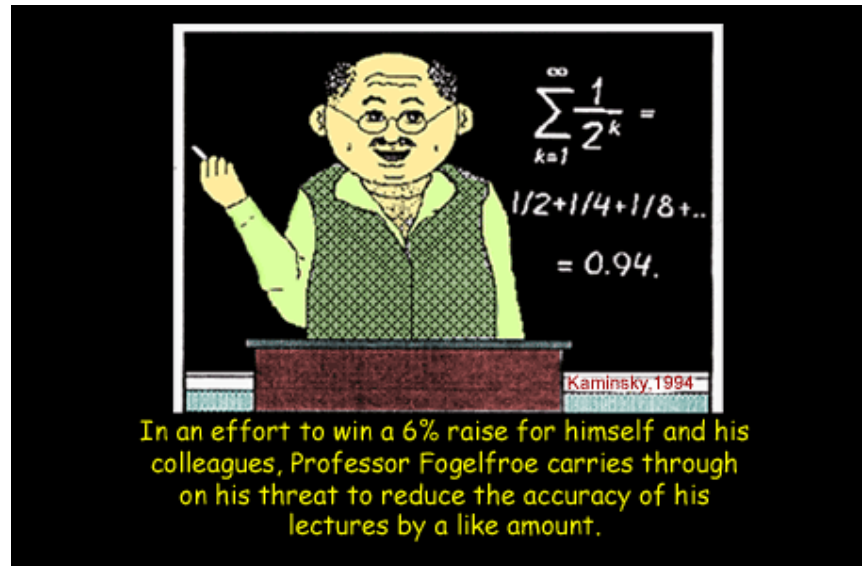
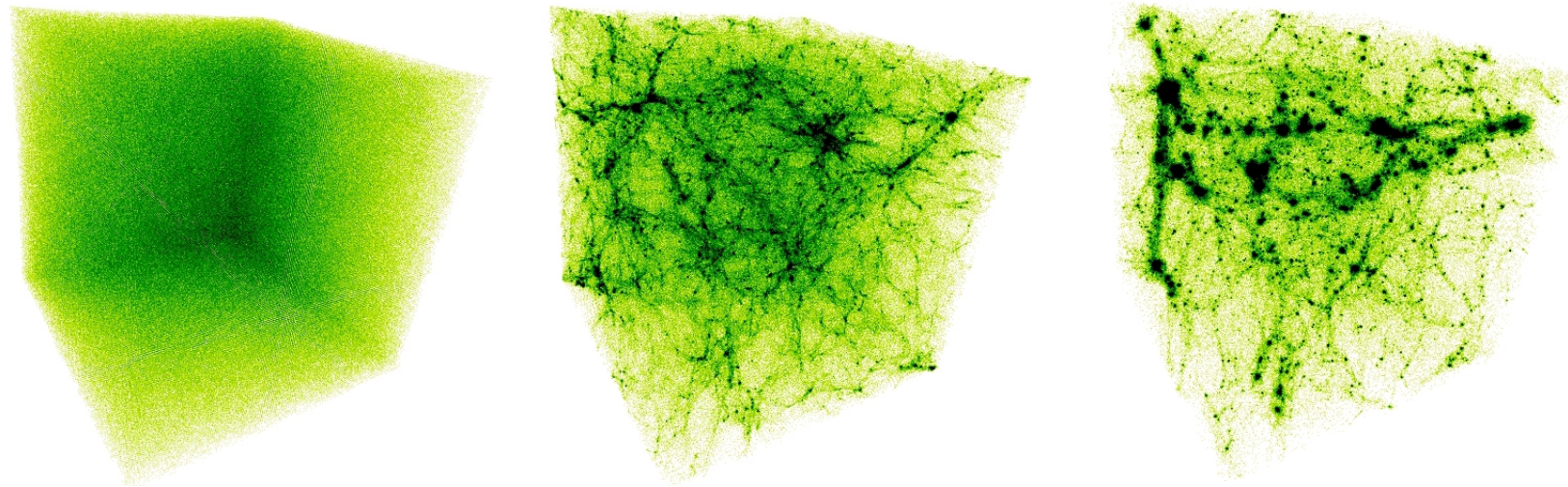


COMPUTATIONAL COSMOLOGY

Alexander Knebe, *Universidad Autonoma de Madrid*

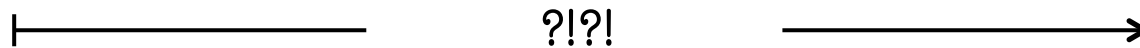
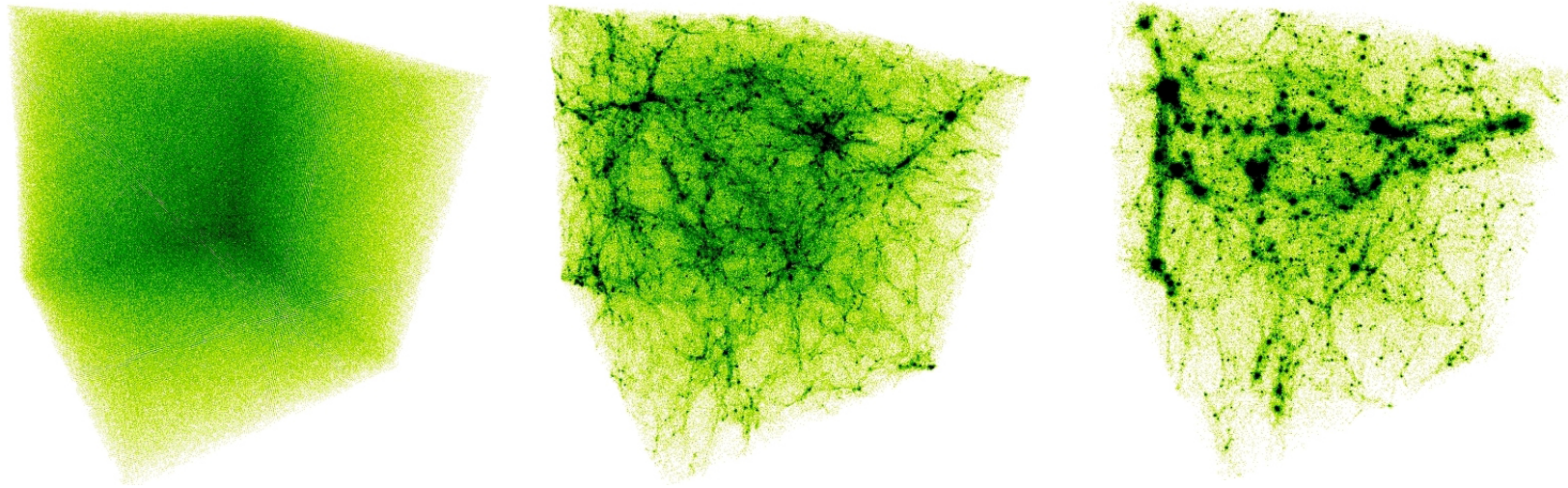


CODE TESTING



?!?

CODE TESTING



how can we be sure to actually model the Universe?

▪ full set of equations

- collisionless matter (e.g. dark matter)

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

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

- collisional matter (e.g. gas)

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

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

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

- Poisson's equation

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

- ideal gas equations

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

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

- Maxwell's equation

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

▪ full set of equations

- collisionless matter (e.g. dark matter)

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

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time integration lecture

gravity solvers lectures

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

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

time integration lecture

gravity solvers lectures

2 possible error sources!

- Poisson's equation

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

- collisional matter (e.g. gas)

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

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

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CODE TESTING

- the time integration
 - how to verify the time integration scheme?

- stationary problems
 - how accurate is the Poisson solver?

- evolutionary problems
 - how do both act together?

- code cross-comparison

- convergence studies

CODE TESTING

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- time step criteria

- cosmological criterion

$$\Delta t \leq \frac{1}{H}$$

≈ the time step should be smaller than the age of the Universe

- acceleration/velocity criterion

$$\Delta t \leq \sqrt{\frac{\varepsilon}{a_{\max}}} \quad \Delta t \leq \frac{\varepsilon}{v_{\max}}$$

≈ particles should not move farther than some preselected threshold ε

ε of order the force resolution

▪ time step criteria

• cosmological criterion

$$\Delta t \leq \frac{1}{H} = \frac{a}{\dot{a}} = \frac{a}{\Delta a} \Delta t \Rightarrow 1 \leq \frac{a}{\Delta a}$$

$$\Delta t \leq \frac{1}{H} \quad \Leftrightarrow \quad \frac{\Delta a}{a} \leq 1$$

