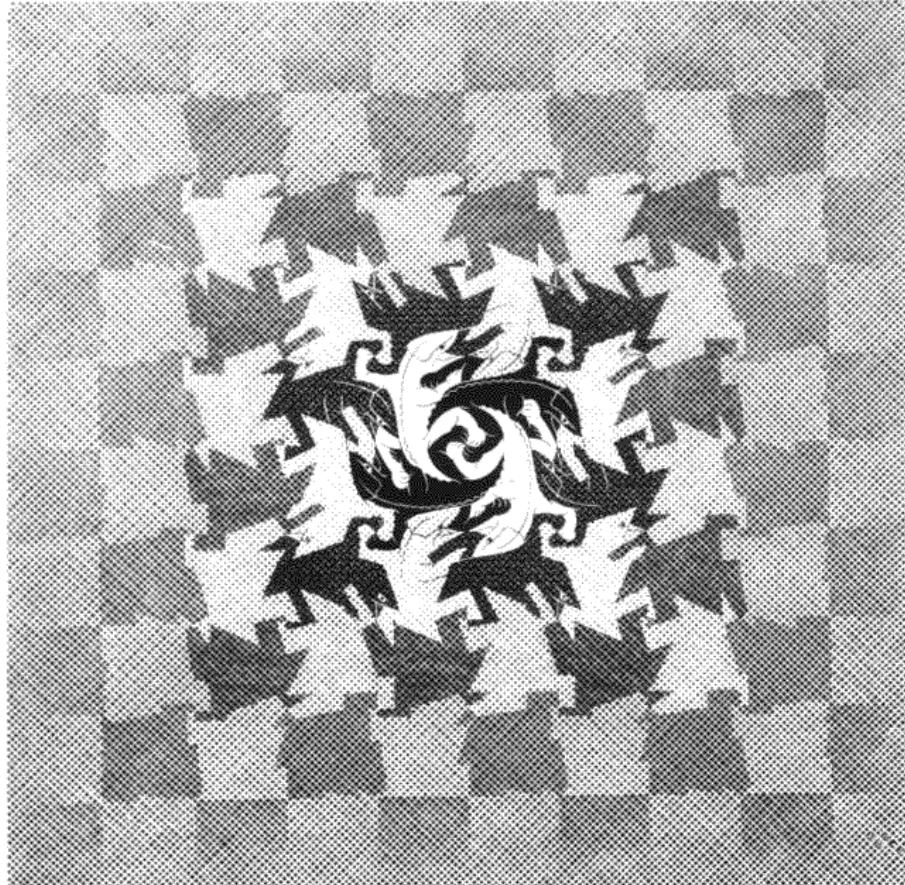


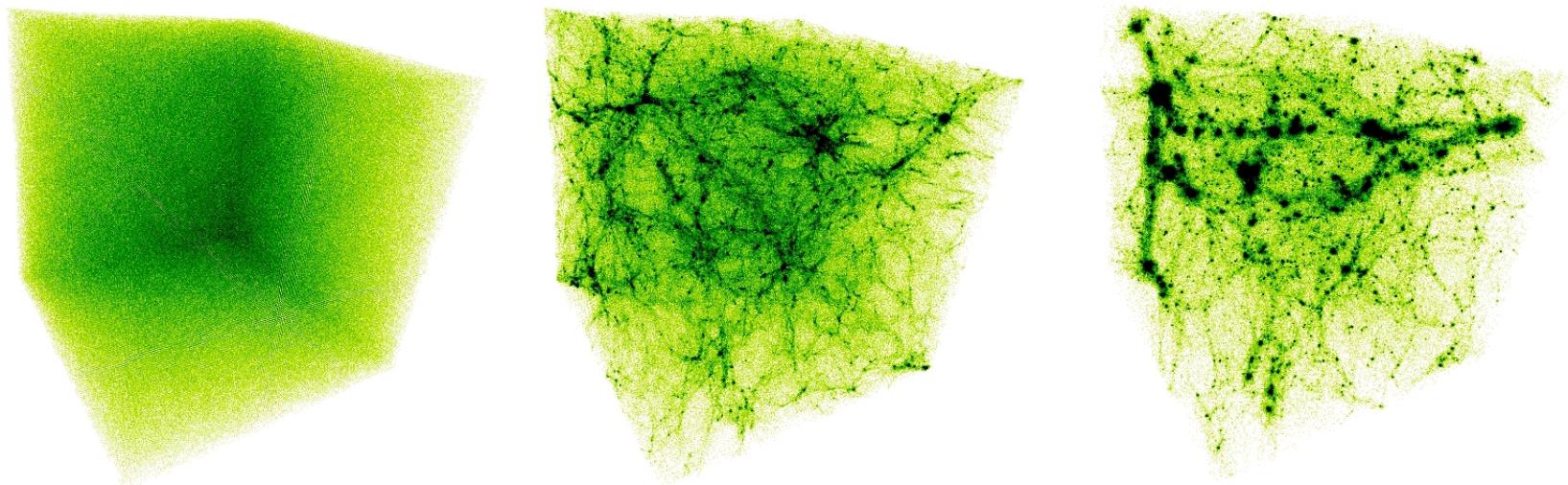
PM CODES

Alexander Knebe, *Universidad Autonoma de Madrid*



Platynota-Mesh code?

PM CODES



↔ particle mesh (PM) codes →

- 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

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

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

particle approach

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

grid approach ($\vec{x}_{i,j,k}$ = 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

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

grid approach ($\vec{x}_{i,j,k}$ = 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

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

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

particle approach

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

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

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

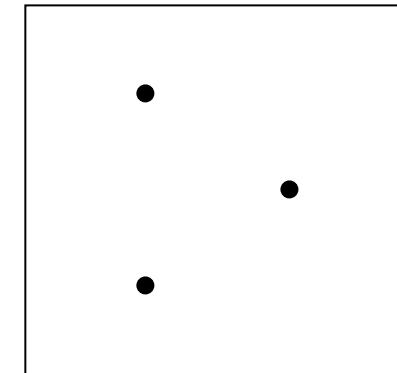
$$\vec{F}(\vec{x}_{i,j,k}) = -m \nabla \Phi(\vec{x}_{i,j,k})$$

weapon of choice: AMR codes – based upon PM!

- numerically integrate Poisson's equation

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

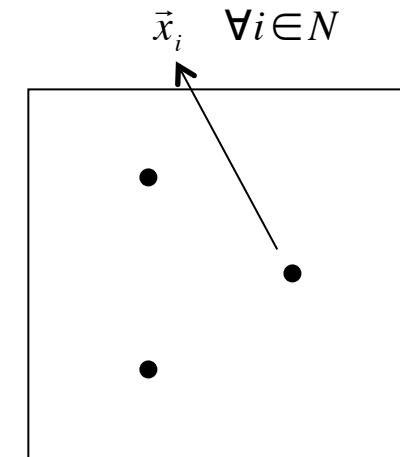
$$\vec{F}(\vec{g}_{k,l,m}) = -m \nabla \Phi(\vec{g}_{k,l,m})$$



- numerically integrate Poisson's equation

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

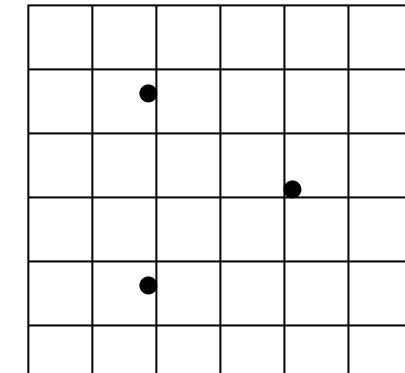
$$\vec{F}(\vec{g}_{k,l,m}) = -m \nabla \Phi(\vec{g}_{k,l,m})$$



- numerically integrate Poisson's equation

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

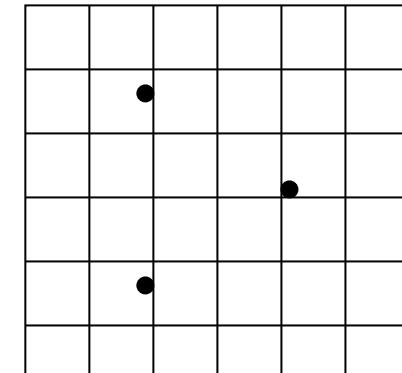
$$\vec{F}(\vec{g}_{k,l,m}) = -m \nabla \Phi(\vec{g}_{k,l,m})$$



- numerically integrate Poisson's equation

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

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

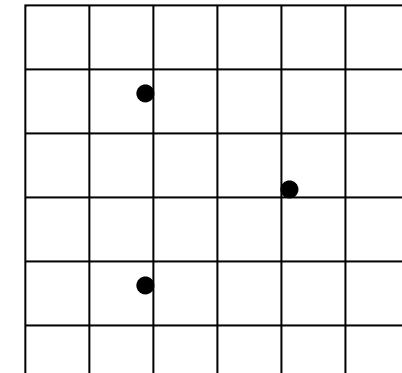


- calculate mass density on grid $\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$
- solve Poisson's equation on grid $\Phi(\vec{g}_{k,l,m})$
- differentiate potential to get forces $\vec{F}(\vec{g}_{k,l,m})$
- interpolate forces back to particles $\vec{F}(\vec{g}_{k,l,m}) \rightarrow \vec{F}(\vec{x}_i)$

