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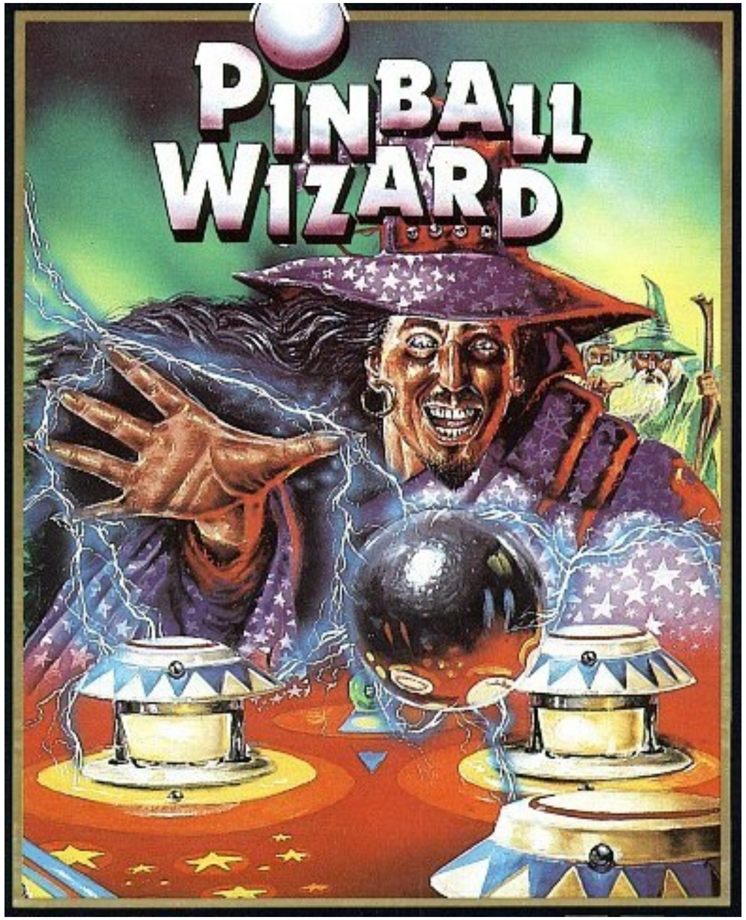
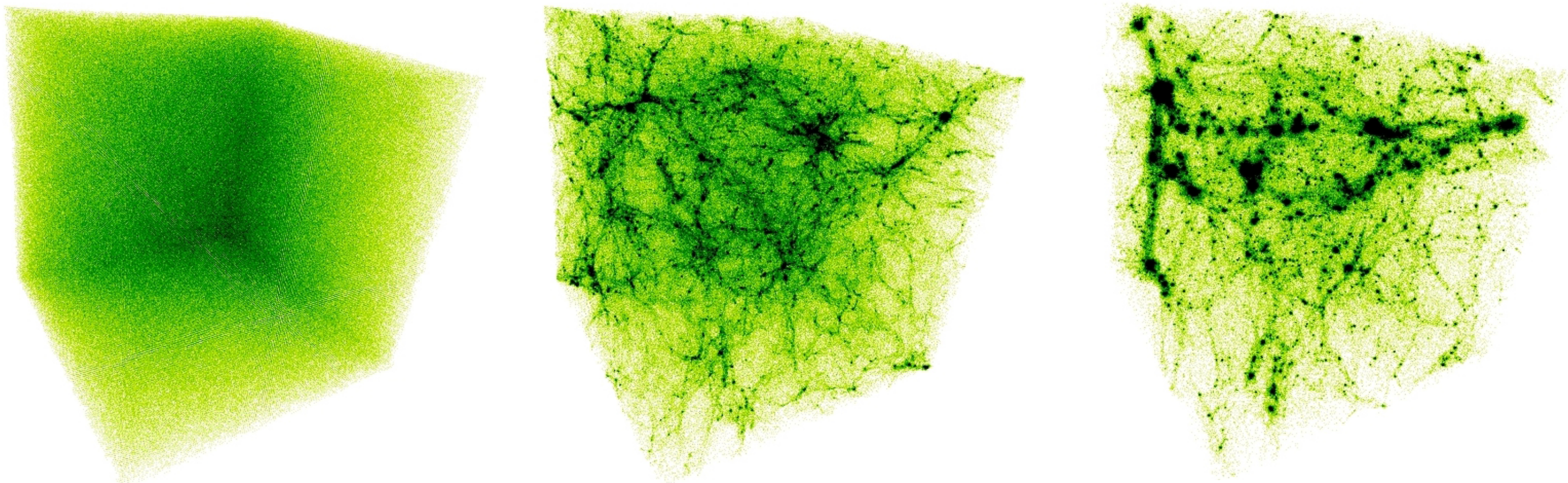


Tree Codes



tree codes

▪ 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)

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

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

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

• ideal gas equations

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

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

• Maxwell's equation

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

▪ full set of equations

- collisionless matter (e.g. dark matter)

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

time integration lecture

- Poisson's equation

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

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

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• collisional matter (e.g. gas)

later...

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\vec{v}) = 0$$
$$\frac{\partial(\rho\vec{v})}{\partial t} + \nabla\cdot\left(\rho\vec{v}\otimes\vec{v} + \left(p + \frac{1}{2\mu}B^2\right)\vec{1} - \frac{1}{\mu}\vec{B}\otimes\vec{B}\right) = \rho\ (-\nabla\phi)$$
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• ideal gas equations

$$p = (\gamma - 1)\rho\varepsilon$$
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• Maxwell's equation

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

hyperbolic partial differential equations:
solutions are wave-like, i.e. perturbations need time to travel...

- 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

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

physics lecture...

  - ideal gas equations

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

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

  - collisional matter (e.g. gas)

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

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

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  - Maxwell's equation

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

- full set of equations

now!

- Poisson's equation

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

elliptical partial differential equation:
solution obtainable via FFT (for constant coefficients)

- collisionless matter (e.g. dark matter)

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

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- Maxwell's equation

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- Poisson's equation

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

- Poisson's equation

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

- general 2nd order partial differential equation:

$$A\,\Phi_{xx} + 2B\,\Phi_{xy} + C\,\Phi_{yy} \quad + D\,\Phi_x + E\,\Phi_y + F = 0$$

  - $\begin{pmatrix} A & B \\ B & C \end{pmatrix}$ is positive definite => elliptical equation
  - if the coefficients A,B,C are constant => solutions via Fourier transforms

- Poisson's equation

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

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

- Poisson's equation

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

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

→

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

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

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

- Poisson's equation

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weapon of choice: AMR codes

- Poisson's equation

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

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

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))

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

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

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

weapon of choice: tree codes

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))

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

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

- Poisson's equation

...but where is this formula actually coming from?

weapon of choice: tree codes

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

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

<u>particle approach</u>

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

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

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

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

- Poisson's equation

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

Green's function method

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

- Poisson's equation – Green's function method

$$\Delta\Phi = S \qquad \rightarrow \text{ equation we wish to solve}$$

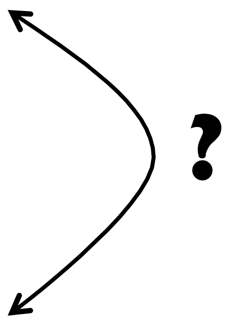
- Poisson's equation – Green's function method

$$\Delta\Phi = S$$ → equation we wish to solve

$$\Delta\mathcal{G} = \delta$$ → equation way easier to solve…

- Poisson's equation – Green's function method

$$\Delta\Phi = S$$



$$\Delta\mathcal{G} = \delta$$

- Poisson's equation – Green's function method

$$\Delta\Phi = S$$

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

$$\Delta\mathcal{G} = \delta$$

- Poisson's equation – Green's function method

$$\Delta\Phi = S$$

$$\Delta\mathcal{G} = \delta$$

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

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

- Poisson's equation – Green's function method

$$\Delta \mathcal{G} = \delta$$

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

- Poisson's equation – Green's function method

$$\Delta \mathcal{G} = \delta$$

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

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

- Poisson's equation – Green's function method

$$\Delta \mathcal{G} = \delta$$

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

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

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

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

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

- Poisson's equation – Green's function method

$$\Delta \mathcal{G} = \delta$$

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

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

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

- Poisson's equation – Green's function method

$$\Delta\mathcal{G} = \delta$$

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

- Poisson's equation – Green's function method

$$\Delta \mathcal{G} = \delta$$

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

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

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

- Poisson's equation – Green's function method

$$\Delta \mathcal{G} = \delta$$

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

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

$$= \iiint \hat{\mathcal{G}}(\vec{k})\,(-k^2)\delta(\vec{k}-\vec{k}')d^3k$$

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

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

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

- Poisson's equation – Green's function method

$$\Delta \mathcal{G} = \delta$$

$$\hat{\mathcal{G}}(\vec{k}) = -\frac{1}{k^2} \qquad\qquad \mathcal{G}(\vec{x}) = \frac{1}{4\pi\, x}$$

- Poisson's equation – Green's function method

$$\Delta\mathcal{G} = \delta$$

$$\hat{\mathcal{G}}(\vec{k}) = -\frac{1}{k^2} \qquad\qquad \mathcal{G}(\vec{x}) = \frac{1}{4\pi\, x}$$

$$\Delta\Phi = S$$

=>

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

- Poisson's equation – Green's function method

$$\Delta\Phi = S$$

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

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

- Poisson's equation – Green's function method

$$\Delta\Phi = 4\pi G\rho \longrightarrow \rho(\vec{r}) = \sum_{i=1}^{N} m_i \delta_{\text{Dirac}}(\vec{r} - \vec{r}_i)$$

particle approach

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

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

remember:
we are already using particles to sample phase-space!

- direct particle-particle summation (PP)

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

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

analytical solution to Poisson's equation

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

- direct particle-particle summation (PP)

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

$$\begin{aligned}
\Phi(\vec{r}) &= 4\pi G \iiint \mathcal{G}(\vec{r} - \vec{r}')\ \rho(\vec{r}') d^3r' \\
&= 4\pi G \iiint \mathcal{G}(\vec{r} - \vec{r}') \sum_{i=1}^{N} m_i \delta_{\texttt{Dirac}}(\vec{r}' - \vec{r}_i) d^3r' \\
&= 4\pi G \sum_{i=1}^{N} m_i \iiint \mathcal{G}(\vec{r} - \vec{r}') \delta_{\texttt{Dirac}}(\vec{r}' - \vec{r}_i)\ d^3r' \\
&= \sum_{i=1}^{N} m_i \iiint \frac{G}{|\vec{r} - \vec{r}'|} \delta_{\texttt{Dirac}}(\vec{r}' - \vec{r}_i)\ d^3r' \\
&= \sum_{i=1}^{N} m_i \iiint \frac{G}{|(\vec{r} - \vec{r}_i) - (\vec{r}' - \vec{r}_i)|} \delta_{\texttt{Dirac}}(\vec{r}' - \vec{r}_i)\ d^3r' \\
&= -\sum_{i=1}^{N} m_i \iiint \frac{G}{|(\vec{r}' - \vec{r}_i) - (\vec{r} - \vec{r}_i)|} \delta_{\texttt{Dirac}}(\vec{r}' - \vec{r}_i)\ d^3r' \\
&= -\sum_{i=1}^{N} m_i \iiint \frac{G}{|\vec{y} - (\vec{r} - \vec{r}_i)|} \delta_{\texttt{Dirac}}(\vec{y})\ d^3y = -\sum_{i=1}^{N} \frac{Gm_i}{|\vec{r} - \vec{r}_i|}
\end{aligned}$$

$$\begin{aligned}
\vec{F}_i(\vec{r}_i) &= -m_i \vec{\nabla} \Phi(\vec{r}_i) \\
&= -m_i \vec{\nabla} \left(-\sum_{j=1}^{N} \frac{Gm_j}{|\vec{r}_i - \vec{r}_j|} \right) \\
&= \sum_{j=1}^{N} Gm_i m_j \vec{\nabla} \frac{1}{|\vec{r}_i - \vec{r}_j|} \\
&= -\sum_{j=1}^{N} Gm_i m_j \frac{(\vec{r}_i - \vec{r}_j)}{|\vec{r}_i - \vec{r}_j|^3} \\
&= -\sum_{j=1}^{N} \frac{Gm_i m_j}{|\vec{r}_i - \vec{r}_j|^3} (\vec{r}_i - \vec{r}_j)
\end{aligned}$$

Note: $|\vec{r}_i - \vec{r}_j| \rightarrow (r_i - r_j)$

- direct particle-particle summation (PP)

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

analytical solution to Poisson's equation

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

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✓ advantage:	easy to code
drawback:	extremely time consuming (N^2 operations)

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$$N \times N = N^2$$

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analytical solution to Poisson's equation

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overcoming the "N^2" issue?!

✓ advantage:	easy to code
⌁ drawback:	extremely time consuming (N^2 operations)

- 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

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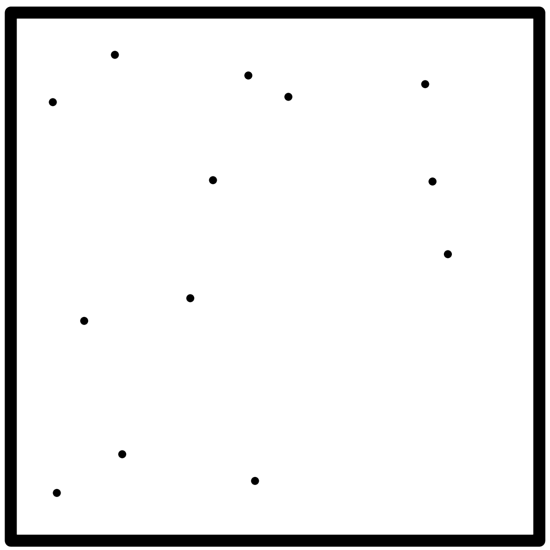

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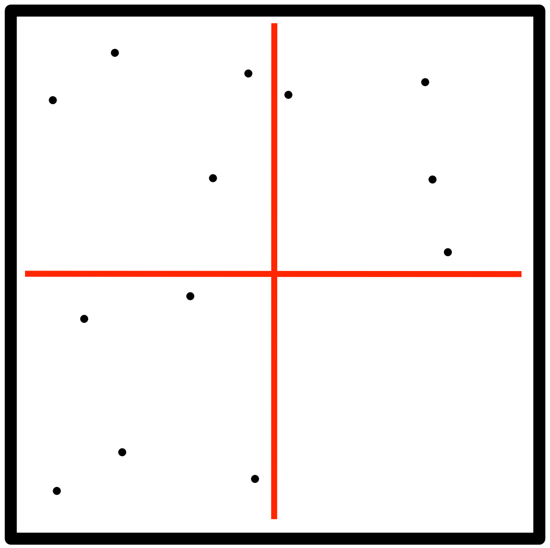

