

full set of equations

• collisionless matter (e.g. dark matter)

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

$$\frac{d\vec{v}_{DM}}{dt} = -\nabla\phi$$

Poisson's equation

$$\Delta \phi = 4\pi G \rho_{tot}$$

• collisional matter (e.g. gas)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0$$

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot \left(\rho \vec{v} \otimes \vec{v} + \left(p + \frac{1}{2\mu} B^2 \right) \vec{1} - \frac{1}{\mu} \vec{B} \otimes \vec{B} \right) = \rho \left(-\nabla \phi \right)$$

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot \left(\left[\rho E + p + \frac{1}{2\mu} B^2 \right] \vec{v} - \frac{1}{\mu} \left[\vec{v} \cdot \vec{B} \right] \vec{B} \right) = \rho \vec{v} \cdot \left(-\nabla \phi \right) + \left(\Gamma - L \right)$$
 • Maxwell's equation

• ideal gas equations

$$p = (\gamma - 1)\rho\varepsilon$$

$$\rho\varepsilon = \rho E - \frac{1}{2}\rho v^2$$

$$\frac{\partial \vec{B}}{\partial t} = -\nabla \times \left(\vec{v} \times \vec{B} \right)$$

full set of equations

• collisionless matter (e.g. dark matter)

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

$$\frac{d\vec{v}_{DM}}{dt} = -\nabla \phi \quad ... \text{ and the force}$$

• collisional matter (e.g. gas)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \qquad p = (\gamma - 1)\rho \varepsilon$$

$$\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot \left(\rho \vec{v} \otimes \vec{v} + \left(p + \frac{1}{2\mu}B^2\right)\vec{1} - \frac{1}{\mu}\vec{B} \otimes \vec{B}\right) = \rho \left(-\nabla \phi\right)$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot \left(\left[\rho E + p + \frac{1}{2\mu}B^2\right]\vec{v} - \frac{1}{\mu}\left[\vec{v} \cdot \vec{B}\right]\vec{B}\right) = \rho \vec{v} \cdot \left(-\nabla \phi\right) + (\Gamma - L) \qquad \bullet \text{ Maxwell's equation}$$

• Poisson's equation

$$\Delta \phi = 4\pi G \rho_{tot}$$

• ideal gas equations

$$p = (\gamma - 1)\rho\varepsilon$$

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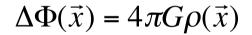
■ Poisson's equation

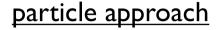
$$\vec{F}(\vec{x}) = -m\nabla\Phi(\vec{x})$$

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

Poisson's equation

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





$$\vec{F}(\vec{x}_i) = -\sum_{i \neq j} \frac{Gm_i m_j}{(x_i - x_j)^3} (\vec{x}_i - \vec{x}_j)$$

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

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

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

Poisson's equation

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

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

weapon of choice: tree codes

particle approach

$$\vec{F}(\vec{x}_i) = -\sum_{i \neq j} \frac{Gm_i m_j}{(x_i - x_j)^3} (\vec{x}_i - \vec{x}_j)$$

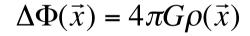
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■ Poisson's equation

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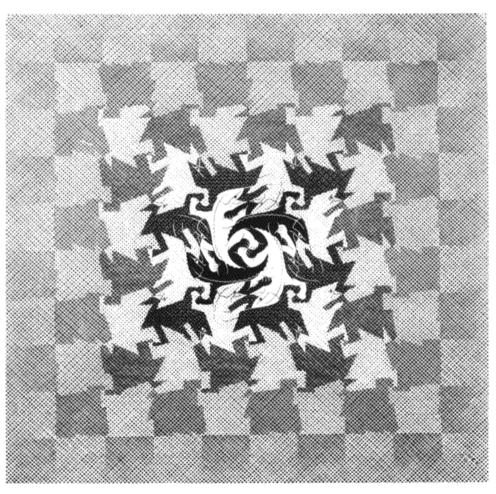
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weapon of choice: AMR codes

Computational Astrophysics

Solving for Gravity



the particle-mesh (PM) method

numerically integrate Poisson's equation

$$\Delta\Phi(\vec{g}_{k,l,m}) = 4\pi G \rho(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m}) = -m\nabla\Phi(\vec{g}_{k,l,m})$$

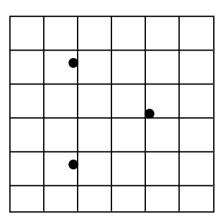
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numerically integrate Poisson's equation

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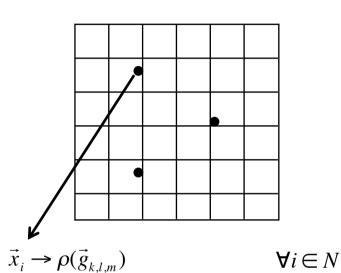


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I. calculate mass density on grid



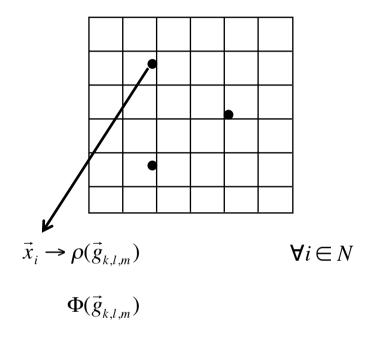
numerically integrate Poisson's equation

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$$\vec{F}(\vec{g}_{k,l,m}) = -m\nabla\Phi(\vec{g}_{k,l,m})$$



2. solve Poisson's equation on grid



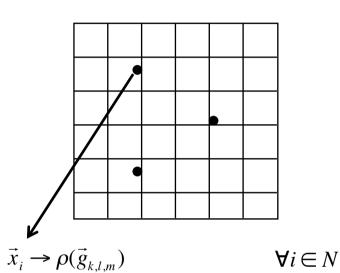
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$$\vec{F}(\vec{g}_{k,l,m}) = -m\nabla\Phi(\vec{g}_{k,l,m})$$



- 2. solve Poisson's equation on grid
- 3. differentiate potential to get forces



$$\Phi(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m})$$

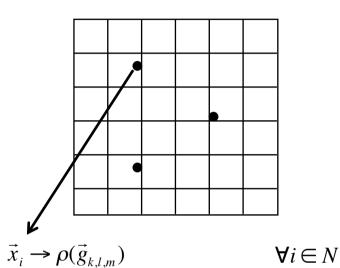
numerically integrate Poisson's equation

$$\Delta\Phi(\vec{g}_{k,l,m}) = 4\pi G \rho(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m}) = -m\nabla\Phi(\vec{g}_{k,l,m})$$