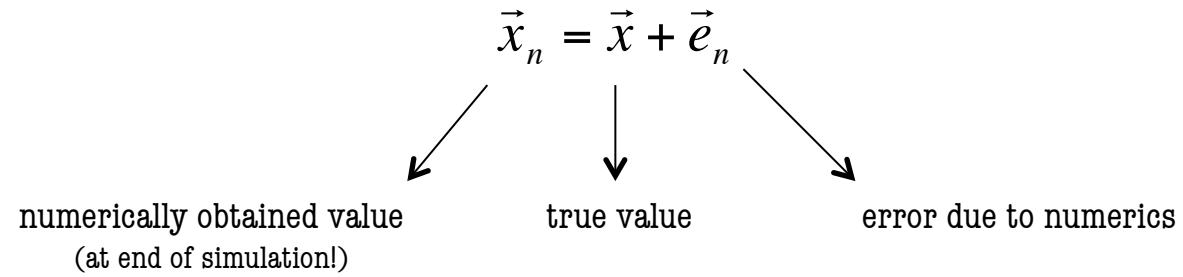
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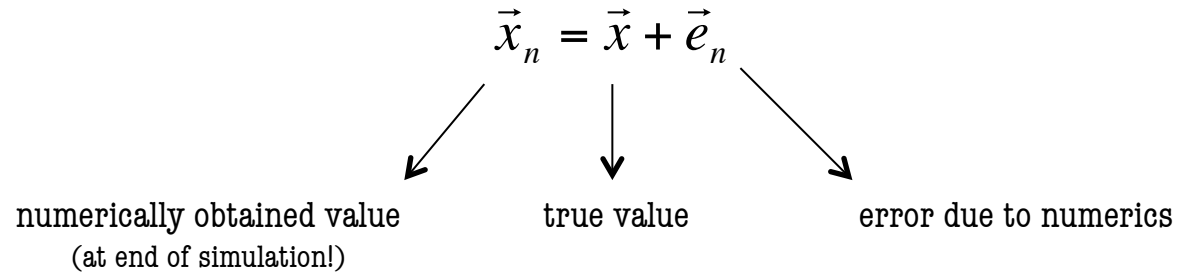
$$\Delta t \leq \sqrt{\frac{\epsilon}{a_{\max}}} \quad \Delta t \leq \frac{\epsilon}{v_{\max}}$$

≈ particles should not move farther than some preselected threshold ϵ

- the time integration



- the time integration



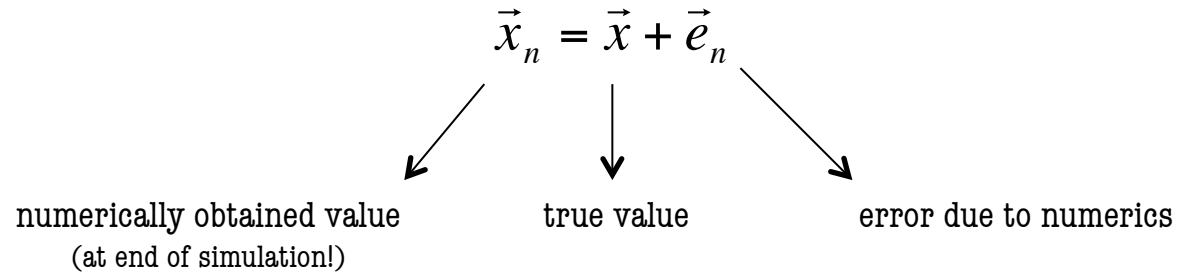
- second order accurate leap-frog:

$$\vec{e}_n = C(\Delta t_n)^2$$

$$\begin{aligned}\vec{x}_n - \vec{x}_m &= \vec{x} + \vec{e}_n - (\vec{x} + \vec{e}_m) \\ &= \vec{e}_n - \vec{e}_m \\ &= C(\Delta t_n^2 - \Delta t_m^2)\end{aligned}$$

$$\begin{aligned}\vec{x}_m - \vec{x}_l &= \vec{x} + \vec{e}_m - (\vec{x} + \vec{e}_l) \\ &= \vec{e}_m - \vec{e}_l \\ &= C(\Delta t_m^2 - \Delta t_l^2)\end{aligned}$$

- the time integration



- second order accurate leap-frog:

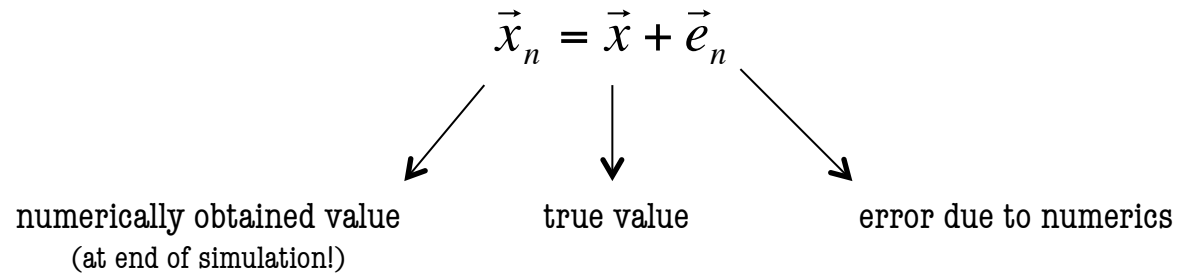
$$\vec{e}_n = C(\Delta t_n)^2$$

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$$\begin{aligned}\vec{x}_m - \vec{x}_l &= \vec{x} + \vec{e}_m - (\vec{x} + \vec{e}_l) \\ &= \vec{e}_m - \vec{e}_l \\ &= C(\Delta t_m^2 - \Delta t_l^2)\end{aligned}$$

$$\text{let: } \Delta t_l = k\Delta t_m = k^2\Delta t_n$$

- the time integration



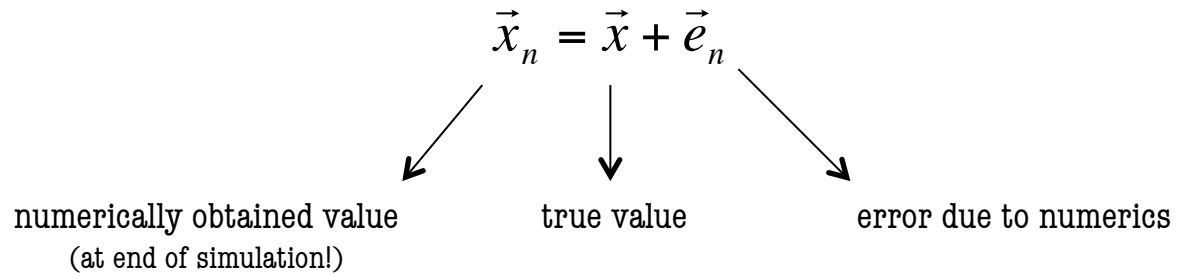
- second order accurate leap-frog:

$$\vec{e}_n = C(\Delta t_n)^2$$

$$\frac{\vec{x}_n - \vec{x}_m}{\vec{x}_m - \vec{x}_l} = \dots = \frac{1}{k^2}$$

$$\text{let: } \Delta t_l = k\Delta t_m = k^2\Delta t_n$$

- the time integration



- second order accurate leap-frog:

$$\vec{e}_n = C(\Delta t_n)^2$$

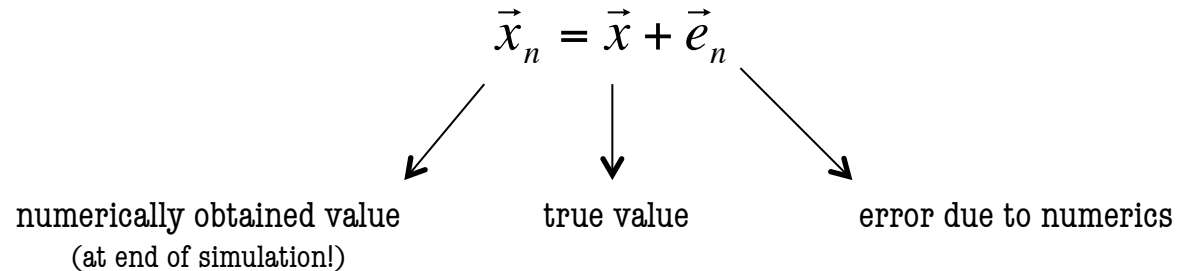
applicable to test any scheme...

$$\frac{\vec{x}_n - \vec{x}_m}{\vec{x}_m - \vec{x}_l} = \dots = \frac{1}{k^2}$$

let : $\Delta t_l = k\Delta t_m = k^2\Delta t_n$

(most obvious choice: $k=2$)

- the time integration



- second order accurate leap-frog – test in practice:

- run full simulation with three different choices for (constant!) time step:

Δt , $2\Delta t$, and $4\Delta t$

- calculate $\frac{\vec{x}_{\Delta t} - \vec{x}_{2\Delta t}}{\vec{x}_{2\Delta t} - \vec{x}_{4\Delta t}} \stackrel{?}{=} \frac{1}{4}$

- repeat exercise for $(2\Delta t, 4\Delta t, \text{ and } 8\Delta t)$, $(4\Delta t, 8\Delta t, \text{ and } 16\Delta t)$, ...

CODE TESTING

- the time integration
 - how to verify the time integration scheme?

- **stationary problems**
 - how accurate is the Poisson solver?

