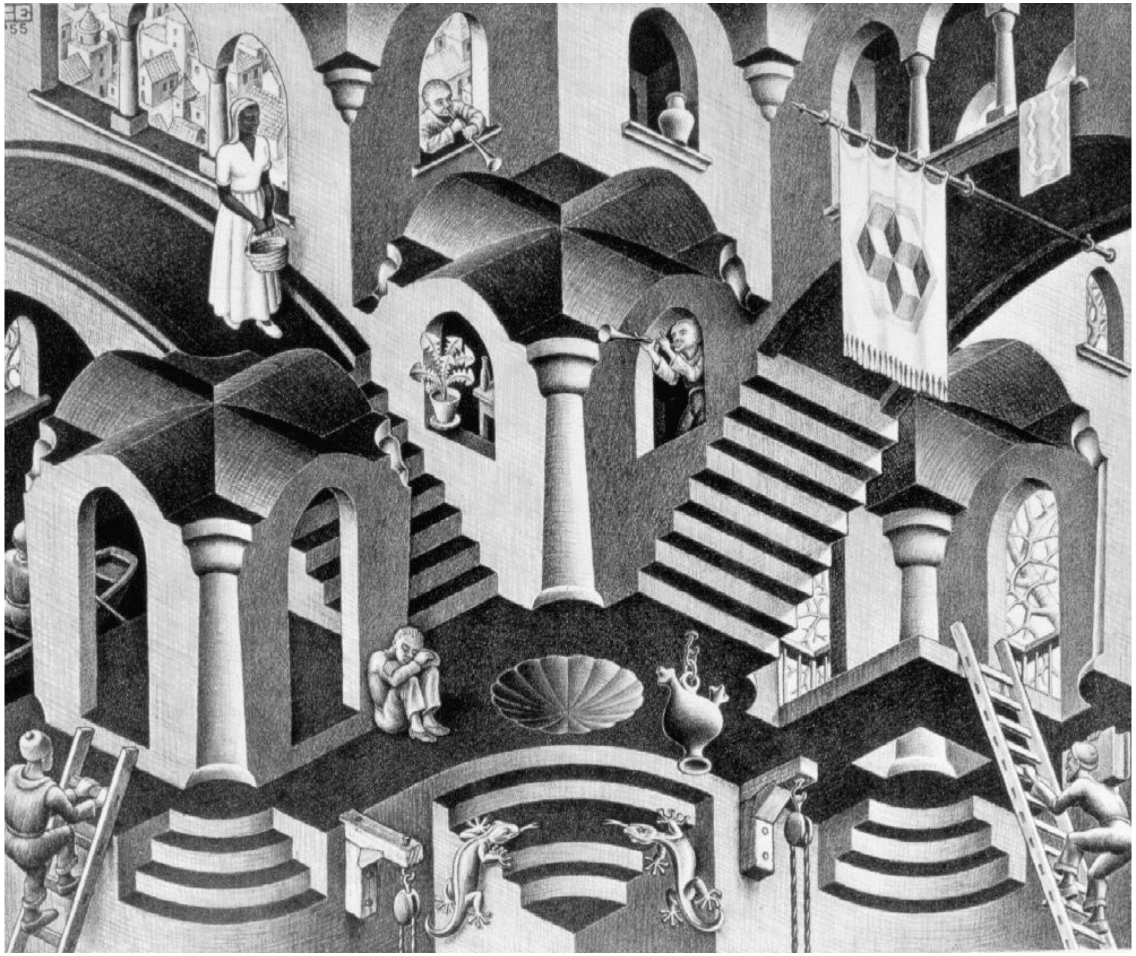
Alexander Knebe, *Universidad Autonoma de Madrid*



- Poisson's equation

$$\Delta\Phi(\vec{r}) = 4\pi G\rho(\vec{r})$$

$$\vec{F}(\vec{r}) = -m\nabla\Phi(\vec{r})$$

Solving for Gravity

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→

grid approach ($\vec{r}_{i,j,k}$ =position of centre of grid cell (i,j,k))

$$\Delta\Phi(\vec{r}_{i,j,k}) = 4\pi G\rho(\vec{r}_{i,j,k})$$

$$\vec{F}(\vec{r}_{i,j,k}) = -m\nabla\Phi(\vec{r}_{i,j,k})$$

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particle approach

$$\vec{F}(\vec{r}_i) = -\sum_{i\neq j}\frac{Gm_i m_j}{(r_i - r_j)^3}(\vec{r}_i - \vec{r}_j)$$

grid approach ($\vec{r}_{i,j,k}$ =position of centre of grid cell (i,j,k))

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$$\vec{F}(\vec{r}_{i,j,k}) = -m\nabla\Phi(\vec{r}_{i,j,k})$$

- direct particle-particle summation (PP)

$$\vec{F}_i(\vec{r}_i) = -\sum_{i \neq j} \frac{G m_i m_j}{(r_i - r_j)^3} (\vec{r}_i - \vec{r}_j) \quad \forall i \in N$$

organizing particles into a "tree structure" will give $N \log(N)$ operations

- direct particle-particle summation (PP)

the tree

Solving for Gravity

- direct particle-particle summation (PP)