- numerically integrate Poisson's equation

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

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



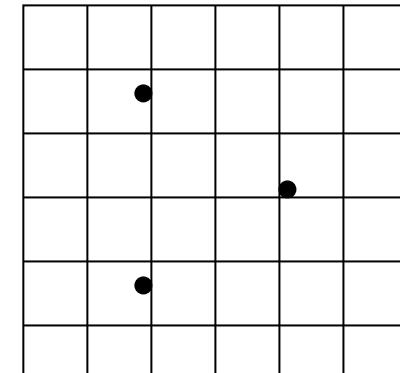
- calculate mass density on grid $\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$
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- differentiate potential to get forces $\vec{F}(\vec{g}_{k,l,m})$
- interpolate forces back to particles $\vec{F}(\vec{g}_{k,l,m}) \rightarrow \vec{F}(\vec{x}_i)$

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

- numerically integrate Poisson's equation

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

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



1. 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

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

- density assignment schemes

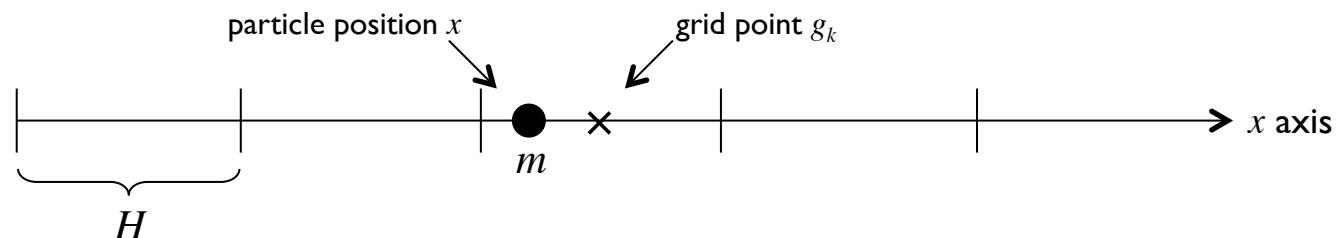
$$\vec{x}_i \rightarrow \rho(\vec{g}_{k,l,m})$$

example: 1 particle on 1 dimensional grid

$$M(g_k) = m W(d) \quad d = |x - g_k|$$

mass assignment function

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



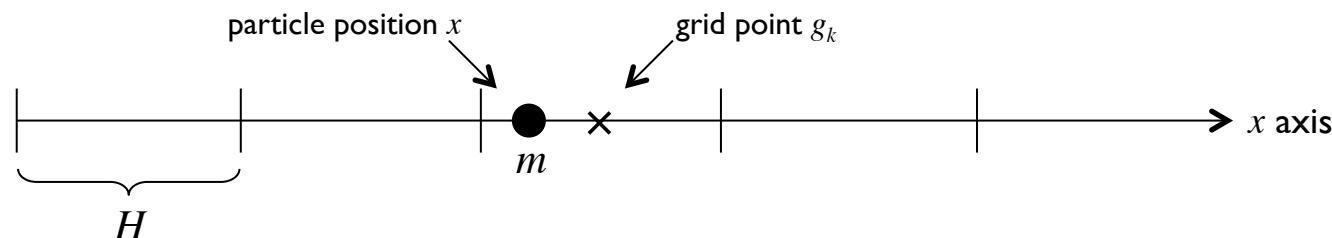
- density assignment schemes

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

example: 1 particle on 1 dimensional grid

- hierarchy of mass assignment schemes:

- Nearest-Grid-Point NGP
- Could-In-Cell CIC
- Triangular-Shaped Cloud TSC
- ...



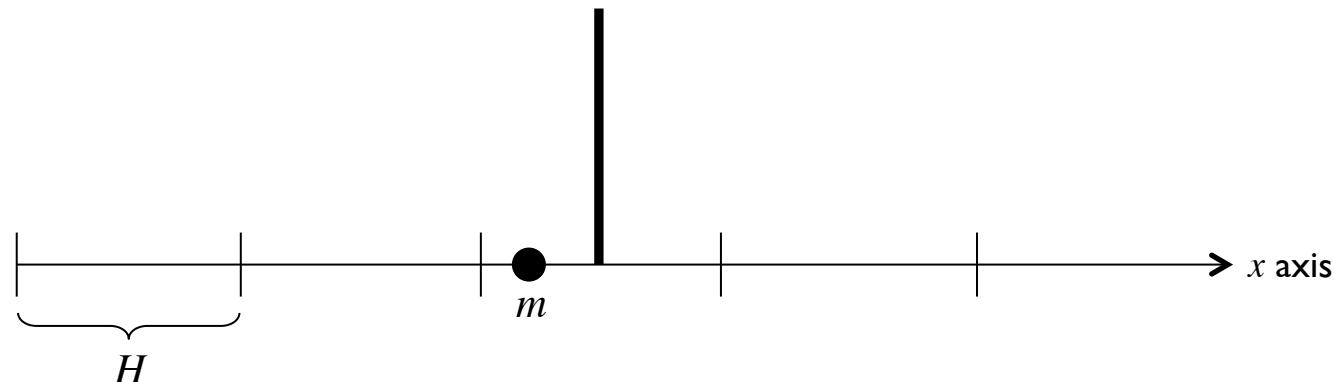
- density assignment schemes

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

Nearest-Grid-Point (NGP):

mass assignment function:

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



- density assignment schemes

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

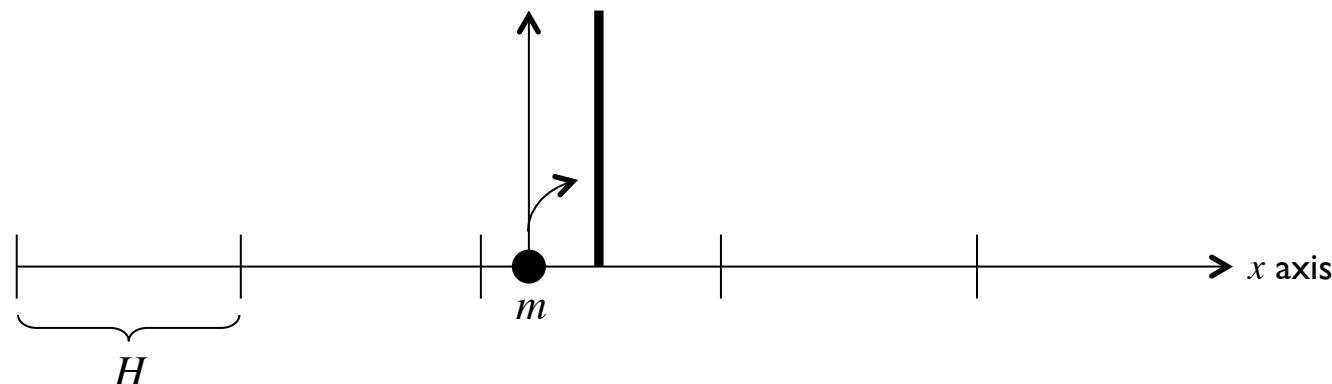
Nearest-Grid-Point (NGP):

particle shape:

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

mass assignment function:

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



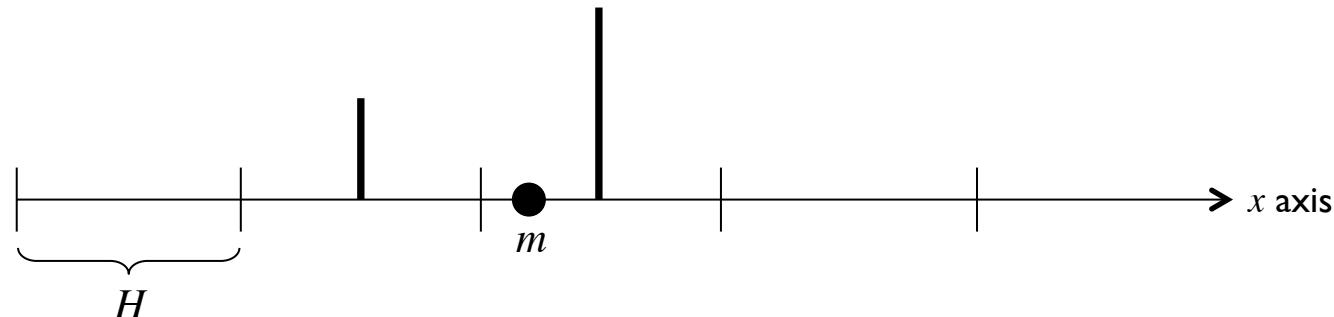
- density assignment schemes

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

Cloud-In-Cell (CIC):

mass assignment function:

$$W(d) = \begin{cases} 1 - \frac{d}{H} & d \leq H \\ 0 & \text{otherwise} \end{cases}$$



- density assignment schemes

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

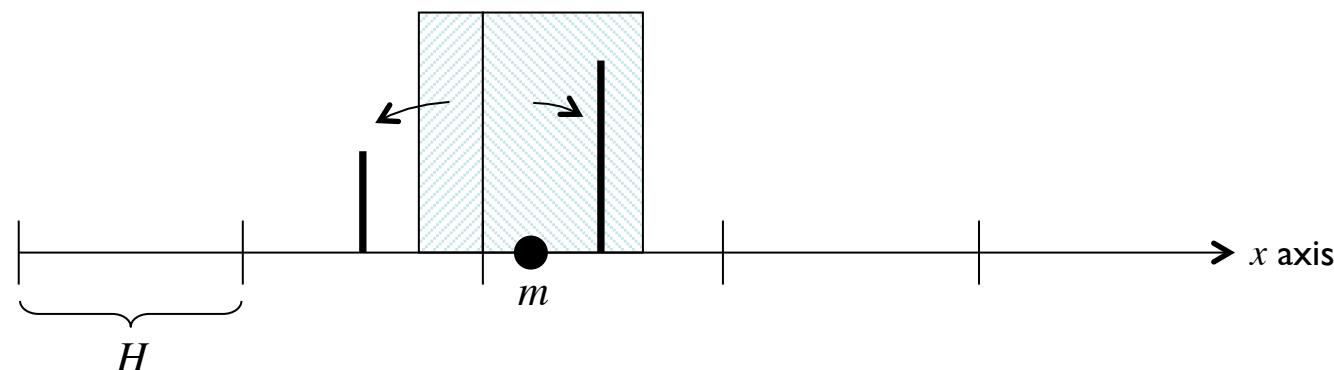
Cloud-In-Cell (CIC):

particle shape:

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

mass assignment function:

$$W(d) = \begin{cases} 1 - \frac{d}{H} & d \leq H \\ 0 & \text{otherwise} \end{cases}$$



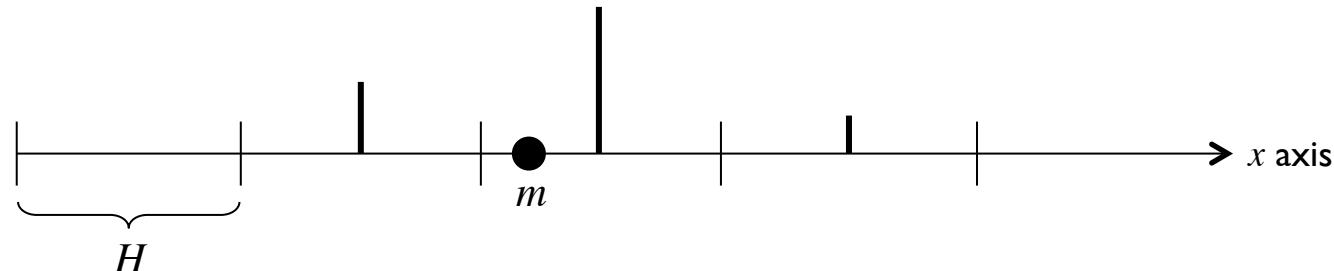
- density assignment schemes

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

Triangular-Shaped-Cloud (TSC):

mass assignment function:

$$W(d) = \begin{cases} \frac{3}{4} - \left(\frac{d}{H}\right)^2 & d \leq \frac{H}{2} \\ \frac{1}{2} \left(\frac{3}{2} - \frac{d}{H} \right)^2 & \frac{H}{2} \leq d \leq \frac{3H}{2} \\ 0 & \text{otherwise} \end{cases}$$



- density assignment schemes

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

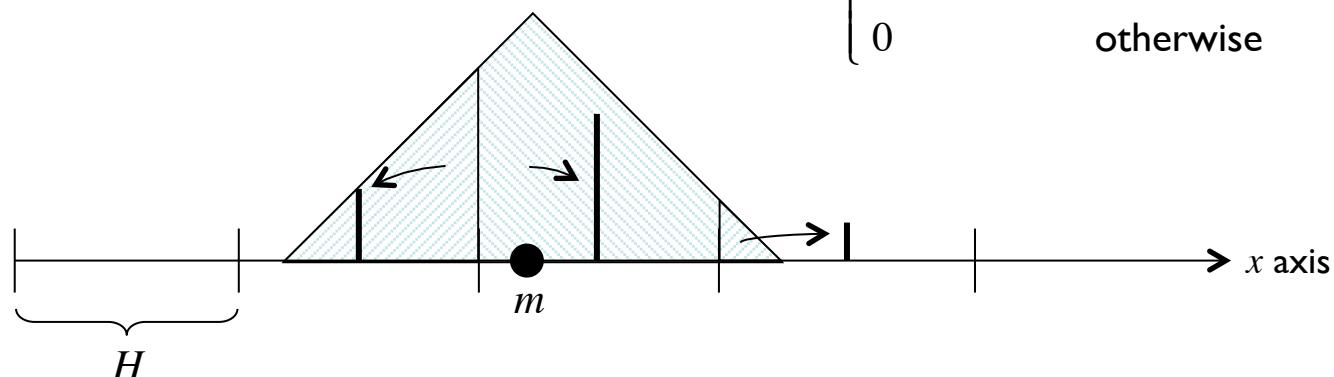
Triangular-Shaped-Cloud (TSC):

particle shape:

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

mass assignment function:

$$W(d) = \begin{cases} \frac{3}{4} - \left(\frac{d}{H}\right)^2 & d \leq \frac{H}{2} \\ \frac{1}{2} \left(3 - \frac{d}{H}\right)^2 & \frac{H}{2} \leq d \leq \frac{3H}{2} \\ 0 & \text{otherwise} \end{cases}$$



- 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

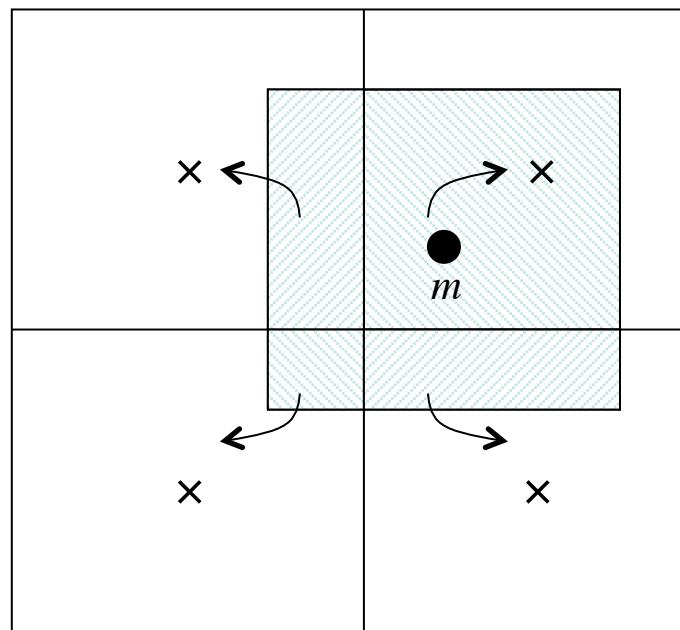
assign them to the appropriate grid points,
because the mapping $x_i \rightarrow g_k$ is rather easy

- 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 :

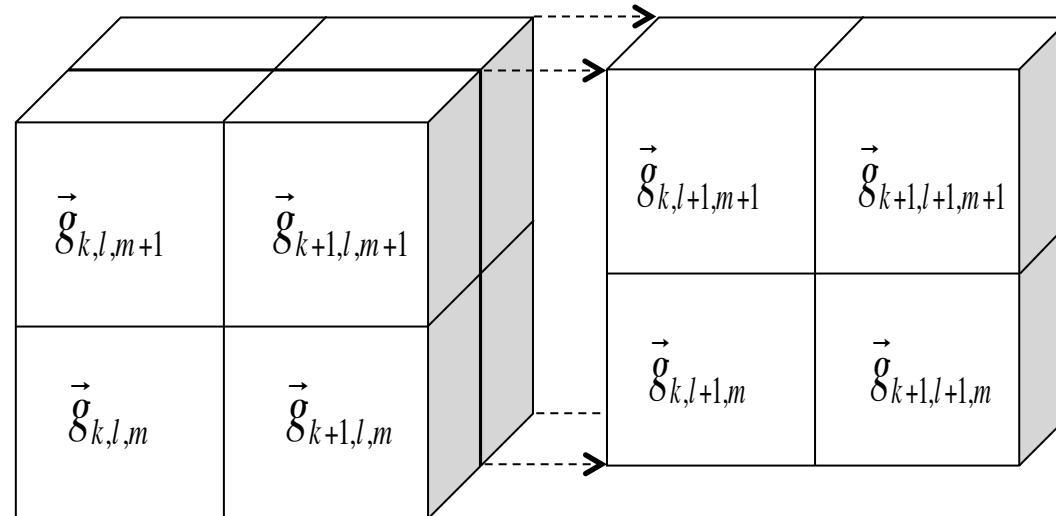


- density assignment schemes - in practice

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

- 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 (1 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

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

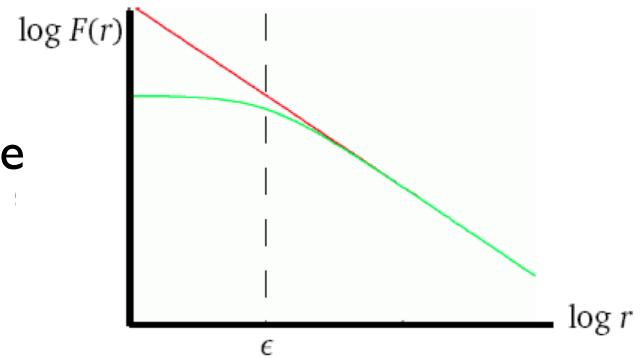
- density assignment schemes
 - which scheme to choose?

interplay between N and ϵ : $N\epsilon^3 = \text{const.}$

NGP = too crude

CIC = common choice

TSC = pretty smooth



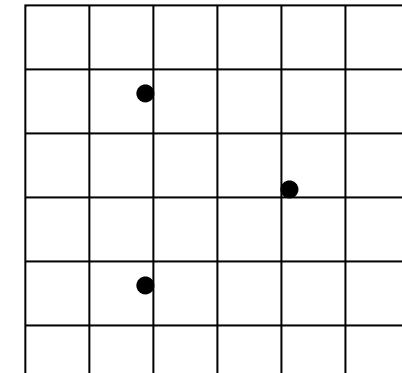
smoothing the density field will lead to a “bias” in the forces
but at the same time decrease the “variance”!