- evolutionary problems
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- code cross-comparison

- convergence studies

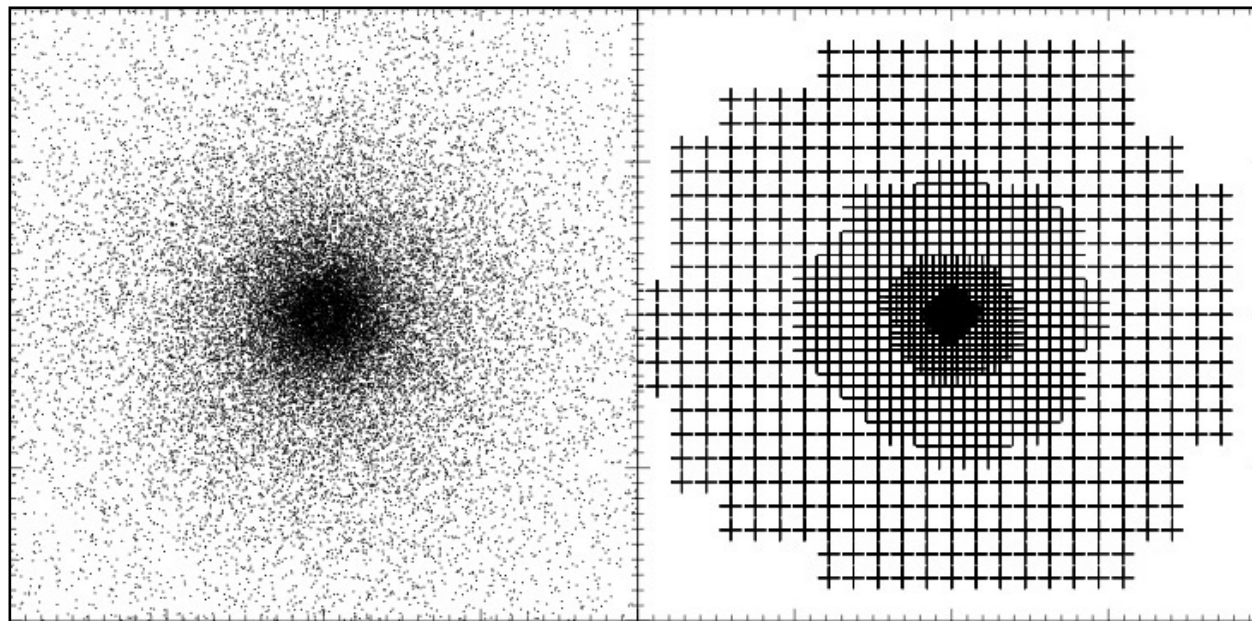
- static test scenarios
 - Hernquist sphere
 - Zel'dovich wave

- Hernquist sphere
 - analytic representation

$$\rho(x) = \frac{Mx_0}{2\pi} \frac{1}{x(x_0 + x)^3}$$
$$\nabla \cdot \vec{F}(\vec{x}) = 4\pi G(\rho - \bar{\rho})$$
$$\vec{F}(\vec{x}) = -\left(\frac{GM}{(x_0 + x)^2} \frac{1}{x} + \frac{4\pi G}{3} \bar{\rho} \right) \vec{x}$$