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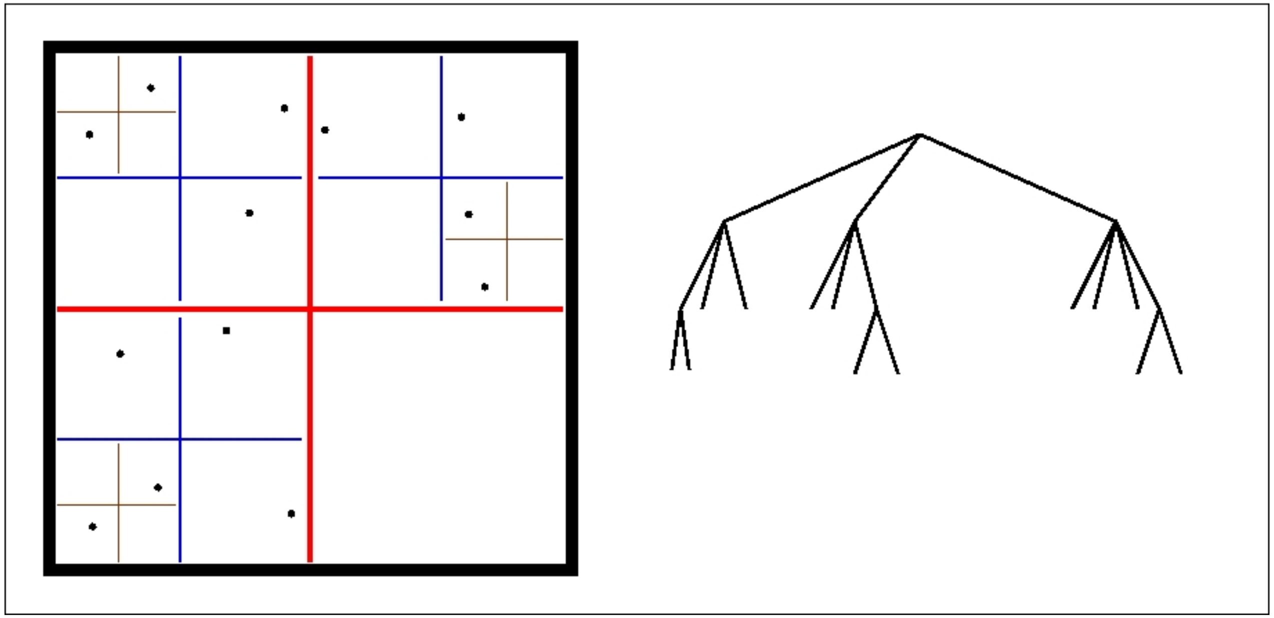
- generating the tree:



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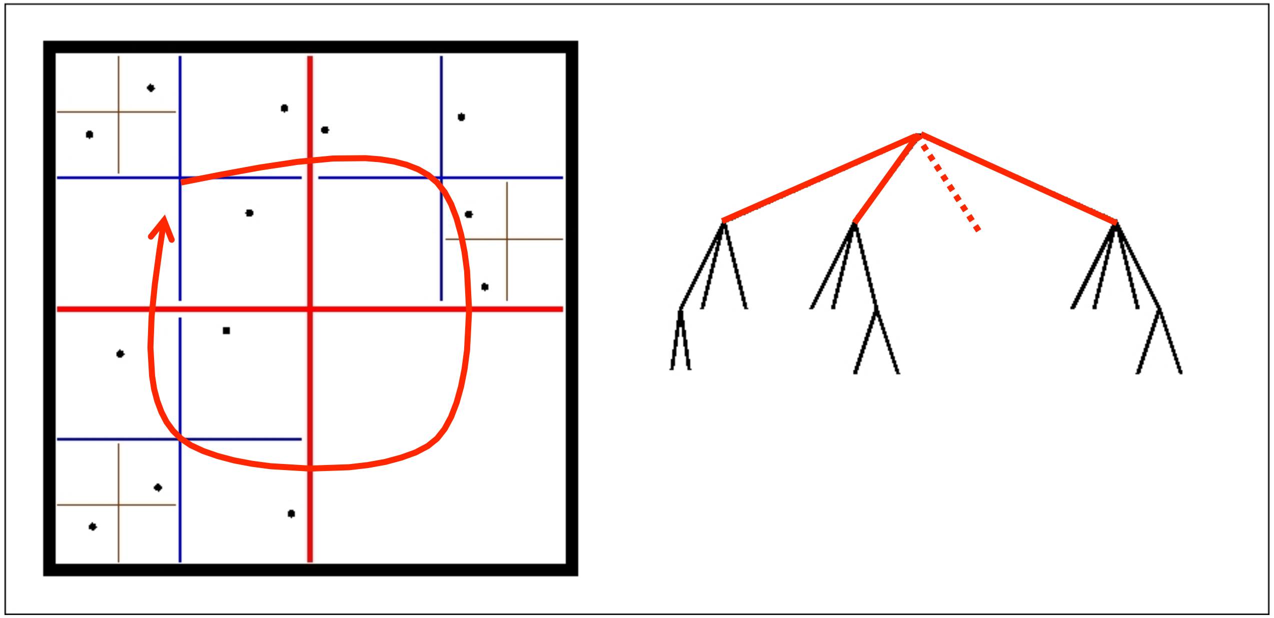