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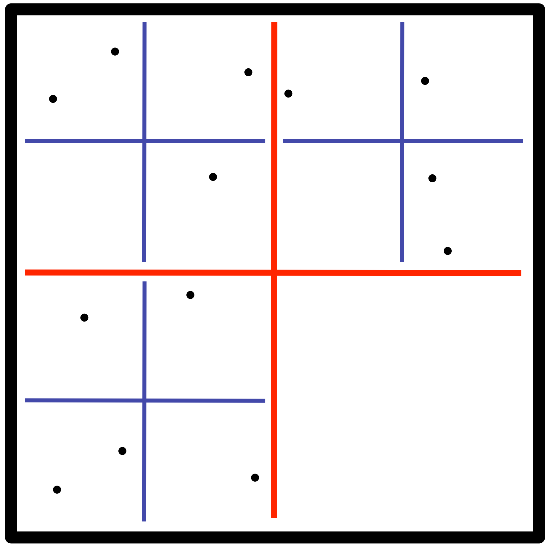

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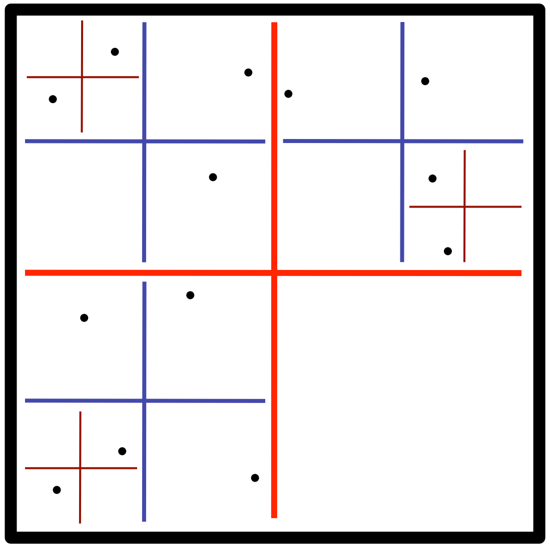

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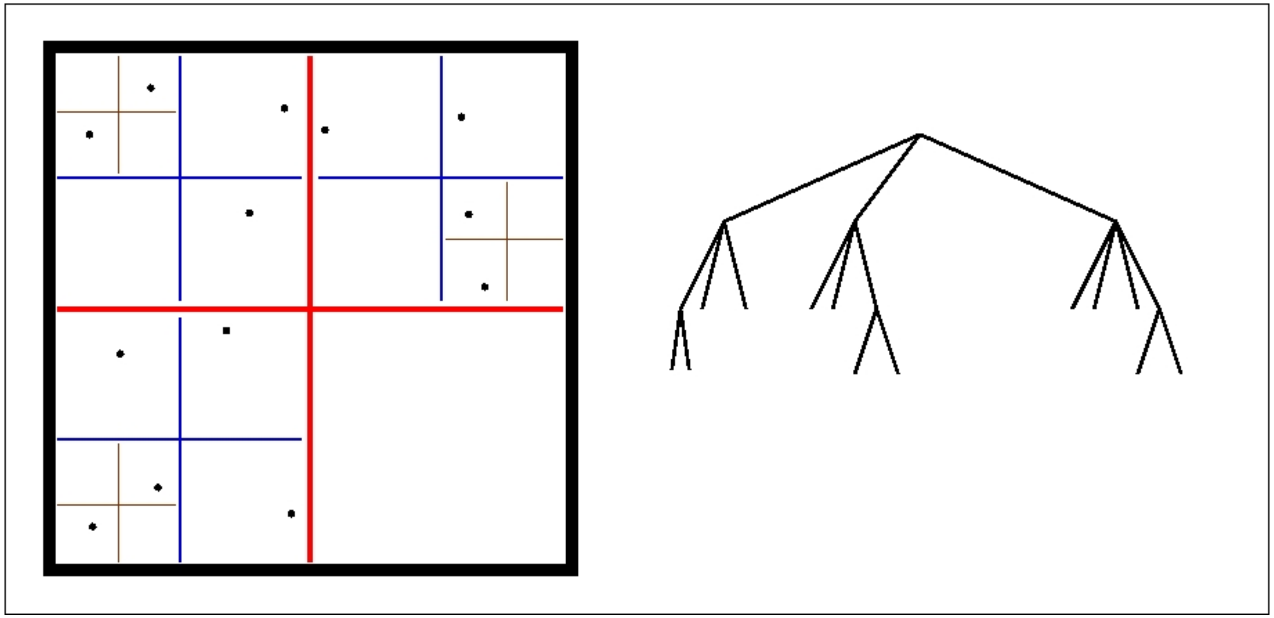

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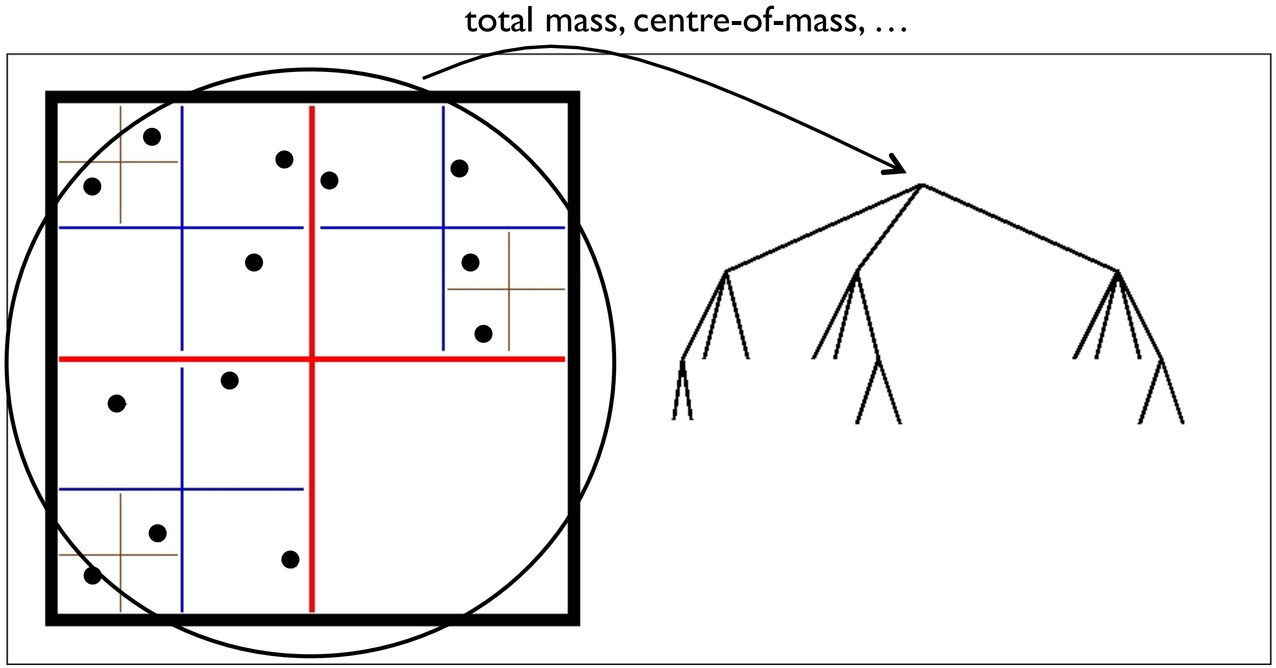

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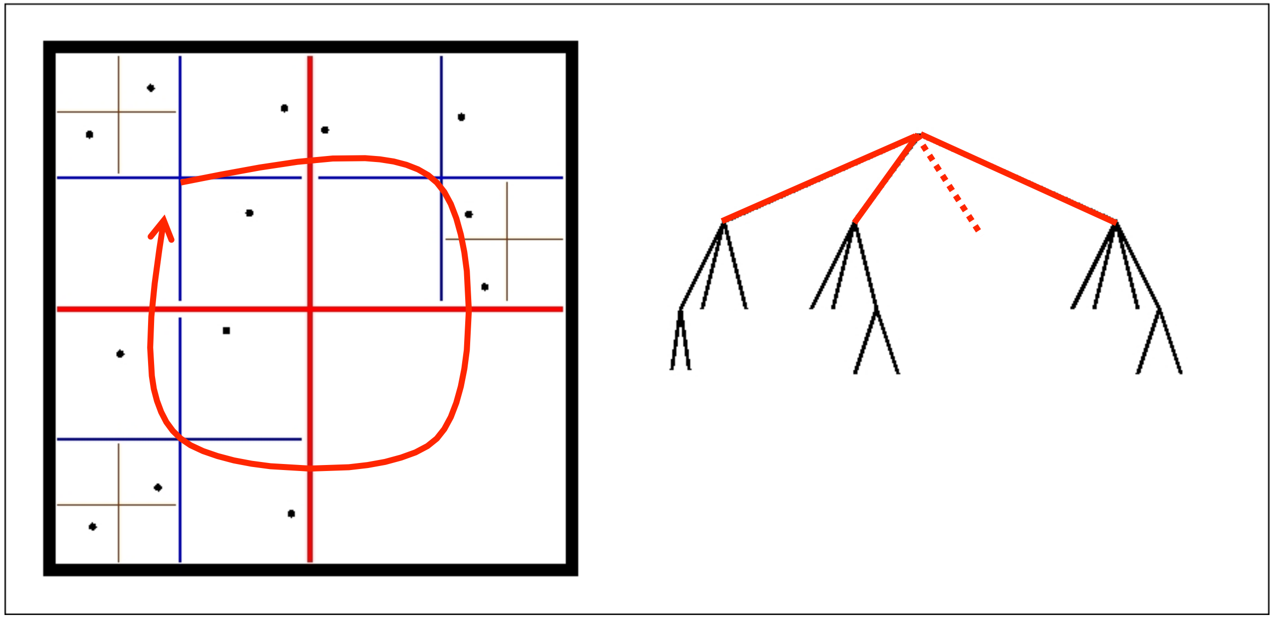

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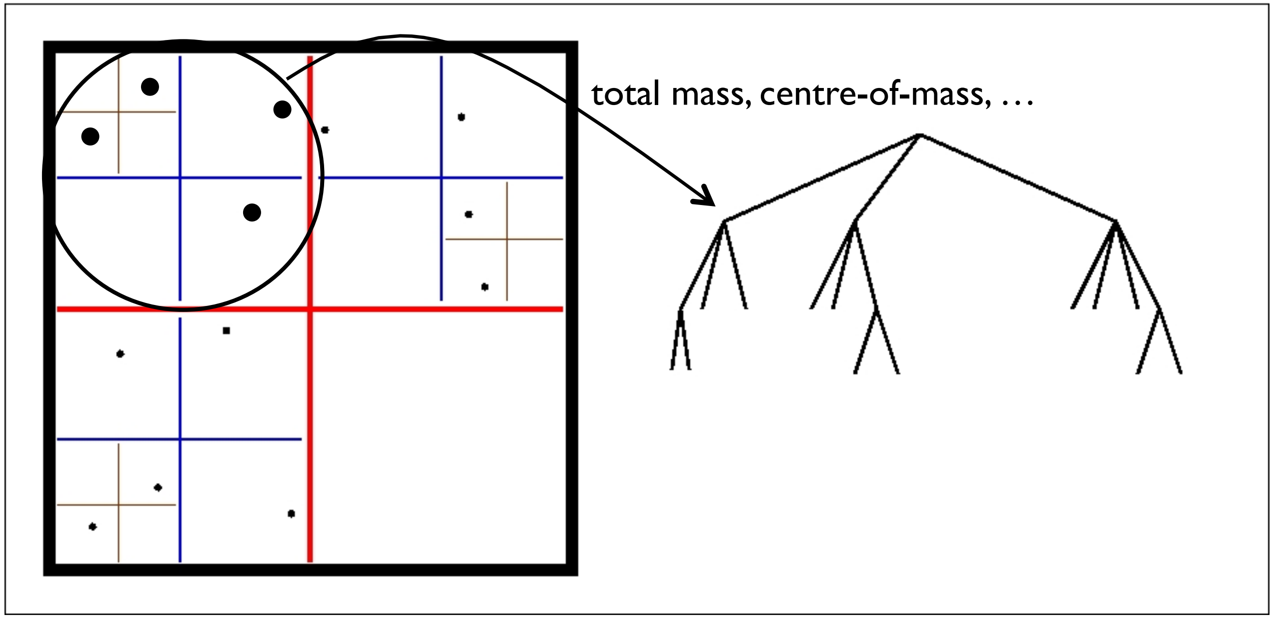

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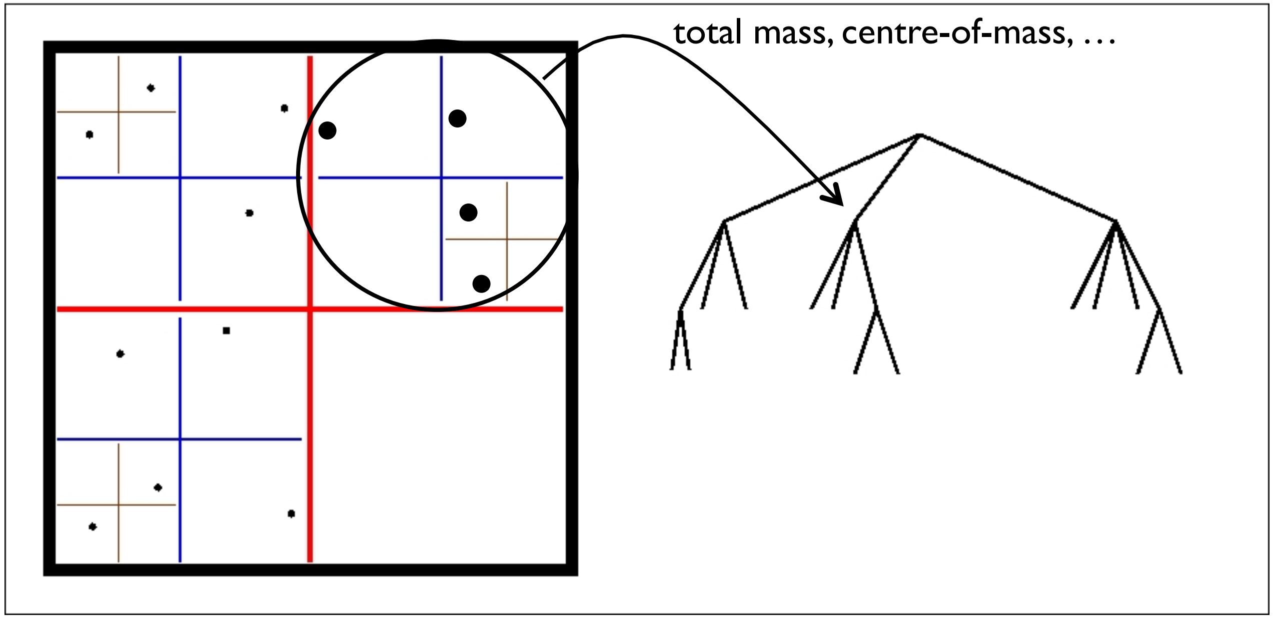