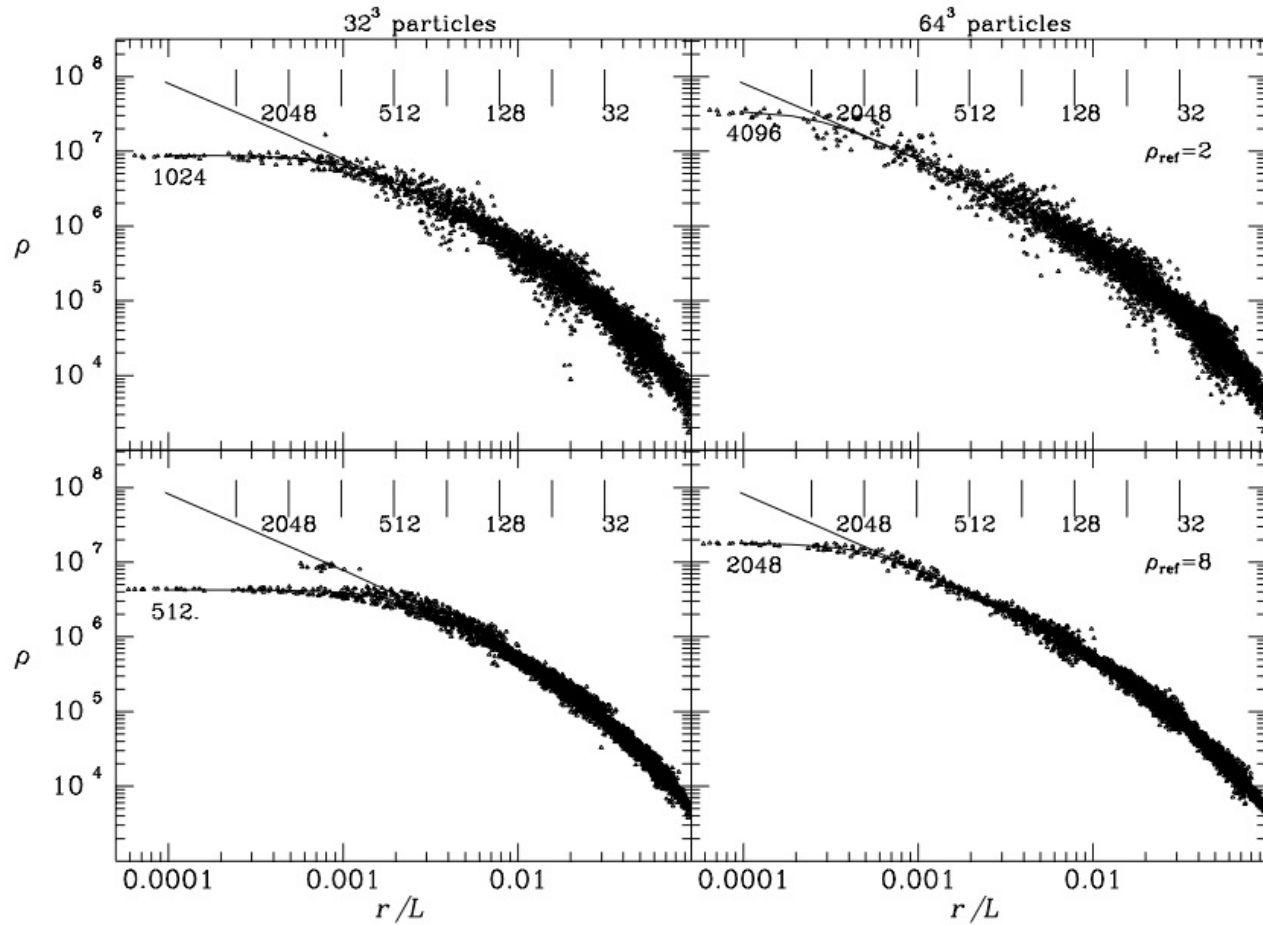
- Hernquist sphere

- particle representation and AMR refinement hierarchy



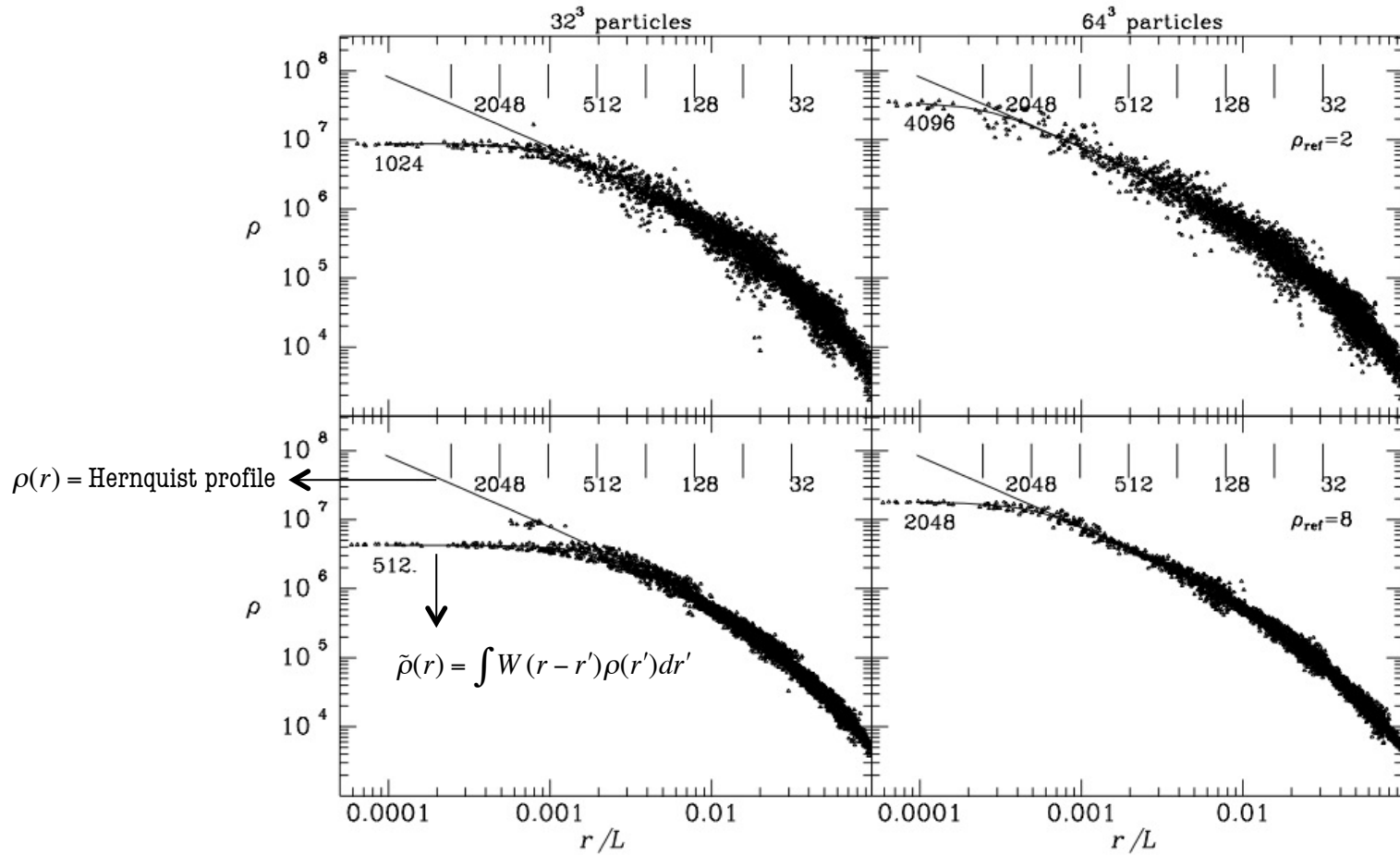
- Hernquist sphere

- recovering densities



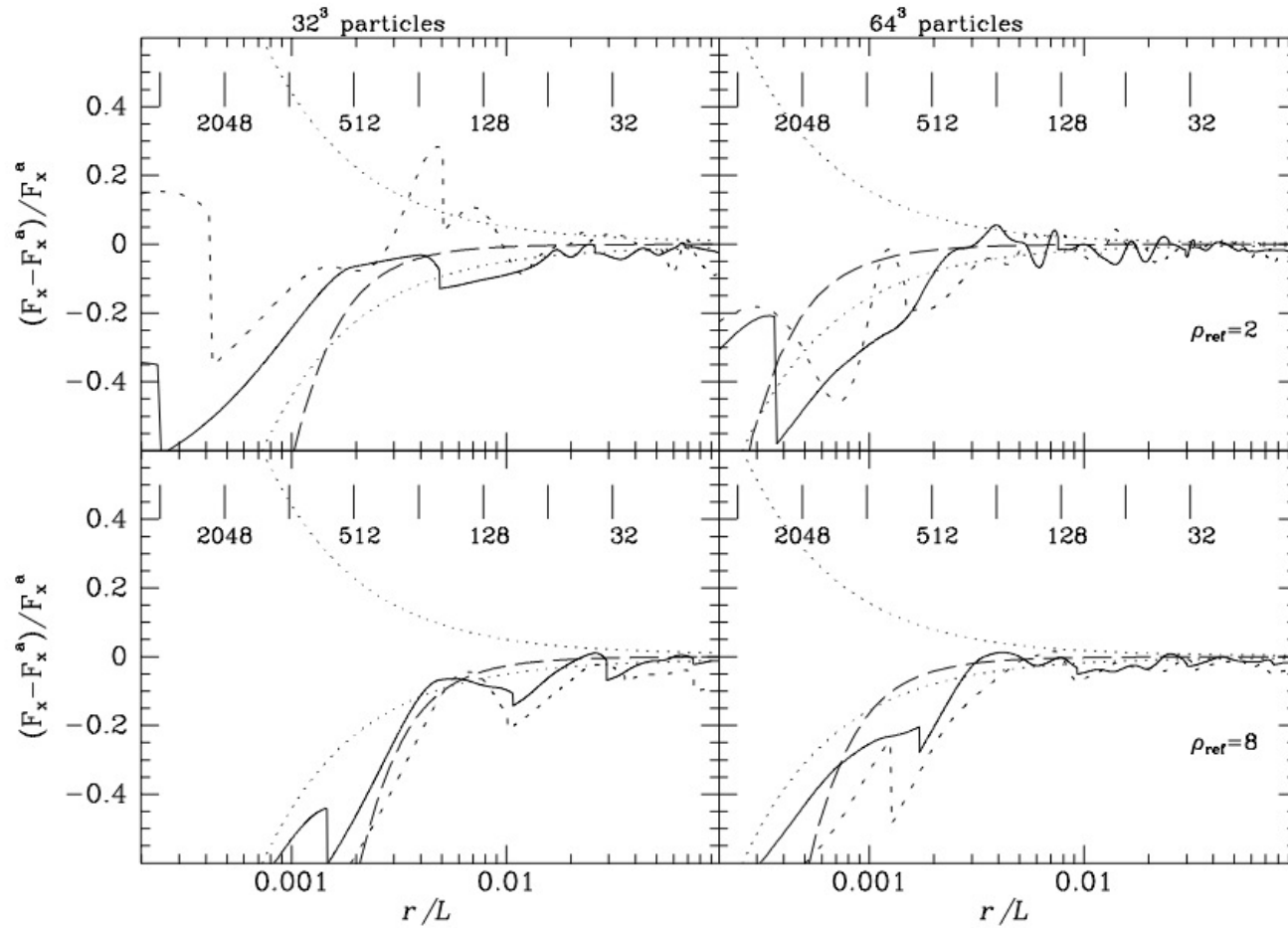
- Hernquist sphere

- recovering densities



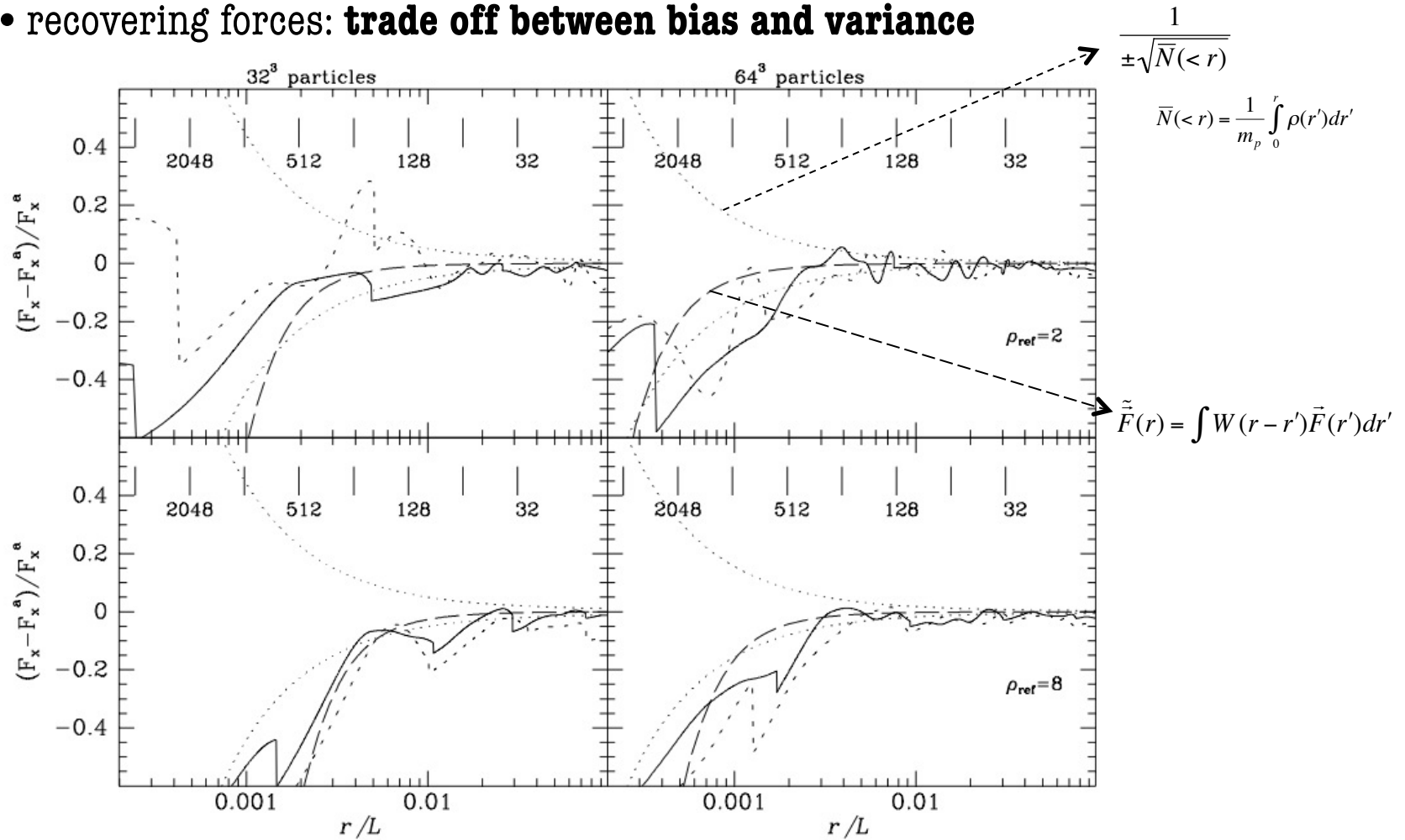
