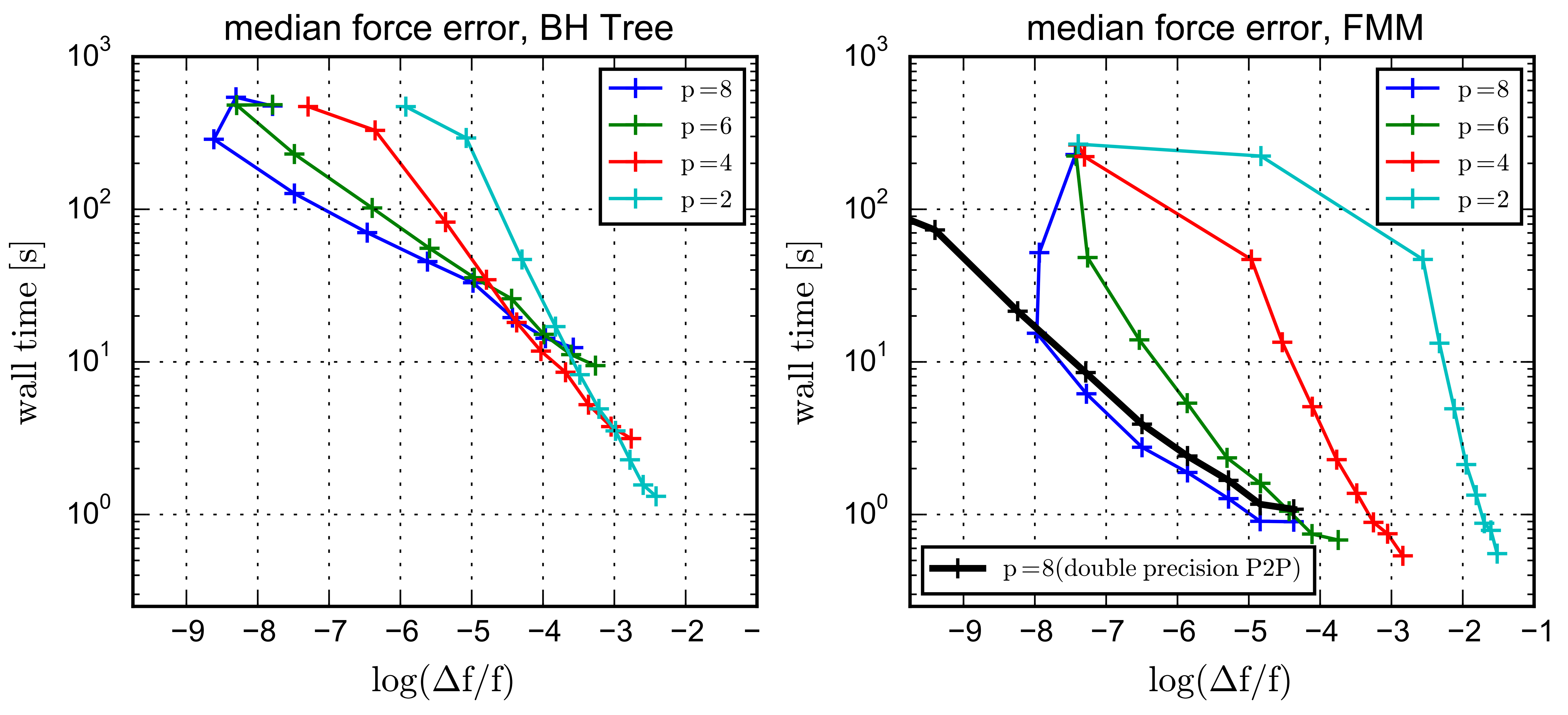
Evaluations of simple but cumbersome polynomials; simple + and *, no complex numbers…

```
L[1]+= M[10]*d[20]+M[11]*d[21]+M[12]*d[22]+M[13]*d[23]+M[14]*d[25]+M[15]*d[26]+M[16]*d[27]+M[17]*d[29]+M[18]*d[30]+M[19]*d[32];
L[2]+= M[10]*d[21]+M[11]*d[22]+M[12]*d[23]+M[13]*d[24]+M[14]*d[26]+M[15]*d[27]+M[16]*d[28]+M[17]*d[30]+M[18]*d[31]+M[19]*d[33];
L[3]+= M[10]*d[25]+M[11]*d[26]+M[12]*d[27]+M[13]*d[28]+M[14]*d[29]+M[15]*d[30]+M[16]*d[31]+M[17]*d[32]+M[18]*d[33]+M[19]*d[34];
```