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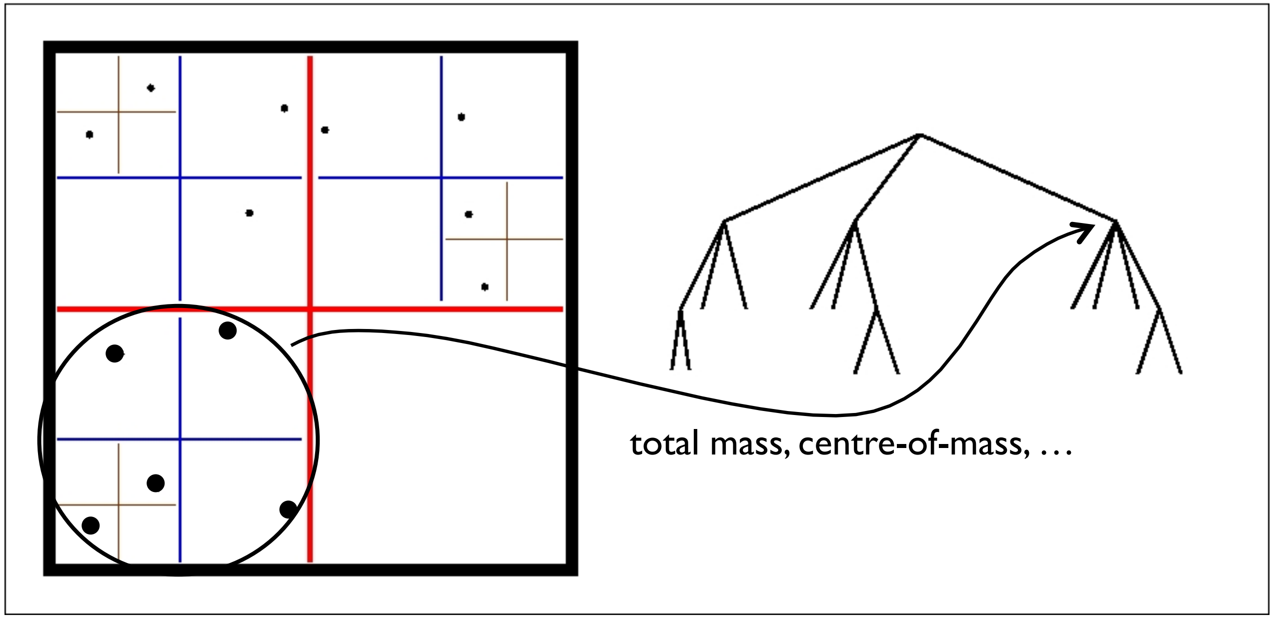

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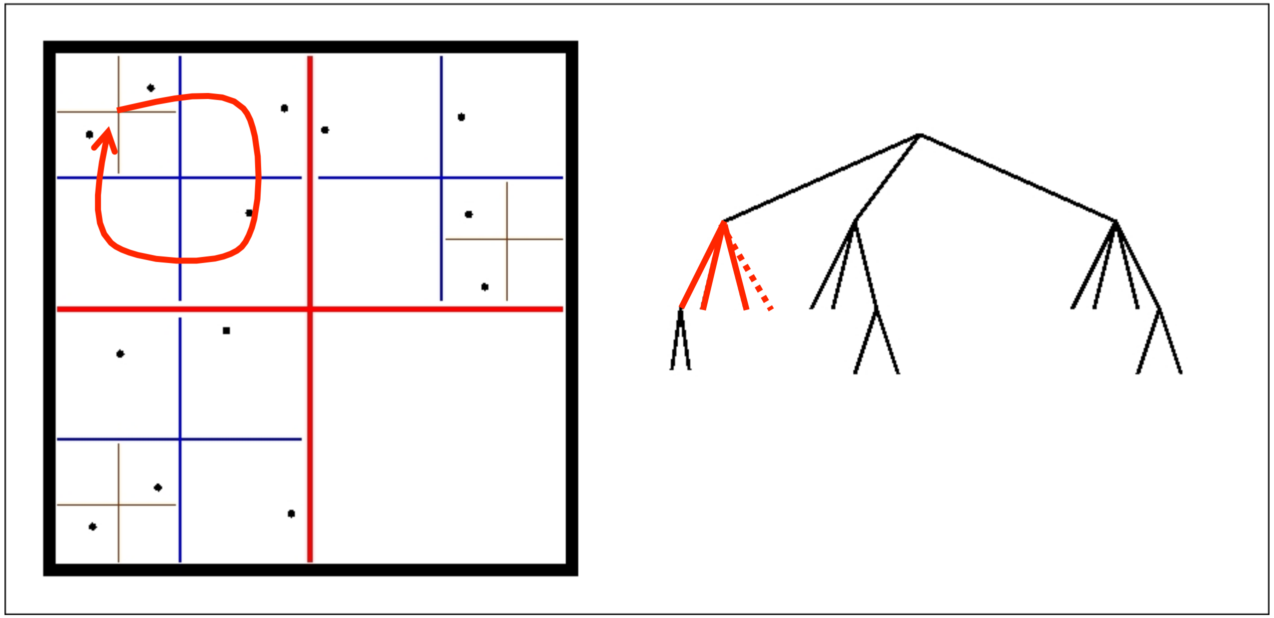

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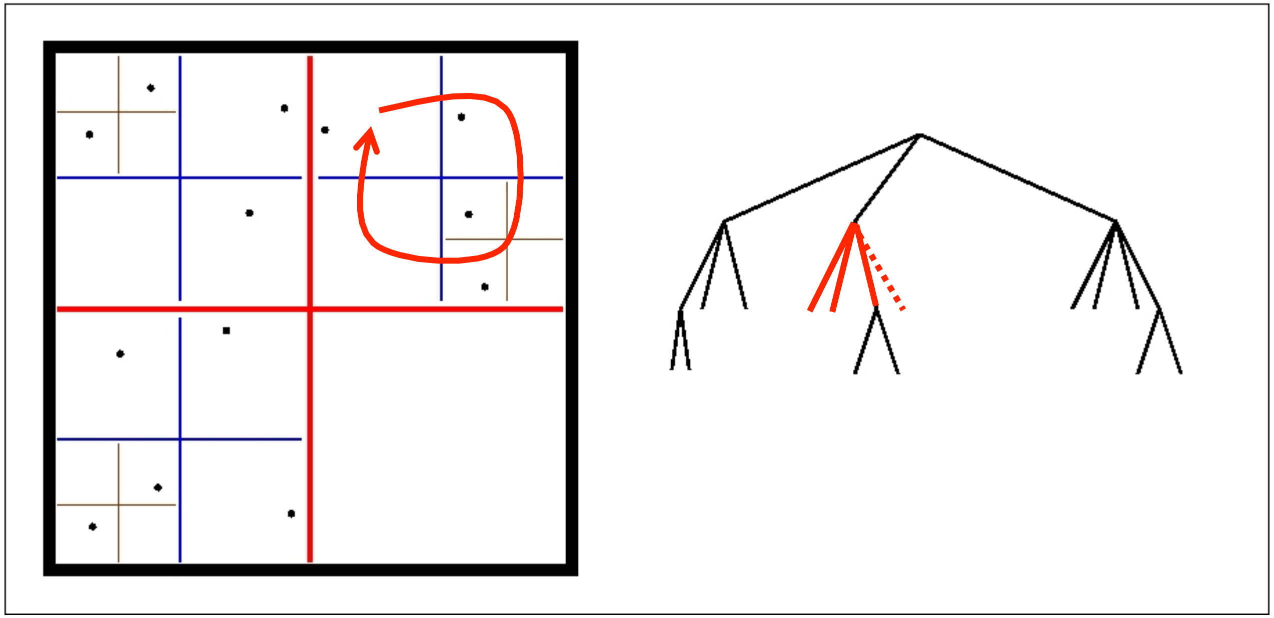

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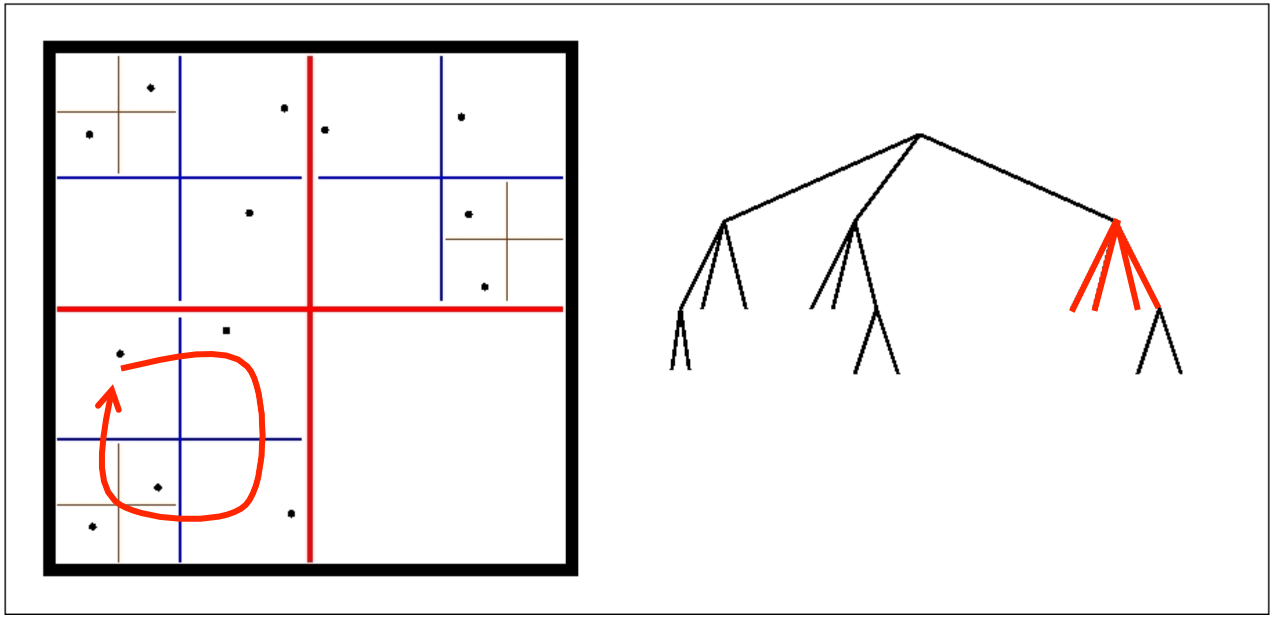

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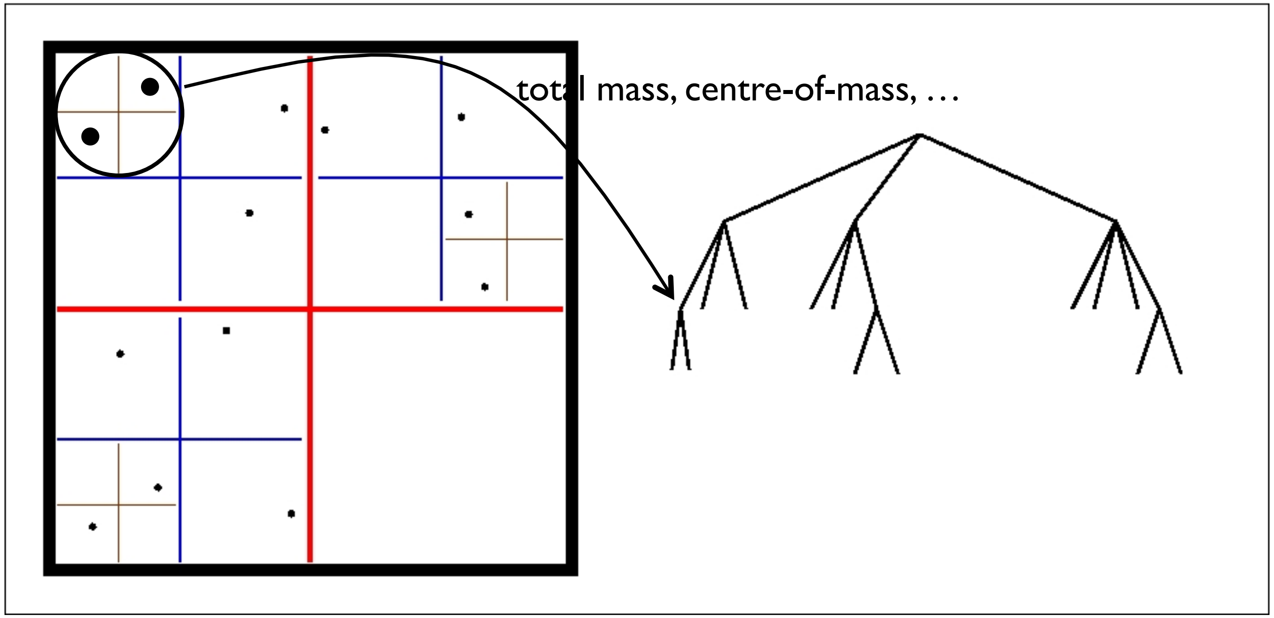

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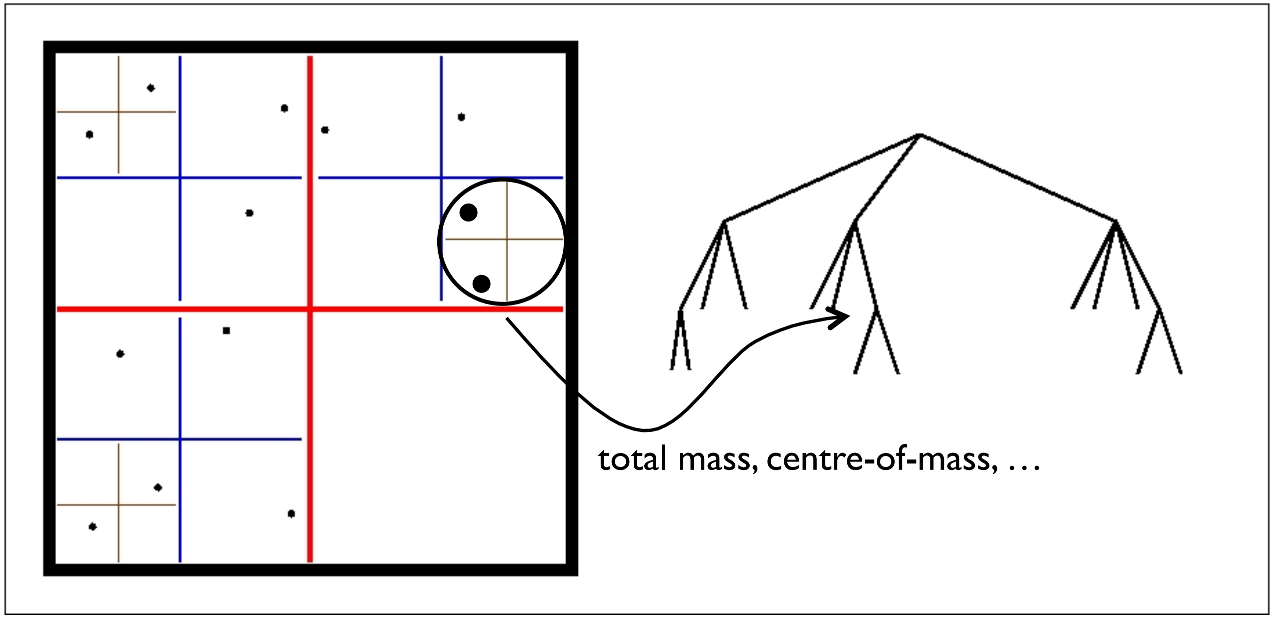