(more later when studying the accuracy...)

- numerically integrate Poisson's equation

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

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



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

- numerically integrate Poisson's equation

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

- relaxation technique:
 - obtain iterative solver by discretizing differential equation
 - applicable and usable for **any** differential equation

- numerically integrate Poisson's equation

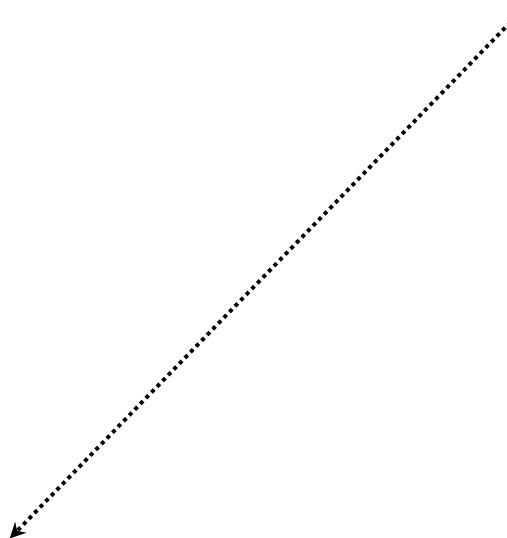
relaxation technique

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

- numerically integrate Poisson's equation

relaxation technique

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



discretized Poisson's equation

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

- numerically integrate Poisson's equation

relaxation technique

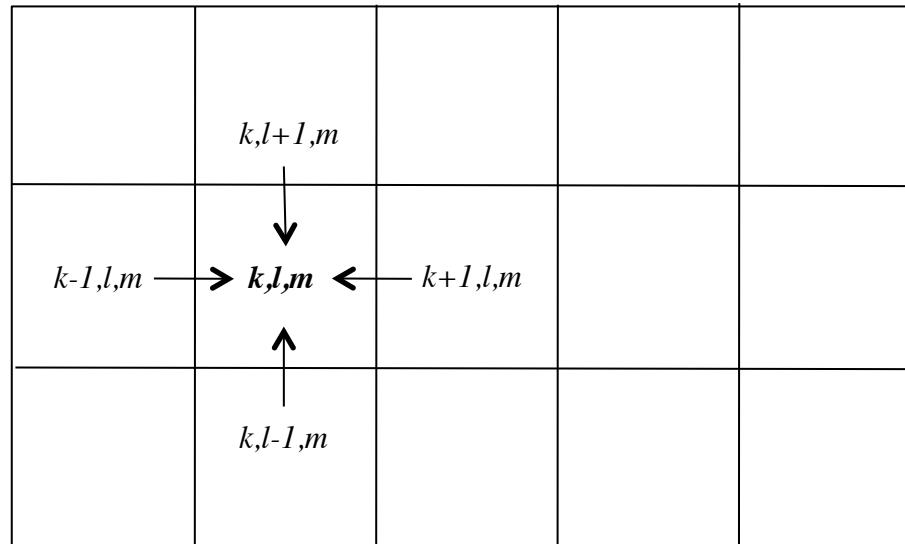
$$\Delta\Phi_{k,l,m} = \rho_{k,l,m}$$

iterative solution: $\Phi_{k,l,m}^i \rightarrow \Phi_{k,l,m}^{i+1}$

discretized Poisson's equation

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

- numerically integrate Poisson's equation *relaxation technique*
- how to sweep through the grid?

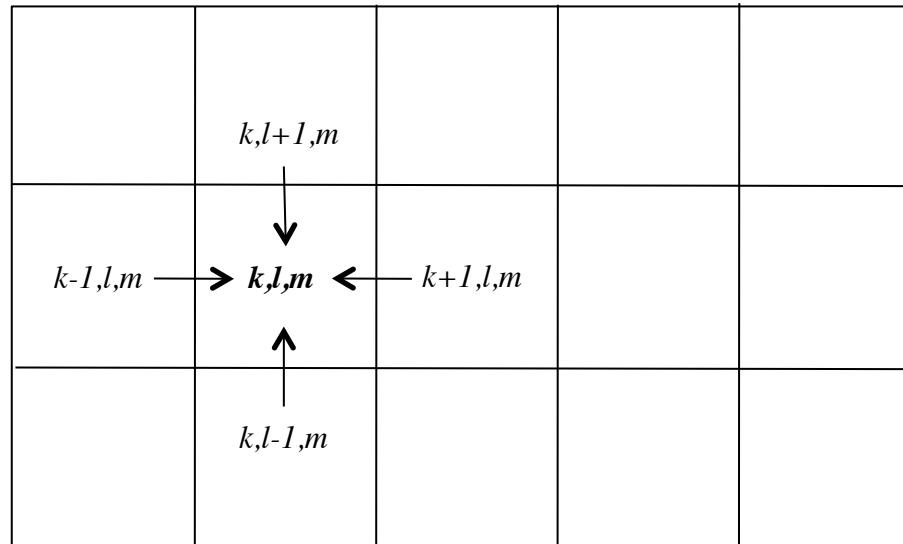


discretized Poisson's equation

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

- numerically integrate Poisson's equation *relaxation technique*
- how to sweep through the grid?

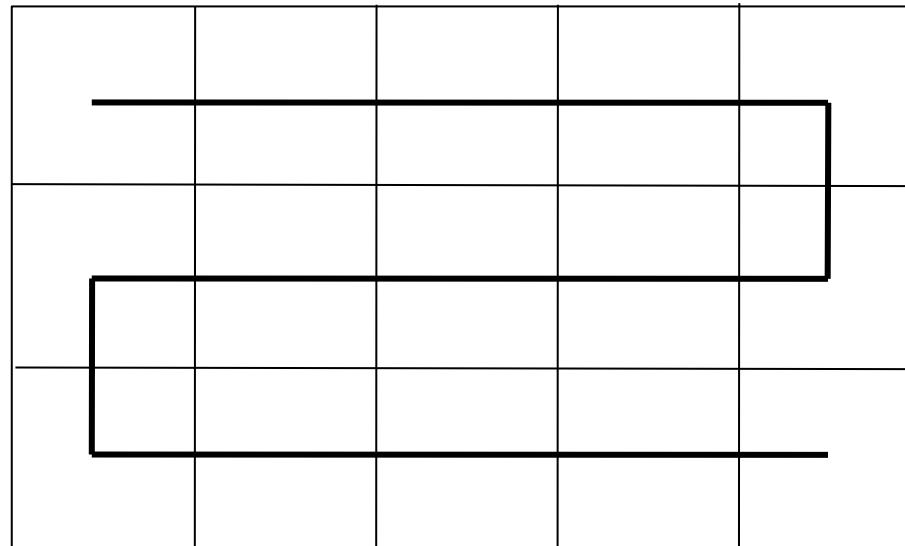
applicable to grids of **arbitrary** geometry!



discretized Poisson's 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?

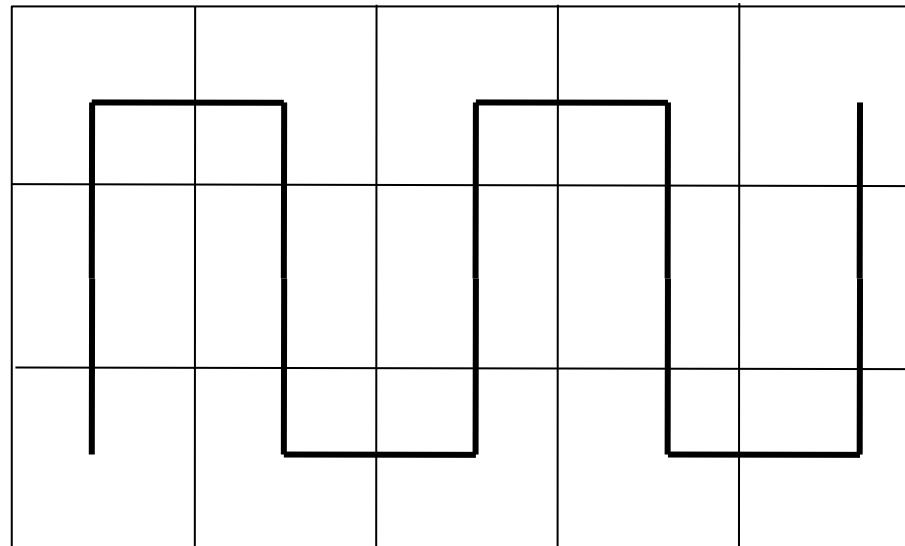


discretized Poisson's equation

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

- numerically integrate Poisson's equation
 - how to sweep through the grid?

