$$\nabla^2 \Phi = 4\pi G\rho$$

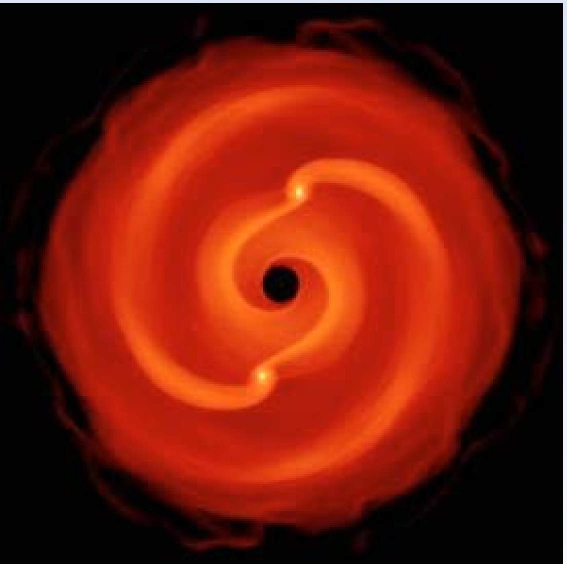
Self-Gravity: Open Boundary Condition
- The James's Algorithm

2019. 03. 19
In *Athena*++ developer meeting, Las Vegas

Sanghyuk Moon (Seoul National University)
Woong-Tae Kim (Seoul National University)
Eve C. Ostriker (Princeton University)

Motivation : Lack of efficient 3D cylindrical Poisson solver

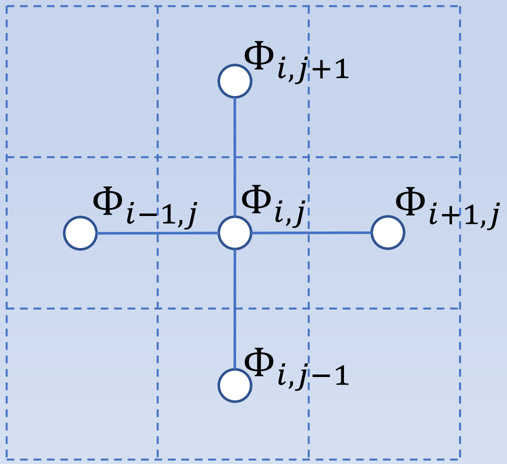
- FFT + direct summation (2D) : $O\left(N^3 + N^2 \log N\right)$
- Kalnajs logarithmic spiral (2D, logarithmic spacing): $O(N^2 \log N)$
- FFT + direct summation (3D) : $O\left(N^4 + N^3 \log N\right)$
- CCGF (3D; Cohl & Tohline 1999) : $O(m_{\max} N^3 + N^3 \log N)$



MRI+GI simulation in 3D cylindrical grid (Fromang 2005)
Self-gravity with CCGF method
Resolution : $128 \times 256 \times 64$ with $m_{\max} = 128$

In general, there are two approaches to solve the Poisson equation.

1. Finite difference methods (FFT, Multigrid, …)



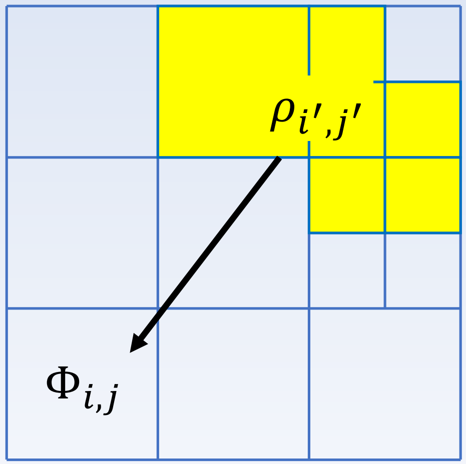
$$\nabla^2\Phi = 4\pi G\rho$$

- *Very efficient.*
- *Need to provide an appropriate boundary condition.*

2. Green's function methods (zero-padding FFT, multipole expansion, …)

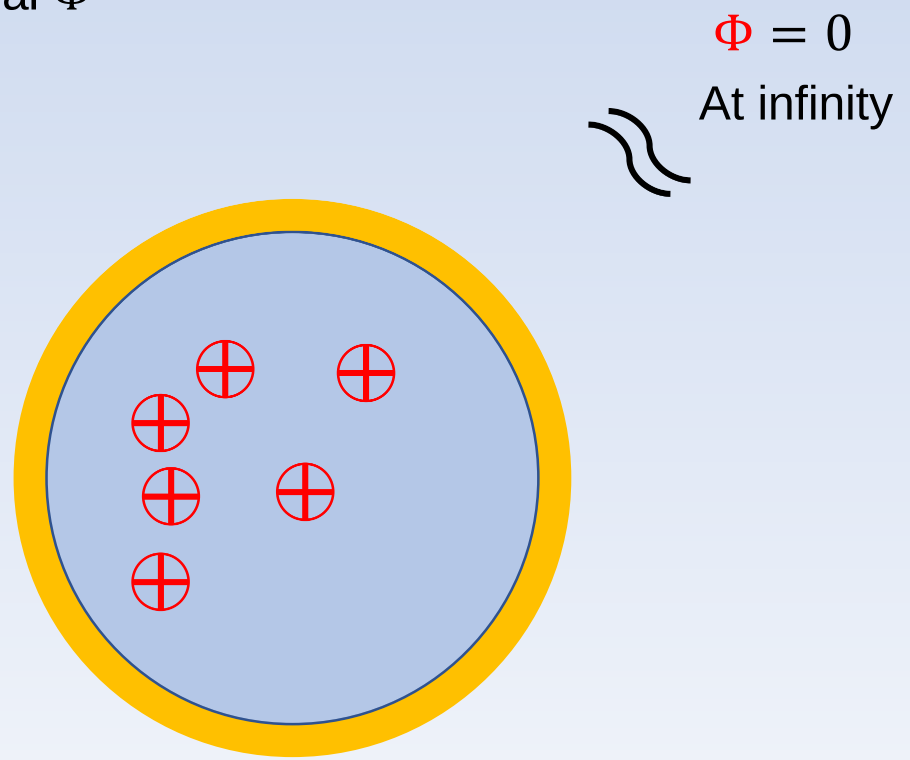
$$\Phi(\vec{x}) = -\iiint \frac{G\rho}{|\vec{x}-\vec{x}'|} d^3x'$$