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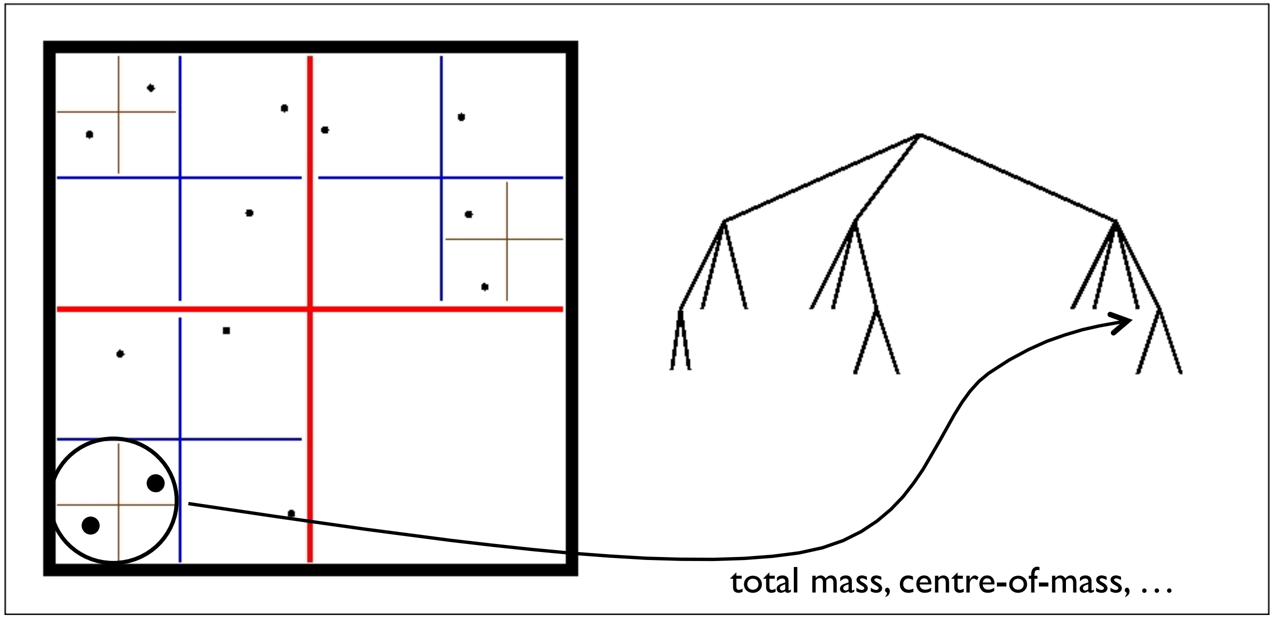

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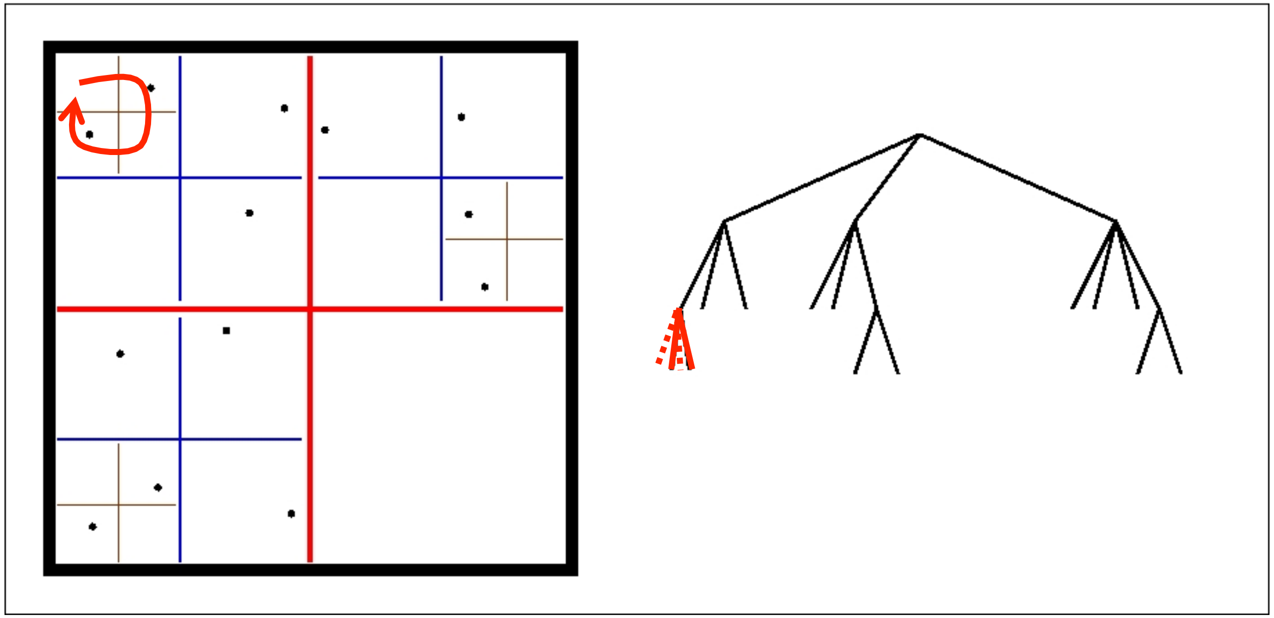

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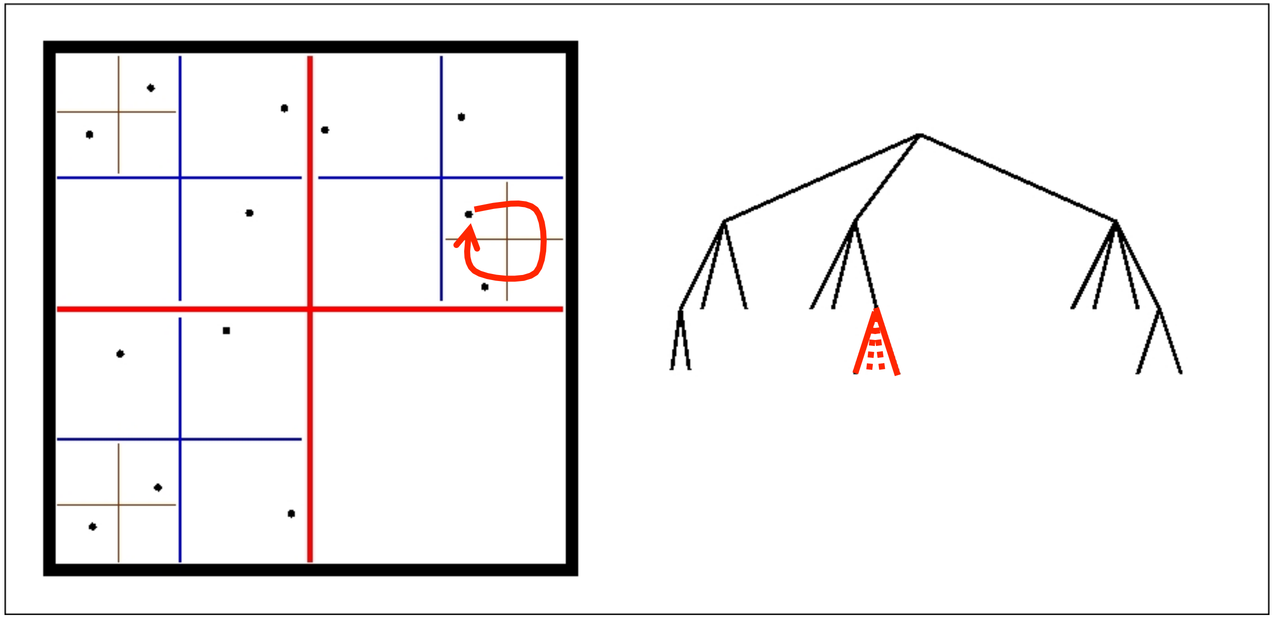

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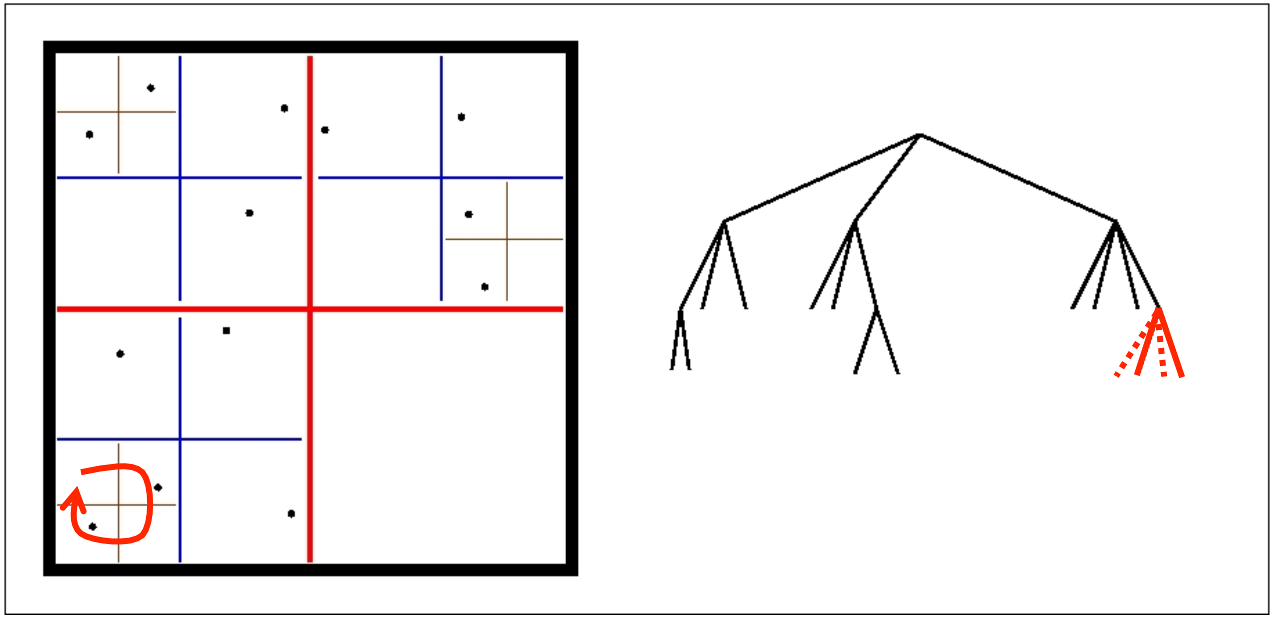

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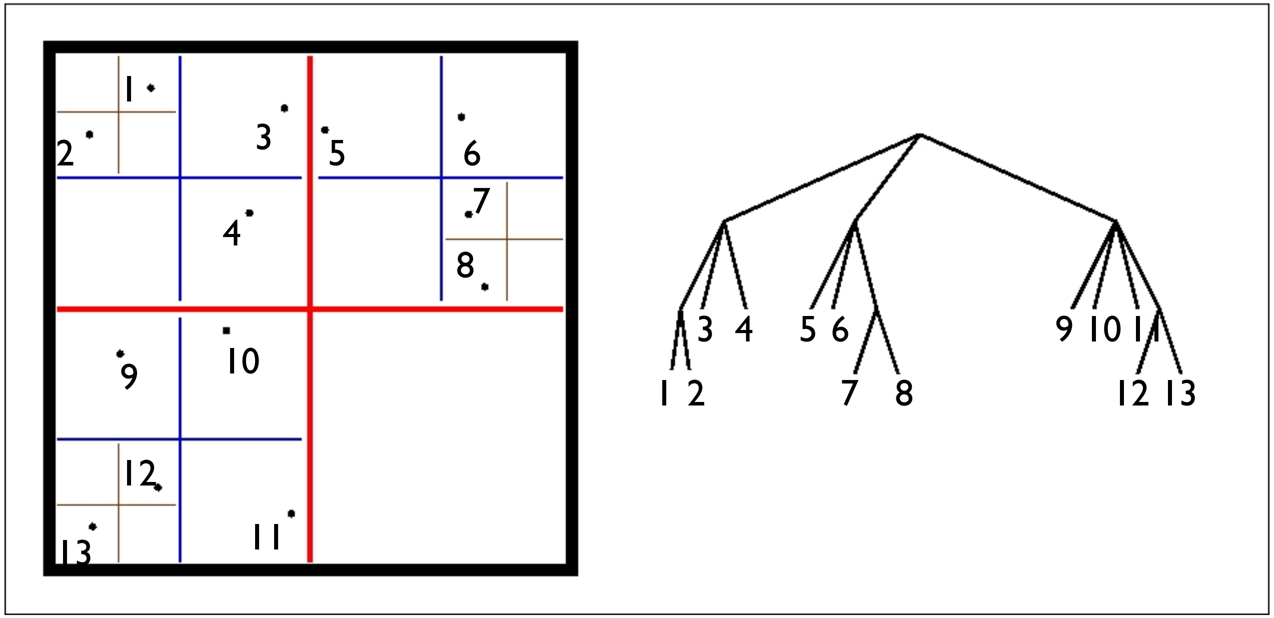

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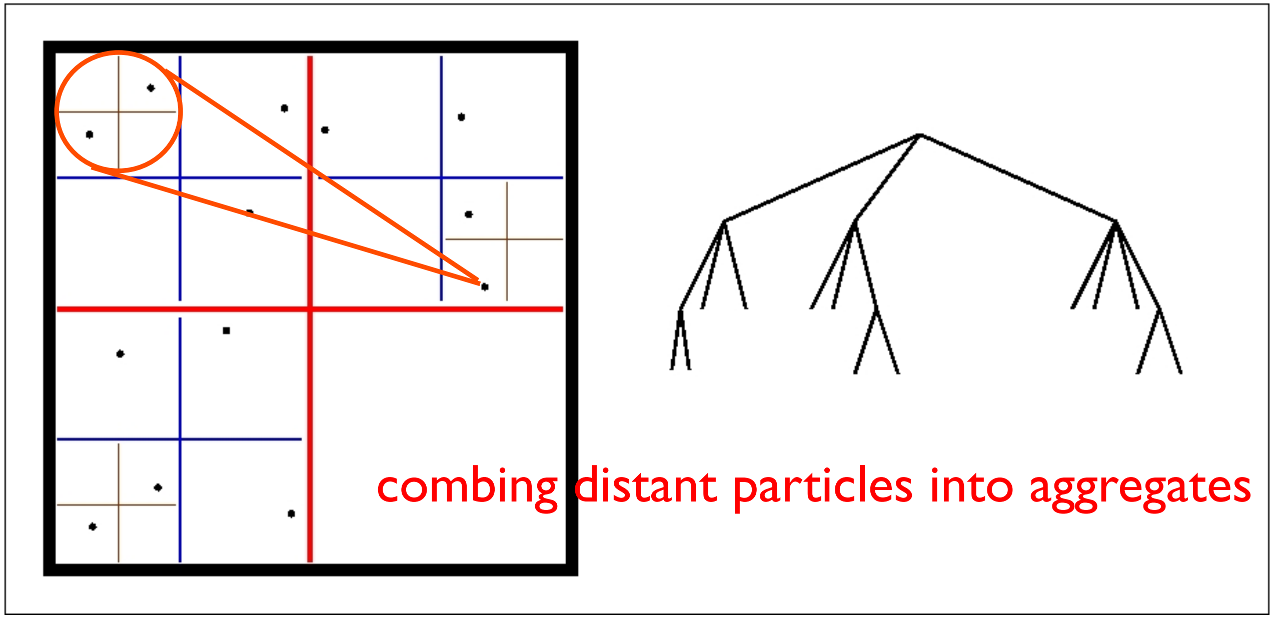