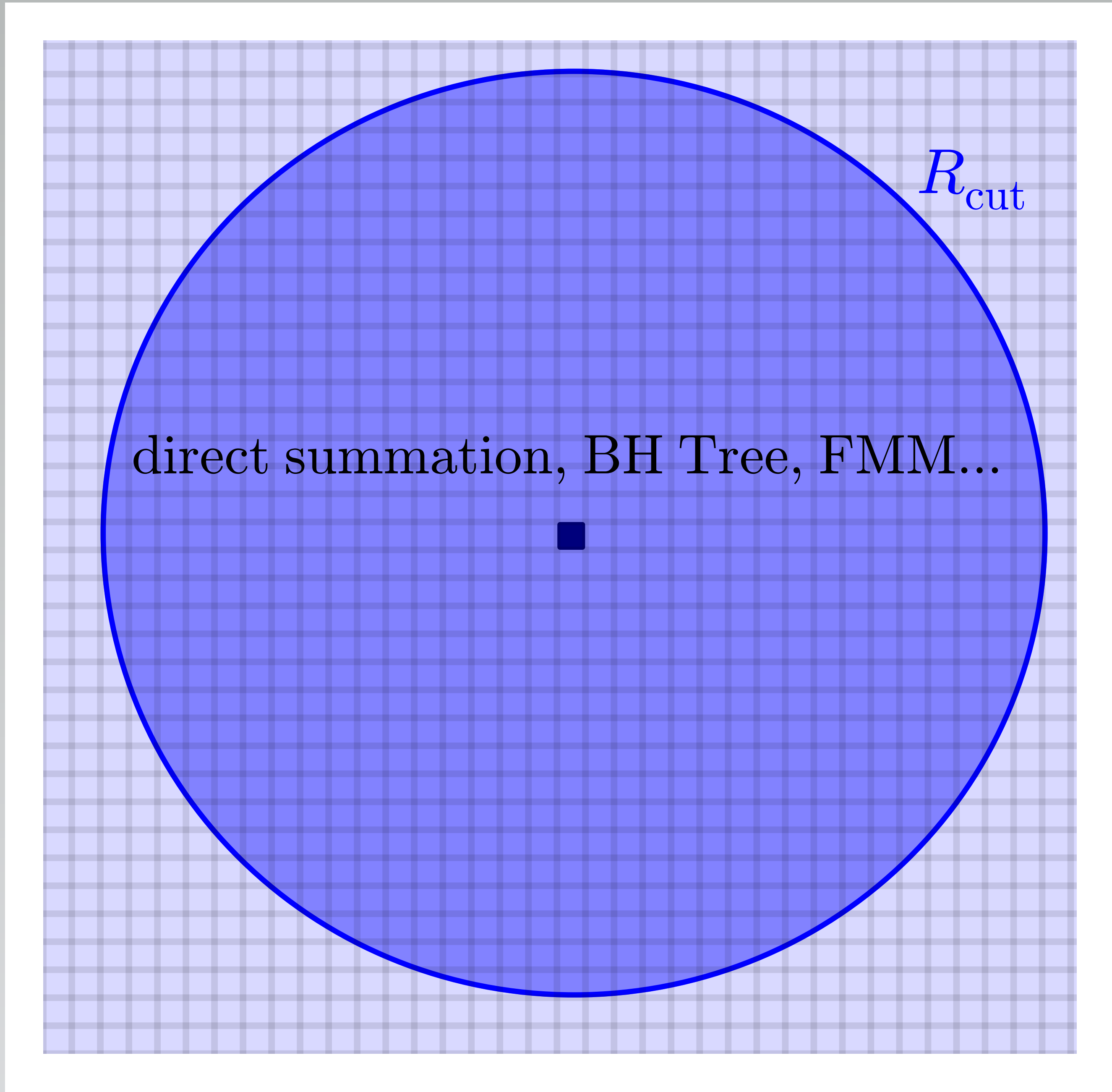
High order expansion with FMM

Cost to obtain median force error for an isolated Hernquist profile



PBC with real-space force solvers

cut-off error: $\mathcal{O}(R^{-5})$

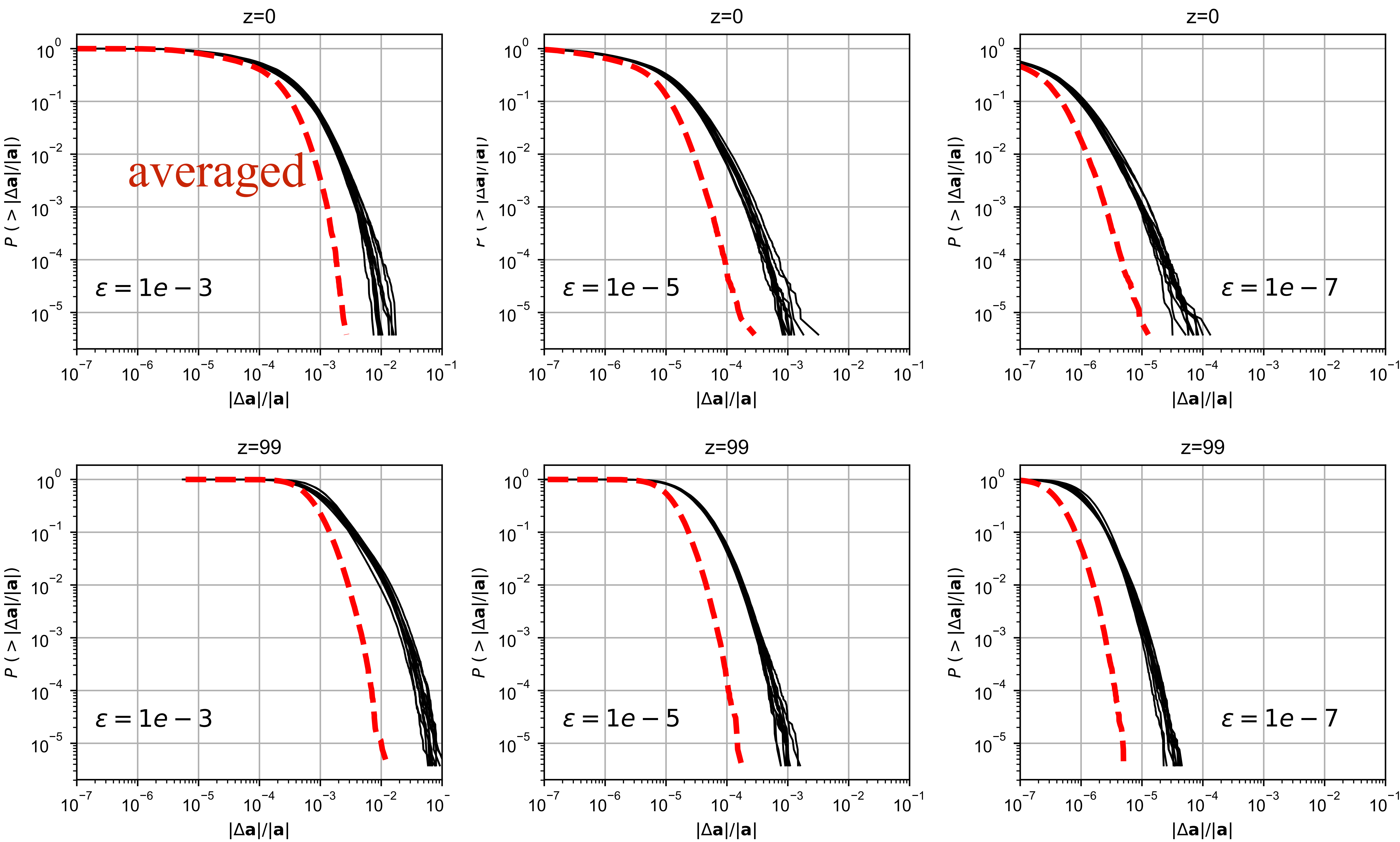


A. Arrange replicas spherically with original box in the center;