- *Computationally expensive.*
- *Open BC is automatically satisfied.*
- ***Possible to calculate Φ only along the boundary.***



The James Algorithm (R. A. James 1977, JCoPh)

Let’s find electrostatic potential Φ



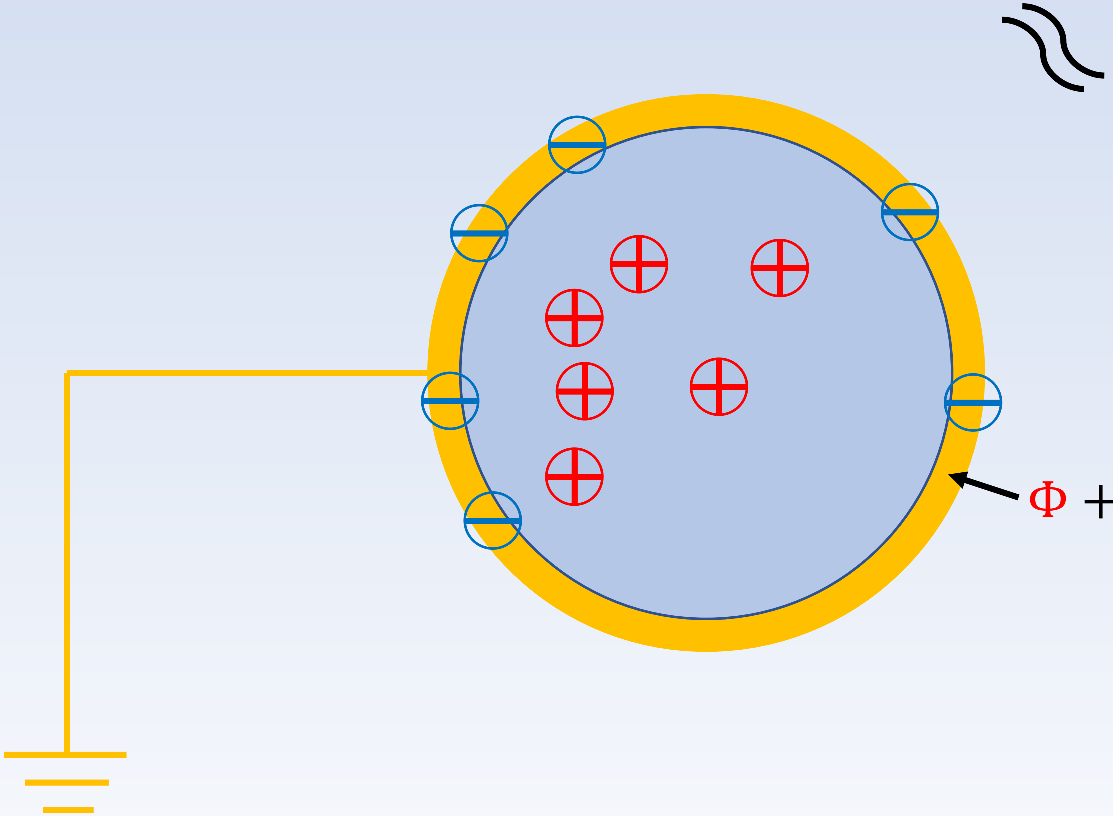
The James Algorithm (R. A. James 1977, JCoPh)

Let’s find electrostatic potential Φ

$\Phi = 0$

$\Theta = 0$

At infinity



$\Phi + \Theta = 0$

The James Algorithm (R. A. James 1977, JCoPh)

Let’s find electrostatic potential Φ

Green’s function method

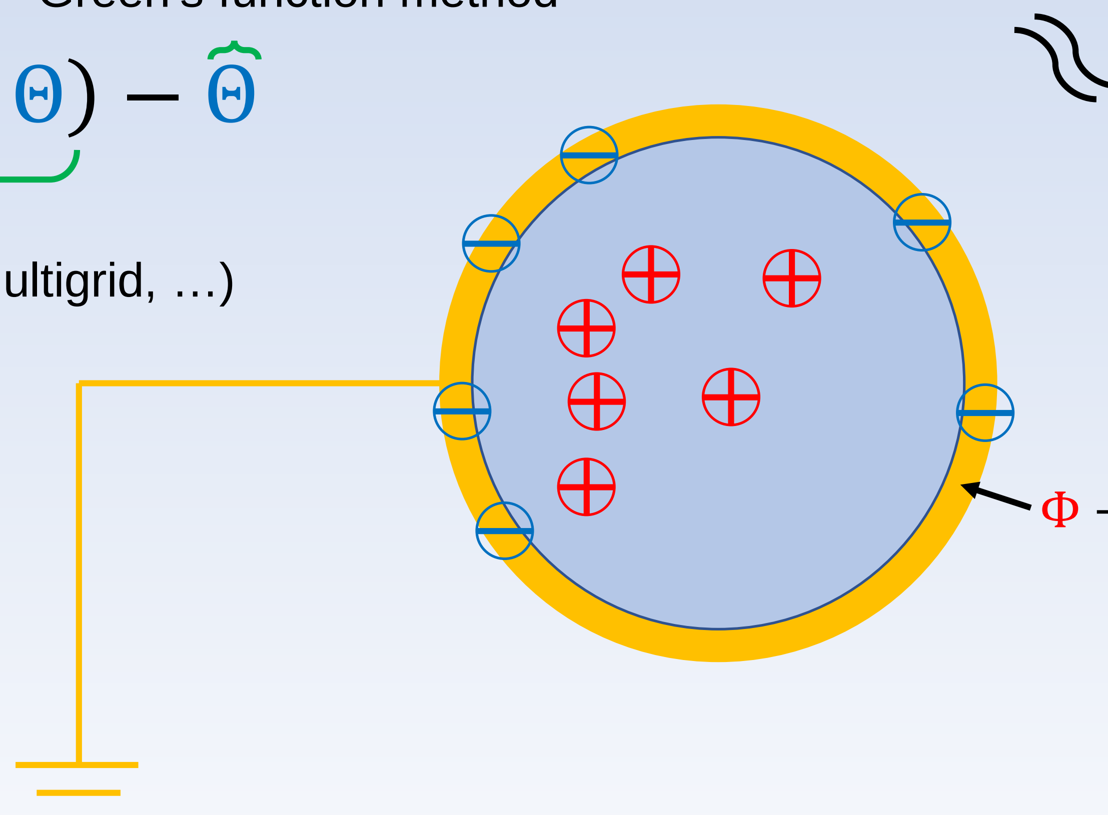
$$\Phi = \underbrace{(\Phi + \Theta)} - \overbrace{\Theta}$$