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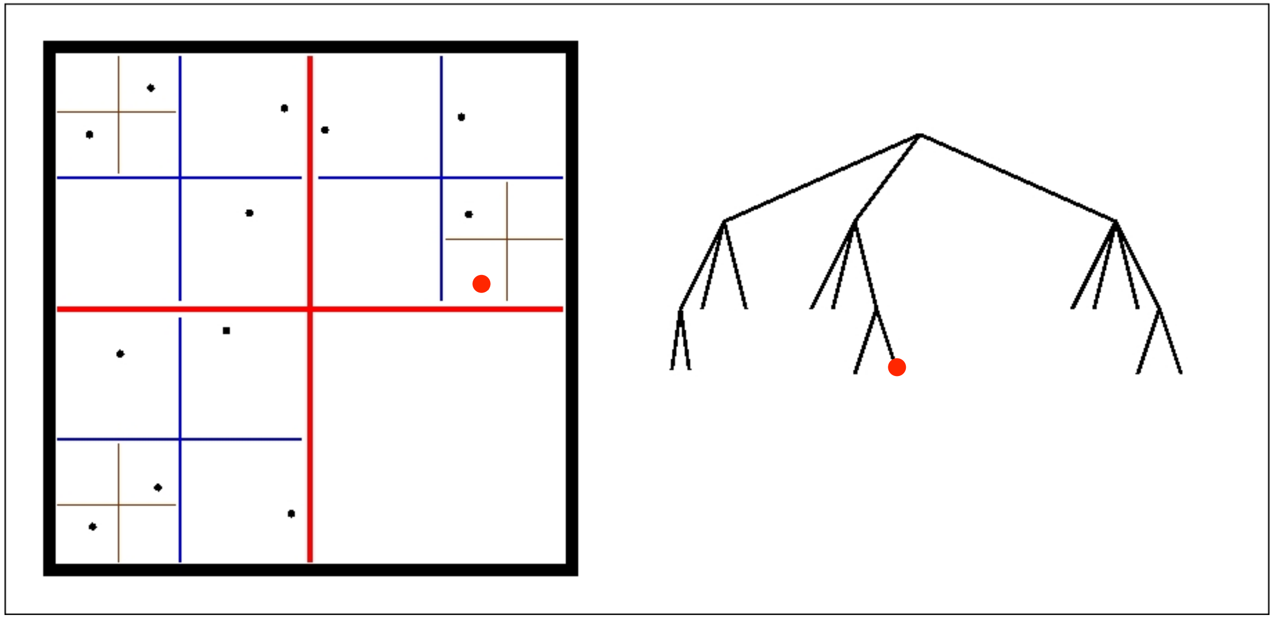

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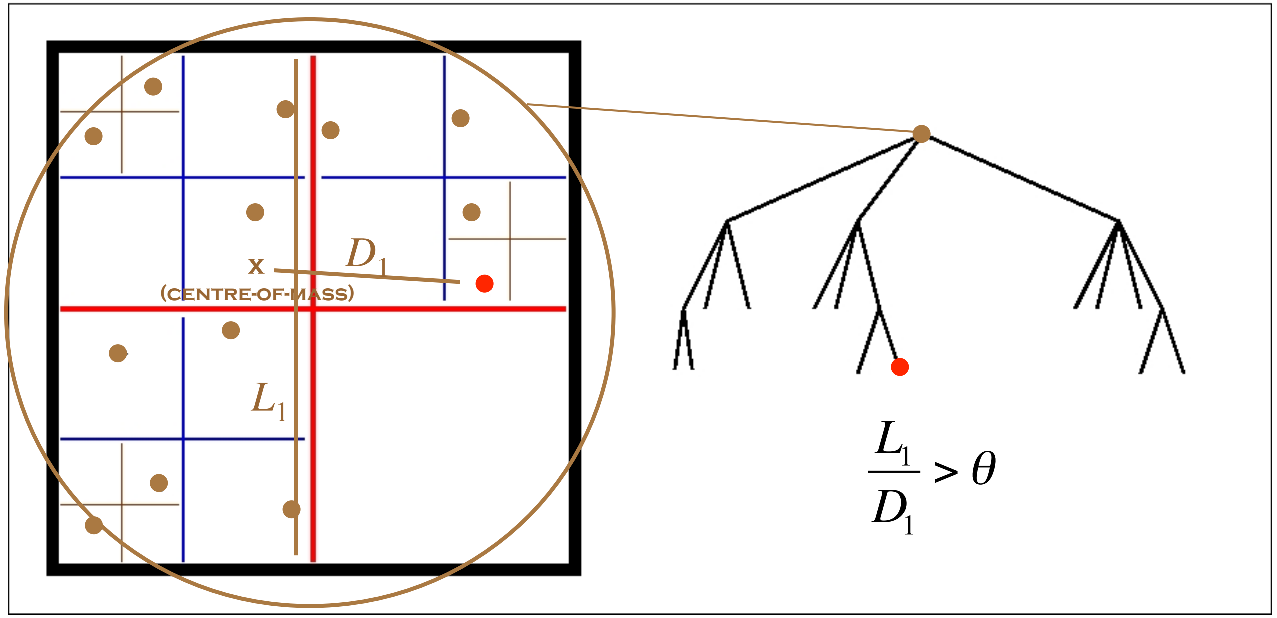

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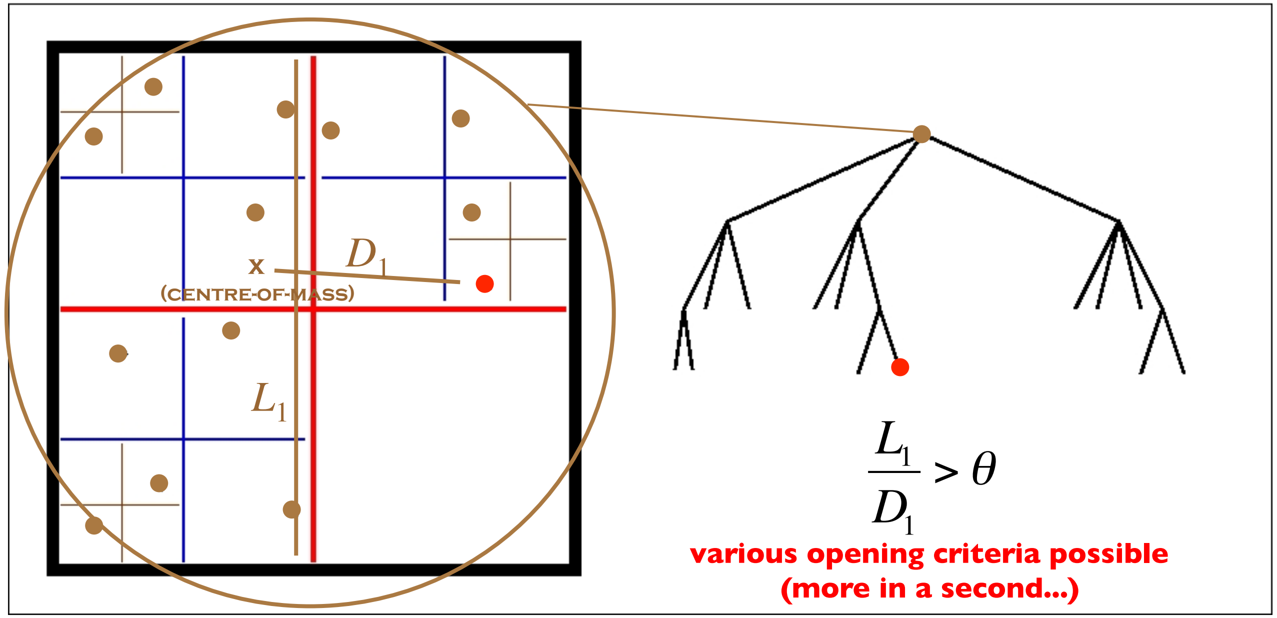

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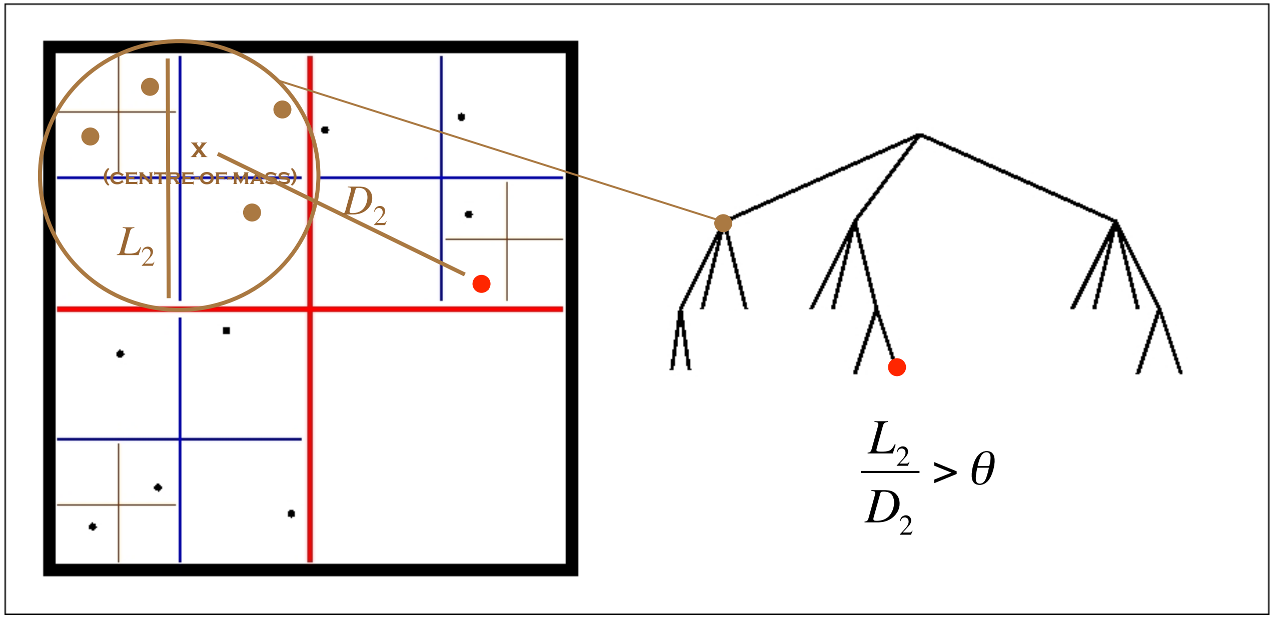

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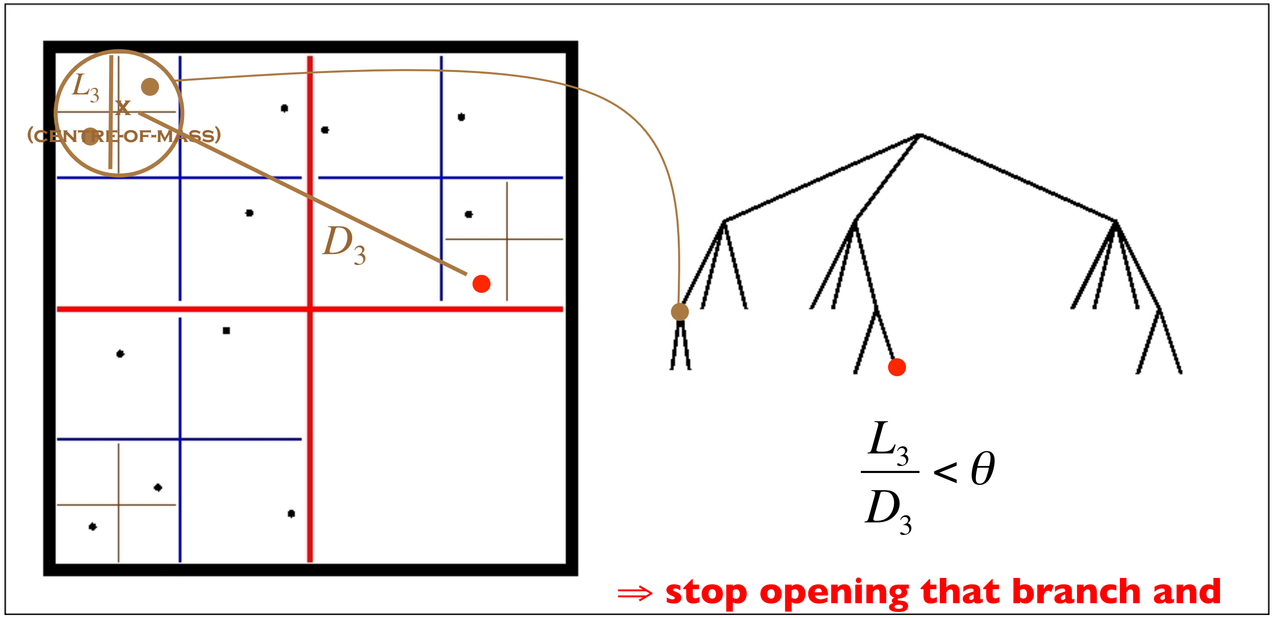

⇒ stop opening that branch and add force contribution from "super-particle"