- 2. solve Poisson's equation on grid
- 3. differentiate potential to get forces
- 4. interpolate forces back to particles



$$\Phi(\vec{g}_{k,l,m})$$

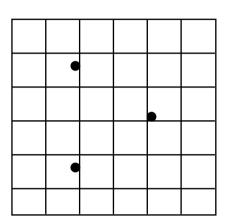
$$\vec{F}(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m}) \to \vec{F}(\vec{x}_i) \qquad \forall i \in N$$

numerically integrate Poisson's equation

$$\Delta\Phi(\vec{g}_{k,l,m}) = 4\pi G \rho(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m}) = -m\nabla\Phi(\vec{g}_{k,l,m})$$



$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

$$\Phi(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m})$$

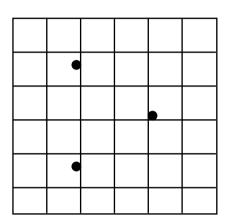
$$\vec{F}(\vec{g}_{k,l,m}) \to \vec{F}(\vec{x}_i)$$

sounds like a waste of time and computer resources, but **exceptionally fast** in practice

numerically integrate Poisson's equation

$$\Delta\Phi(\vec{g}_{k,l,m}) = 4\pi G \rho(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m}) = -m\nabla\Phi(\vec{g}_{k,l,m})$$



$$\vec{x}_i \to \rho(\vec{g}_{k,l,m})$$

2. solve Poisson's equation on grid

$$\Phi(\vec{g}_{k,l,m})$$

3. differentiate potential to get forces

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4. interpolate forces back to particles

$$\vec{F}(\vec{g}_{k,l,m}) \to \vec{F}(\vec{x}_i)$$

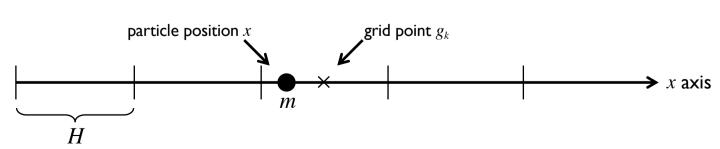
density assignment schemes

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

example: I particle on I dimensional grid

$$M(g_k) = mW(d)$$
 $d = |x - g_k|$

$$\rho(g_k) = \frac{M(g_k)}{H}$$



density assignment schemes

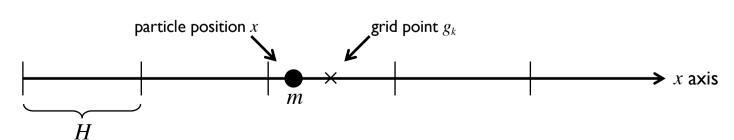
$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

example: I particle on I dimensional grid

$$M(g_k) = mW(d) \qquad d = |x - g_k|$$

mass assignment function

$$\rho(g_k) = \frac{M(g_k)}{H}$$



density assignment schemes

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

example: I particle on I dimensional grid

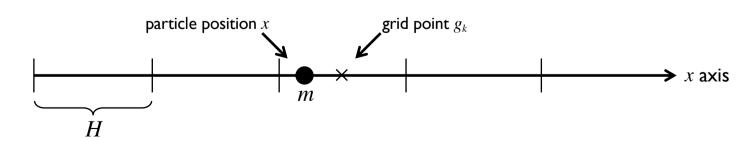
hierarchy of mass assignment schemes:

Nearest-Grid-PointNGP

Could-In-CellCIC

Triangular-Shaped CloudTSC

– ...



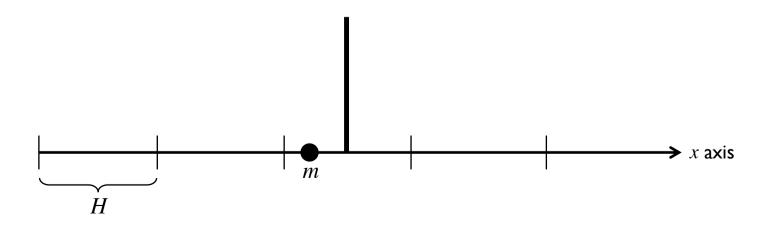
density assignment schemes

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

Nearest-Grid-Point (NGP):

mass assignment function:

$$W(d) = \begin{cases} 1 & d \le H/2 \\ 0 & \text{otherwise} \end{cases}$$



density assignment schemes

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

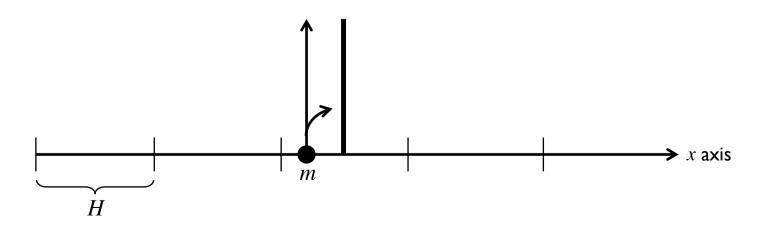
Nearest-Grid-Point (NGP):

particle shape:

mass assignment function:

$$S(x) = \delta(x)$$

$$W(d) = \begin{cases} 1 & d \le H/2 \\ 0 & \text{otherwise} \end{cases}$$

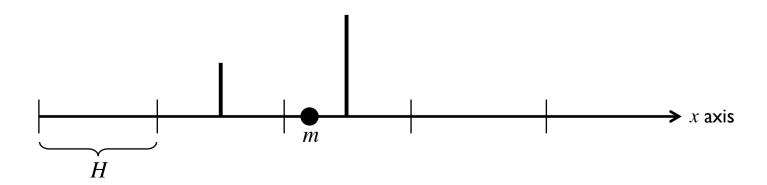


density assignment schemes

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

Cloud-In-Cell (CIC):

mass assignment function:
$$W(d) = \begin{cases} 1 - \frac{d}{H} & d \le H \\ 0 & \text{otherwise} \end{cases}$$



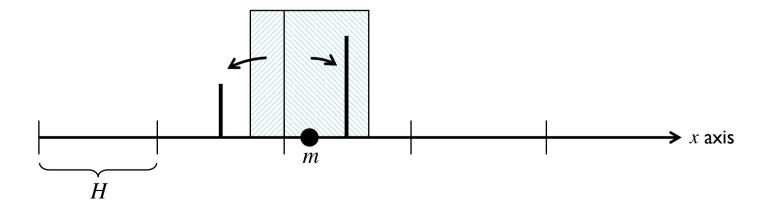
density assignment schemes

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

Cloud-In-Cell (CIC):

$$S(x) = \begin{cases} 1 & |x| \le H/2 \\ 0 & \text{otherwise} \end{cases}$$

particle shape: mass assignment function: $S(x) = \begin{cases} 1 & |x| \le H/2 \\ 0 & \text{otherwise} \end{cases}$ mass assignment function: $W(d) = \begin{cases} 1 - \frac{d}{H} & d \le H \\ 0 & \text{otherwise} \end{cases}$