B. R_cut: 100L~1000L;
C. Compute forces onto the original box from all the replicas;
D. Apply correction for boundary conditions:

$$\frac{4\pi G\rho}{3}(\mathbf{r}-\mathbf{r}_{\rm com})$$

Does it work?

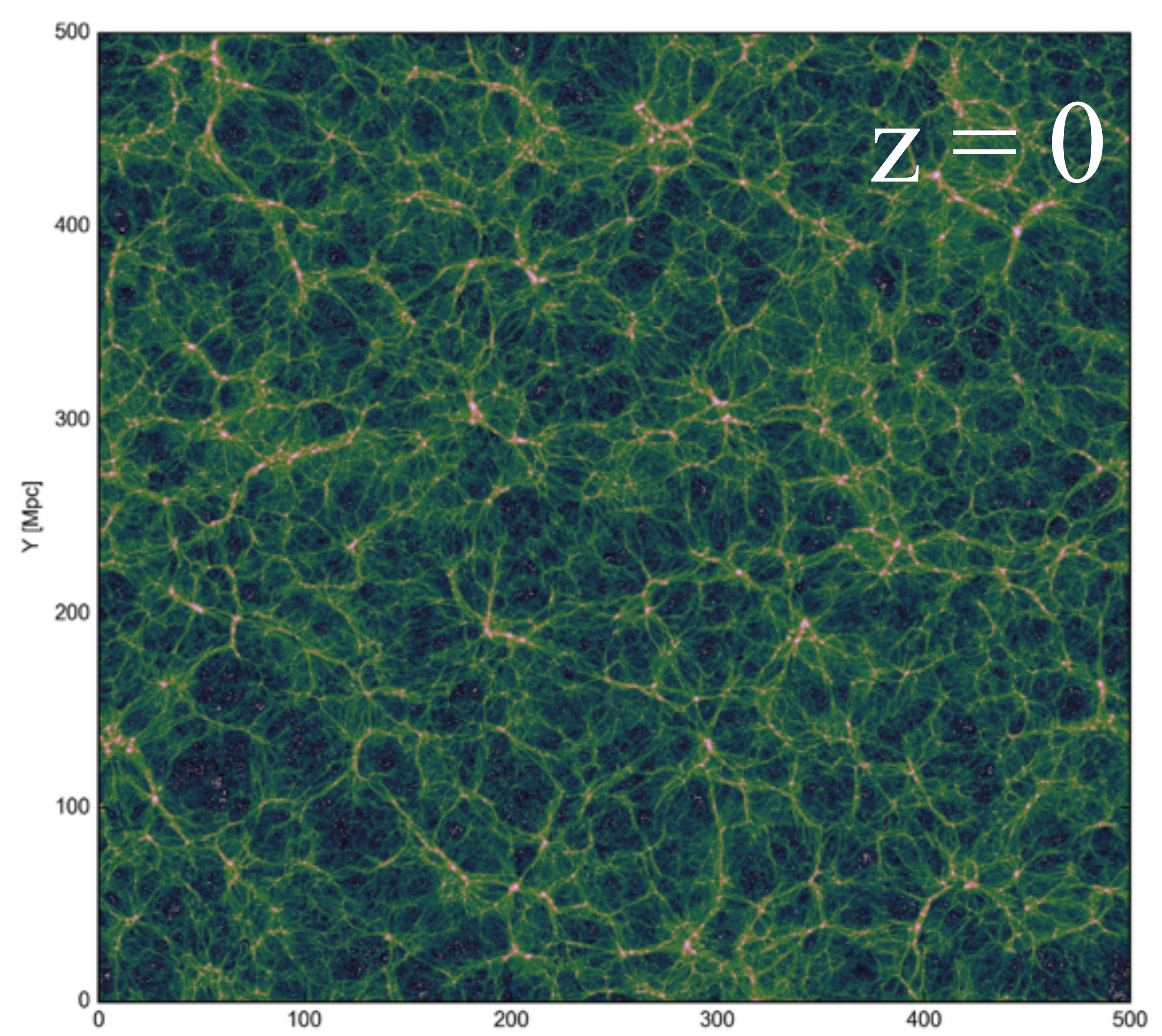
Compare FMM with high-precision Ewald sums