Zero-BC solver (FFT, multigrid, …)

$\Phi = 0$

$\Theta = 0$

At infinity



$\Phi + \Theta = 0$

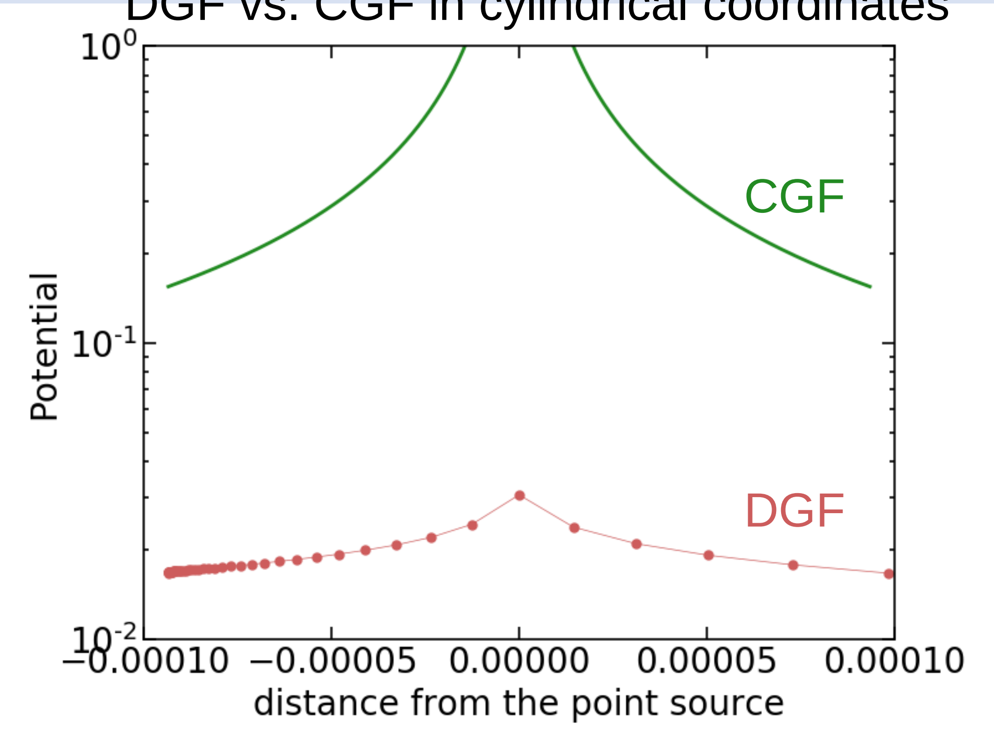
Discrete Green's Function

- **Because the screening charges are computed using the discrete Laplace operator, the corresponding Green's function is different from $1/|\vec{x} - \vec{x}'|$**

"Continuous" Green's function : $\nabla^2 G(\vec{x} - \vec{x}') = 4\pi \mathrm{G} \delta(\vec{x} - \vec{x}')$

"Discrete" Green's function : $\Delta_h^2 G_h(i, i', j, j', k, k') = 4\pi \mathrm{G} \delta_{i,i'} \delta_{j,j'} \delta_{k,k'}$