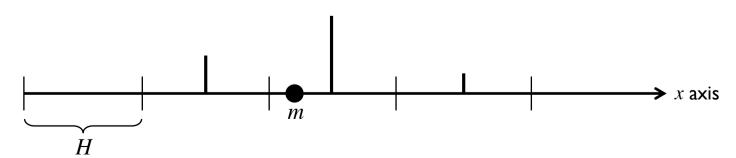
density assignment schemes

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

Triangular-Shaped-Cloud (TSC):

mass assignment function:
$$W(d) = \begin{cases} \frac{3}{4} - \left(\frac{d}{H}\right)^2 & d \le \frac{H}{2} \\ \frac{1}{2} \left(\frac{3}{2} - \frac{d}{H}\right)^2 & \frac{H}{2} \le d \le \frac{3H}{2} \end{cases}$$

$$0 \quad \text{otherwise}$$



density assignment schemes

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

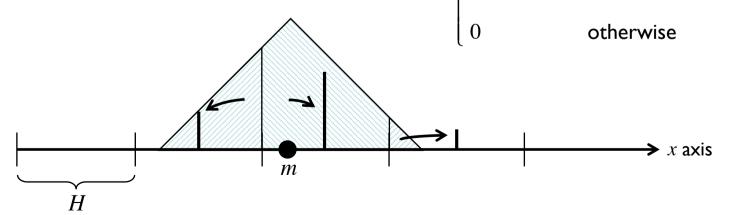
Triangular-Shaped-Cloud (TSC):

particle shape: mass assignment function:

 $S(x) = \begin{cases} 1 - \frac{|x|}{H} & |x| \le H \\ 0 & \text{otherwise} \end{cases}$

$$\left[\frac{3}{4} - \left(\frac{d}{H}\right)^2 \quad d \le \frac{H}{2}\right]$$

$$W(d) = \begin{cases} \frac{1}{2} \left(\frac{3}{2} - \frac{d}{H} \right)^2 & \frac{H}{2} \le d \le \frac{3H}{2} \end{cases}$$



density assignment schemes

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

N particles on 3 dimensional grid

$$\vec{d} = \vec{x}_i - \vec{g}_{k,l,m}$$

$$M(\vec{g}_{k,l,m}) = \sum_{i=1}^{N} m_i W(|d_x|) W(|d_y|) W(|d_z|)$$

$$\rho(\vec{g}_{k,l,m}) = \frac{M(\vec{g}_{k,l,m})}{H^3}$$

density assignment schemes

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

N particles on 3 dimensional grid

$$\vec{d} = \vec{x}_i - \vec{g}_{k,l,m}$$

$$M(\vec{g}_{k,l,m}) = \sum_{i=1}^{N} m_i W(|d_x|) W(|d_y|) W(|d_z|)$$

for every grid point we need to loop over all N particles...

$$\rho(\vec{g}_{k,l,m}) = \frac{M(\vec{g}_{k,l,m})}{H^3}$$

density assignment schemes - in practice

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

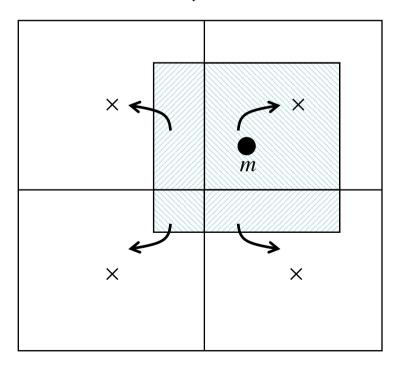
...rather loop over all particles and assign them to the appropriate grid points, because the mapping $x_i \rightarrow g_k$ is rather easy

density assignment schemes - in practice

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

• example for CIC assignment in 2D:

 \vec{x}_i contributes its mass m_i to the 4 closest grid points:

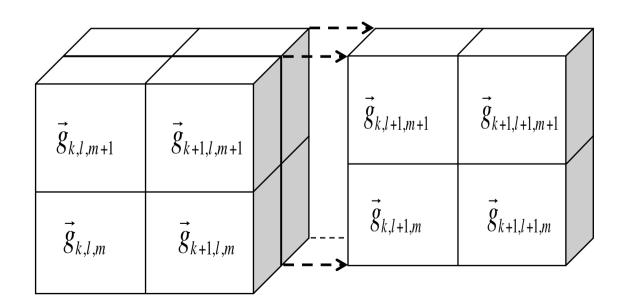


density assignment schemes - in practice

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

• example for CIC assignment in 3D:

 \vec{x}_i contributes its mass m_i to the 8 closest grid points:



- density assignment schemes
 - which scheme to choose?

NGP = stepwise force (I grid point)

CIC = continuous piecewise linear force (8 grid points)

TSC = continuous force and first derivative (27 grid points)

- density assignment schemes
 - which scheme to choose?

NGP = too crude

CIC = common choice

TSC = pretty smooth ↓

increased smoothing of density field

- density assignment schemes
 - which scheme to choose?

CIC = common choice

increased smoothing of density field

smoothing the density field will lead to a "bias" in the forces but at the same time decrease the "variance"!

bias =
$$\left(\left\langle \vec{F}(\vec{x})\right\rangle - \vec{F}_{true}(\vec{x})\right) \propto \varepsilon^{\alpha}$$

$$\operatorname{var} = \langle \vec{F}^{2}(\vec{x}) \rangle - \langle \vec{F}(\vec{x}) \rangle^{2} \propto N^{-\beta}$$

- density assignment schemes
 - which scheme to choose?

NGP = too crude
$$\log F(r)$$

CIC = common choice

TSC = pretty smooth

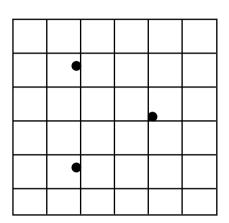
smoothing the density field will lead to a "bias" in the forces but at the same time decrease the "variance"!

bias =
$$\left(\left\langle \vec{F}(\vec{x})\right\rangle - \vec{F}_{true}(\vec{x})\right) \propto \varepsilon^{\alpha}$$
 (interplay between N and ε : $N\varepsilon^{\beta}$ =const.)
$$\text{var} = \left\langle \vec{F}^{2}(\vec{x})\right\rangle - \left\langle \vec{F}(\vec{x})\right\rangle^{2} \propto N^{-\beta}$$

numerically integrate Poisson's equation

$$\Delta\Phi(\vec{g}_{k,l,m}) = 4\pi G \rho(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m}) = -m\nabla\Phi(\vec{g}_{k,l,m})$$