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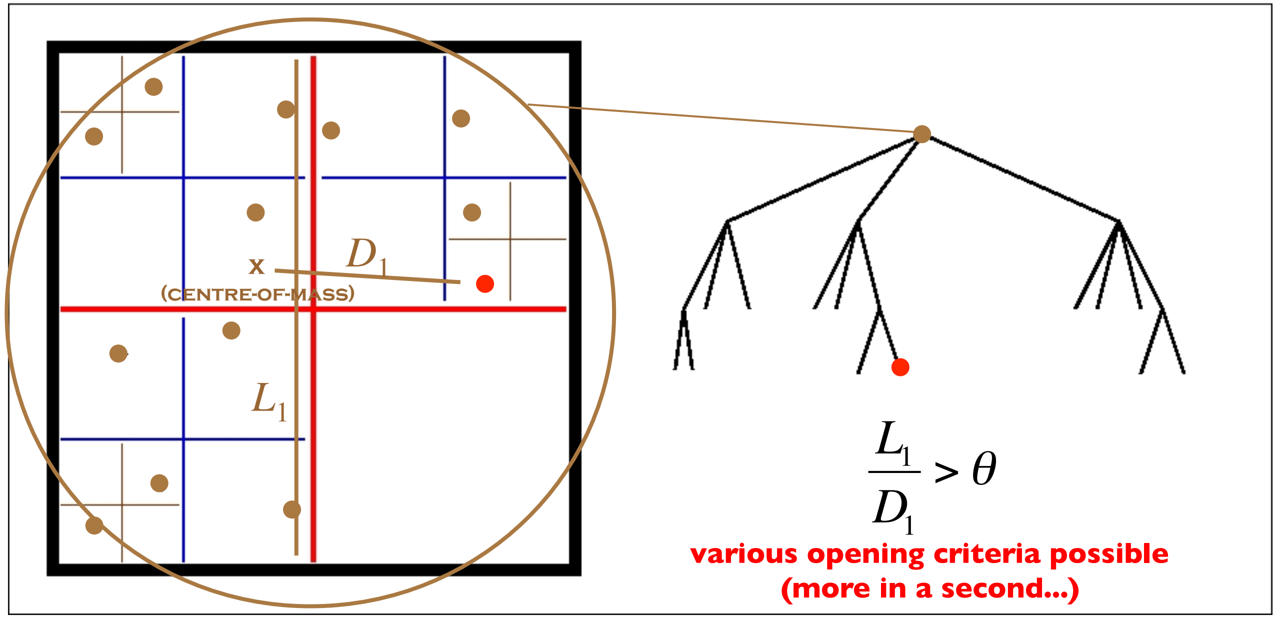
- walking the tree ($\forall i \in N$):



requirements to perform Cosmological Simulations

Solving for Gravity

- specific requirements for cosmological simulations:

  - periodic boundary conditions
  - equations-of-motion in comoving coordinates

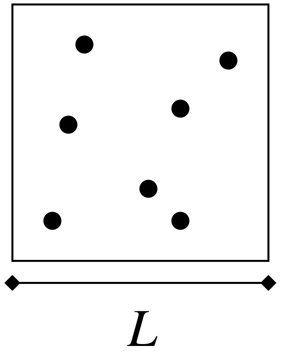
Solving for Gravity

- specific requirements for cosmological simulations:

  - **periodic boundary conditions**
  - equations-of-motion in comoving coordinates