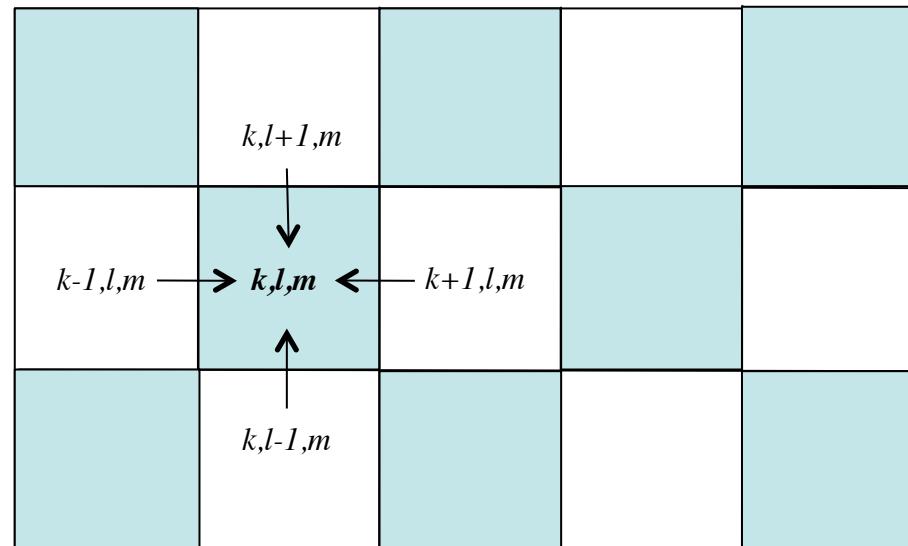
relaxation technique



discretized Poisson's 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*
- Gauss-Seidel sweeps:



discretized Poisson's 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*
- Gauss-Seidel sweeps:

• loop over all “black” cells
 • loop over all “red” cells

}

one iteration of the potential

$$\Phi_{k,l,m}^i \rightarrow \Phi_{k,l,m}^{i+1}$$

how many iterations i are necessary?

discretized Poisson's equation

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

- numerically integrate Poisson's equation *relaxation technique*
- stopping criterion:

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

discretized Poisson's equation

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

- numerically integrate Poisson's equation *relaxation technique*
- stopping criterion:

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

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

discretized Poisson's 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*
- stopping criterion:

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

residual: $R^i = \|\Delta\Phi_{k,l,m}^i - \rho_{k,l,m}\|$ $\|\cdot\|$ = suitable norm

discretized Poisson's 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*
- stopping criterion:

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

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

↑ ↑
tolerance error estimate

$\|\cdot\|$ = suitable norm

discretized Poisson's 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*
- stopping criterion:

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

– truncation error:

error due to discreteness of grid

discretized Poisson's 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*
- stopping criterion:

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

– truncation error:

error due to discreteness of grid

$\xrightarrow{\text{estimation}}$ compare solution on actual grid
to solution on coarser grid

discretized Poisson's equation

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

- numerically integrate Poisson's equation *relaxation technique*
- stopping criterion:

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

– truncation error: $T_{k,l,m} = \underbrace{\mathcal{P}[\Delta(\mathcal{R}\Phi_{k,l,m}^i)]}_{\mathcal{R}\Phi_{k,l,m}^i} - (\Delta\Phi_{k,l,m}^i)$

$$\mathcal{R}\Phi_{k,l,m}^i = \Phi_{j,n,p}^i \quad \text{restriction to coarser grid}$$

$$\Delta(\mathcal{R}\Phi_{k,l,m}^i) = \rho_{j,n,p}^{i-1}$$

$$\mathcal{P}[\Delta(\mathcal{R}\Phi_{k,l,m}^i)] = \rho_{k,l,m}^i \quad \text{prolongation to finer grid}$$

discretized Poisson's 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*
- stopping criterion:

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

– truncation error: $T_{k,l,m} = \mathcal{P}[\Delta(\mathcal{R}\Phi_{k,l,m}^i)] - \underbrace{(\Delta\Phi_{k,l,m}^i)}$

$$\mathcal{R}\Phi_{k,l,m}^i = \Phi_{j,n,p}^i$$

$$\Delta(\mathcal{R}\Phi_{k,l,m}^i) = \rho_{j,n,p}^{i-1}$$

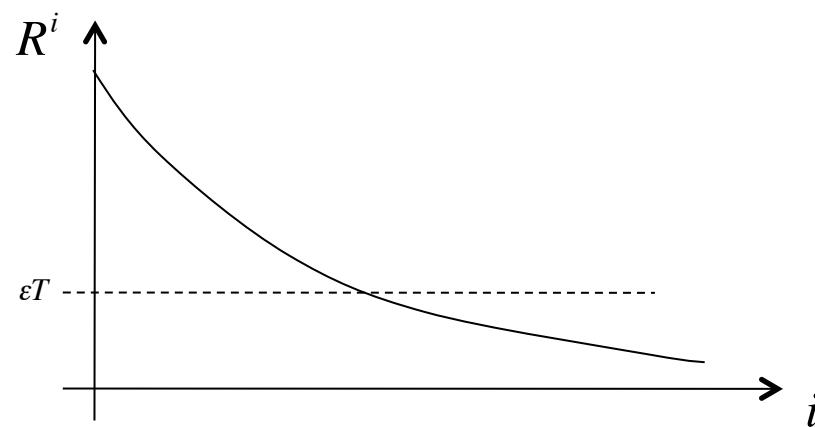
$$\mathcal{P}[\Delta(\mathcal{R}\Phi_{k,l,m}^i)] = \rho_{k,l,m}^i \stackrel{?}{=} \Delta\Phi_{k,l,m}^i$$

discretized Poisson's 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*
- stopping criterion:

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

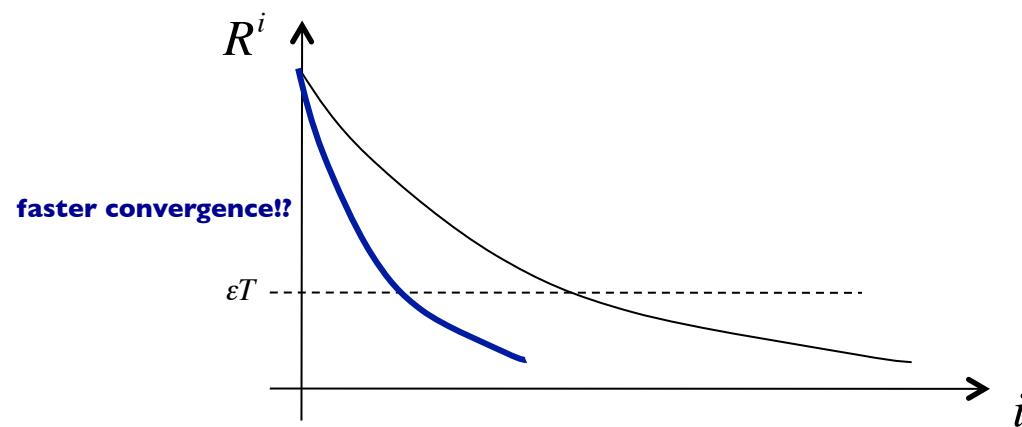


discretized Poisson's equation

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

- numerically integrate Poisson's equation *relaxation technique*
- stopping criterion:

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



discretized Poisson's equation

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

- 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...

discretized Poisson's equation

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

- numerically integrate Poisson's equation *relaxation technique*
- convergence:

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

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

multi-grid relaxation techniques

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

discretized Poisson's 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

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

- 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

$$\Delta\Phi = \rho \quad \rightarrow \text{equation we wish to solve}$$

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

$$\Delta\Phi = \rho \quad \rightarrow \text{equation we wish to solve}$$

$$\Delta G = \delta \quad \rightarrow \text{equation way easier to solve...}$$

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

$$\Delta\Phi = \rho$$

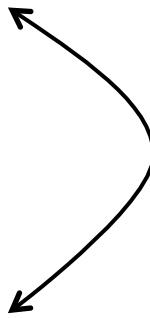
A diagram illustrating the iterative or coupled nature of the numerical integration process. At the top, the equation $\Delta\Phi = \rho$ is shown. A curved arrow originates from this equation and points downwards to the equation $\Delta G = \delta$. From the end of this downward-pointing arrow, another curved arrow curves back upwards towards the $\Delta\Phi = \rho$ equation, ending near the equals sign. A large question mark is positioned to the right of the downward-pointing arrow, indicating a dependency or a step in the process.

$$\Delta G = \delta$$

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

$$\Delta\Phi = \rho$$

$$\Delta G = \delta$$

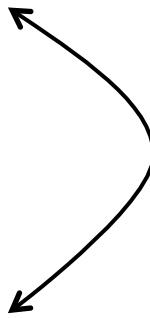


$$\Phi(\vec{x}) = \iiint G(\vec{x} - \vec{x}') \rho(\vec{x}') d^3 x'$$

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

$$\Delta\Phi = \rho$$

$$\Delta G = \delta$$



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

$$\begin{aligned}\Delta\Phi(\vec{x}) &= \Delta \iiint G(\vec{x} - \vec{x}') \rho(\vec{x}') d^3 x' \\ &= \iiint \Delta G(\vec{x} - \vec{x}') \rho(\vec{x}') d^3 x' \\ &= \iiint \delta(\vec{x} - \vec{x}') \rho(\vec{x}') d^3 x' \\ &= \rho(\vec{x})\end{aligned}$$

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

$$\Delta G = \delta$$

Ansatz : $G = \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) e^{i\vec{k}\cdot\vec{x}} d^3k$ (spectral decomposition of G)

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

$$\Delta G = \delta$$

Ansatz : $G = \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) e^{i\vec{k}\cdot\vec{x}} d^3k$

$$\begin{aligned} \delta &= \Delta \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) e^{i\vec{k}\cdot\vec{x}} d^3k \\ &= \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) \Delta e^{i\vec{k}\cdot\vec{x}} d^3k \\ &= \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) (-k^2) e^{i\vec{k}\cdot\vec{x}} d^3k \end{aligned}$$