Does it work?

- Euclid code comparison ICs (Schneider+2015), 2048^3 particles.
- Parallel FMM using locally essential tree based on ExaFMM.
- Momentum-conserving integration.

For median force error ~10^{-5}
with 1024 CPUs
400 sec/step (high-z),
200 sec/step (low-z).



Approximation with first three multipoles

$$\text{Monopole (total mass/charge)}: Q_{\text{tot}} = \sum q_j$$

M
(multipoles)

$$\text{Dipole } \mathbf{P}: P_x = -\sum q_j x_j,\ P_y = -\sum q_j y_j,\ P_z = -\sum q_j z_j$$

$$\text{Quadrupole } \mathbb{Q}: Q_{xx} = \sum q_j x_j x_j/2,\ Q_{xy} = \sum q_j x_j y_j,\ Q_{xz} = \sum q_j x_j z_j \ldots$$

*****

d
(derivatives of 1/r)

$$\frac{1}{R},\ \frac{1}{R^3}(-R_x, -R_y, -R_z),\ \mathbb{D} = \frac{1}{R^5}\begin{bmatrix} 3R_x^2 - R^2 & 3R_xR_y & 3R_xR_z \\ 3R_xR_y & 3R_y^2 - R^2 & 3R_yR_z \\ 3R_xR_z & 3R_yR_z & 3R_z^2 - R^2 \end{bmatrix}$$

$$\Phi \approx \frac{Q_{\text{tot}}}{R} - \frac{Q_{\text{tot}}}{R^3}(xR_x + yR_y + zR_z) + \frac{1}{R^3}(P_{\text{x}}R_x + P_{\text{y}}R_y + P_{\text{z}}R_z)$$

$$+ Q_{\text{tot}}\{\frac{xx}{2}D_{xx} + xyD_{xy} + xzD_{xz} + \frac{yy}{2}D_{yy} + yzD_{yz} + \frac{zz}{2}D_{zz}\}$$
$$- x(P_xD_{xx} + P_yD_{xy} + P_zD_{xz})$$
$$- y(P_xD_{xy} + P_yD_{yy} + P_zD_{yz})$$
$$- z(P_xD_{xz} + P_yD_{yz} + P_zD_{zz})$$
$$+ \{Q_{xx}D_{xx} + Q_{xy}D_{xy} + Q_{xz}D_{xz} + Q_{yy}D_{yy} + Q_{yz}D_{yz} + Q_{zz}D_{zz}\} + \ldots$$