DGF vs. CGF in cylindrical coordinates



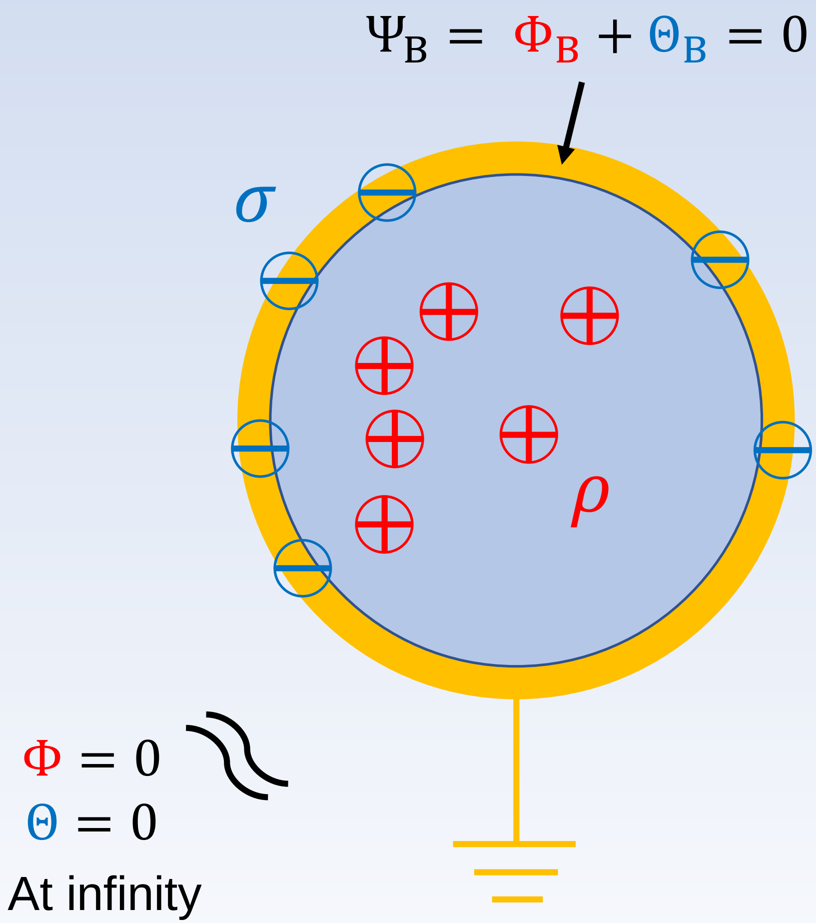
Flowchart

Main loop

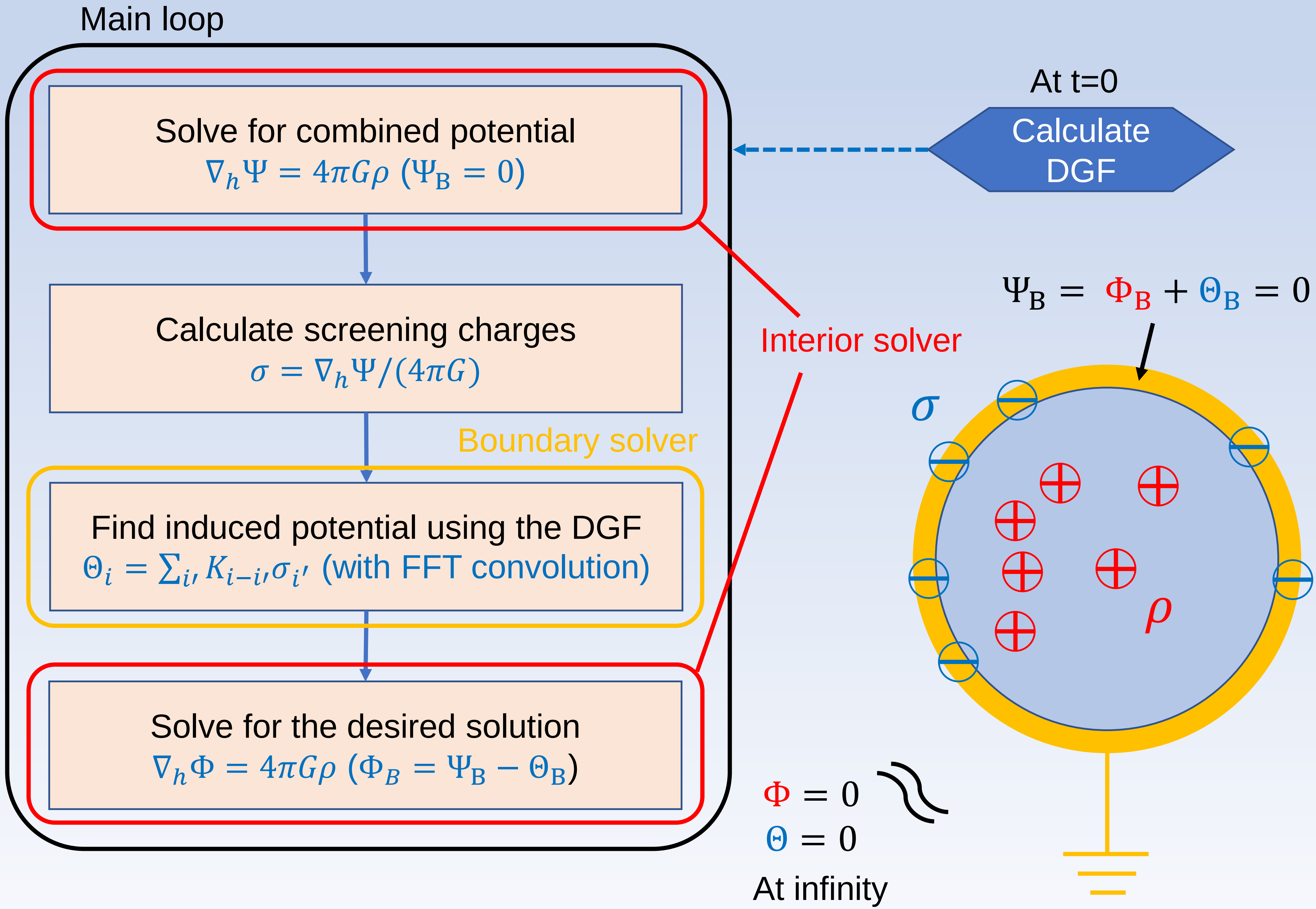
1. Solve for combined potential
   $\nabla_h \Psi = 4\pi G \rho \; (\Psi_{\mathrm{B}} = 0)$
2. Calculate screening charges
   $\sigma = \nabla_h \Psi / (4\pi G)$
3. Find induced potential using the DGF
   $\Theta_i = \sum_{i'} K_{i-i'} \sigma_{i'}$ (with FFT convolution)
4. Solve for the desired solution
   $\nabla_h \Phi = 4\pi G \rho \; (\Phi_B = \Psi_{\mathrm{B}} - \Theta_{\mathrm{B}})$