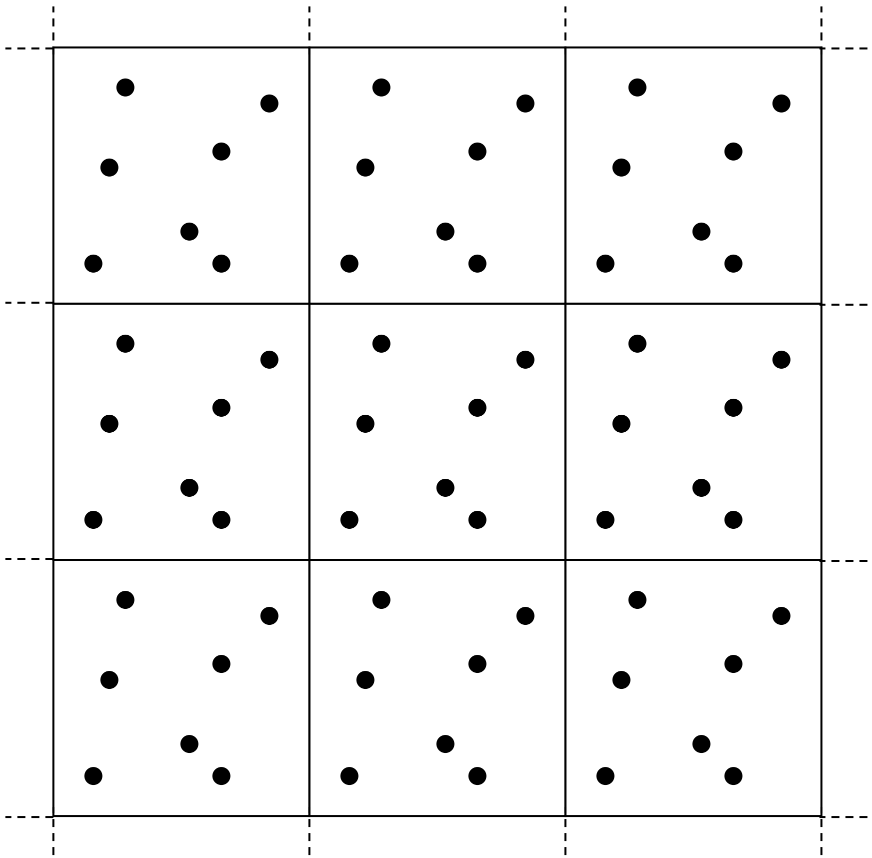
Solving for Gravity

- periodic boundary conditions



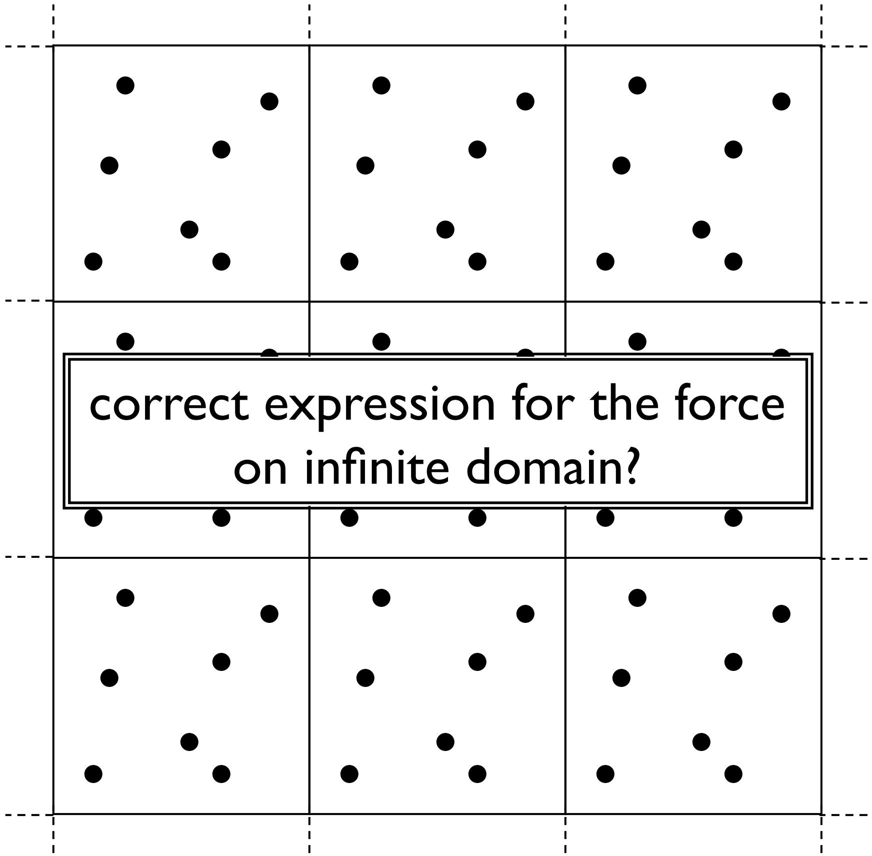
Solving for Gravity

- periodic boundary conditions



Solving for Gravity

- periodic boundary conditions



correct expression for the force on infinite domain?

Solving for Gravity

- periodic boundary conditions

$$\Delta_x \Phi(\vec{x}) = 4\pi G\left(\rho_x(\vec{x}) - \overline{\rho}_x\right)$$

Solving for Gravity

- periodic boundary conditions

$$\Delta_x \Phi(\vec{x}) = 4\pi G\left(\rho_x(\vec{x}) - \bar{\rho}_x\right)$$

we need to subtract the mean background density
in order for the solution to converge!

Solving for Gravity

- periodic boundary conditions

$$\Delta_x \Phi(\vec{x}) = 4\pi G\left(\rho_x(\vec{x}) - \overline{\rho}_x\right)$$

↓ general solution

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

Solving for Gravity

- periodic boundary conditions

$$\Delta_x \Phi(\vec{x}) = 4\pi G\left(\rho_x(\vec{x}) - \overline{\rho}_x\right)$$

$\downarrow$ general solution

$$\Phi(\vec{x}) = G \iiint \frac{\rho_x(\vec{x}\,') - \overline{\rho}_x}{\left|\vec{x} - \vec{x}\,'\right|} d^3x'$$

periodicity automatically taken care of when using PM solver!

Solving for Gravity

- periodic boundary conditions

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periodicity automatically taken care of when using PM solver!

...but needs to be properly implemented for tree codes!

Solving for Gravity

- periodic boundary conditions

$$\Delta_x \Phi(\vec{x}) = 4\pi G\left(\rho_x(\vec{x}) - \overline{\rho}_x\right)$$

↓ general solution

fluctuates about zero!