I. calculate mass density on grid

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

2. solve Poisson's equation on grid

$$\Phi(\vec{g}_{k,l,m})$$

3. differentiate potential to get forces

$$\vec{F}(\vec{g}_{k,l,m})$$

4. interpolate forces back to particles

$$\vec{F}(\vec{g}_{k,l,m}) \to \vec{F}(\vec{x}_i)$$

numerically integrate Poisson's equation

$$\Delta\Phi_{k,l,m}=\rho_{k,l,m}$$

• relaxation technique: applicable and usable for **any** differential equation

• FTT technique: only applicable and usable for *linear* differential equation

numerically integrate Poisson's equation

$$\Delta\Phi_{k,l,m}=\rho_{k,l,m}$$

• relaxation technique: applicable and usable for **any** differential equation

• FTT technique: only applicable and usable for *linear* differential equation

$$\Delta\Phi_{k,l,m}=\rho_{k,l,m}$$

- Green's function method:
 - solve differential equation by Fourier transformation
 - applicable and usable for *linear* differential equations

- numerically integrate Poisson's equation fast fourier transform method
 - Green's function method

$$\Delta\Phi = \rho$$

$$\Phi(\vec{x}) = \iiint G(\vec{x} - \vec{x}') \rho(\vec{x}') d^3 x'$$
; $G(\vec{x}) = \frac{1}{4\pi x}$

- numerically integrate Poisson's equation fast fourier transform method
 - Green's function method

$$\Delta\Phi = \rho$$

$$\Phi(\vec{x}) = \iiint G(\vec{x} - \vec{x}') \rho(\vec{x}') d^3 x'$$
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- numerically integrate Poisson's equation fast fourier transform method
 - Green's function method

$$\Delta\Phi = \rho$$

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; $G(\vec{x}) = \frac{1}{4\pi x}$

- numerically integrate Poisson's equation fast fourier transform method
 - discretized Green's function

$$\hat{\mathcal{G}}(\vec{k}) = -\frac{1}{k^2} \qquad \Longrightarrow \qquad \hat{\mathcal{G}}(\vec{g}_{k,l,m}) = -\frac{1}{\sin^2\left(\frac{k_x}{2}\right) + \sin^2\left(\frac{k_y}{2}\right) + \sin^2\left(\frac{k_z}{2}\right)}$$

compensates for grid anisotropies...

$$\hat{G}(\vec{g}_{0,0,0}) = 0$$
, $k_x = \frac{2\pi k}{L}$, $k_y = \frac{2\pi l}{L}$, $k_y = \frac{2\pi m}{L}$

$$\Delta\Phi_{k,l,m}=\rho_{k,l,m}$$

- relaxation technique: applicable and usable for any differential equation
- FTT technique: only applicable and usable for *linear* differential equation

numerically integrate Poisson's equation

relaxation technique

obtain iterative solver by discretizing differential equation

$$\Delta\Phi_{{\scriptscriptstyle k,l,m}}=\rho_{{\scriptscriptstyle k,l,m}}$$

numerically integrate Poisson's equation

relaxation technique

obtain iterative solver by discretizing differential equation

$$\Delta\Phi_{k,l,m} = \rho_{k,l,m}$$

$$\begin{split} & \Delta \Phi_{k,l,m} = \nabla \cdot \nabla \Phi_{k,l,m} \\ & = \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \cdot \begin{pmatrix} \frac{\partial \Phi_{k,l,m}}{\partial x} \\ \frac{\partial \Phi_{k,l,m}}{\partial y} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \\ & = \frac{1}{H} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} \end{pmatrix} \cdot \begin{pmatrix} \Phi_{k+\frac{1}{2},l,m} - \Phi_{k-\frac{1}{2},l,m} \\ \Phi_{k,l+\frac{1}{2},m} - \Phi_{k,l-\frac{1}{2},m} \\ \Phi_{k,l,m+\frac{1}{2}} - \Phi_{k,l,m-\frac{1}{2}} \end{pmatrix} \\ & = \frac{1}{H} \begin{pmatrix} \frac{\partial}{\partial x} + \frac{1}{2} \\ \frac{\partial}{\partial z} \\ \frac{\partial}{\partial z} \end{pmatrix} \cdot \begin{pmatrix} \Phi_{k+\frac{1}{2},l,m} - \Phi_{k,l-\frac{1}{2},l,m} \\ \Phi_{k,l,m+\frac{1}{2}} - \Phi_{k,l,m-\frac{1}{2}} \\ \frac{\partial}{\partial z} \end{pmatrix} \\ & = \frac{1}{H^2} \left(\Phi_{k+1,l,m} - 2\Phi_{k,l,m} + \Phi_{k-1,l,m} + \Phi_{k,l+1,m} - 2\Phi_{k,l,m} + \Phi_{k,l-1,m} + \Phi_{k,l-1,m} + \Phi_{k,l-1,m} + \Phi_{k,l,m+1} - 2\Phi_{k,l,m} + \Phi_{k,l,m-1} \right) \end{split}$$

numerically integrate Poisson's equation

relaxation technique

obtain iterative solver by discretizing differential equation

$$\Delta\Phi_{k,l,m}=\rho_{k,l,m}$$

$$\Phi_{k,l,m} = \frac{1}{6} (\Phi_{k+1,l,m} + \Phi_{k-1,l,m} + \Phi_{k,l+1,m} + \Phi_{k,l-1,m} + \Phi_{k,l,m+1} + \Phi_{k,l,m-1} - \rho_{k,l,m} H^2)$$

numerically integrate Poisson's equation

relaxation technique

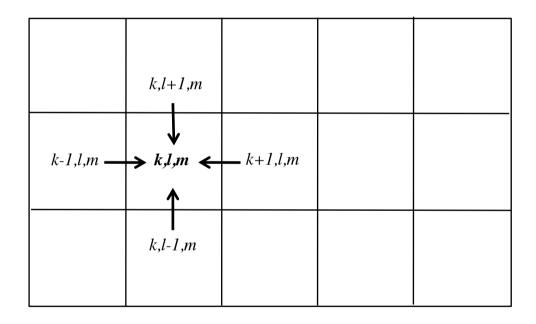
obtain iterative solver by discretizing differential equation

$$\Phi_{k,l,m}^{(+)} = \frac{1}{6} (\Phi_{k+1,l,m}^{(i)} + \Phi_{k-1,l,m}^{(i)} + \Phi_{k,l+1,m}^{(i)} + \Phi_{k,l-1,m}^{(i)} + \Phi_{k,l,m+1}^{(i)} + \Phi_{k,l,m-1}^{(i)} - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