- Hernquist sphere

- recovering forces



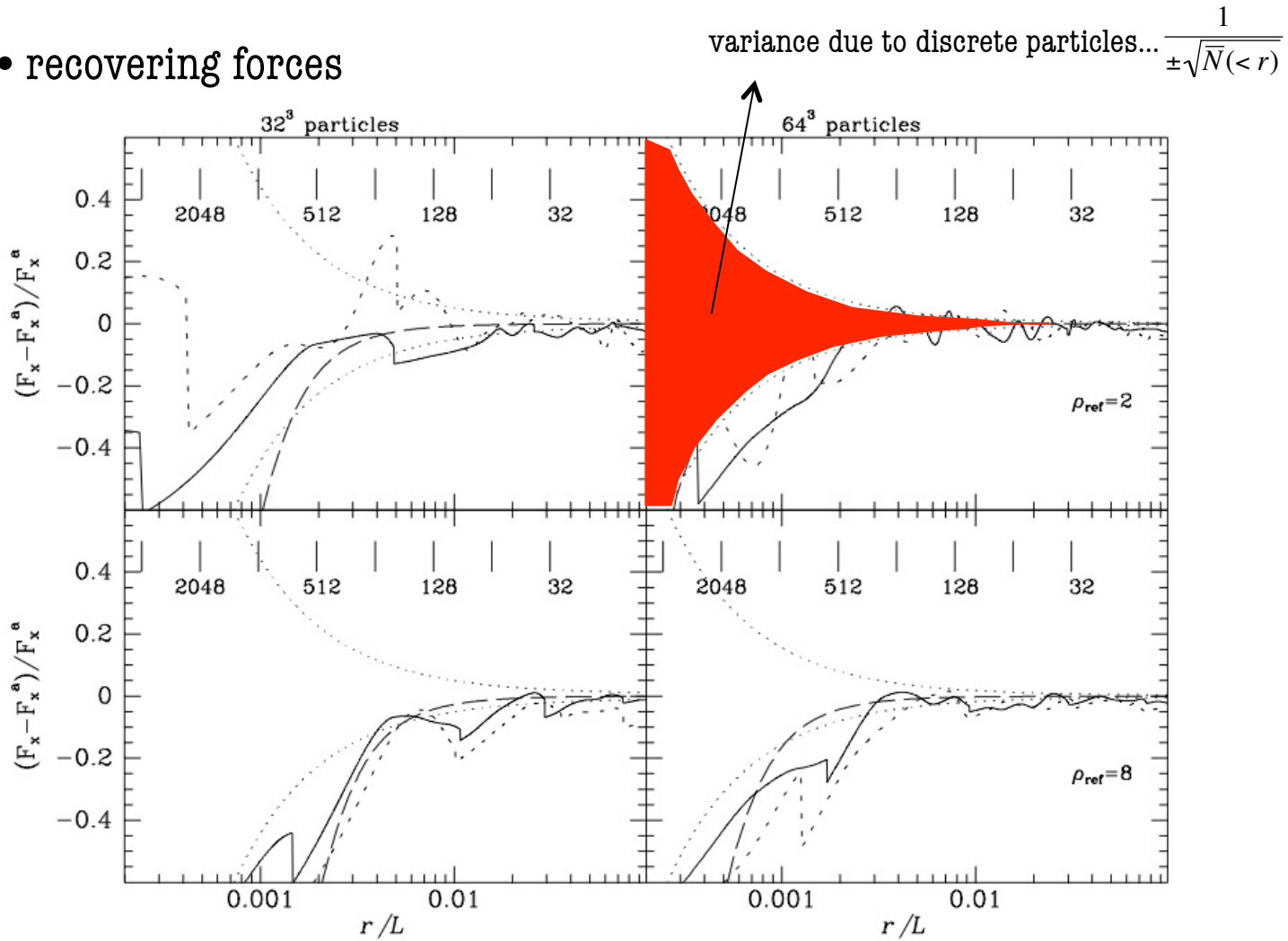
■ Hernquist sphere

- recovering forces: **trade off between bias and variance**



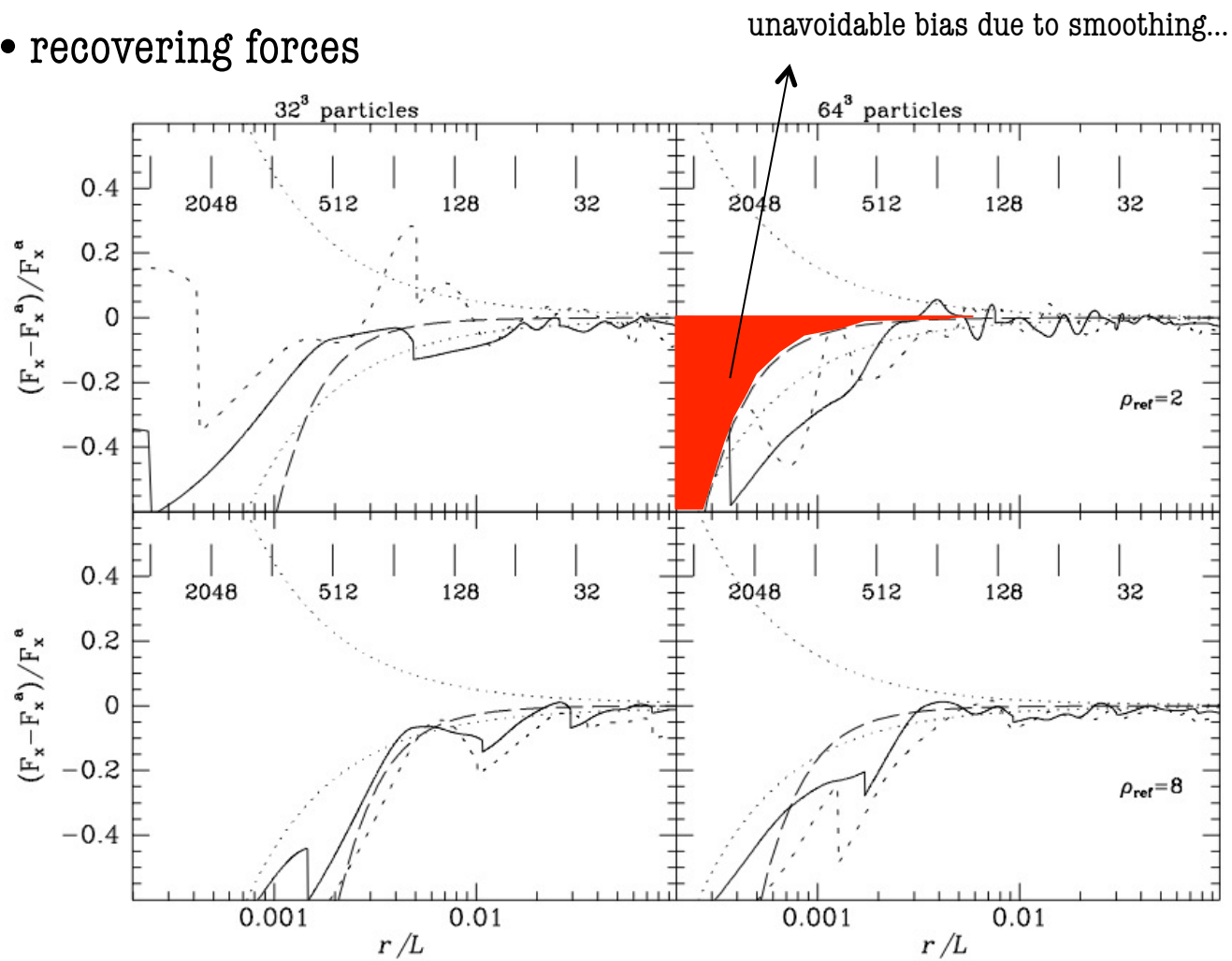
■ Hernquist sphere

- recovering forces

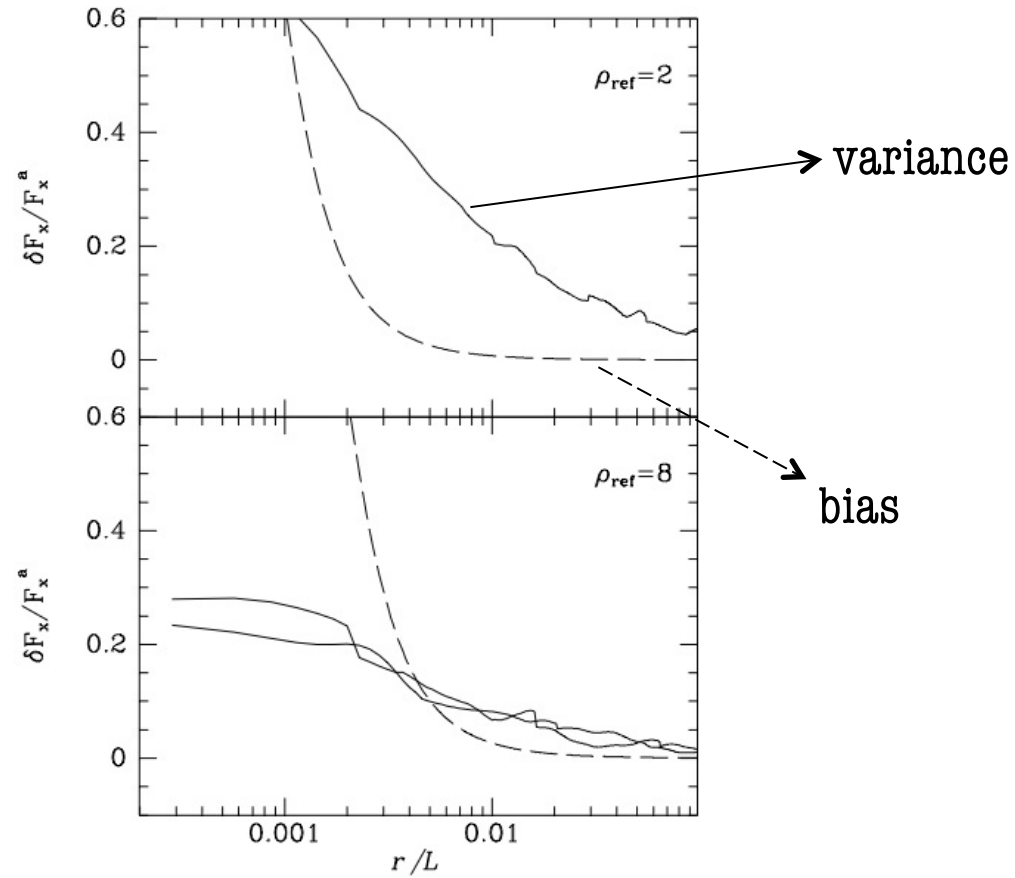


- Hernquist sphere