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

$$i.e., \Phi(\vec{0}) = -G \iiint \frac{\left(\rho_x(\vec{x}) - \overline{\rho}_x\right)}{\left|\vec{x}\right|} d^3x$$

$$= -G \int_{x=0}^{\infty} \frac{1}{\left|\vec{x}\right|} x^2 \iint_{\vartheta,\varphi} \left(\rho_x(\vec{x}) - \overline{\rho}_x\right) \sin\vartheta \, d\vartheta \, d\varphi$$

$$= -G \int_{x=0}^{\infty} x \left\langle \rho_x(\vec{x}) - \overline{\rho}_x \right\rangle_{\left|\vec{x}\right| = x} dx$$

$\Rightarrow$ convergence to **finite value**, as $\langle \; \rangle \rightarrow 0$ for $x \rightarrow \infty$

Note: what is true to x=0 is true for any point as the origin of the coordinate system is arbitrary for periodic boundaries...

Solving for Gravity

- periodic boundary conditions

$$\Delta_x \Phi(\vec{x}) = 4\pi G\left(\rho_x(\vec{x}) - \overline{\rho}_x\right)$$

↓ general solution

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

↓ desired (peculiar) force field

$$\vec{F}(\vec{x}) = -G \iiint \frac{\rho_x(\vec{x}') - \overline{\rho}_x}{|\vec{x} - \vec{x}'|^3} (\vec{x} - \vec{x}') d^3x'$$

Solving for Gravity

- periodic boundary conditions

$$\vec{F}(\vec{x}) = -G\iiint \frac{\rho_x(\vec{x}\,') - \overline{\rho}_x}{\left|\vec{x} - \vec{x}\,'\right|^3}(\vec{x} - \vec{x}\,')d^3x'$$

Solving for Gravity

- periodic boundary conditions

...but in the end it will not contribute to F!

$$\vec{F}(\vec{x}) = -G \iiint \frac{\rho_x(\vec{x}') - \bar{\rho}_x}{|\vec{x} - \vec{x}'|^3} (\vec{x} - \vec{x}') d^3 x'$$

Solving for Gravity

- periodic boundary conditions

...but in the end it will not contribute to *F*!

$$\vec{F}(\vec{x}) = -G \iiint \frac{\rho_x(\vec{x}') - \bar{\rho}_x}{|\vec{x}-\vec{x}'|^3}(\vec{x}-\vec{x}')d^3x'$$

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$$= -G \iiint \frac{\rho_x(\vec{x})}{|\vec{x}|^3}\vec{x}d^3x + G \iiint \frac{\bar{\rho}_x}{|\vec{x}|^3}\vec{x}d^3x$$

$$\iiint \frac{\vec{x}}{|\vec{x}|^3}d^3x = \iiint_{x,\vartheta,\varphi} \frac{1}{x^3}\begin{pmatrix} x\cos\varphi\sin\vartheta \\ x\sin\varphi\sin\vartheta \\ x\cos\vartheta \end{pmatrix} x^2\sin\vartheta dx d\vartheta d\varphi = \iiint_{x,\vartheta,\varphi} \begin{pmatrix} \cos\varphi\sin\vartheta \\ \sin\varphi\sin\vartheta \\ \cos\vartheta \end{pmatrix} \sin\vartheta dx d\vartheta d\varphi = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Solving for Gravity

- periodic boundary conditions

$$\vec{F}(\vec{x}) = -G \iiint \frac{\rho_x(\vec{x}\,')}{\left|\vec{x} - \vec{x}\,'\right|^3} (\vec{x} - \vec{x}\,') d^3 x'$$

Solving for Gravity

- periodic boundary conditions

$$\vec{F}(\vec{x}) = -G \iiint \frac{\rho_x(\vec{x}')}{\left|\vec{x}-\vec{x}'\right|^3}(\vec{x}-\vec{x}')d^3x'$$

↓ particle/discrete picture

$$\vec{F}(\vec{x}) = -G \sum_{i=1}^{N} \sum_{\vec{R}} \frac{m_i}{\left|\vec{x}-(\vec{x}_i+\vec{R})\right|^3}\left(\vec{x}-(\vec{x}_i+\vec{R})\right)$$

$$\vec{R} = \vec{n}L$$

Solving for Gravity

- periodic boundary conditions

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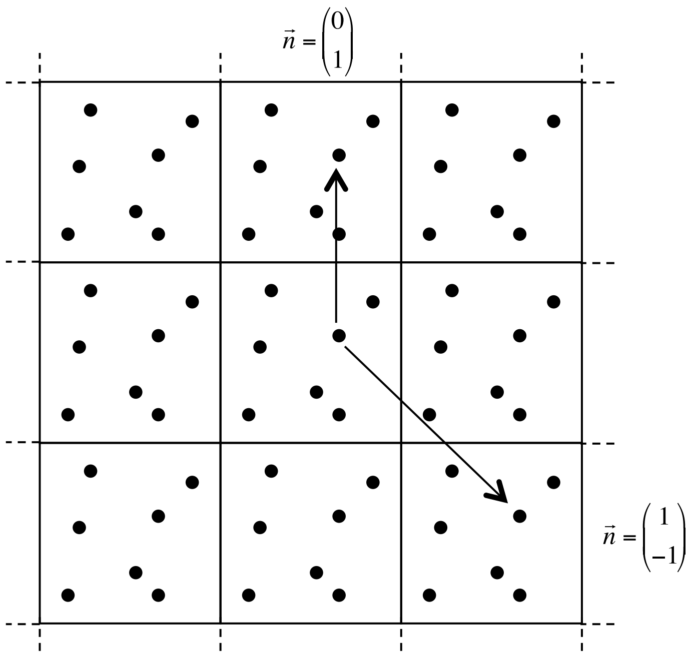
correct expression for the force on infinite domain!