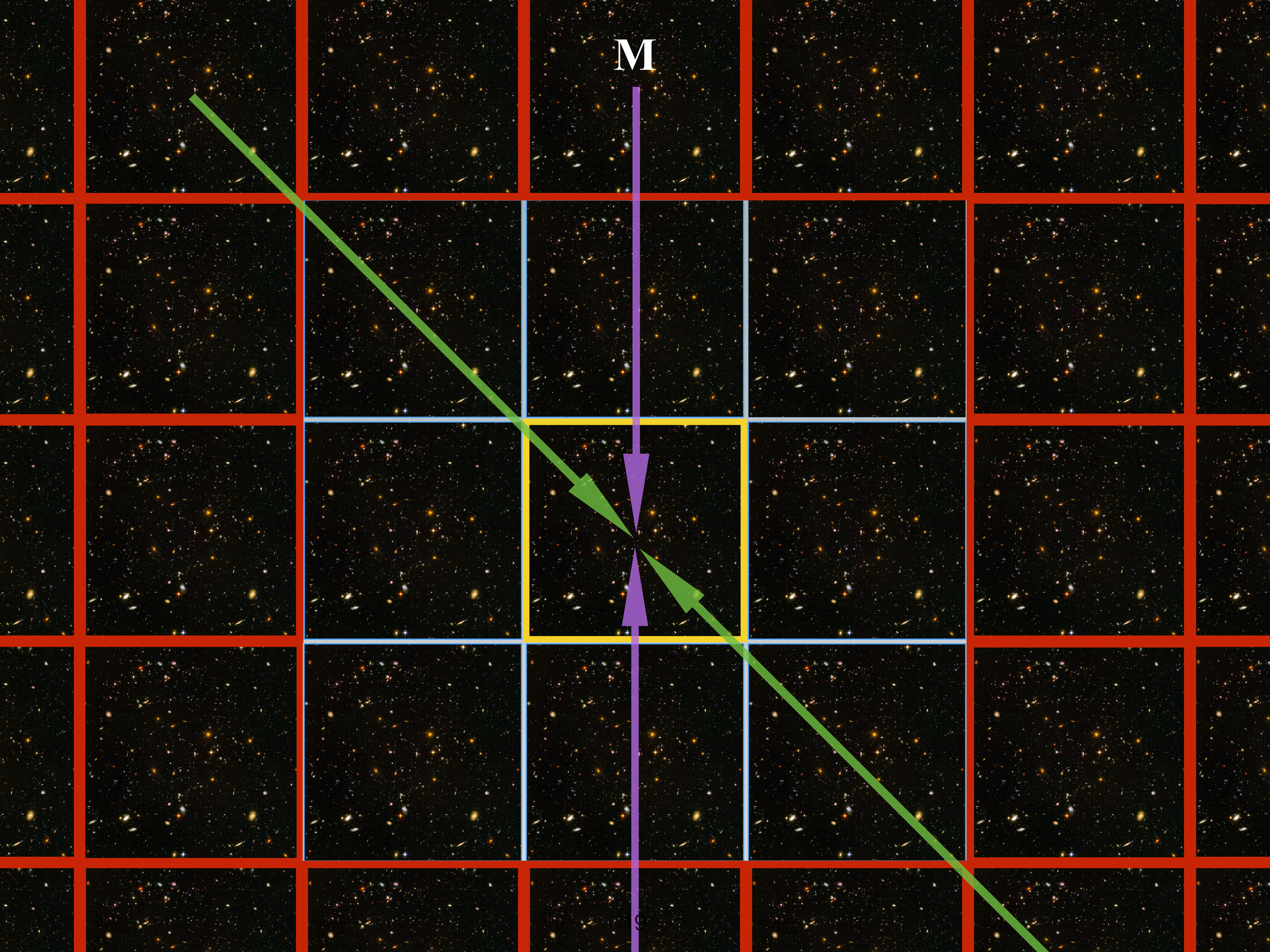
~1/R^2

~1/R^3

Only monopoles are causing troubles

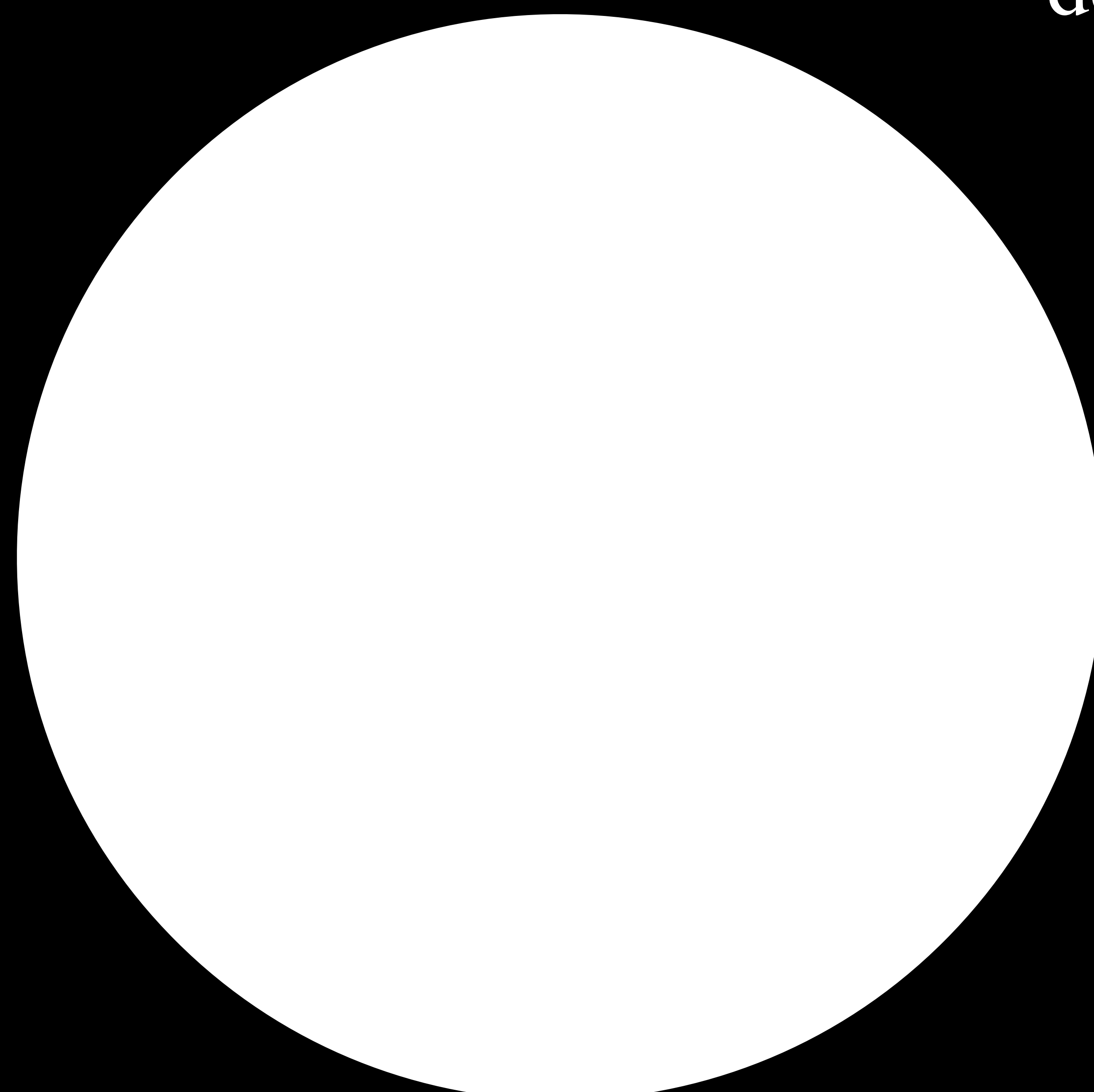
$$\begin{bmatrix} f_x \\ f_y \\ f_z \end{bmatrix} = -\nabla\Phi = -\frac{Q_{\text{tot}}}{R^3}\begin{bmatrix} R_x \\ R_y \\ R_z \end{bmatrix} - \mathbb{D}\begin{bmatrix} P_x \\ P_y \\ P_z \end{bmatrix} + Q_{\text{tot}}\mathbb{D}\begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

$$\mathbb{D} = \frac{1}{R^5}\begin{bmatrix} 3R_x^2 - R^2 & 3R_xR_y & 3R_xR_z \\ 3R_xR_y & 3R_y^2 - R^2 & 3R_yR_z \\ 3R_xR_z & 3R_yR_z & 3R_z^2 - R^2 \end{bmatrix}$$


M

Only monopoles are causing troubles

density = Q_tot/L^3



Replace summation with integration (R_cut >>L)

Conclusions

- Periodic boundary conditions can be imposed without Fourier method; solve the integral form instead of the differential form of Poisson's equation.
- The correction takes very similar form as the open (vacuum) boundary condition.
- Only need one (Gadget-like) force error tolerance parameter.