- recovering forces

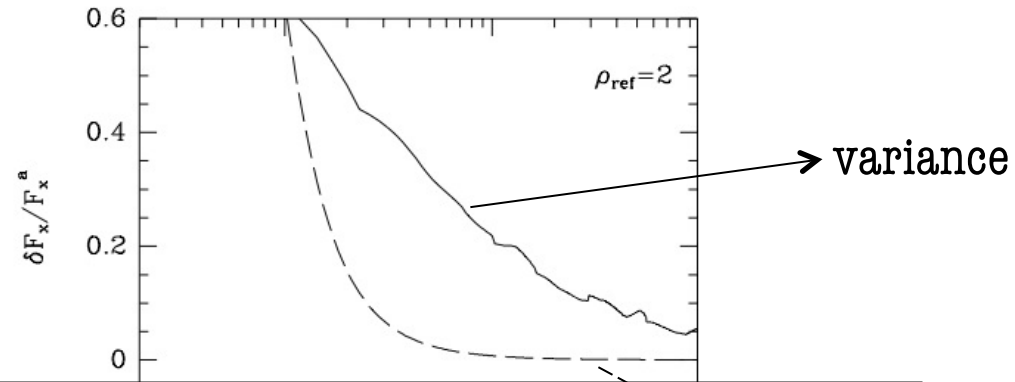


- Hernquist sphere
 - recovering forces

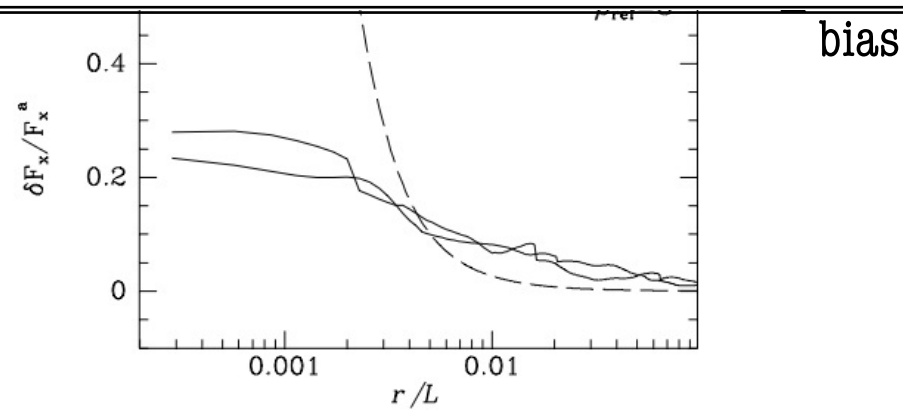


- Hernquist sphere

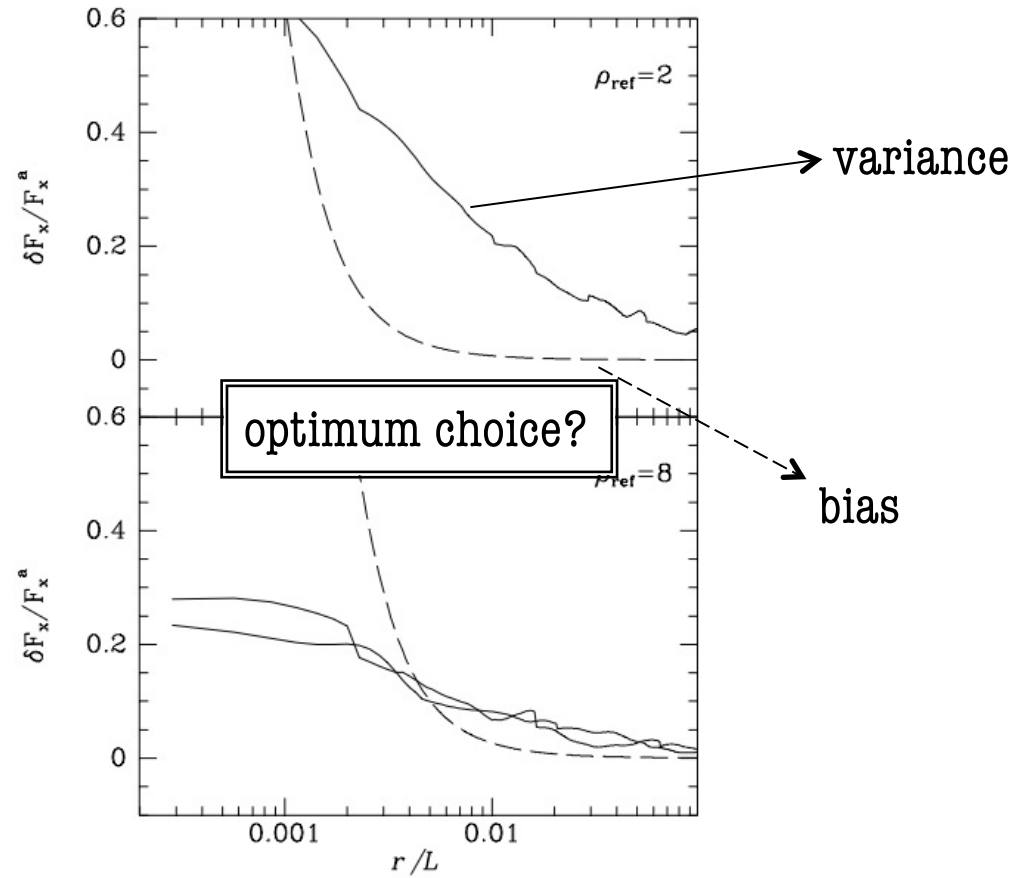
- recovering forces



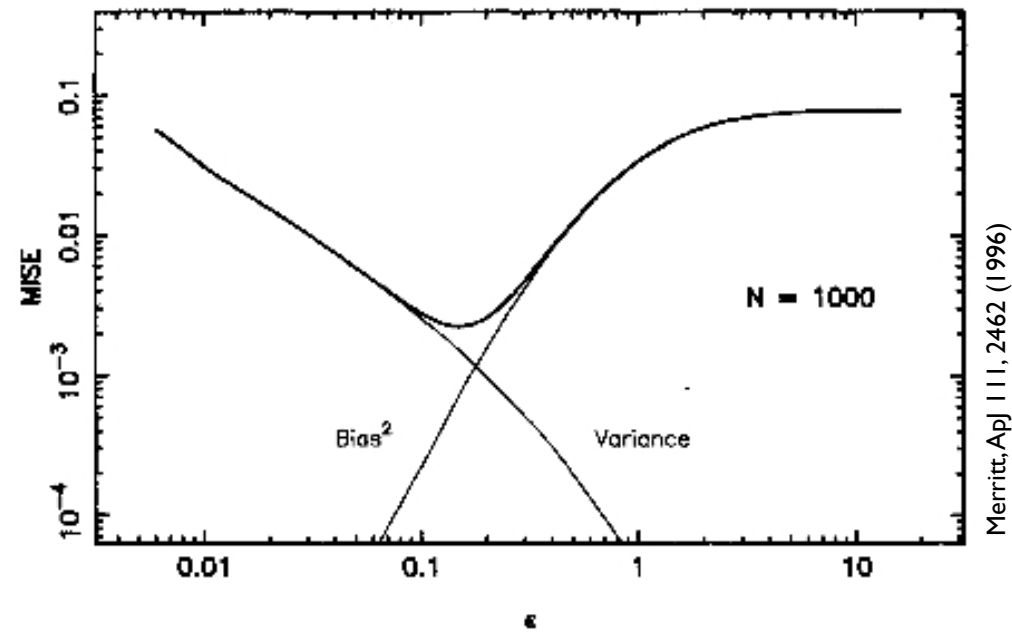
softer forces -> stronger bias, lower variance