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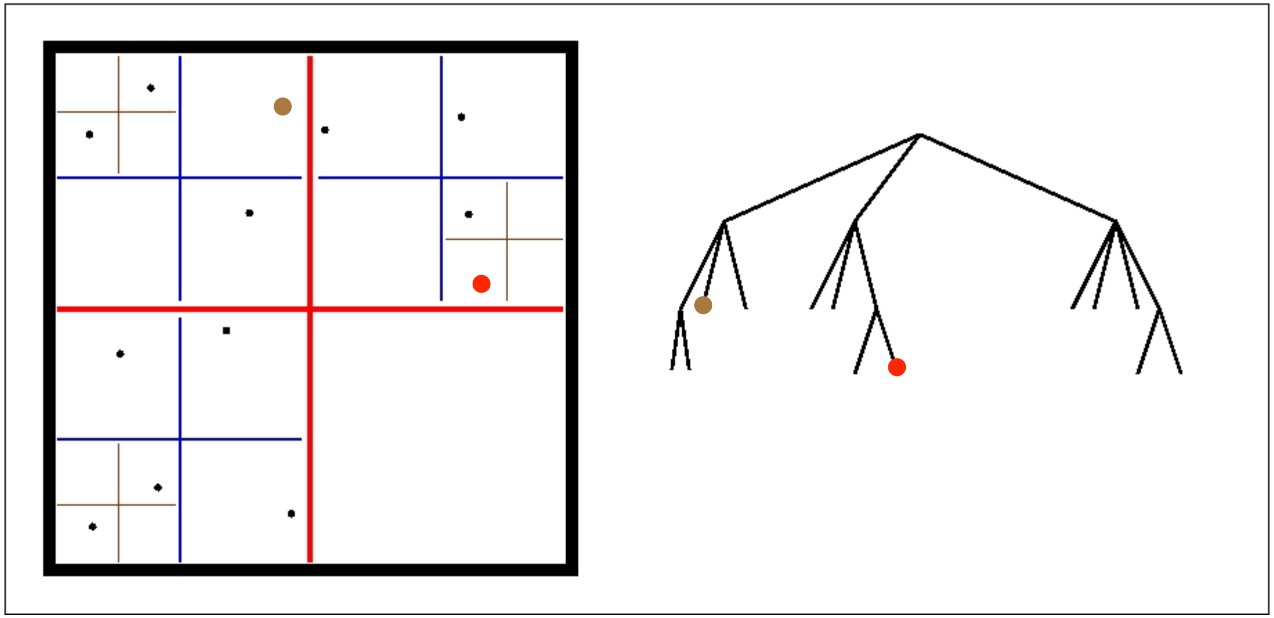

we still need to add the remaining contributions from that branch…

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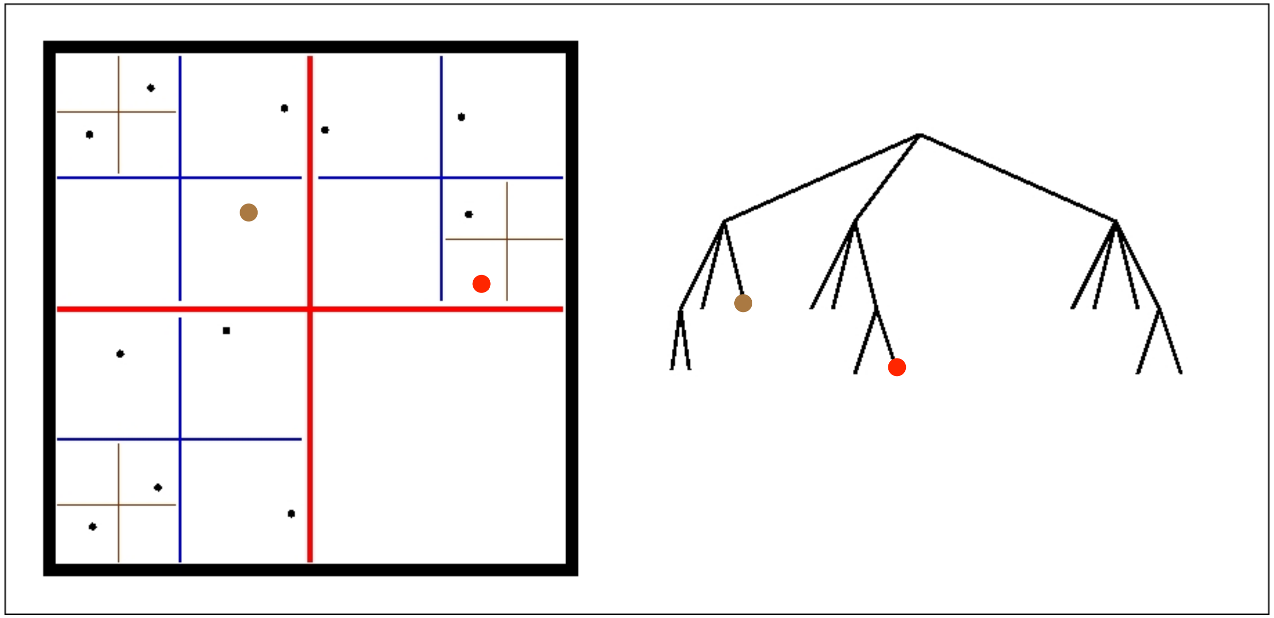

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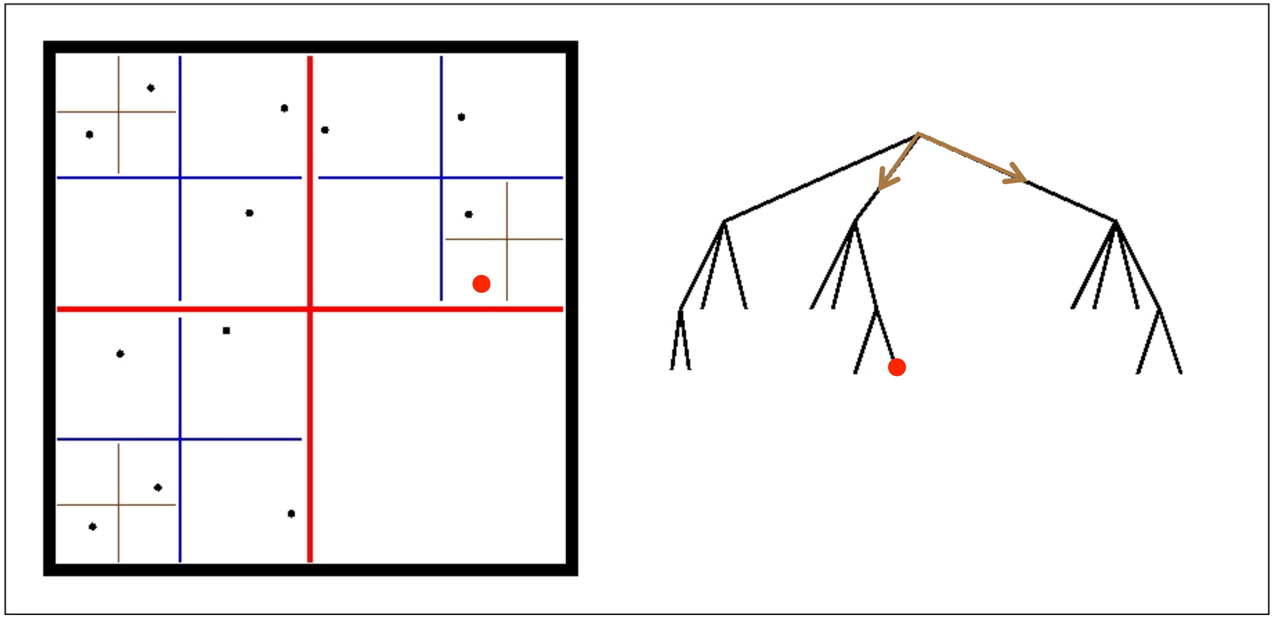

...as well as walking the other branches!

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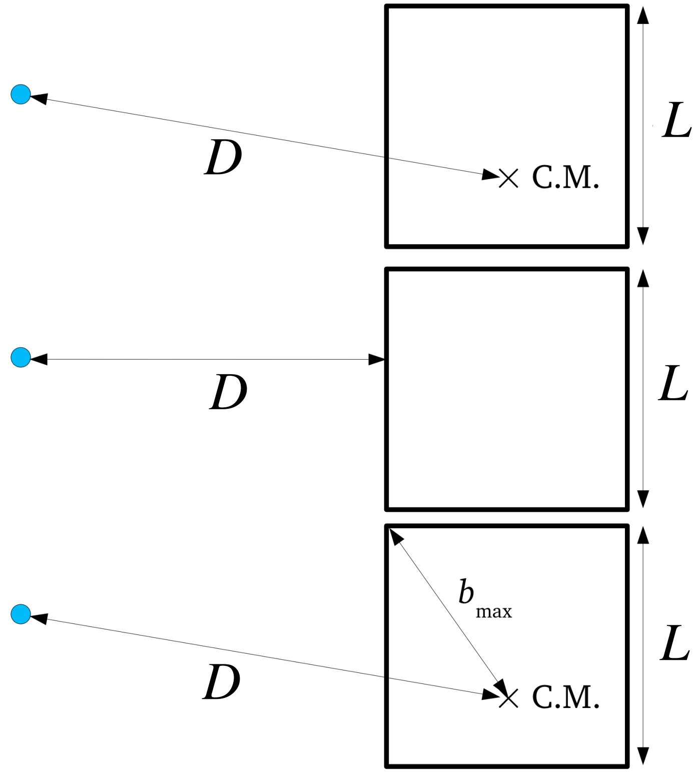
  - opening criteria:
    - Barnes-Hut $\quad L/D < \theta$
    - Min-distance $\quad L/D < \theta$
    - Bmax $\quad b_{\max}/D < \theta$



- direct particle-particle summation (PP)

other speed-ups?

- direct particle-particle summation (PP)

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GRAPE (**GRA**vity **P**ip**E**):

- particle-particle summation hardwired into motherboard
- combination with tree possible

- direct particle-particle summation (PP)

force resolution

vs.

softening

- direct particle-particle summation (PP)

$$\vec{F}_i(\vec{r}_i) = -\sum_{i \neq j} \frac{G m_i m_j}{\left((r_i - r_j)^2 + \varepsilon^2\right)^{3/2}} (\vec{r}_i - \vec{r}_j) \quad \forall i \in N$$

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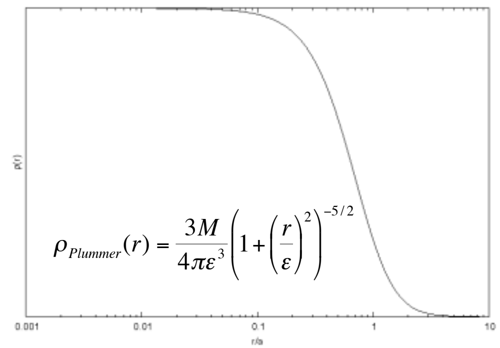
"soften" the force to…

1. avoid the singularity for $r_i = r_j$
2. smooth mass density on small scales

- direct particle-particle summation (PP)

$$\vec{F}_i(\vec{r}_i) = -\sum_{i \neq j} \frac{G m_i m_j}{\left((r_i - r_j)^2 + \varepsilon^2\right)^{3/2}} (\vec{r}_i - \vec{r}_j) \quad \forall i \in N$$

- Plummer softening



- S2 softening

- spline softening

- …

for an exhaustive discussion please refer to Dehnen, MNRAS 324, 273 (2001)

- direct particle-particle summation (PP)

$$\vec{F}_i(\vec{r}_i) = -\sum_{i \neq j} \frac{G m_i m_j}{\left((r_i - r_j)^2 + \varepsilon^2\right)^{3/2}} (\vec{r}_i - \vec{r}_j) \quad \forall i \in N$$

for collisionless simulations even more important:
each particle should only feel the mean field generated by all particles!

- direct particle-particle summation (PP)

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for collisionless simulations even more important:
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ε determines the overall force resolution of the simulation

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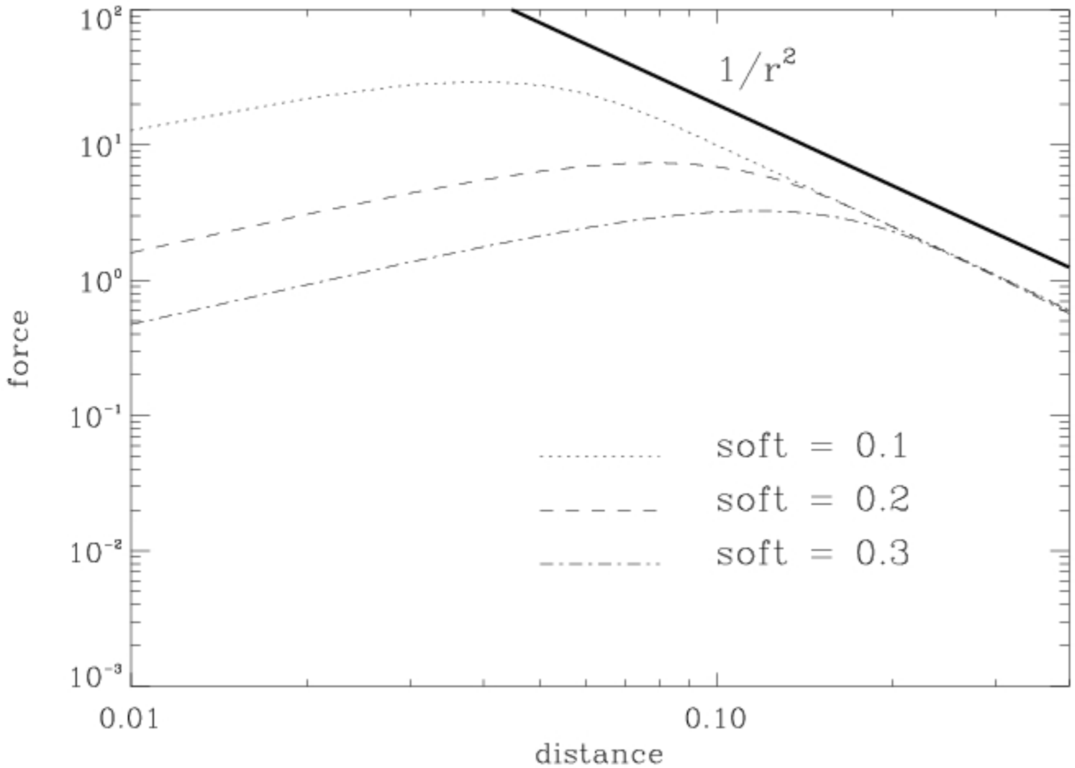

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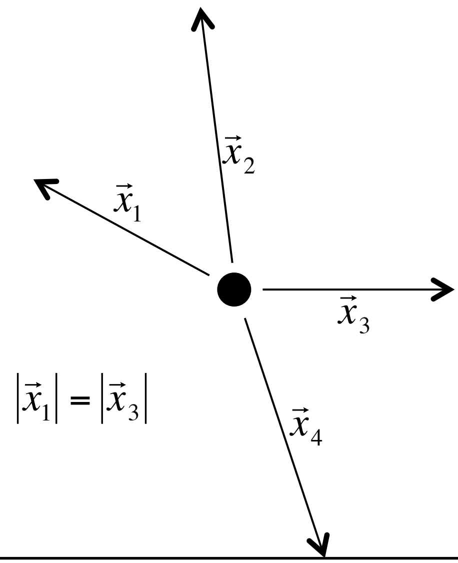
$$e^2 = \left\langle \left| \vec{F}(\vec{x}) - \vec{F}_{true}(\vec{x}) \right|^2 \right\rangle_{\vec{x}}$$