At t=0

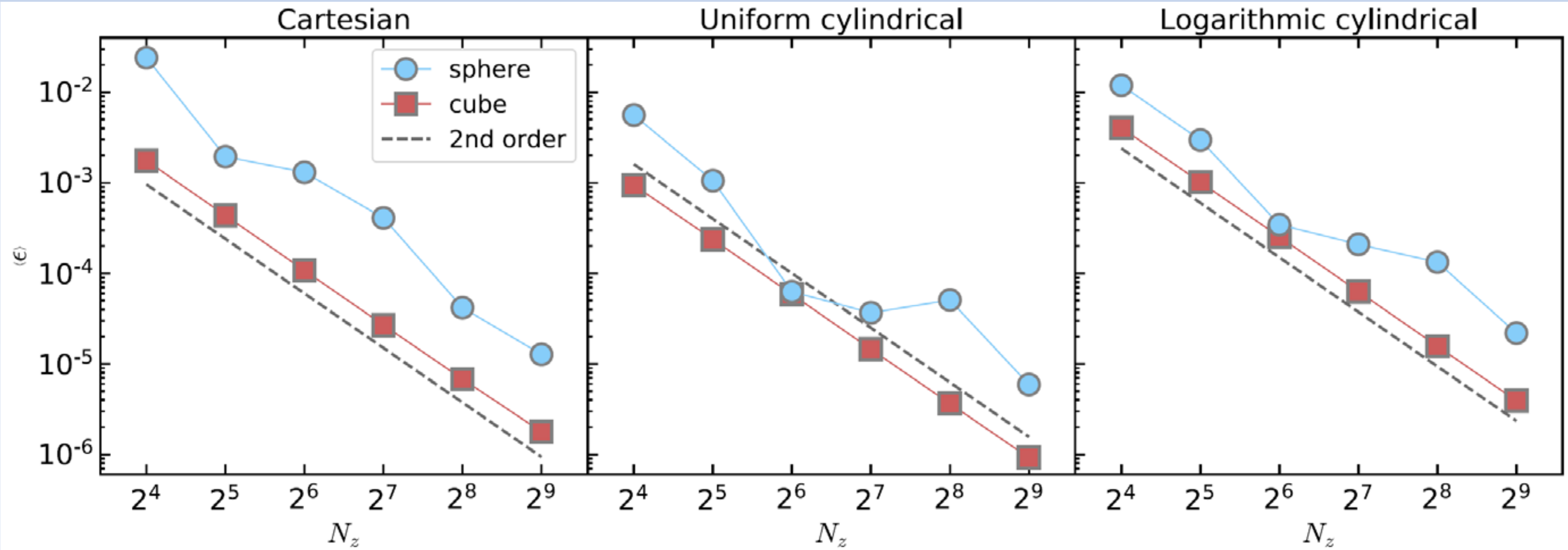
Calculate DGF



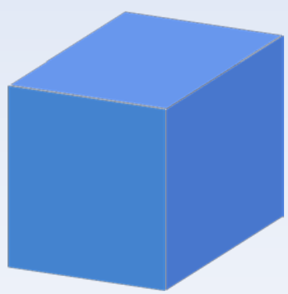
Flowchart


Main loop
Solve for combined potential
$\nabla_h \Psi = 4\pi G\rho \ (\Psi_B = 0)$
Calculate screening charges
$\sigma = \nabla_h \Psi / (4\pi G)$
Boundary solver
Find induced potential using the DGF
$\Theta_i = \sum_{i'} K_{i-i'} \sigma_{i'}$ (with FFT convolution)
Solve for the desired solution
$\nabla_h \Phi = 4\pi G\rho \ (\Phi_B = \Psi_B - \Theta_B)$
At t=0
Calculate DGF
Interior solver
$\Psi_B = \Phi_B + \Theta_B = 0$
σ
ρ
$\Phi = 0$
$\Theta = 0$
At infinity