Solving for Gravity

- periodic boundary conditions

$$\vec{F}(\vec{x}) = -G\sum_{i=1}^{N}\sum_{\vec{R}} \frac{m_i}{\left|\vec{x} - (\vec{x}_i + \vec{R})\right|^3}\left(\vec{x} - (\vec{x}_i + \vec{R})\right)$$



Solving for Gravity

- periodic boundary conditions

$$\vec{F}(\vec{x}) = -G\sum_{i=1}^{N}\sum_{\vec{R}}\frac{m_i}{\left|\vec{x}-(\vec{x}_i+\vec{R})\right|^3}\left(\vec{x}-(\vec{x}_i+\vec{R})\right)$$

=> slow convergence and hence not feasible…

=> Ewald summation instead…

Solving for Gravity

- periodic boundary conditions

$$\Delta_x \Phi(\vec{x}) = 4\pi G \rho(\vec{x})$$

Solving for Gravity

- periodic boundary conditions

$$\Delta_x \Phi(\vec{x}) = 4\pi G \rho(\vec{x})$$

$$\rho(\vec{x}) = \sum_{i=1}^{N} m_i \delta_{\mathrm{Dirac}}(\vec{x} - \vec{x}_i)$$

$$\downarrow$$

"peculiar" density

$$\rho(\vec{x}) = \sum_{i=1}^{N} m_i \delta_{\mathrm{Dirac}}(\vec{x} - \vec{x}_i) - \overline{\rho}$$

$$\downarrow$$

periodic, peculiar density

$$\rho_{periodic}(\vec{x}) = \sum_{i=1}^{N} \sum_{\vec{R}} m_i \delta_{\mathrm{Dirac}}(\vec{x} - (\vec{x}_i + \vec{R})) - \overline{\rho}$$

$\vec{R} = \vec{n}L$ ($\vec{n}$ = integer vector)

Solving for Gravity

- periodic boundary conditions

$$\rho_{periodic}(\vec{x}) = \sum_{i=1}^{N} \sum_{\vec{R}} m_i \delta_{\mathrm{Dirac}}(\vec{x} - \vec{x}_i - \vec{R}) - \overline{\rho}$$

Solving for Gravity

- periodic boundary conditions

$$\rho_{periodic}(\vec{x}) = \sum_{i=1}^{N} \sum_{\vec{R}} \underbrace{m_i \delta_{\text{Dirac}}(\vec{x} - \vec{x}_i - \vec{R})}_{\rho_1(\vec{x},\vec{x}_i)} \underbrace{- \overline{\rho}}_{\rho_2(\vec{x},\vec{x}_i)}$$

$$\rho_{periodic}(\vec{x}) = \sum_{i=1}^{N} \rho_1(\vec{x},\vec{x}_i) + \rho_2(\vec{x},\vec{x}_i)$$

Solving for Gravity

- periodic boundary conditions

$$\rho_{periodic}(\vec{x}) = \sum_{i=1}^{N} \rho_1(\vec{x},\vec{x}_i) + \rho_2(\vec{x},\vec{x}_i)$$

$$\rho_1(\vec{x},\vec{x}_i) = \sum_{\vec{R}} m_i \delta_{\mathrm{Dirac}}(\vec{x} - \vec{x}_i - \vec{R})$$

$$\rho_2(\vec{x},\vec{x}_i) = -\overline{\rho}$$

Solving for Gravity

- periodic boundary conditions

$$\rho_{periodic}(\vec{x}) = \sum_{i=1}^{N} \rho_1(\vec{x},\vec{x}_i) + \rho_2(\vec{x},\vec{x}_i)$$

$$\rho_1(\vec{x},\vec{x}_i) = -\sum_{\vec{R}} \frac{1}{\sqrt{\mu^2\pi}} e^{-\frac{(\vec{x}-\vec{x}_i-\vec{R})^2}{\mu^2}} + \sum_{\vec{R}} m_i \delta_{\mathrm{Dirac}}(\vec{x}-\vec{x}_i-\vec{R})$$

$$\rho_2(\vec{x},\vec{x}_i) = +\sum_{\vec{R}} \frac{1}{\sqrt{\mu^2\pi}} e^{-\frac{(\vec{x}-\vec{x}_i-\vec{R})^2}{\mu^2}} - \bar{\rho}$$

Ewald introduced (Gaussian) "screening charges"