- The cut-off error can be made arbitrarily small, falls off as O(R^-5).
- The above approach is best realized with FMM; one single translation for almost the entire spherical volume.

Magic tricks by Lord Rayleigh

$$
\begin{aligned}
\sum \mathbb{D} &= \sum \frac{1}{R^5} \begin{bmatrix} 3R_x^2 - R^2 & 3R_xR_y & 3R_xR_z \\ 3R_xR_y & 3R_y^2 - R^2 & 3R_yR_z \\ 3R_xR_z & 3R_yR_z & 3R_z^2 - R^2 \end{bmatrix} \\
&= \sum \frac{1}{R^5} \begin{bmatrix} 3R_x^2 - R^2 & 0 & 0 \\ 0 & 3R_y^2 - R^2 & 0 \\ 0 & 0 & 3R_z^2 - R^2 \end{bmatrix} \\
&= \frac{4\pi}{3L^3} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}
\end{aligned}
$$

LVI. *On the Influence of Obstacles arranged in Rectangular Order upon the Properties of a Medium.* *By* Lord RAYLEIGH, *Sec. R.S.**

Magic tricks by Lord Rayleigh

We now proceed to the calculation of S_2. We have

$$S_2 = \Sigma \frac{3\mu^2 - 1}{2\rho^3} = \Sigma \frac{2\xi^2 - \eta^2 - \zeta^2}{2\rho^5} = -\tfrac{1}{2}\Sigma \frac{d}{d\xi}\left(\frac{\xi}{\rho^3}\right).$$