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

$$\Delta G = \delta$$

Ansatz : $G = \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) e^{i\vec{k} \cdot \vec{x}} d^3k$

$$\begin{aligned}
 \delta &= \Delta \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) e^{i\vec{k} \cdot \vec{x}} d^3k \\
 &= \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) \Delta e^{i\vec{k} \cdot \vec{x}} d^3k \\
 &= \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) (-k^2) e^{i\vec{k} \cdot \vec{x}} d^3k \quad \xrightarrow{e^{-i(\vec{k}' \cdot \vec{x})}} \quad \delta e^{-i(\vec{k}' \cdot \vec{x})} = e^{-i(\vec{k}' \cdot \vec{x})} \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) (-k^2) e^{i\vec{k} \cdot \vec{x}} d^3k \\
 &\quad = \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) (-k^2) e^{i(\vec{k} - \vec{k}') \cdot \vec{x}} d^3k
 \end{aligned}$$

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

$$\Delta G = \delta$$

$$\text{Ansatz : } \mathcal{G} = \frac{1}{(2\pi)^3} \iiint \hat{\mathcal{G}}(\vec{k}) e^{i\vec{k} \cdot \vec{x}} d^3k$$

$$\delta = \Delta \frac{1}{(2\pi)^3} \iiint \hat{\mathcal{G}}(\vec{k}) e^{i\vec{k}\cdot\vec{x}} d^3k$$

$$= \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) \Delta e^{i\vec{k}\cdot\vec{x}} d^3k$$

$$= \frac{1}{(2\pi)^3} \iiint \hat{\mathcal{G}}(\vec{k}) (-k^2) e^{i\vec{k}\cdot\vec{x}} d^3 k$$

$$\overrightarrow{e}^{-i(\vec{k}' \cdot \vec{x})}$$

$$\delta e^{-i(\vec{k}' \cdot \vec{x})} = e^{-i(\vec{k}' \cdot \vec{x})} \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) (-k^2) e^{i\vec{k} \cdot \vec{x}} d^3 k$$

$$= \frac{1}{(2\pi)^3} \iiint \hat{\mathcal{G}}(\vec{k}) (-k^2) e^{i(\vec{k}-\vec{k}') \cdot \vec{x}} d^3 k$$

$$\overrightarrow{\iiint d^3x}$$

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

$$\Delta G = \delta$$

$$\iiint \delta e^{-i(\vec{k}' \cdot \vec{x})} d^3x = \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) (-k^2) \iiint e^{i(\vec{k} - \vec{k}') \cdot \vec{x}} d^3x d^3k$$

$$\begin{aligned} 1 &= \iiint \hat{G}(\vec{k}) (-k^2) \frac{1}{(2\pi)^3} \iiint e^{i(\vec{k} - \vec{k}') \cdot \vec{x}} d^3x d^3k \\ &= \iiint \hat{G}(\vec{k}) (-k^2) \delta(\vec{k} - \vec{k}') d^3k \\ &= -k^2 \hat{G}(\vec{k}) \end{aligned}$$

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

$$\Delta G = \delta$$

$$\iiint \delta e^{-i(\vec{k}' \cdot \vec{x})} d^3x = \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) (-k^2) \iiint e^{i(\vec{k} - \vec{k}') \cdot \vec{x}} d^3x d^3k$$

$$\begin{aligned} 1 &= \iiint \hat{G}(\vec{k}) (-k^2) \frac{1}{(2\pi)^3} \iiint e^{i(\vec{k} - \vec{k}') \cdot \vec{x}} d^3x d^3k \\ &= \iiint \hat{G}(\vec{k}) (-k^2) \delta(\vec{k} - \vec{k}') d^3k \\ &= \underline{-k^2 \hat{G}(\vec{k})} \end{aligned}$$

$$\hat{G}(\vec{k}) = -\frac{1}{k^2}$$

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

$$\Delta G = \delta$$

$$\iiint \delta e^{-i(\vec{k}' \cdot \vec{x})} d^3x = \frac{1}{(2\pi)^3} \iiint \hat{G}(\vec{k}) (-k^2) \iiint e^{i(\vec{k} - \vec{k}') \cdot \vec{x}} d^3x d^3k$$

$$\begin{aligned} 1 &= \iiint \hat{G}(\vec{k}) (-k^2) \frac{1}{(2\pi)^3} \iiint e^{i(\vec{k} - \vec{k}') \cdot \vec{x}} d^3x d^3k \\ &= \iiint \hat{G}(\vec{k}) (-k^2) \delta(\vec{k} - \vec{k}') d^3k \\ &= \underline{-k^2 \hat{G}(\vec{k})} \end{aligned}$$

$$\hat{G}(\vec{k}) = -\frac{1}{k^2}$$

$\xrightarrow{\text{FFT}^{-1}(\hat{G}(\vec{k}))}$

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

$$\Delta G = \delta$$

$$\hat{G}(\vec{k}) = -\frac{1}{k^2}$$

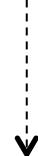
$$G(\vec{x}) = \frac{1}{4\pi x}$$

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

$$\Phi = \rho \otimes G$$

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

$$\Phi = \rho \otimes G$$



FFT \rightarrow convolution becomes multiplication

$$\hat{\Phi} = \hat{\rho} \quad \hat{G} \quad (\text{with } \hat{G} = -\frac{1}{k^2} \text{ for Poisson's equation})$$

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

$$\Phi = \rho \otimes G$$

FFT → convolution becomes multiplication

$$\hat{\Phi} = \hat{\rho} \quad \hat{G} \quad (\text{with } \hat{G} = -\frac{1}{k^2} \text{ for Poisson's equation})$$

FFT⁻¹

$$\Phi$$

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

$$\Phi = \rho \otimes G$$

FFT → convolution becomes multiplication

$$\hat{\Phi} = \hat{\rho} \quad \hat{G} \quad (\text{with } \hat{G} = -\frac{1}{k^2} \text{ for Poisson's equation})$$

FFT⁻¹

$$\Phi$$

FFT demands a *regular grid* though!