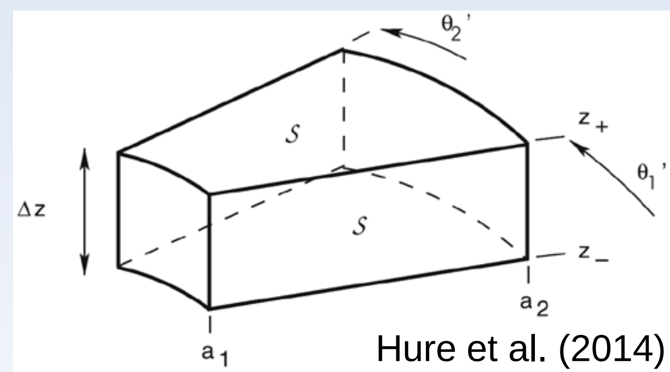
Second-Order Convergence



Uniform sphere

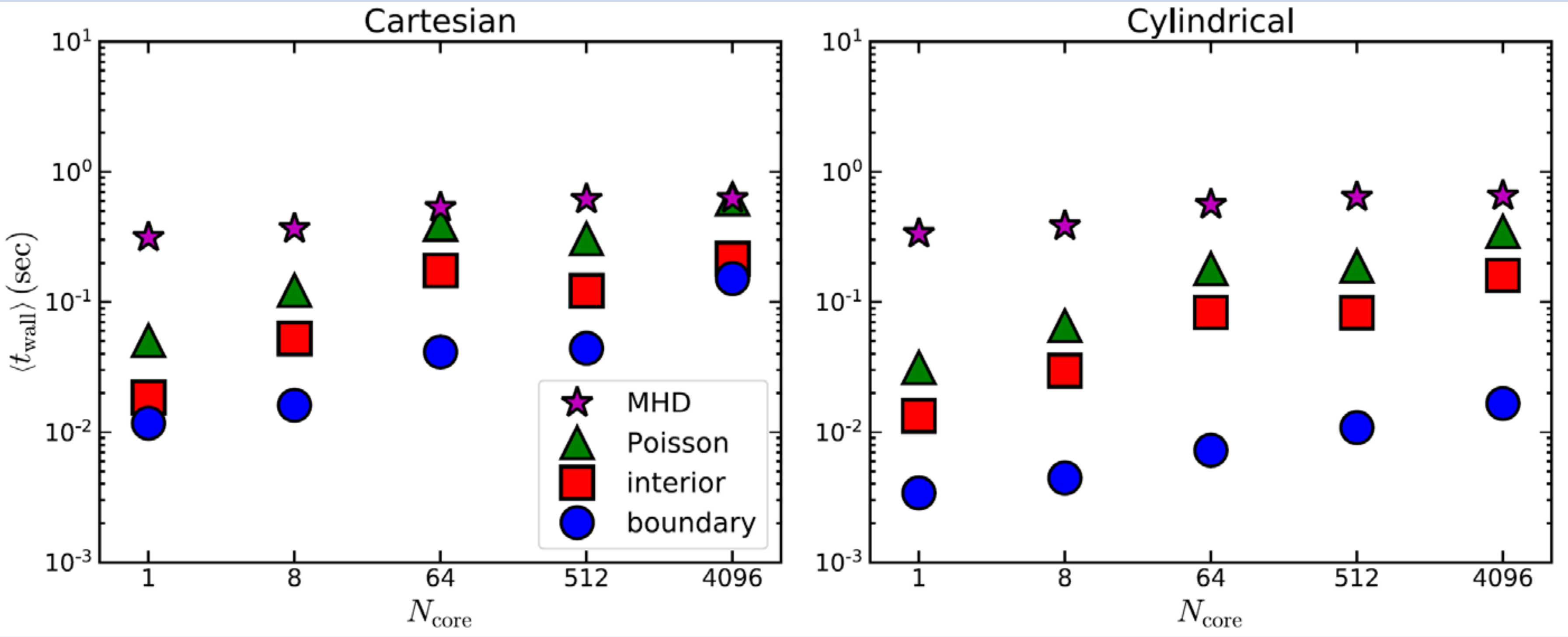


Uniform cube (in Cartesian)



Rectangular torus (in cylindrical)

Weak Scaling Test



- Mesh size : 64^3 $(N_{\rm core} = 1) \sim 1024^3$ $(N_{\rm core} = 4096)$
- **Poisson** = 2 x **interior** + **boundary**
- Poisson solver takes less time than MHD solver up to 4096 cores.
- James's algorithm is more efficient in cylindrical coordinates.

GravityBoundaryValues::ApplyPhysicalBoundaries()

Supplements

FFT Poisson Solver

1. Periodic boundary condition

$$\nabla^2 \Phi = 4\pi G \rho \quad \xrightarrow{\text{FT}} \quad -k^2 \hat{\Phi} = 4\pi G \hat{\rho}$$

The equation being solved is different;
FFT is used only as a computational aid.

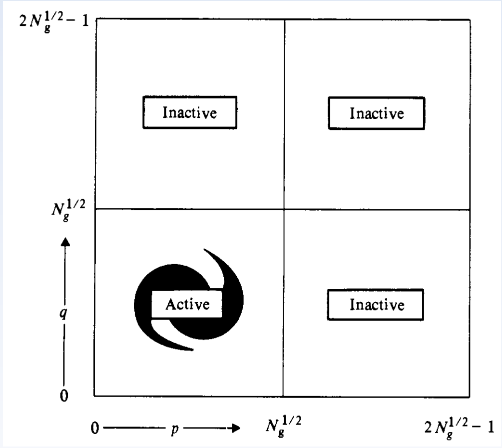
2. Open boundary condition

$$\Phi(\vec{x}) = -\iiint \frac{G\rho}{|\vec{x} - \vec{x}'|} d^3x'$$

$$\xrightarrow{\text{FT}} \quad \hat{\Phi} = \hat{K} \hat{\rho}$$

“Convolution theorem”

Hockney & Eastwood, 1988



The multipole expansion method has been widely used in Cartesian, cylindrical, and spherical coordinates to provide open BC at the domain boundary.

(e.g., Stone & Norman 1992; Boley & Durisen 2008; Katz et al. 2016)

$$\Phi_{\mathrm{B}} = -\mathrm{G}\sum_{l} P_l(\cos\theta)\left[\frac{M_l^{(\mathrm{int})}(r_{\mathrm{B}})}{r_{\mathrm{B}}^{l+1}} + r_{\mathrm{B}}^{l} M_l^{(\mathrm{ext})}(r_{\mathrm{B}})\right]$$

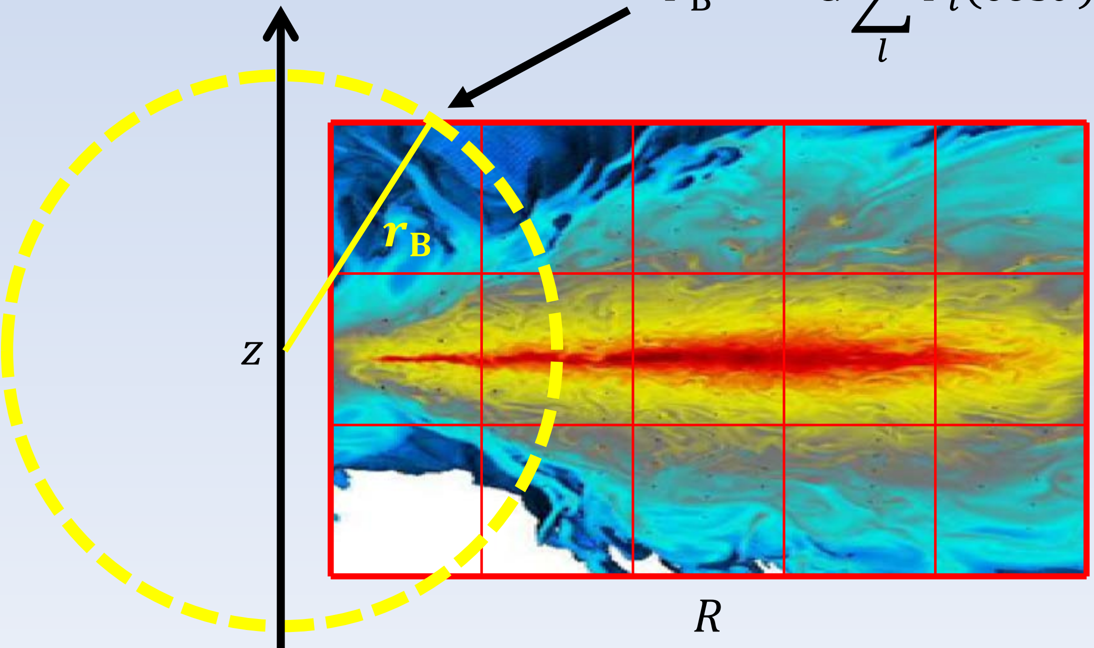


Image taken from Jiang et al. (2014)