- periodic boundary conditions

$$\rho_{periodic}(\vec{x}) = \sum_{i=1}^{N} \rho_1(\vec{x},\vec{x}_i) + \rho_2(\vec{x},\vec{x}_i)$$

$$\rho_1(\vec{x},\vec{x}_i) = -\sum_{\vec{R}} \frac{1}{\sqrt{\mu^2\pi}} e^{-\frac{(\vec{x}-\vec{x}_i-\vec{R})^2}{\mu^2}} + \sum_{\vec{R}} m_i \delta_{\mathrm{Dirac}}(\vec{x}-\vec{x}_i-\vec{R})$$

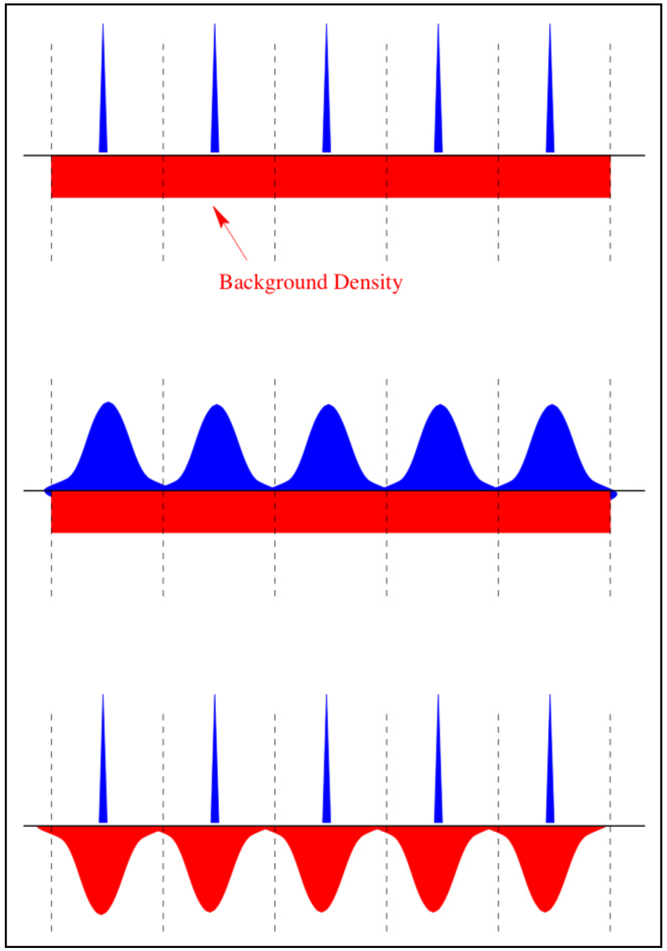
➔ **real-space**

$$\rho_2(\vec{x},\vec{x}_i) = +\sum_{\vec{R}} \frac{1}{\sqrt{\mu^2\pi}} e^{-\frac{(\vec{x}-\vec{x}_i-\vec{R})^2}{\mu^2}} - \overline{\rho}$$

➔ **Fourier-space**

Solving for Gravity

- periodic boundary conditions



$$\rho_{periodic}(\vec{x}) = \sum_{i=1}^{N} \rho_1(\vec{x},\vec{x}_i) + \rho_2(\vec{x},\vec{x}_i)$$

potential obtained in…

$$\rho_2(\vec{x},\vec{x}_i) = \sum_{\vec{R}} \frac{1}{\sqrt{\mu^2\pi}} e^{-\frac{(\vec{x}-\vec{x}_i-\vec{R})^2}{\mu^2}} - \overline{\rho}$$

Fourier-space

$$\rho_1(\vec{x},\vec{x}_i) = \sum_{\vec{R}} m_i \delta_{\mathrm{Dirac}}(\vec{x}-\vec{x}_i-\vec{R}) - \frac{1}{\sqrt{\mu^2\pi}} e^{-\frac{(\vec{x}-\vec{x}_i-\vec{R})^2}{\mu^2}}$$

real-space

=> exponential convergence and hence feasible!

Solving for Gravity

- periodic boundary conditions

detailed calculation…

Solving for Gravity

- periodic boundary conditions

  - force due to particles in computational box:

$$\vec{F}(\vec{x}) = -G\sum_{i=1}^{N} \frac{m_i}{\left|\vec{x}-\vec{x}_i\right|^3}\left(\vec{x}-\vec{x}_i\right)$$

  - *additional* force due to periodic images:

$$\vec{F}_{Ewald}(\vec{x}) = \frac{\vec{x}}{x^3} - \sum_{\vec{R}} \frac{\vec{x}-\vec{R}}{\left|\vec{x}-\vec{R}\right|^3} \times \left[erfc\left(\frac{\left|\vec{x}-\vec{R}\right|}{\mu}\right) + \frac{2\left|\vec{x}-\vec{R}\right|}{\sqrt{\mu^2\pi}} e^{-\frac{\left|\vec{x}-\vec{R}\right|^2}{\mu^2}} \right] - \frac{2}{L^2}\sum_{\vec{n}\neq 0} \frac{\vec{n}}{n} \sin\left(\frac{2\pi}{L}\vec{n}\cdot\left(\vec{x}-\vec{R}\right)\right) e^{-\frac{(\mu\pi)^2 n^2}{L^2}}$$