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$$\begin{aligned}
e^2(\vec{x}) &= \left\langle \left| \vec{F}(\vec{x}) - \vec{F}_{true}(\vec{x}) \right|^2 \right\rangle \\
&= \left\langle \vec{F}^2(\vec{x}) \right\rangle - 2\left\langle \vec{F}(\vec{x}) \vec{F}_{true}(\vec{x}) \right\rangle + \left\langle \vec{F}^2{}_{true}(\vec{x}) \right\rangle \\
&= \left\langle \vec{F}^2(\vec{x}) \right\rangle - 2\left\langle \vec{F}(\vec{x}) \right\rangle \vec{F}_{true}(\vec{x}) + \vec{F}^2{}_{true}(\vec{x}) \\
&= \left\langle \vec{F}^2(\vec{x}) \right\rangle - 2\left\langle \vec{F}(\vec{x}) \right\rangle \vec{F}_{true}(\vec{x}) + \vec{F}^2{}_{true}(\vec{x}) + \left\langle \vec{F}(\vec{x}) \right\rangle^2 - \left\langle \vec{F}(\vec{x}) \right\rangle^2 \\
&= \left(\left\langle \vec{F}(\vec{x}) \right\rangle - \vec{F}_{true}(\vec{x}) \right)^2 + \left\langle \vec{F}^2(\vec{x}) \right\rangle - \left\langle \vec{F}(\vec{x}) \right\rangle^2
\end{aligned}$$

- direct particle-particle summation (PP)

$$\vec{F}_i(\vec{r}_i) = -\sum_{i\neq j} \frac{G m_i m_j}{\left((r_i - r_j)^2 + \varepsilon^2\right)^{3/2}} (\vec{r}_i - \vec{r}_j) \quad \forall i \in N$$

$$\begin{aligned} e^2 &= \left\langle \left| \vec{F}(\vec{x}) - \vec{F}_{true}(\vec{x}) \right|^2 \right\rangle \\ &= \left\langle \vec{F}^2(\vec{x}) \right\rangle - 2\left\langle \vec{F}(\vec{x})\vec{F}_{true}(\vec{x}) \right\rangle + \left\langle \vec{F}^2{}_{true}(\vec{x}) \right\rangle \\ &= \left\langle \vec{F}^2(\vec{x}) \right\rangle - 2\left\langle \vec{F}(\vec{x}) \right\rangle \vec{F}_{true}(\vec{x}) + \vec{F}^2{}_{true}(\vec{x}) \\ &= \left\langle \vec{F}^2(\vec{x}) \right\rangle - 2\left\langle \vec{F}(\vec{x}) \right\rangle \vec{F}_{true}(\vec{x}) + \vec{F}^2{}_{true}(\vec{x}) + \left\langle \vec{F}(\vec{x}) \right\rangle^2 - \left\langle \vec{F}(\vec{x}) \right\rangle^2 \\ &= \left(\left\langle \vec{F}(\vec{x}) \right\rangle - \vec{F}_{true}(\vec{x}) \right)^2 + \left\langle \vec{F}^2(\vec{x}) \right\rangle - \left\langle \vec{F}(\vec{x}) \right\rangle^2 \end{aligned}$$

comparing numerical and analytical force at a given point

scatter of numerical force for a given point (note, F only depends on $|x|$)

- direct particle-particle summation (PP)

$$\vec{F}_i(\vec{r}_i) = -\sum_{i\neq j} \frac{G m_i m_j}{\left((r_i - r_j)^2 + \varepsilon^2\right)^{3/2}} (\vec{r}_i - \vec{r}_j) \quad \forall i \in N$$

$$\begin{aligned}
e^2 &= \left\langle \left| \vec{F}(\vec{x}) - \vec{F}_{true}(\vec{x}) \right|^2 \right\rangle \\
&= \left\langle \vec{F}^2(\vec{x}) \right\rangle - 2\left\langle \vec{F}(\vec{x}) \vec{F}_{true}(\vec{x}) \right\rangle + \left\langle \vec{F}^2{}_{true}(\vec{x}) \right\rangle \\
&= \left\langle \vec{F}^2(\vec{x}) \right\rangle - 2\left\langle \vec{F}(\vec{x}) \right\rangle \vec{F}_{true}(\vec{x}) + \vec{F}^2{}_{true}(\vec{x}) \\
&= \left\langle \vec{F}^2(\vec{x}) \right\rangle - 2\left\langle \vec{F}(\vec{x}) \right\rangle \vec{F}_{true}(\vec{x}) + \vec{F}^2{}_{true}(\vec{x}) + \left\langle \vec{F}(\vec{x}) \right\rangle^2 - \left\langle \vec{F}(\vec{x}) \right\rangle^2 \\
&= \left(\left\langle \vec{F}(\vec{x}) \right\rangle - \vec{F}_{true}(\vec{x}) \right)^2 + \left\langle \vec{F}^2(\vec{x}) \right\rangle - \left\langle \vec{F}(\vec{x}) \right\rangle^2 \\
&= \mathtt{bias}^2 + \mathtt{var}
\end{aligned}$$

- direct particle-particle summation (PP)

$$\vec{F}_i(\vec{r}_i) = -\sum_{i \neq j} \frac{G m_i m_j}{\left((r_i - r_j)^2 + \varepsilon^2\right)^{3/2}} (\vec{r}_i - \vec{r}_j) \quad \forall i \in N$$

$$\texttt{bias} = \left(\left\langle \vec{F}(\vec{x}) \right\rangle - \vec{F}_{true}(\vec{x})\right)$$

$$\texttt{var} = \left\langle \vec{F}^{\,2}(\vec{x}) \right\rangle - \left\langle \vec{F}(\vec{x}) \right\rangle^2$$

- direct particle-particle summation (PP)

$$\vec{F}_i(\vec{r}_i) = -\sum_{i \neq j} \frac{G m_i m_j}{\left((r_i - r_j)^2 + \varepsilon^2\right)^{3/2}} (\vec{r}_i - \vec{r}_j) \quad \forall i \in N$$

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

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

α, β = non-trivial power-law indices…
$N\varepsilon^3$ = const.

- direct particle-particle summation (PP)

$$\vec{F}_i(\vec{r}_i) = -\sum_{i \neq j} \frac{G m_i m_j}{\left((r_i - r_j)^2 + \varepsilon^2\right)^{3/2}} (\vec{r}_i - \vec{r}_j) \quad \forall i \in N$$

  - error estimate:

$$MISE = \left\langle \iiint \rho(\vec{x}) \left| \vec{F}(\vec{x}) - \vec{F}_{true}(\vec{x}) \right|^2 d^3x \right\rangle$$

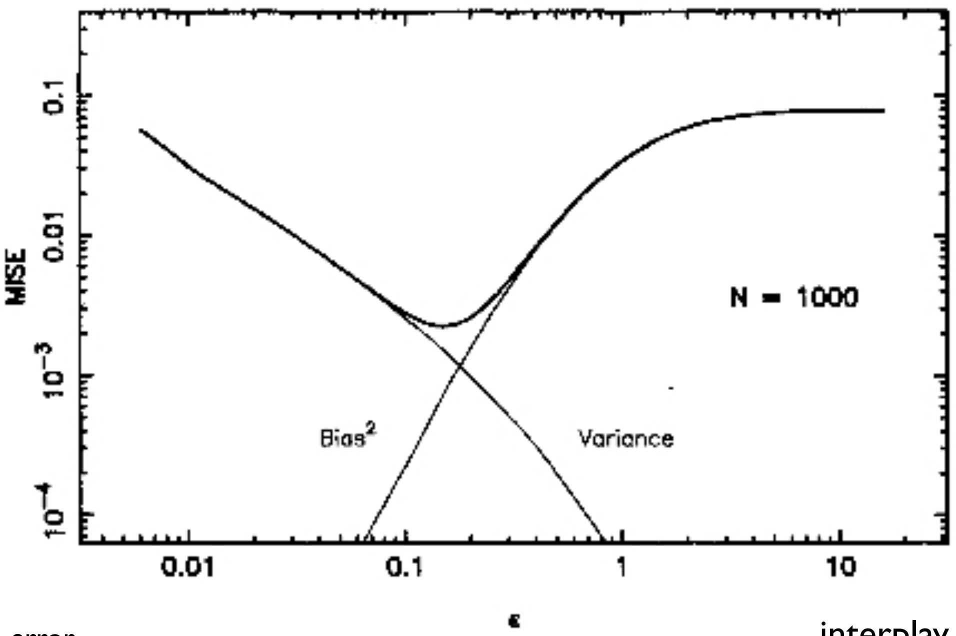
MISE = mean integrated square error

- direct particle-particle summation (PP)

$$\vec{F}_i(\vec{r}_i) = -\sum_{i \neq j} \frac{G m_i m_j}{\left((r_i - r_j)^2 + \varepsilon^2\right)^{3/2}} (\vec{r}_i - \vec{r}_j) \quad \forall i \in N$$

- error estimate:

$$MISE = \left\langle \iiint \rho(\vec{x}) \left| \vec{F}(\vec{x}) - \vec{F}_{true}(\vec{x}) \right|^2 d^3x \right\rangle$$



Merritt, ApJ 111, 2462 (1996)

MISE = mean integrated square error

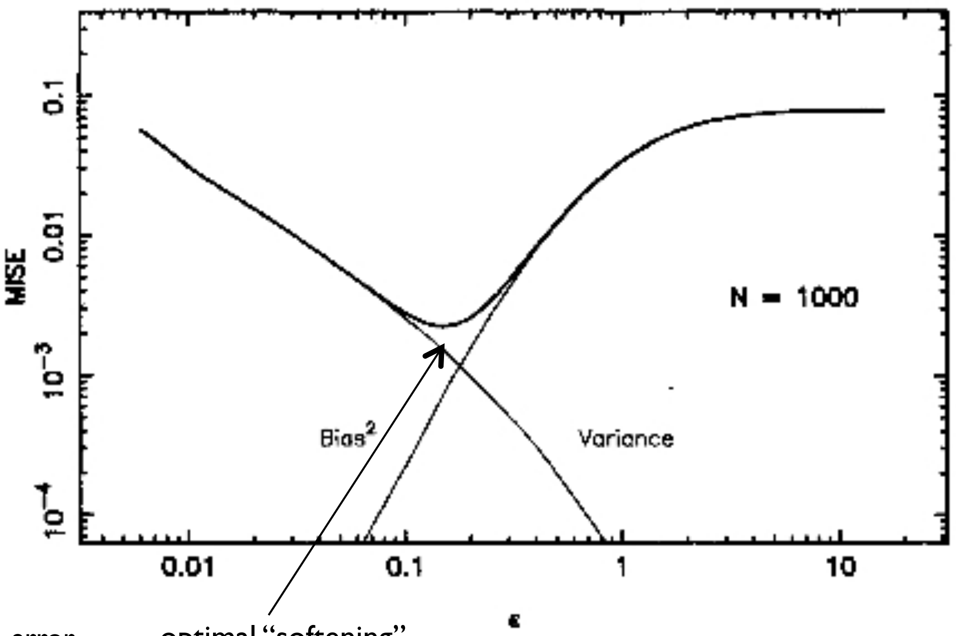
interplay between N and ε: $N\varepsilon^3$=const.

- direct particle-particle summation (PP)

$$\vec{F}_i(\vec{r}_i) = -\sum_{i \neq j} \frac{G m_i m_j}{\left((r_i - r_j)^2 + \varepsilon^2\right)^{3/2}} (\vec{r}_i - \vec{r}_j) \quad \forall i \in N$$

- error estimate:

$$MISE = \left\langle \iiint \rho(\vec{x}) \left| \vec{F}(\vec{x}) - \vec{F}_{true}(\vec{x}) \right|^2 d^3x \right\rangle$$



Merritt, ApJ 111, 2462 (1996)

MISE = mean integrated square error

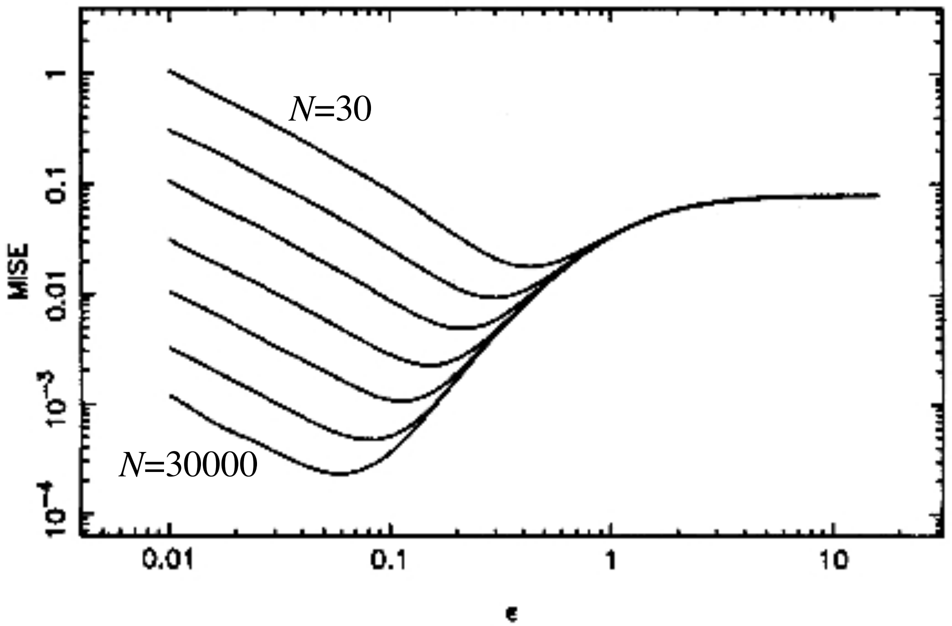
optimal "softening"

- direct particle-particle summation (PP)

$$\vec{F}_i(\vec{r}_i) = -\sum_{i \neq j} \frac{G m_i m_j}{\left((r_i - r_j)^2 + \varepsilon^2\right)^{3/2}} (\vec{r}_i - \vec{r}_j) \quad \forall i \in N$$

  - error estimate:

$$MISE = \left\langle \iiint \rho(\vec{x}) \left| \vec{F}(\vec{x}) - \vec{F}_{true}(\vec{x}) \right|^2 d^3x \right\rangle$$



Merritt, ApJ 111, 2462 (1996)

MISE = mean integrated square error

requirements to perform

Cosmological Simulations

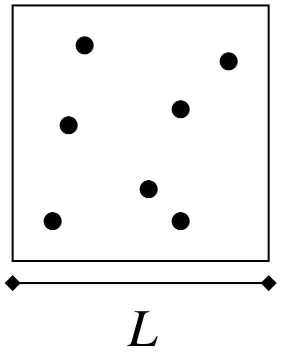
- specific requirements for cosmological simulations:

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

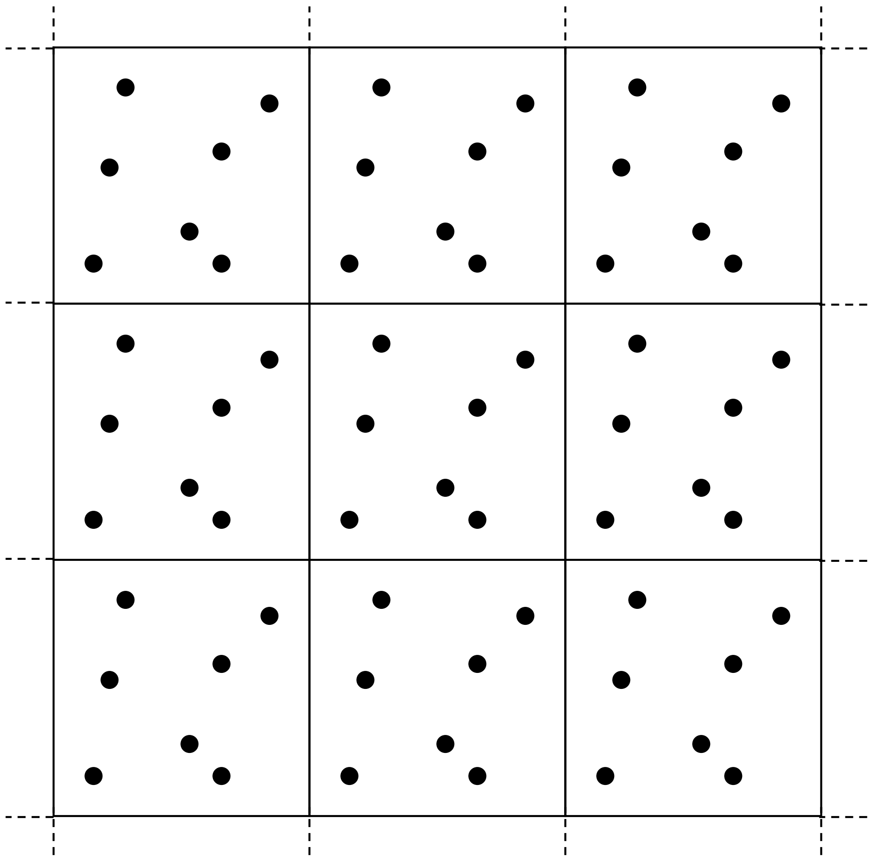
- specific requirements for cosmological simulations:

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

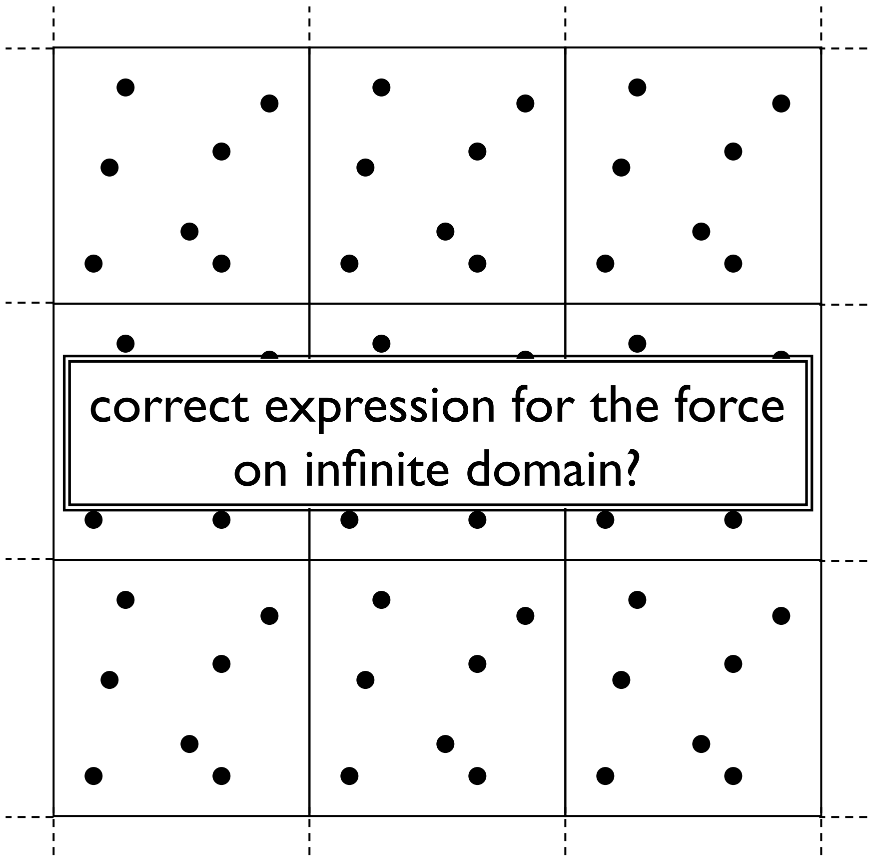
- periodic boundary conditions



- periodic boundary conditions



- periodic boundary conditions



- periodic boundary conditions

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

- 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!

- periodic boundary conditions

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

↓ general solution

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

- periodic boundary conditions

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

↓ general solution

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

periodicity automatically taken care of when using PM solver!

- periodic boundary conditions

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

↓ general solution

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

periodicity automatically taken care of when using PM solver!

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

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

- periodic boundary conditions

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

↓ general solution

fluctuates about zero!

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

$$\begin{aligned} i.e., \Phi(\vec{0}) &= -G \iiint \frac{\left(\rho_x(\vec{x}) - \bar{\rho}_x\right)}{\left|\vec{x}\right|} d^3x \\ &= -G \int_{x=0}^{\infty} \frac{1}{\left|\vec{x}\right|} x^2 \iint_{\vartheta\,\varphi} \left(\rho_x(\vec{x}) - \bar{\rho}_x\right) \sin\vartheta\, d\vartheta\, d\varphi \\ &= -G \int_{x=0}^{\infty} x \left\langle \rho_x(\vec{x}) - \bar{\rho}_x \right\rangle_{\left|\vec{x}\right|=x} dx \end{aligned}$$

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

- periodic boundary conditions

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

↓ general solution

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

↓ desired (peculiar) force field

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

- periodic boundary conditions

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

- periodic boundary conditions

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

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

- periodic boundary conditions

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

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

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

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

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

- periodic boundary conditions

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

- periodic boundary conditions

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

↓ particle/discrete picture

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

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

- 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

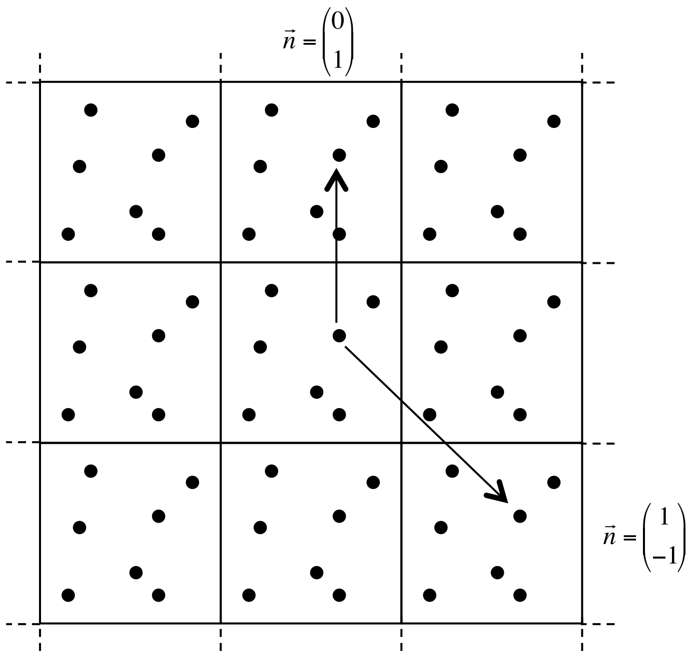
$$\vec{F}(\vec{x}) = -G\sum_{i=1}^{N}\sum_{\vec{R}} \frac{m_i}{\left|\vec{x}-(\vec{x}_i+\vec{R})\right|^3}\left(\vec{x}-(\vec{x}_i+\vec{R})\right)$$

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

correct expression for the force on infinite domain!

- periodic boundary conditions

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



- 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…

- periodic boundary conditions

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

- 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)

- periodic boundary conditions

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

- periodic boundary conditions

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

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

- periodic boundary conditions

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

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

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

- 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"

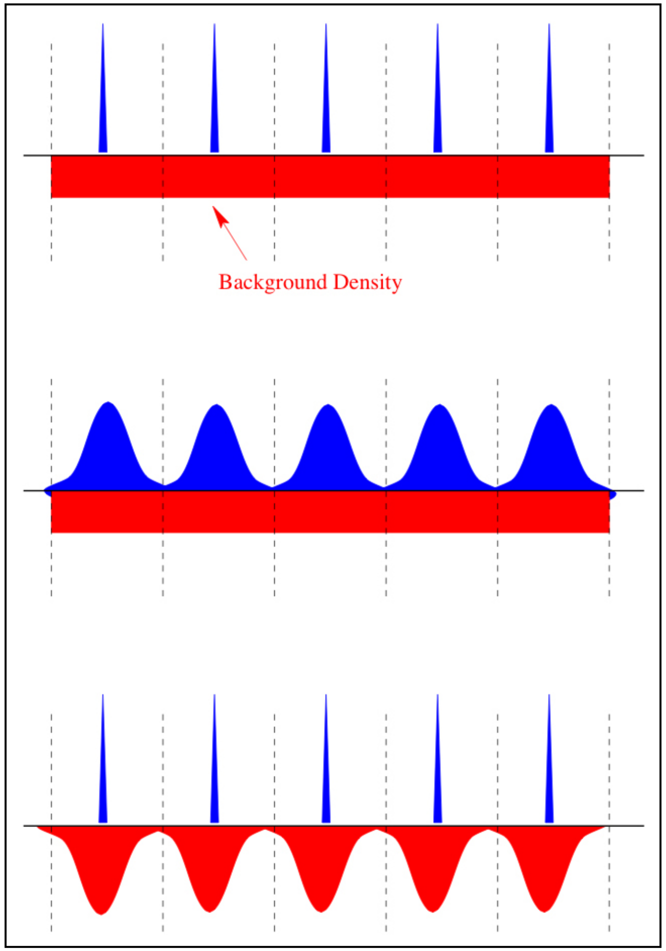
- periodic boundary conditions

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

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

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

- 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

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

real-space

=> exponential convergence and hence feasible!

- periodic boundary conditions

detailed calculation…

- 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…

- specific requirements for cosmological simulations:

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

(cf. "gastrophysics in supercomoving coordinates" lecture...)

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

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

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

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

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

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

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

additional/closure equations:

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

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

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

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

- 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:

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

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

- comoving coordinates

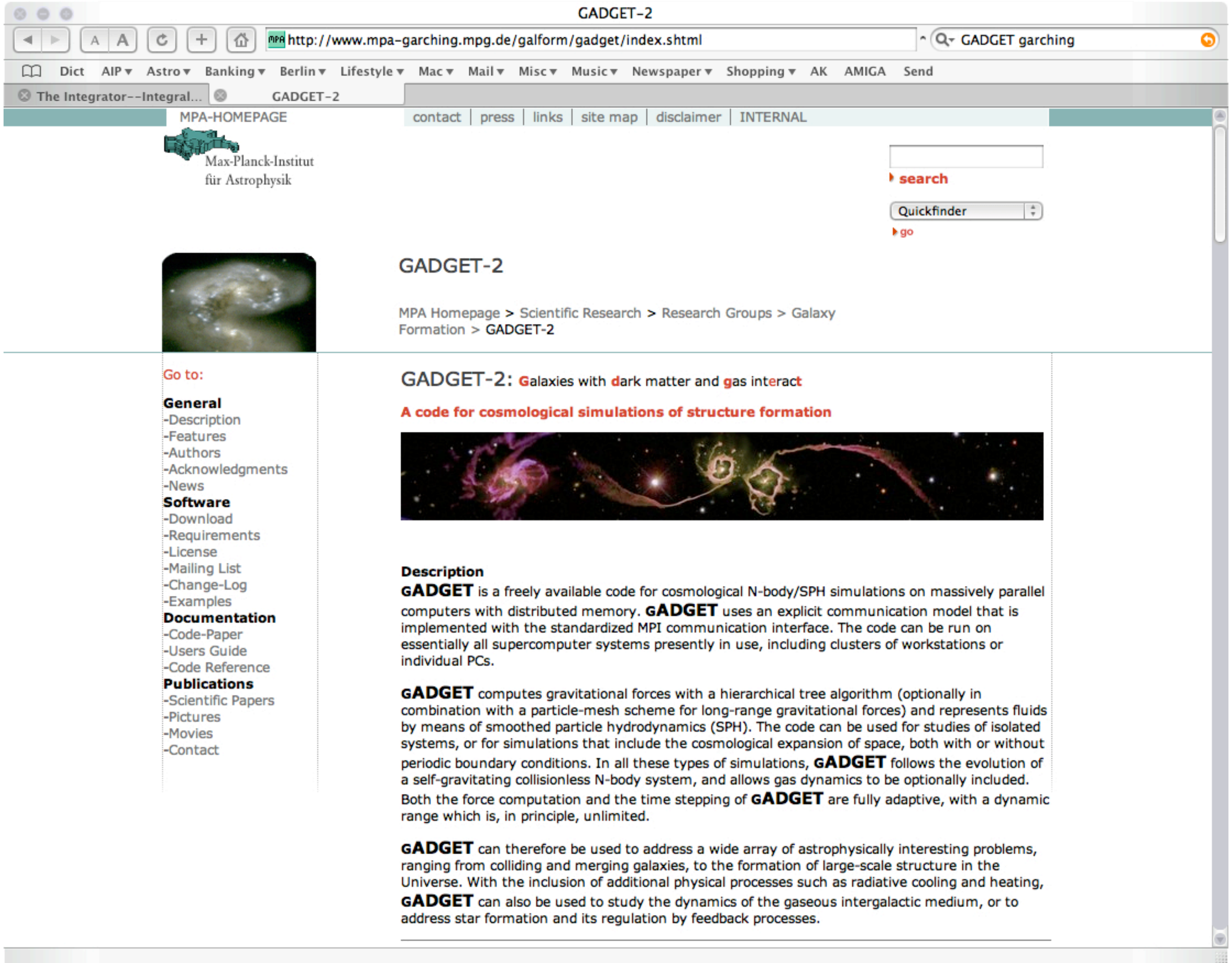
  - isolated boundaries:

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

  - 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…)



GADGET-2

http://www.mpa-garching.mpg.de/galform/gadget/index.shtml

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GADGET-2: Galaxies with dark matter and gas interact

A code for cosmological simulations of structure formation

Description

GADGET is a freely available code for cosmological N-body/SPH simulations on massively parallel computers with distributed memory. **GADGET** uses an explicit communication model that is implemented with the standardized MPI communication interface. The code can be run on essentially all supercomputer systems presently in use, including clusters of workstations or individual PCs.

GADGET computes gravitational forces with a hierarchical tree algorithm (optionally in combination with a particle-mesh scheme for long-range gravitational forces) and represents fluids by means of smoothed particle hydrodynamics (SPH). The code can be used for studies of isolated systems, or for simulations that include the cosmological expansion of space, both with or without periodic boundary conditions. In all these types of simulations, **GADGET** follows the evolution of a self-gravitating collisionless N-body system, and allows gas dynamics to be optionally included. Both the force computation and the time stepping of **GADGET** are fully adaptive, with a dynamic range which is, in principle, unlimited.

GADGET can therefore be used to address a wide array of astrophysically interesting problems, ranging from colliding and merging galaxies, to the formation of large-scale structure in the Universe. With the inclusion of additional physical processes such as radiative cooling and heating, **GADGET** can also be used to study the dynamics of the gaseous intergalactic medium, or to address star formation and its regulation by feedback processes.