obtain iterative solver by discretizing differential equation

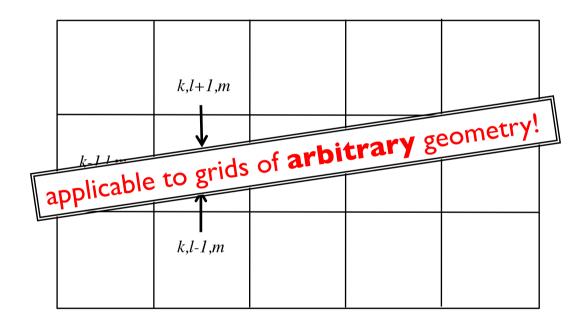


$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m} H^2)$$

numerically integrate Poisson's equation

relaxation technique

obtain iterative solver by discretizing differential equation

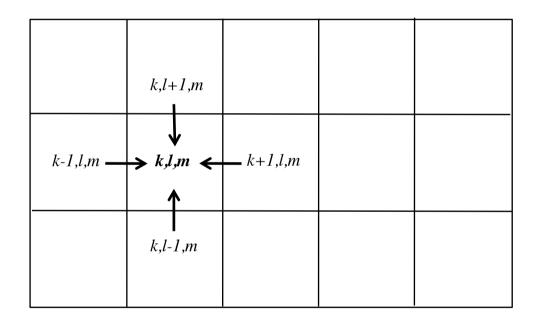


$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

how to sweep through the grid?

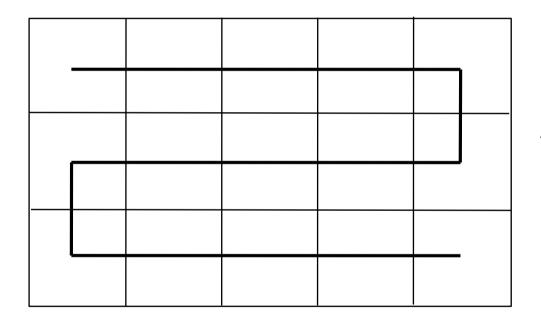


$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m} H^2)$$

numerically integrate Poisson's equation

relaxation technique

• how to sweep through the grid?



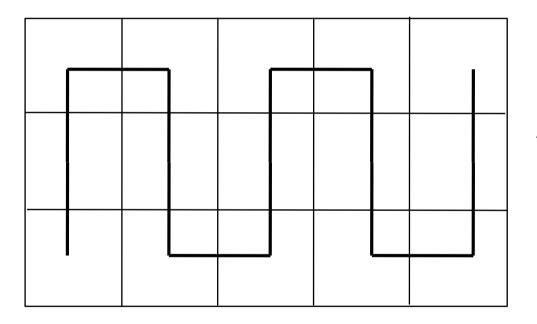
?

$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

how to sweep through the grid?



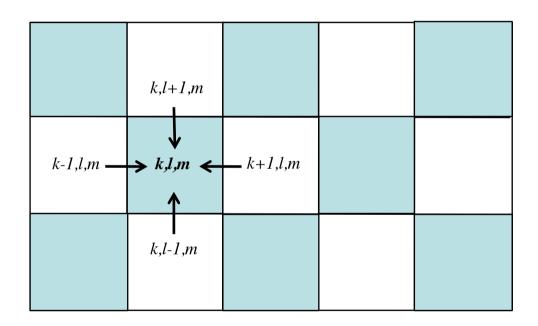
?

$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

• Gauss-Seidel sweeps:



$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m} H^2)$$

numerically integrate Poisson's equation

relaxation technique

- Gauss-Seidel sweeps:
 - loop over all "black" cells $\Phi^i_{k,l,m} \to \Phi^{i+1}_{k,l,m}$ one iteration of the potential

$$\Phi^{i}_{k,l,m} \longrightarrow \Phi^{i+1}_{k,l,m}$$

how many iterations i are necessary?

$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

• stopping criterion:

$$\Delta\Phi^i_{k,l,m}=\rho_{k,l,m}$$

$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

• stopping criterion:

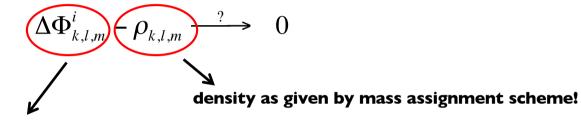
$$\Delta\Phi_{k,l,m}^i - \rho_{k,l,m} \xrightarrow{?} 0$$

$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

• stopping criterion:



density as given by currently best guess for Φ^i !

$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m} H^2)$$

numerically integrate Poisson's equation

relaxation technique

• stopping criterion:

$$\Delta\Phi_{k,l,m}^i - \rho_{k,l,m} \xrightarrow{?} 0$$

residual:
$$R^i = \left\| \Delta \Phi^i_{k,l,m} - \rho_{k,l,m} \right\|$$

 $\|\bullet\|$ = suitable norm

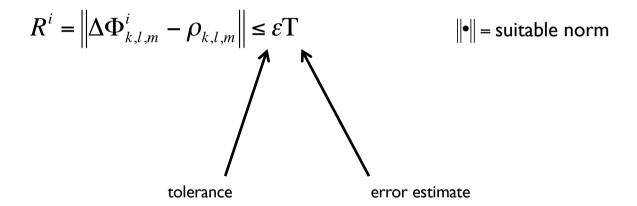
$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

• stopping criterion:

$$\Delta\Phi_{k,l,m}^i - \rho_{k,l,m} \xrightarrow{?} 0$$

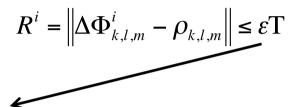


$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

• stopping criterion:



– truncation error:

error due to discreteness of grid

$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

• stopping criterion:

$$R^{i} = \left\| \Delta \Phi_{k,l,m}^{i} - \rho_{k,l,m} \right\| \le \varepsilon T$$

- truncation error:

error due to discreteness of grid

compare solution on actual grid to solution on coarser grid

$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

• stopping criterion:

$$R^{i} = \left\| \Delta \Phi_{k,l,m}^{i} - \rho_{k,l,m} \right\| \le \varepsilon \Gamma = \varepsilon \left\| T_{k,l,m} \right\|$$

$$\begin{array}{ll} - \text{ truncation error: } & T_{k,l,m} = \underbrace{\mathcal{P}\!\!\left[\Delta\!\left(\mathcal{R}\Phi^{i}_{k,l,m}\right)\right]} - \!\left(\Delta\Phi^{i}_{k,l,m}\right) \\ & \mathcal{R}\Phi^{i}_{k,l,m} = \pmb{\varPhi}^{i}_{j,n,p} & \text{restriction to coarser grid} \\ & \Delta\!\left(\mathcal{R}\Phi^{i}_{k,l,m}\right) = \rho^{i-1}_{j,n,p} \\ & \mathcal{P}\!\!\left[\Delta\!\left(\mathcal{R}\Phi^{i}_{k,l,m}\right)\right] = \rho^{i}_{k,l,m} & \text{prolongation to finer grid} \end{array}$$