Now when ρ is sufficiently great, the summation may be replaced by an integration; thus

$$S_2 = -\iiint \frac{d}{d\xi}\left(\frac{\xi}{\rho^3}\right) d\xi \, d\eta \, d\zeta.$$

In this,

$$\int_v^\infty \frac{d}{d\xi}\frac{\xi}{\rho^3}\, d\xi = -\frac{v}{(v^2+\eta^2+\zeta^2)^{\frac{3}{2}}},$$

$$\int_{-v}^{+v} \frac{v\, d\eta}{(v^2+\eta^2+\zeta^2)^{\frac{3}{2}}} = \frac{2v^2}{(v^2+\zeta^2)\,(2v^2+\zeta^2)^{\frac{1}{2}}},$$

and finally

$$\int_{-v}^{+v} \frac{v^2 d\zeta}{(v^2+\zeta^2)\,(2v^2+\zeta^2)^{\frac{1}{2}}} = \int_0^1 \frac{2d\theta}{\sqrt{(2+\tan^2\theta)}}$$

$$= \int_0^{1/\sqrt{2}} \frac{2ds}{\sqrt{(2-s^2)}} = \frac{\pi}{3}.$$

Thus

$$S_2 = \frac{2\pi}{3} \quad \ldots\ldots\ldots\ldots \quad (65)$$

Taylor expansion on which side?

Newton

J. Barnes and P. Hut

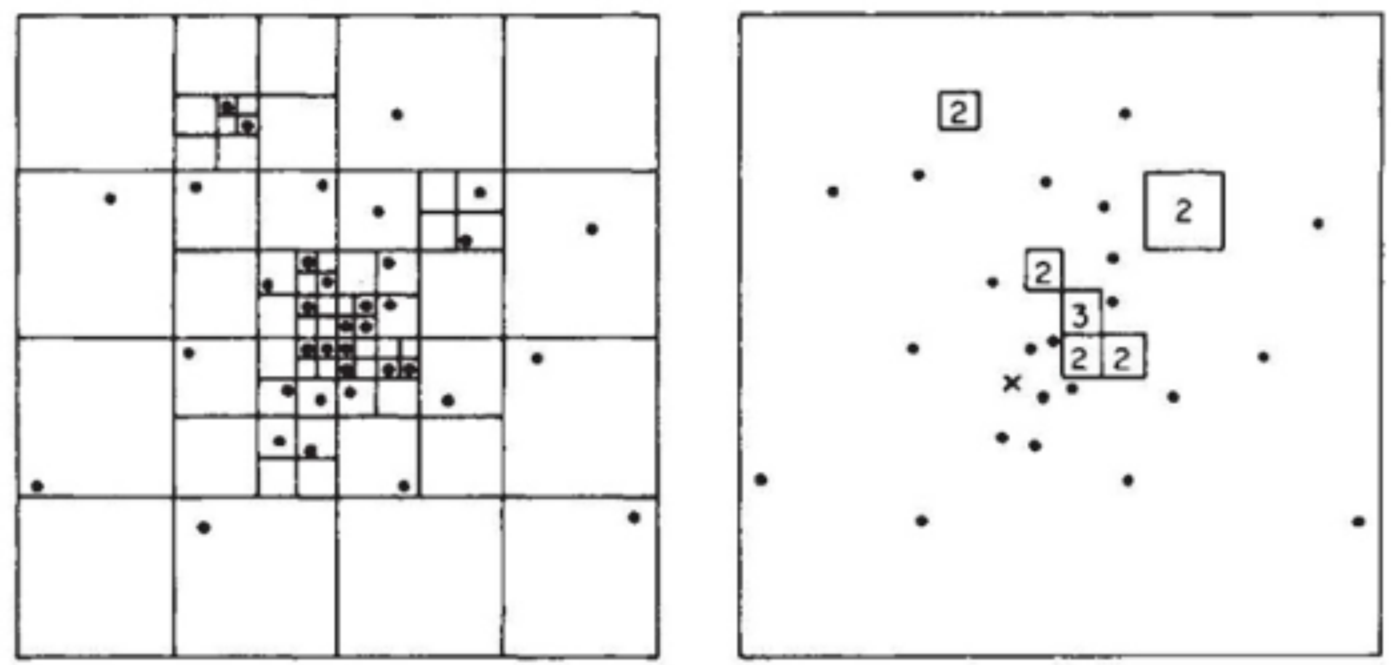


Fig. 1 Hierarchical boxing and force calculation, presented for simplicity in two dimensions. On the left, a system of particles and the recursive subdivision of system space induced by these particles. Our algorithm makes the minimum number of subdivisions necessary to isolate each particle. On the right, how the force on particle *x* is calculated. Fitted cells contain particles that have been lumped together by our 'opening angle' criterion; each such cell represents a single term in the force summation.