Ewald summation in practice…

- periodic boundary conditions

  - additional force due to periodic images:

$$\vec{F}_{Ewald}(\vec{x}) = \frac{\vec{x}}{x^3} - \sum_{\vec{R}} \frac{\vec{x}-\vec{R}}{\left|\vec{x}-\vec{R}\right|^3} \times \left[erfc\left(\frac{\left|\vec{x}-\vec{R}\right|}{\mu} \right) + \frac{2\left|\vec{x}-\vec{R}\right|}{\sqrt{\mu^2\pi}} e^{-\frac{\left|\vec{x}-\vec{R}\right|^2}{\mu^2}} \right] - \frac{2}{L^2} \sum_{\vec{n}\neq 0} \frac{\vec{n}}{n} \sin\left(\frac{2\pi}{L} \vec{n}\cdot\left(\vec{x}-\vec{R}\right) \right) e^{-\frac{(\mu\pi)^2 n^2}{L^2}}$$

  - in practice:

1. $\mu = L/2, \quad \left|\vec{x}-\vec{R}\right| < 3L, \quad n^2 < 10$

2. tabulate $F_{Ewald}(x)$ on a grid and interpolate…

Solving for Gravity

- specific requirements for cosmological simulations:
  - periodic boundary conditions
  - **equations-of-motion in comoving coordinates**

Solving for Gravity *(cf. "gastrophysics in supercomoving coordinates" lecture...)*

$$\frac{\partial \rho_x}{\partial T} + \nabla_x \cdot (\rho_x \vec{v}) = 0$$

$$\frac{\partial (\rho_x \vec{v})}{\partial T} + \nabla_x \cdot \left(\rho_x \vec{v} \otimes \vec{v} + p_x \overleftrightarrow{1}\right) = \rho_x \left(-\nabla_x \phi_x\right)$$

$$\frac{\partial (\rho_x E_x)}{\partial T} + \nabla_x \cdot \left([\rho_x E_x + p_x]\vec{v}\right) = \rho_x \vec{v} \cdot \left(-\nabla_x \phi_x\right) - \mathcal{H} \rho_x \varepsilon_x [3\gamma - 5] + (\Gamma_x - L_x)$$

$$\frac{\partial S_x}{\partial T} + \nabla_x \cdot (S_x \vec{v}) = -\mathcal{H} S_x [3\gamma - 5]$$

$$\Delta_x \phi_x = 4\pi G a \left(\rho_{x,tot} - \bar{\rho}_x\right)$$

$$\frac{d\vec{x}_{DM}}{dT} = \vec{v}_{DM}$$

$$\frac{d\vec{v}_{DM}}{dT} = -\nabla_x \phi_x$$

<u>additional/closure equations:</u>

$$E_x = \varepsilon_x + \frac{1}{2} v^2$$

$$p_x = (\gamma - 1) \rho_x \varepsilon_x$$

$$S_x = \frac{p_x}{\rho_x^{\gamma-1}}$$

$$\varepsilon_x = \frac{1}{(\gamma - 1)} \frac{1}{\mu} \frac{k_B}{m_p} T_x$$

- comoving coordinates

  - recap:

$$\vec{r} = a\vec{x}, \quad \vec{v} = \vec{u} + H\vec{r}$$

$$\dot{\vec{x}} = \vec{u}/a$$

$$\dot{\vec{u}} = \vec{f} - H\vec{u}$$

$$\vec{f} = -G\frac{1}{a^2}\sum_{x \neq x_j}^{N} \frac{m_j}{\left|\vec{x} - \vec{x}_j\right|^3}\left(\vec{x} - \vec{x}_j\right) - \ddot{a}\vec{x}$$

(cf. "Time Integration" lecture…)

- comoving coordinates
  - GADGET notation:

$$\vec{f} = \frac{1}{a^2}\left[-G\sum_{x \neq x_j}^{N}\frac{m_j}{\left|\vec{x}-\vec{x}_j\right|^3}\left(\vec{x}-\vec{x}_j\right) + \frac{1}{2}\Omega_0 H_0^2 \vec{x}\right]$$

$$\ddot{a} = -\frac{4\pi G}{3} a\rho = -\frac{4\pi G}{3} a \frac{\rho_0}{a^3} = -\frac{4\pi G}{3}\frac{\Omega_0 \rho_{crit,0}}{a^2} = -\frac{4\pi G}{3}\frac{\Omega_0}{a^2}\frac{3H_0^2}{8\pi G} = -\frac{1}{a^2}\frac{1}{2}\Omega_0 H_0^2$$

Solving for Gravity

- comoving coordinates

  - isolated boundaries:

$$\vec{f} = -G\frac{1}{a^2}\sum_{x\neq x_j}^{N}\frac{m_j}{\left|\vec{x}-\vec{x}_j\right|^3}\left(\vec{x}-\vec{x}_j\right)-\ddot{a}\vec{x}$$

  - periodic boundaries:

$$\vec{f} = -G\frac{1}{a^2}\sum_{x\neq x_j}^{N}\sum_{\vec{R}}\frac{m_j}{\left|\vec{x}-\vec{x}_j-\vec{R}\right|^3}\left(\vec{x}-\vec{x}_j-\vec{R}\right)$$

(cf. discussion about periodic boundaries earlier…)