$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

• stopping criterion:

$$R^{i} = \left\| \Delta \Phi_{k,l,m}^{i} - \rho_{k,l,m} \right\| \le \varepsilon \mathbf{T} = \varepsilon \left\| T_{k,l,m} \right\|$$

$$\begin{aligned} & - \text{ truncation error: } \quad \mathbf{T}_{k,l,m} = \mathcal{P} \Big[\Delta \Big(\mathcal{R} \Phi^i_{k,l,m} \Big) \Big] - \Big(\Delta \Phi^i_{k,l,m} \Big) \\ & \mathcal{R} \Phi^i_{k,l,m} = \boldsymbol{\varPhi}^i_{j,n,p} \\ & \Delta \Big(\mathcal{R} \Phi^i_{k,l,m} \Big) = \rho^{i-1}_{j,n,p} \\ & \mathcal{P} \Big[\Delta \Big(\mathcal{R} \Phi^i_{k,l,m} \Big) \Big] = \rho^i_{k,l,m} & = \Delta \Phi^i_{k,l,m} \end{aligned}$$

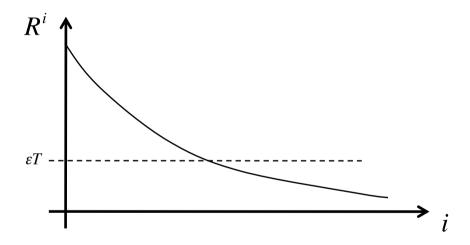
$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

• stopping criterion:

$$R^{i} = \left\| \Delta \Phi_{k,l,m}^{i} - \rho_{k,l,m} \right\| \le \varepsilon \mathbf{T} = \varepsilon \left\| T_{k,l,m} \right\|$$



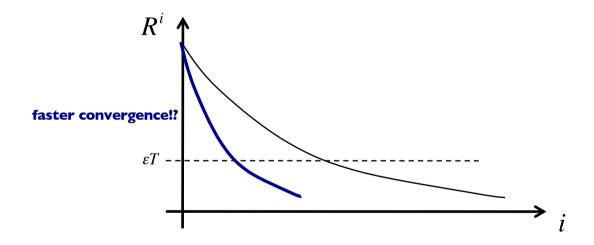
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numerically integrate Poisson's equation

relaxation technique

• stopping criterion:

$$R^{i} = \left\| \Delta \Phi_{k,l,m}^{i} - \rho_{k,l,m} \right\| \le \varepsilon \mathbf{T} = \varepsilon \left\| T_{k,l,m} \right\|$$



$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m} H^2)$$

numerically integrate Poisson's equation

relaxation technique

• convergence:

$$R^{i} = \left\| \Delta \Phi_{k,l,m}^{i} - \rho_{k,l,m} \right\|$$

- slow convergence: $R^{i+1} \approx R^i$

large-scale errors in Φ cannot be "relaxed" sufficiently fast on the actual grid

=> use coarser grids to speed up convergence...

$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

numerically integrate Poisson's equation

relaxation technique

• convergence:

$$R^{i} = \left\| \Delta \Phi_{k,l,m}^{i} - \rho_{k,l,m} \right\|$$

- slow convergence: $R^{i+1} \approx R^i$

$$R^{i+1} \approx R^i$$

multi-grid relaxation techniques

=> beyond the scope of this lecture though...

$$\Phi_{k,l,m}^{i+1} = \frac{1}{6} (\Phi_{k+1,l,m}^i + \Phi_{k-1,l,m}^i + \Phi_{k,l+1,m}^i + \Phi_{k,l-1,m}^i + \Phi_{k,l,m+1}^i + \Phi_{k,l,m-1}^i - \rho_{k,l,m}H^2)$$

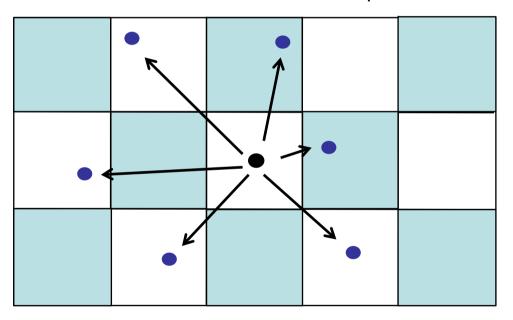
numerically integrate Poisson's equation