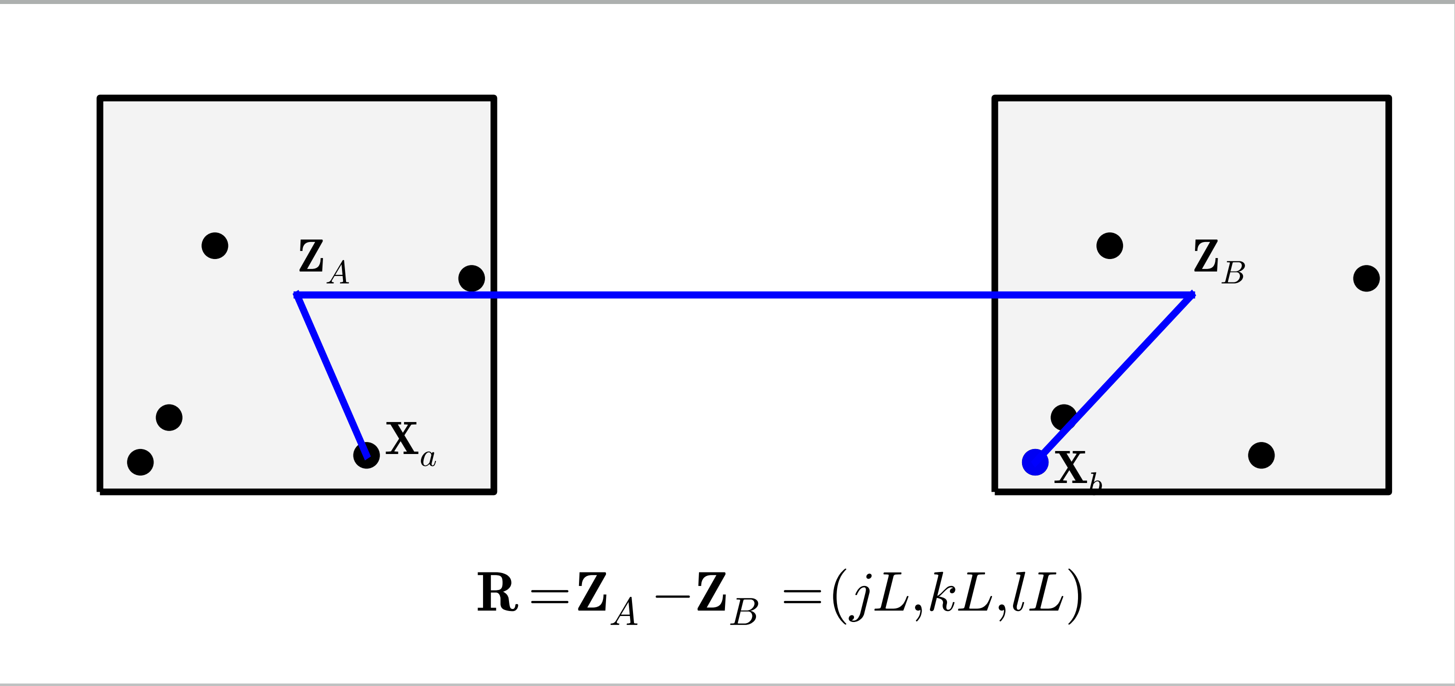
Infinity is reserved solely for God

…it seems to me that if the matter of our sun and planets and all the matter in the universe were evenly scattered throughout all the heavens, and every particle had an innate gravity toward all the rest, and the whole space throughout which this matter was scattered was but **finite**, the matter on the outside of the space would, **by its gravity, tend toward all the matter on the inside**, and by consequence, fall down into the middle of the whole space and there compose one great spherical mass. But if the matter was evenly disposed throughout an **infinite** space, it could never convene into one mass; but **some of it would convene into one mass and some into another**, so as to make an infinite number of great masses, scattered at great distances from one to another…

Infinity is reserved solely for God

…a mathematician will tell you, that if a body stood **in equilibrio between any two equal and contrary attracting infinite forces**; and if to either of these forces you add any new finite attracting force, that new force, how little soever, will destroy their equilibrium, and put the body into the same motion…

Taylor expansion of 1/R on both sides



$$
\begin{aligned}
\Phi \approx \frac{Q_{\text{tot}}}{R} - \frac{Q_{\text{tot}}}{R^3}(xR_x + yR_y + zR_z) + \frac{1}{R^3}(P_{\text{x}}R_x + P_{\text{y}}R_y + P_{\text{z}}R_z) \\
+ Q_{\text{tot}}\{\frac{xx}{2}D_{xx} + xyD_{xy} + xzD_{xz} + \frac{yy}{2}D_{yy} + yzD_{yz} + \frac{zz}{2}D_{zz}\} \\
- x(P_xD_{xx} + P_yD_{xy} + P_zD_{xz}) \\
- y(P_xD_{xy} + P_yD_{yy} + P_zD_{yz}) \\
- z(P_xD_{xz} + P_yD_{yz} + P_zD_{zz}) \\
+ \{Q_{xx}D_{xx} + Q_{xy}D_{xy} + Q_{xz}D_{xz} + Q_{yy}D_{yy} + Q_{yz}D_{yz} + Q_{zz}D_{zz}\} + \ldots
\end{aligned}
$$