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

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

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

- numerically integrate Poisson's equation

accuracy of either

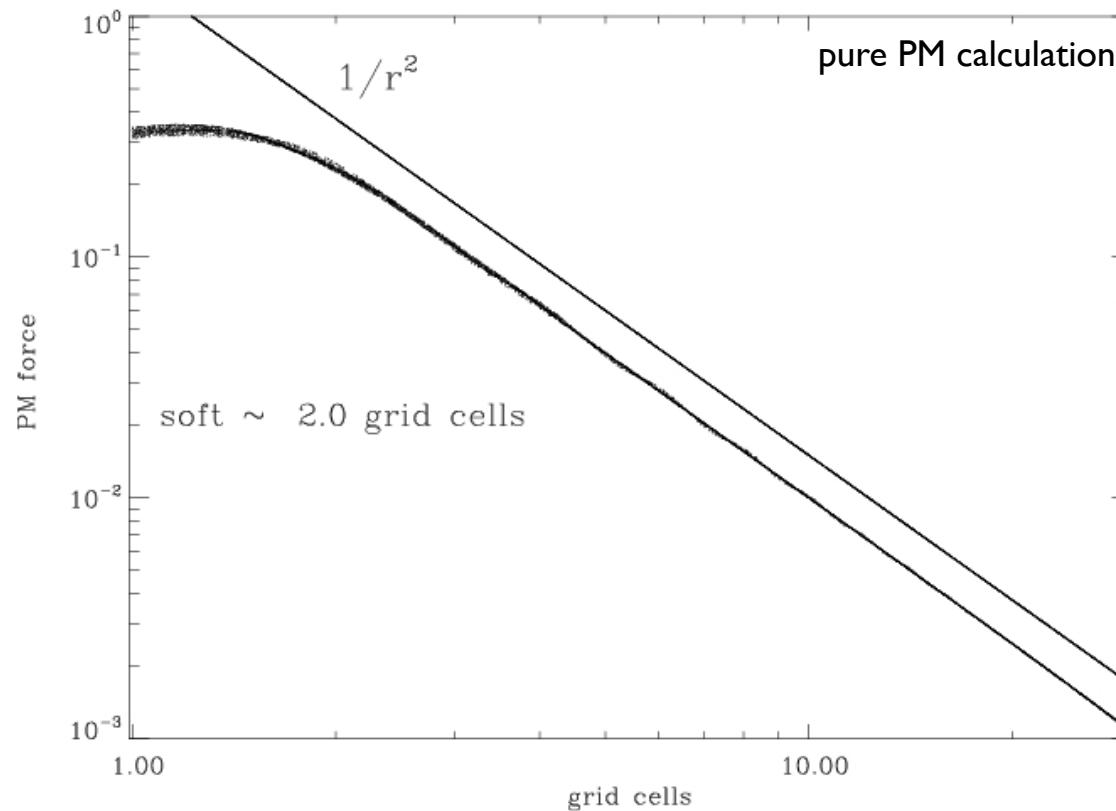
relaxation

or

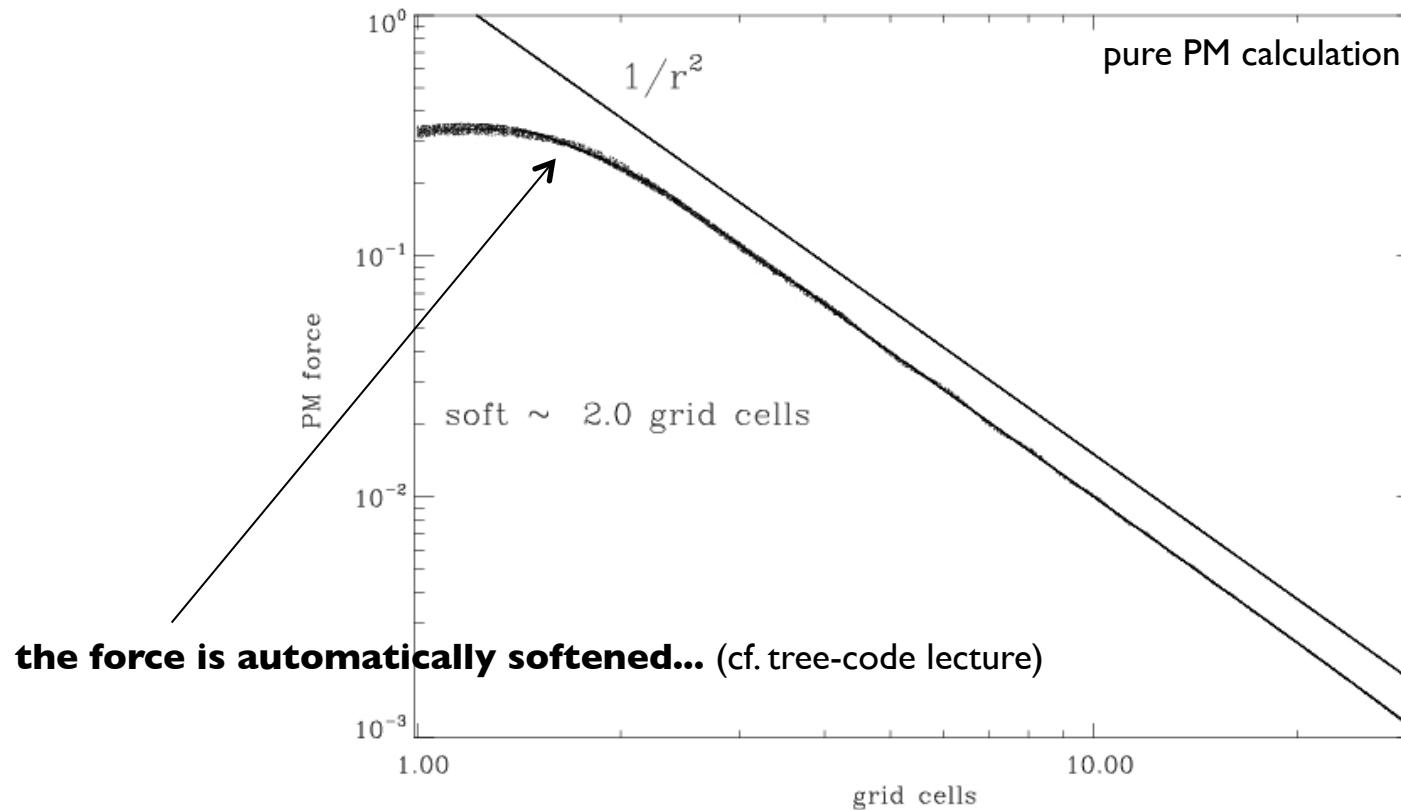
FFT method

to solve Poisson's equation?

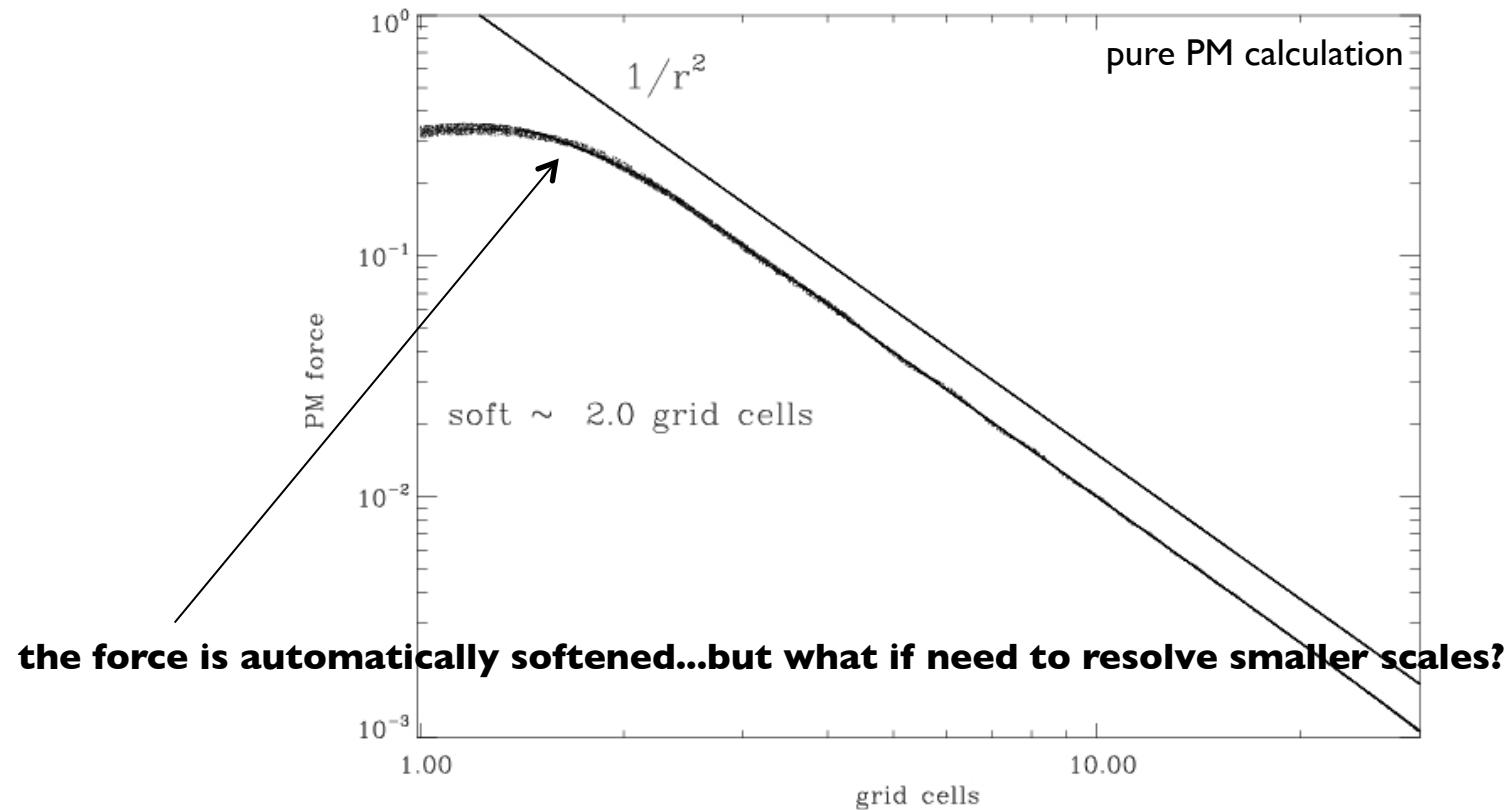
- numerically integrate Poisson's equation



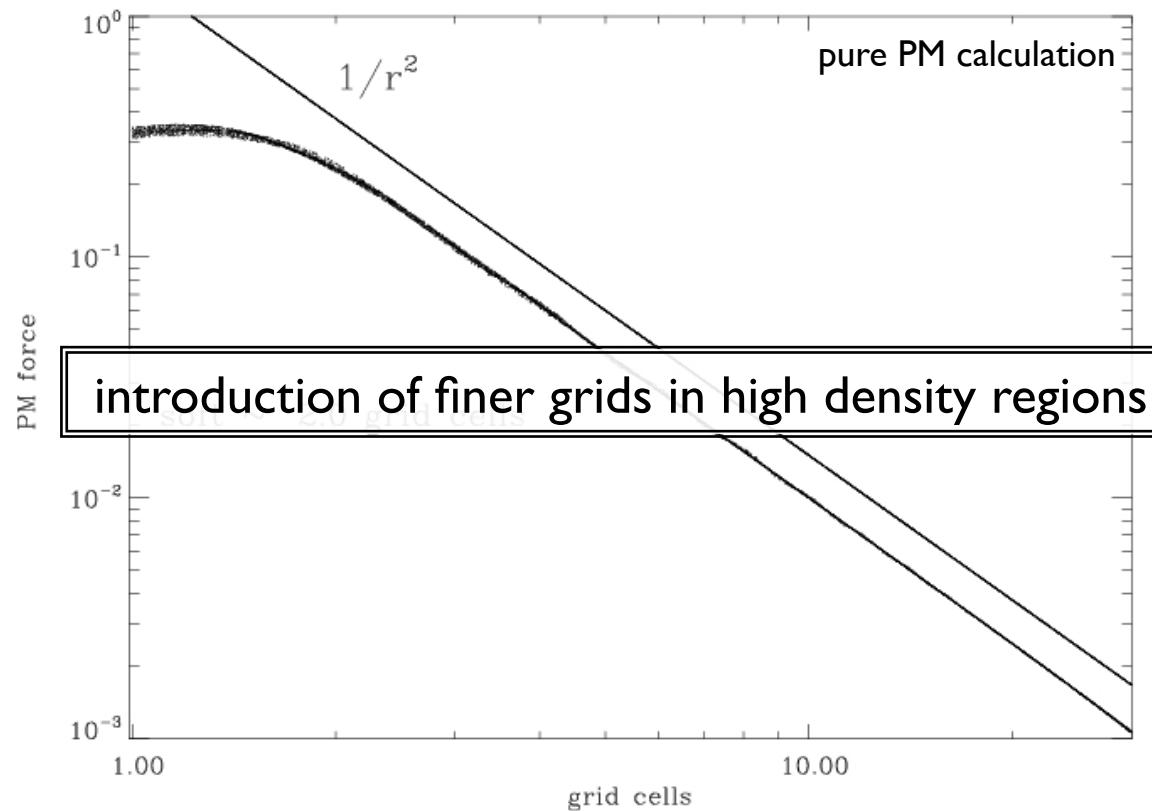
- numerically integrate Poisson's equation