- Hernquist sphere
 - recovering forces



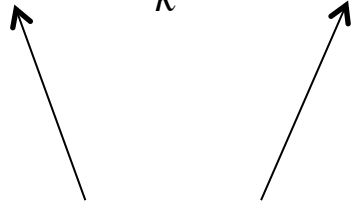
- Hernquist sphere
 - recovering forces



- Zel'dovich wave
 - analytic representation

$$\vec{x} = \vec{q} + a(t) \frac{\vec{k}}{k^2} \cos(\vec{k} \cdot \vec{q})$$

- Zel'dovich wave
 - analytic representation

$$\vec{x} = \vec{q} + a(t) \frac{\vec{k}}{k^2} \cos(\vec{k} \cdot \vec{q})$$


Lagrangian coordinates,
e.g. unperturbed particle positions on a regular grid...

- Zel'dovich wave
 - analytic representation

$$\vec{x} = \vec{q} + a(t) \frac{\vec{k}}{k^2} \cos(\vec{k} \cdot \vec{q})$$

$$\downarrow \vec{F}(\vec{q}) = ?$$

- Zel'dovich wave
 - analytic representation

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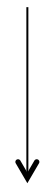
$$\Delta_x \Phi(\vec{x}) = (\rho - \bar{\rho}) \Rightarrow \nabla_x \vec{F}(\vec{x}) = -(\rho - \bar{\rho})$$

$$\nabla_x \vec{F}(\vec{x}) = \frac{1}{\|\partial \vec{x} / \partial \vec{q}\|} \nabla_q \vec{F}(\vec{q}) \quad \rho(\vec{x}) = \frac{1}{\|\partial \vec{x} / \partial \vec{q}\|} \rho(\vec{q}) \quad \rho(\vec{q}) = \bar{\rho}(\vec{q}) = 1$$

- Zel'dovich wave

- analytic representation - 1D

$$x = q + \frac{a(t)}{k} \cos(kq)$$



$F(q) = ?$

$$\frac{d^2\Phi(x)}{dx^2} = (\rho - \bar{\rho}) \Rightarrow \frac{dF(x)}{dx} = -(\rho - \bar{\rho})$$

$$\frac{dF(x)}{dx} = \frac{1}{dx/dq} \frac{dF(q)}{dq}$$

$$\rho(x) = \frac{1}{dx/dq} \rho(q)$$

$$\rho(q) = \bar{\rho}(q) = 1$$

▪ Zel'dovich wave

- analytic representation - 1D

$$x = q + \frac{a(t)}{k} \cos(kq)$$


$$\begin{aligned} \frac{dF(q)}{dq} &= -dx/dq \left(\frac{1}{dq/dq} \rho(q) - \bar{\rho}(q) \right) \\ &= -dx/dq \left(\frac{1}{dx/dq} \bar{\rho}(q) - \rho(q) \right) \\ &= -dx/dq \left(\frac{1}{dx/dq} - 1 \right) \bar{\rho}(q) \\ &= dx/dq - 1 \end{aligned} \quad \left. \begin{array}{l} \downarrow \\ \downarrow \end{array} \right\} \rho(q) = \bar{\rho}(q) = 1$$

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$$dx/dq = 1 - a \sin(kq)$$

▪ Zel'dovich wave

- analytic representation - 1D

$$x = q + \frac{a(t)}{k} \cos(kq)$$

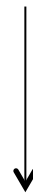
$$\frac{dF(q)}{dq} = 1 - a \sin(kq) - 1 = -a \sin(kq)$$

▪ Zel'dovich wave

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$$x = q + \frac{a(t)}{k} \cos(kq)$$

$$\frac{dF(q)}{dq} = 1 - a \sin(kq) - 1 = -a \sin(kq)$$



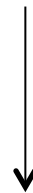
$$F(q) = \frac{a}{k} \cos(kq)$$

▪ Zel'dovich wave

- analytic representation - 1D

$$x = q + \frac{a(t)}{k} \cos(kq)$$

$$\frac{dF(q)}{dq} = 1 - a \sin(kq) - 1 = -a \sin(kq)$$



$$F(q) = \frac{a}{k} \cos(kq)$$

recall "initial conditions" lecture: $\vec{x}(t) = \vec{q} + D(t)\vec{S}(\vec{q})$ $\vec{S}(\vec{q}) = -\nabla\Psi$ $\Delta\Psi = \delta_0$

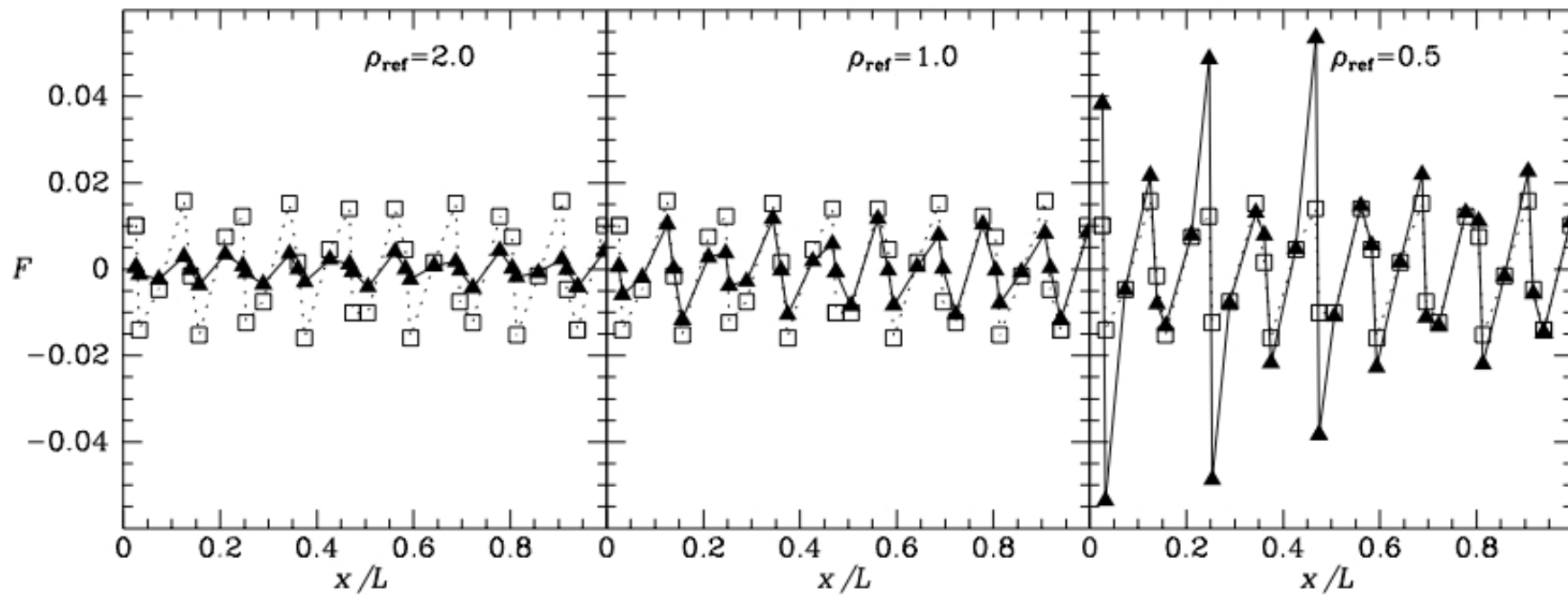
- Zel'dovich wave
 - numerical recovery - 1D

∴ put down particles on regular lattice	q
∴ superimpose Zel'dovich wave	x
∴ numerically calculate forces on lattice	$F(q)$
∴ compare to analytical forces	$F_{\text{true}}(q)$