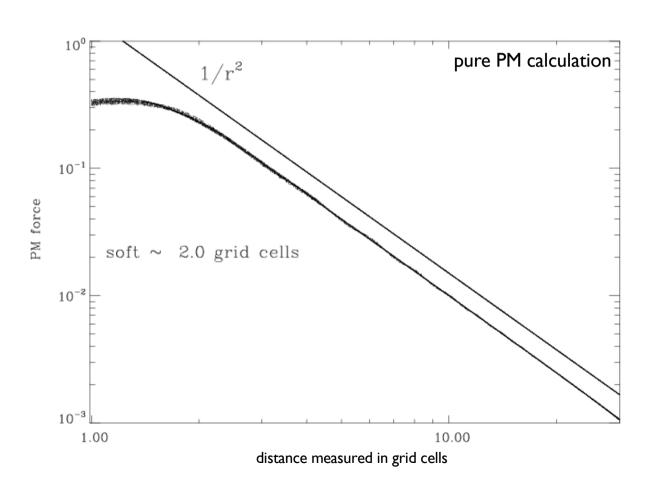
accuracy of either

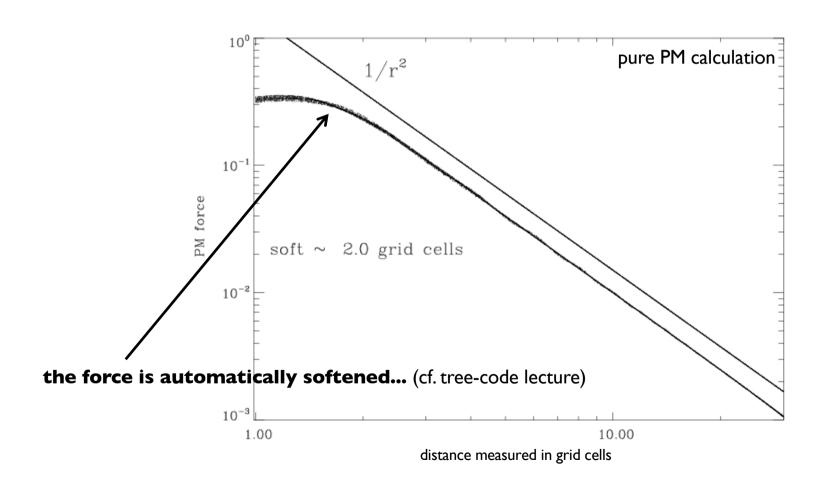
relaxation or FFT method

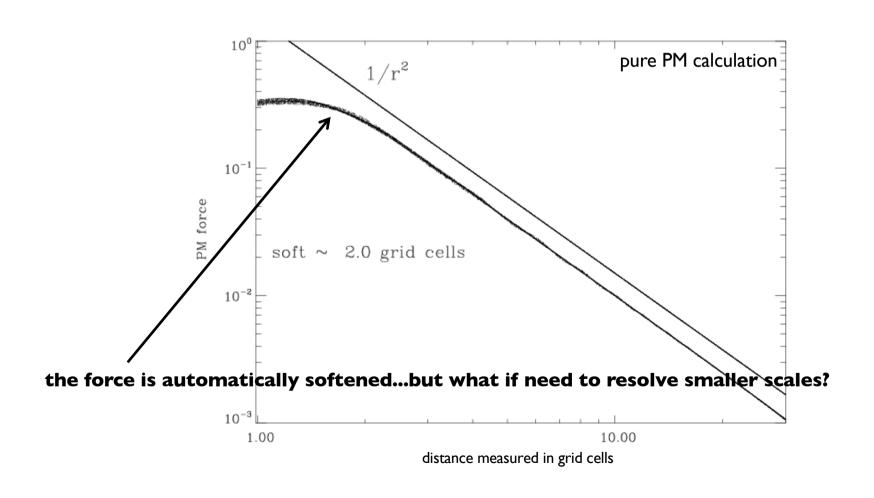
to solve Poisson's equation?

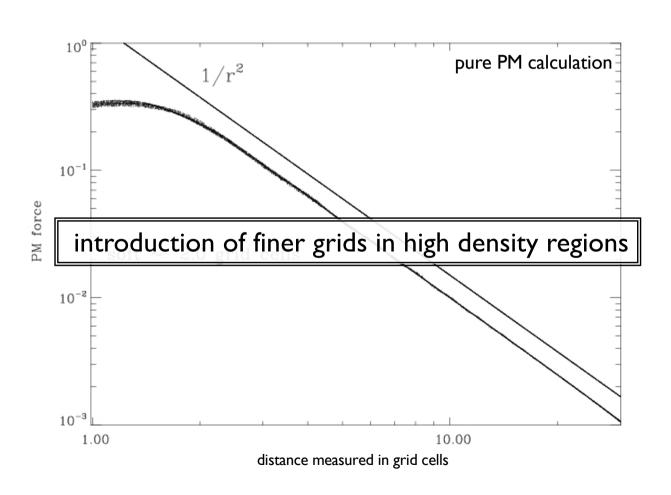
pure PM calculation

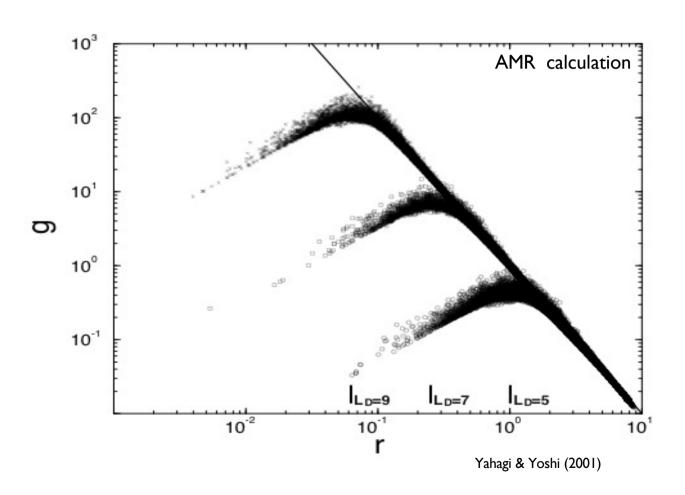


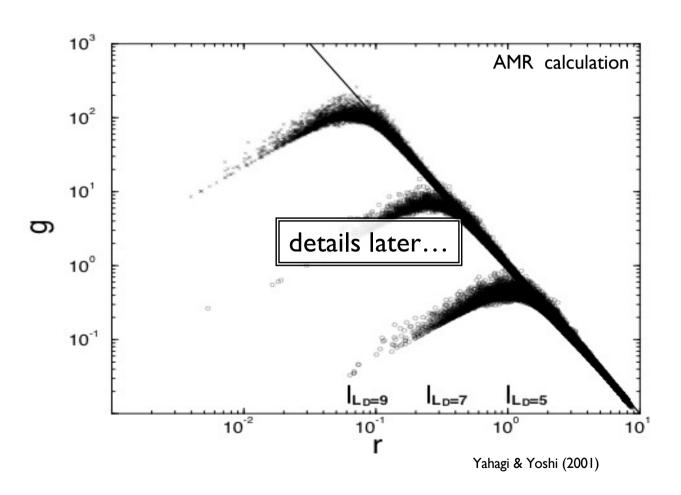


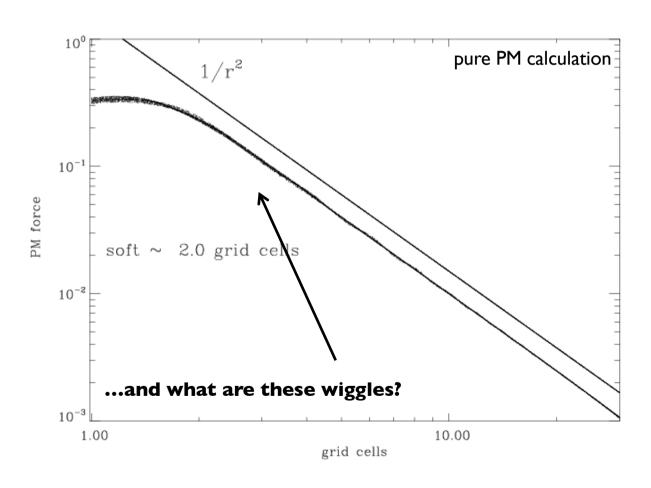


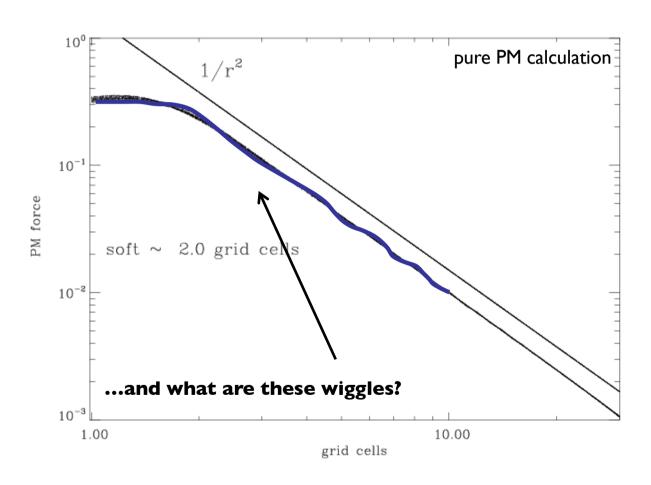






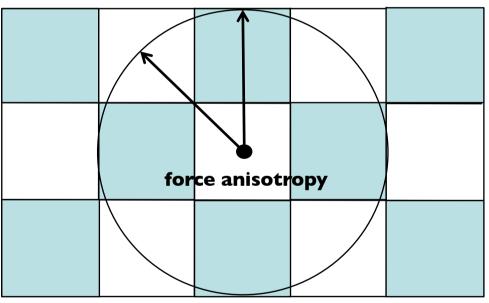






numerically integrate Poisson's equation

pure PM calculation

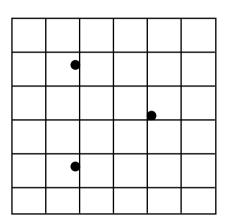


...and what are these wiggles?