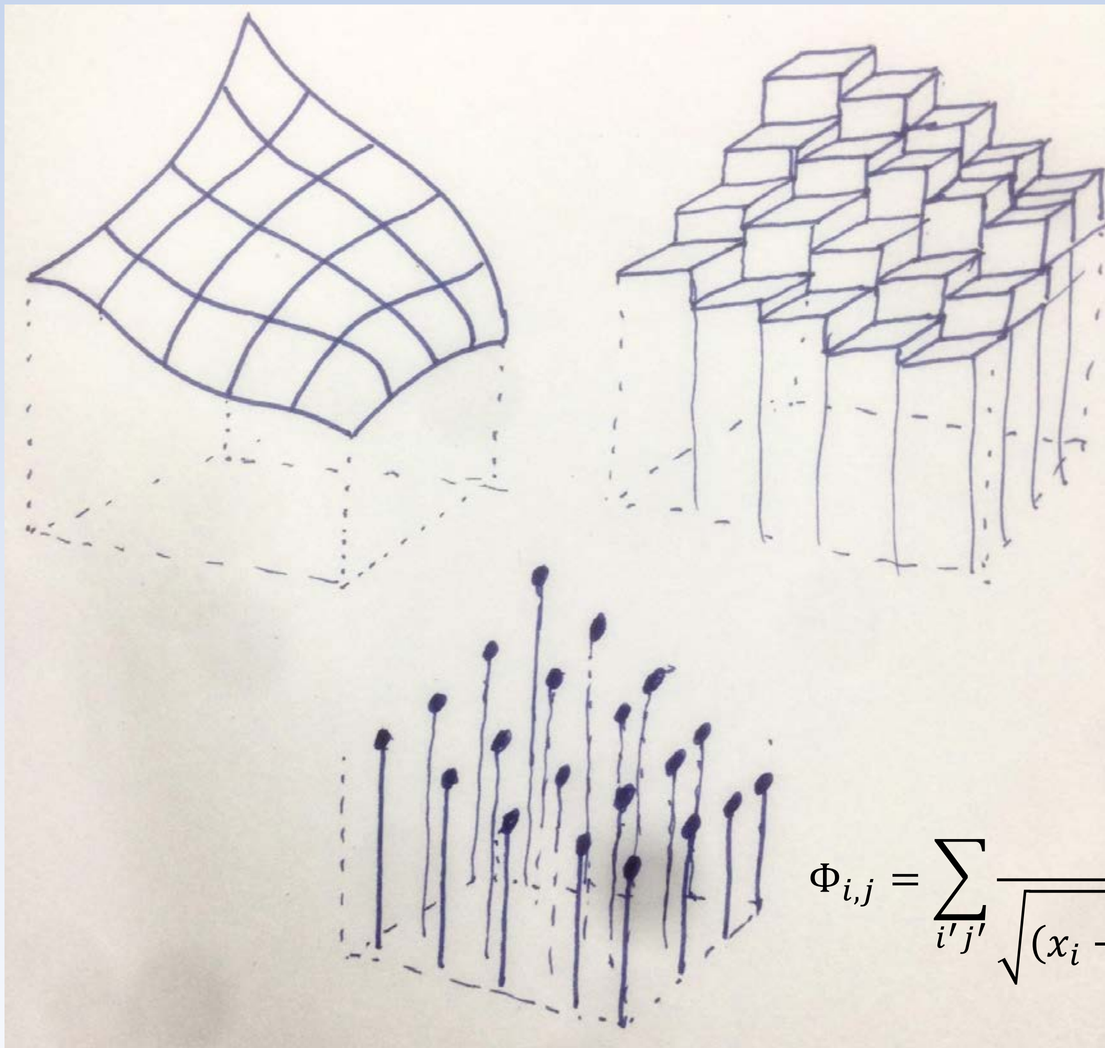
$$M_l^{(\mathrm{int})}(r_{\mathrm{B}}) = \int_0^{r_{\mathrm{B}}} r^l P_l(\mu)\rho(r,\mu)\,d^3x'$$

$$M_l^{(\mathrm{ext})}(r_{\mathrm{B}}) = \int_{r_{\mathrm{B}}}^{\infty} \frac{P_l(\mu)}{r^{l+1}}\rho(r,\mu)\,d^3x'$$

However, for flattened mass distribution, the multipole moments change with r_{B}, requiring $\boldsymbol{O}(\boldsymbol{N}^4)$ operation to fully compute them.