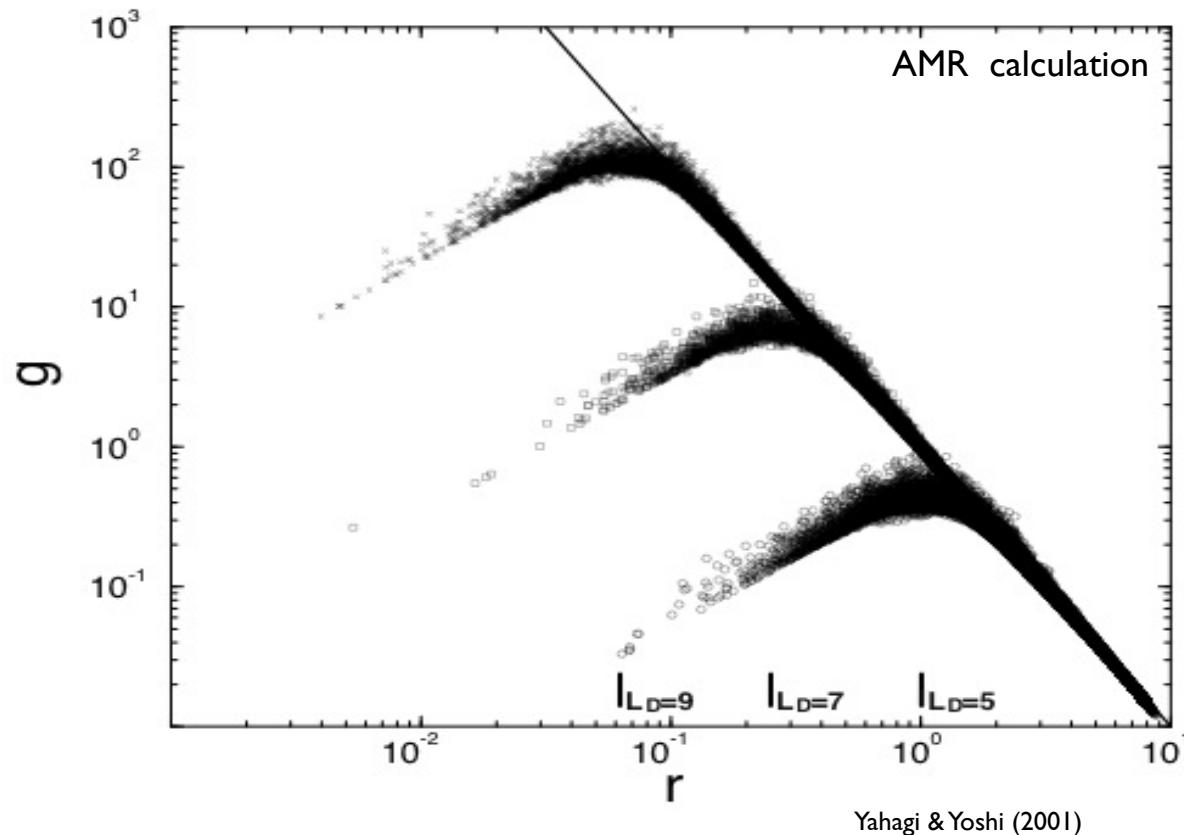
- numerically integrate Poisson's equation



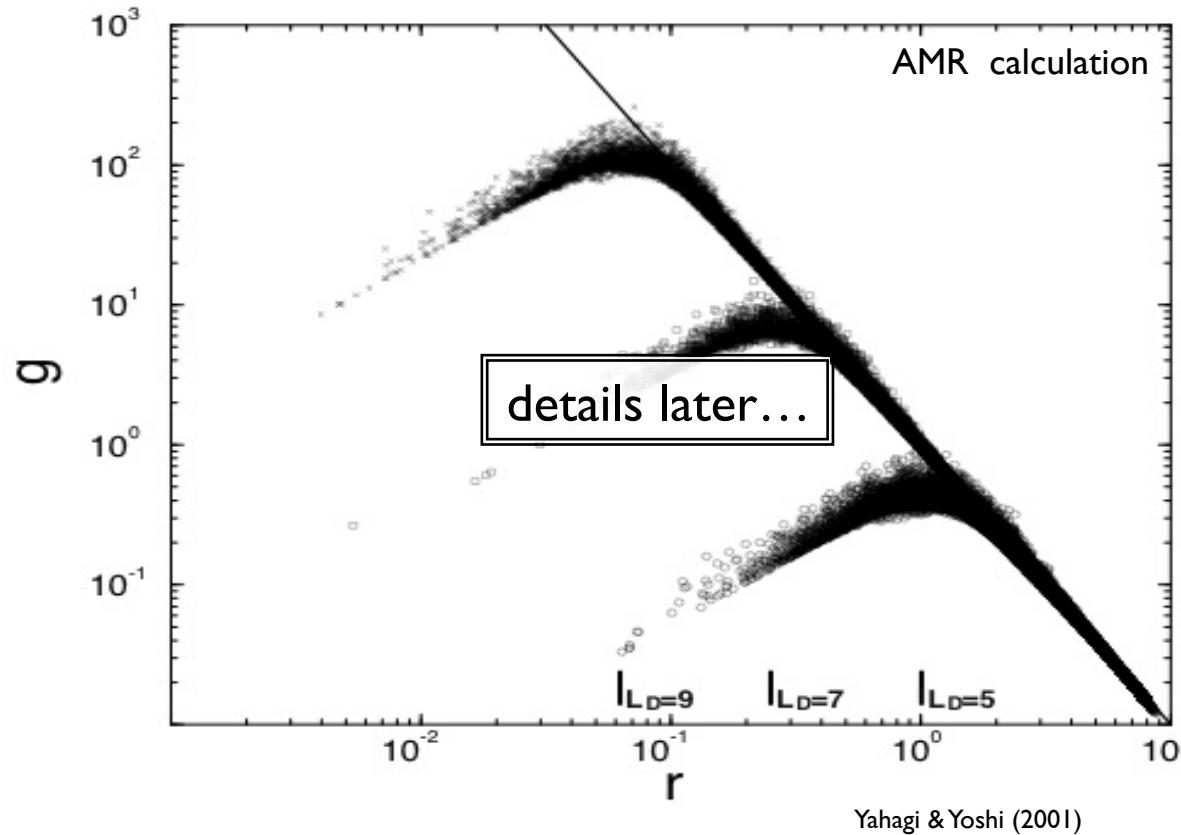
- numerically integrate Poisson's equation



- numerically integrate Poisson's equation



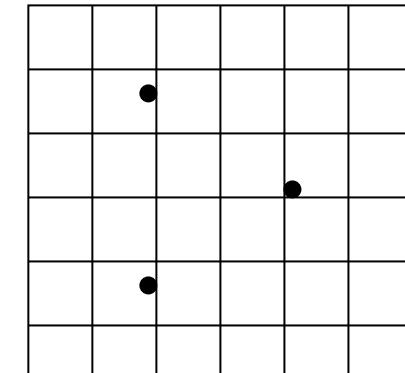
- numerically integrate Poisson's equation



- numerically integrate Poisson's equation

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

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



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

- obtaining the forces

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



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

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

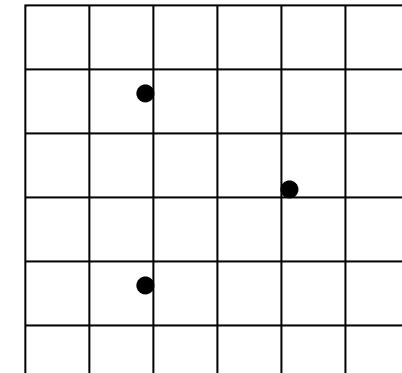
$$F_z(\vec{g}_{k,l,m}) = -m \frac{\Phi(\vec{g}_{k,l,m+1}) - \Phi(\vec{g}_{k,l,m-1})}{2H}$$

H = (current) grid spacing

- numerically integrate Poisson's equation

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

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



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

- interpolating the forces

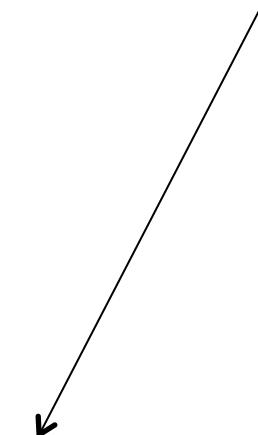
$$\vec{F}(\vec{g}_{k,l,m}) \rightarrow \vec{F}(\vec{r}_i)$$

- 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

$$\vec{F}(\vec{r}_i) = \sum_k \sum_l \sum_m \vec{F}(\vec{g}_{k,l,m}) W(\vec{r}_i - \vec{g}_{k,l,m})$$



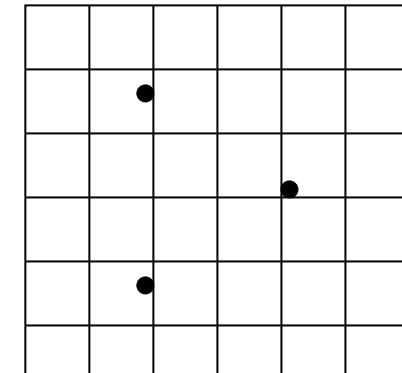
exercise...

in practice the triple sum is “only” over 8 (CIC) or 27 (TCS) cells...

- Particle-Mesh (PM) method

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

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



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

PM CODES

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