numerically integrate Poisson's equation

$$\Delta\Phi(\vec{g}_{k,l,m}) = 4\pi G \rho(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m}) = -m\nabla\Phi(\vec{g}_{k,l,m})$$



I. calculate mass density on grid

$$\vec{x}_i \to \rho(\vec{g}_{k,l,m})$$

2. solve Poisson's equation on grid

$$\Phi(\vec{g}_{k,l,m})$$

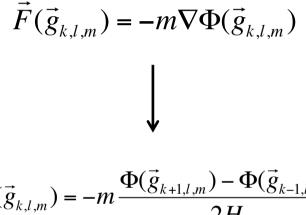
3. differentiate potential to get forces

$$\vec{F}(\vec{g}_{k,l,m})$$

4. interpolate forces back to particles

$$\vec{F}(\vec{g}_{k,l,m}) \rightarrow \vec{F}(\vec{x}_i)$$

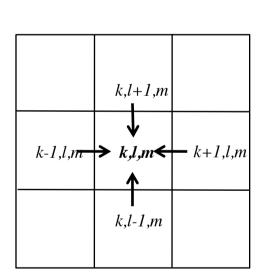
obtaining the forces



$$F_{x}(\vec{g}_{k,l,m}) = -m \frac{\Phi(\vec{g}_{k+1,l,m}) - \Phi(\vec{g}_{k-1,l,m})}{2H}$$

$$F_{y}(\vec{g}_{k,l,m}) = -m \frac{\Phi(\vec{g}_{k,l+1,m}) - \Phi(\vec{g}_{k,l-1,m})}{2H}$$

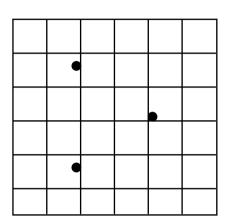
$$F_{z}(\vec{g}_{k,l,m}) = -m \frac{\Phi(\vec{g}_{k,l,m+1}) - \Phi(\vec{g}_{k,l,m-1})}{2H}$$



H = (current) grid spacing

$$\Delta\Phi(\vec{g}_{k,l,m}) = 4\pi G \rho(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m}) = -m\nabla\Phi(\vec{g}_{k,l,m})$$



$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

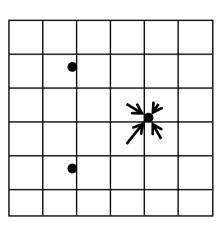
$$\Phi(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m}) \rightarrow \vec{F}(\vec{x}_i)$$

interpolating the forces

$$\vec{F}(\vec{g}_{k,l,m}) \rightarrow \vec{F}(\vec{r}_i)$$



interpolating the forces

$$\vec{F}(\vec{g}_{k,l,m}) \rightarrow \vec{F}(\vec{r}_i)$$

use the inverse of the mass assignment scheme to insure momentum conservation and minimize force anisotropies

$$\vec{F}(\vec{r}_i) = \sum_{k} \sum_{l} \sum_{m} \vec{F}(\vec{g}_{k,l,m}) W(\left| \vec{r}_i - \vec{g}_{k,l,m} \right|)$$

interpolating the forces

$$\vec{F}(\vec{g}_{k,l,m}) \rightarrow \vec{F}(\vec{r}_i)$$

use the inverse of the mass assignment scheme to insure momentum conservation and minimize force anisotropies

$$\vec{F}(\vec{r}_i) = \sum_{k} \sum_{l} \sum_{m} \vec{F}(\vec{g}_{k,l,m}) W(\left| \vec{r}_i - \vec{g}_{k,l,m} \right|)$$

*check by calculating the total (periodic) force:

$$\vec{F}_{tot} = \sum_{i=1}^{N} \vec{F}(\vec{r}_i) = \sum_{i=1}^{N} \sum_{k} \sum_{l} \sum_{m} \vec{F}(\vec{g}_{k,l,m}) W(\vec{r}_i - \vec{g}_{k,l,m})$$

$$= \dots$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k,l,m} \sum_{k',l',m'} \frac{m_i m_j}{H^3} W(\left| \vec{r}_i - \vec{g}_{k,l,m} \right|) \mathcal{G}(\vec{g}_{k,l,m} - \vec{g}_{k',l',m'}) W(\left| \vec{r}_j - \vec{g}_{k',l',m'} \right|)$$
anti-symmetric!
$$= \dots$$

$$= \vec{0} \text{ (because of invariance under coordinate inversion)}$$

PM scheme:

$$F_{x}(\vec{g}_{k,l,m}) = -m \frac{\Phi(\vec{g}_{k+1,l,m}) - \Phi(\vec{g}_{k-1,l,m})}{2H}$$

$$\Phi(\vec{g}_{k,l,m}) = \sum_{k'} \sum_{l'} \sum_{m'} G(\vec{g}_{k,l,m} - \vec{g}_{k',l',m'}) \rho(\vec{g}_{k',l',m'})$$

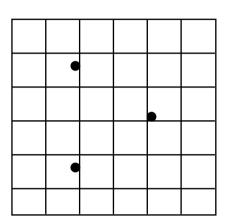
$$\rho(\vec{g}_{k,l,m}) = \frac{M(\vec{g}_{k,l,m})}{H^{3}}$$

$$M(\vec{g}_{k,l,m}) = \sum_{i=1}^{N} m_{i} W(|\vec{r}_{i} - \vec{g}_{k,l,m}|)$$

■ Particle-Mesh (PM) method

$$\Delta\Phi(\vec{g}_{k,l,m}) = 4\pi G \rho(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m}) = -m\nabla\Phi(\vec{g}_{k,l,m})$$



- I. calculate mass density on grid
- 2. solve Poisson's equation on grid
- 3. differentiate potential to get forces
- 4. interpolate forces back to particles

$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

$$\Phi(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m}) \to \vec{F}(\vec{x}_i)$$

anyone fancies to write a PM code as the project?