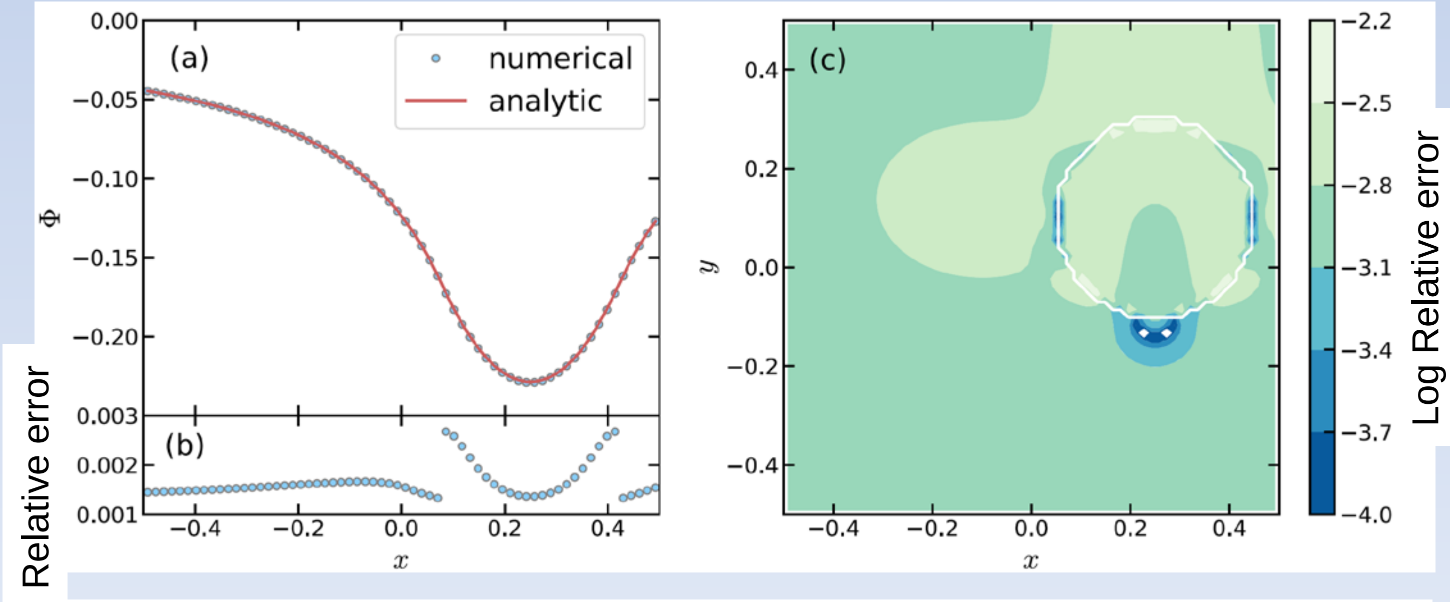
Higher Order with Convolution Method

$$\Phi_{i,j} = \sum_{i'j'} \mathrm{G} \int_{x_{i'-\frac{1}{2}}}^{x_{i'+\frac{1}{2}}} \int_{y_{j'-\frac{1}{2}}}^{y_{j'+\frac{1}{2}}} \frac{-\rho(x',y')}{\sqrt{(x_i - x')^2 + \left(y_j - y'\right)^2}} \, dx'dy'$$



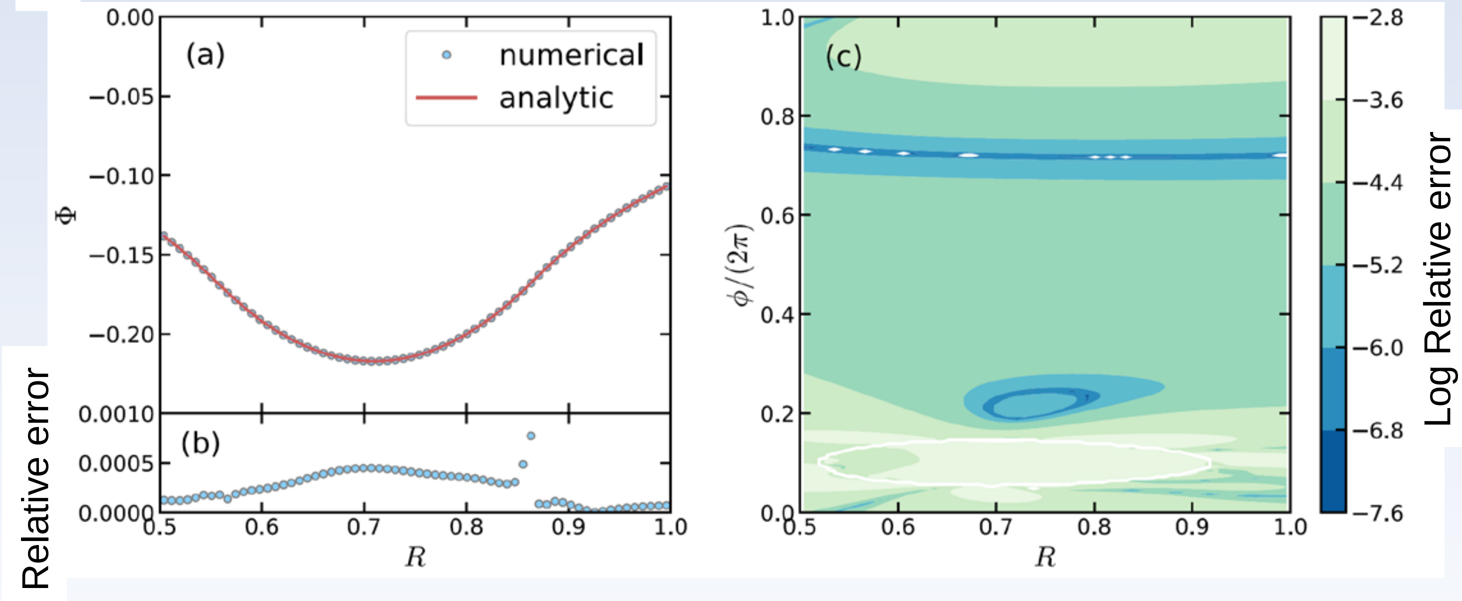
$$\Phi_{i,j} = \sum_{i'j'} \frac{-\mathrm{G}\rho_{i',j'}\Delta x \Delta y}{\sqrt{(x_i - x_{i'})^2 + \left(y_j - y_{j'}\right)^2}}$$

Sample Calculation : Potential of an Uniform Sphere



Cartesian

$64 \times 64 \times 64$



Cylindrical

$64 \times 256 \times 64$