- Zel'dovich wave
 - numerical recovery - 1D

$$F_{true}(q) = \frac{a}{k} \cos(kq)$$

AMR code

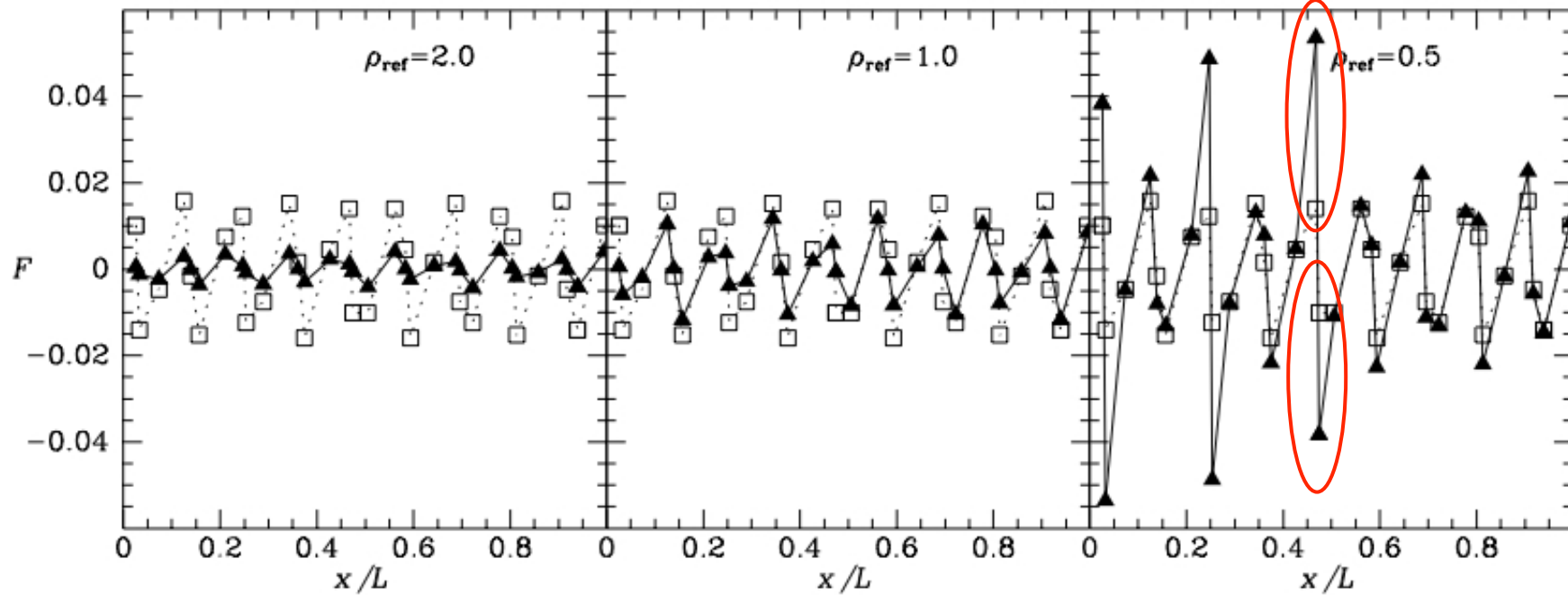


- Zel'dovich wave
 - numerical recovery - 1D

$$F_{true}(q) = \frac{a}{k} \cos(kq)$$

AMR code

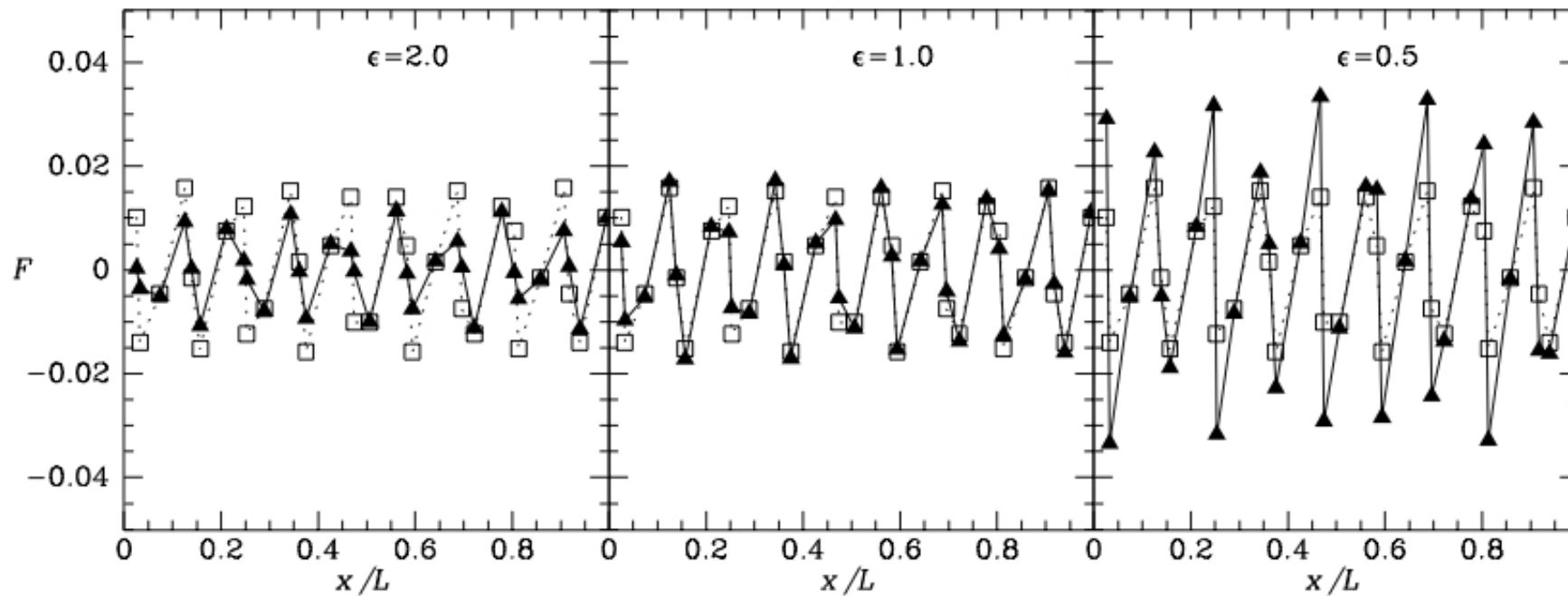
2-body interactions...



- Zel'dovich wave
 - numerical recovery - 1D

$$F_{true}(q) = \frac{a}{k} \cos(kq)$$

AP³M code

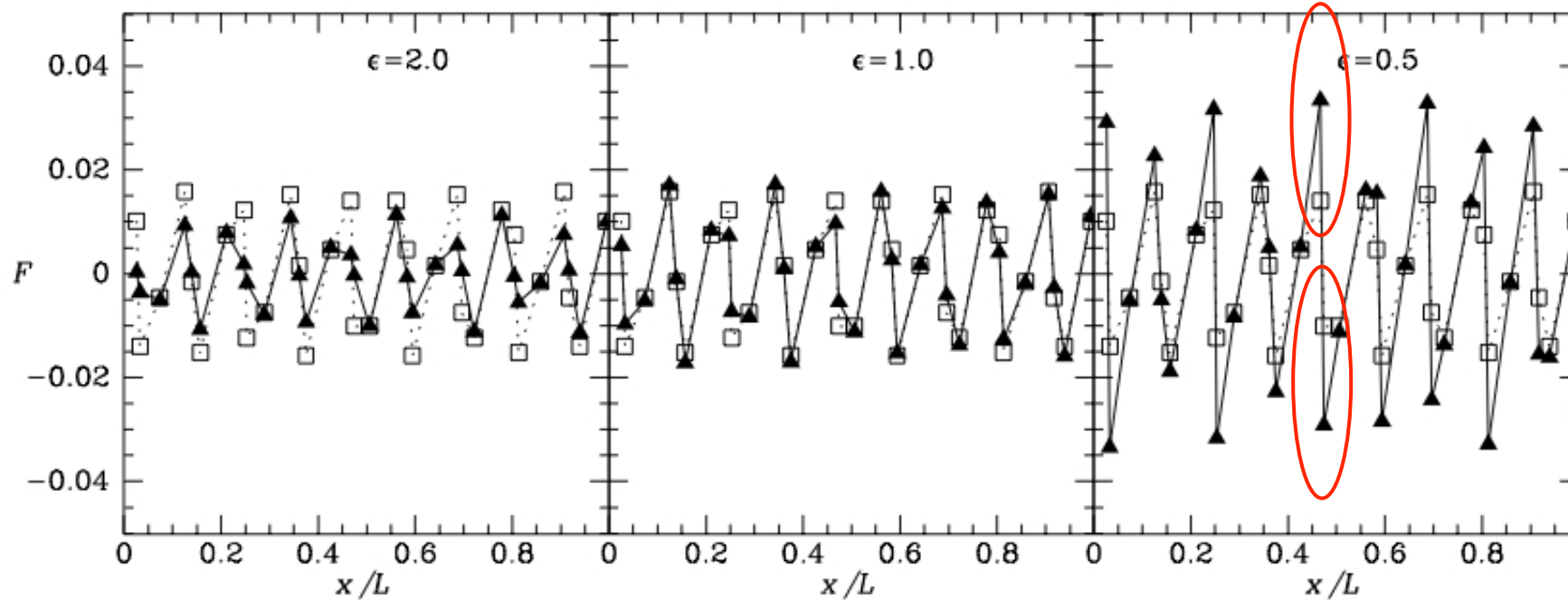


- Zel'dovich wave
 - numerical recovery - 1D

$$F_{true}(q) = \frac{a}{k} \cos(kq)$$

AP³M code

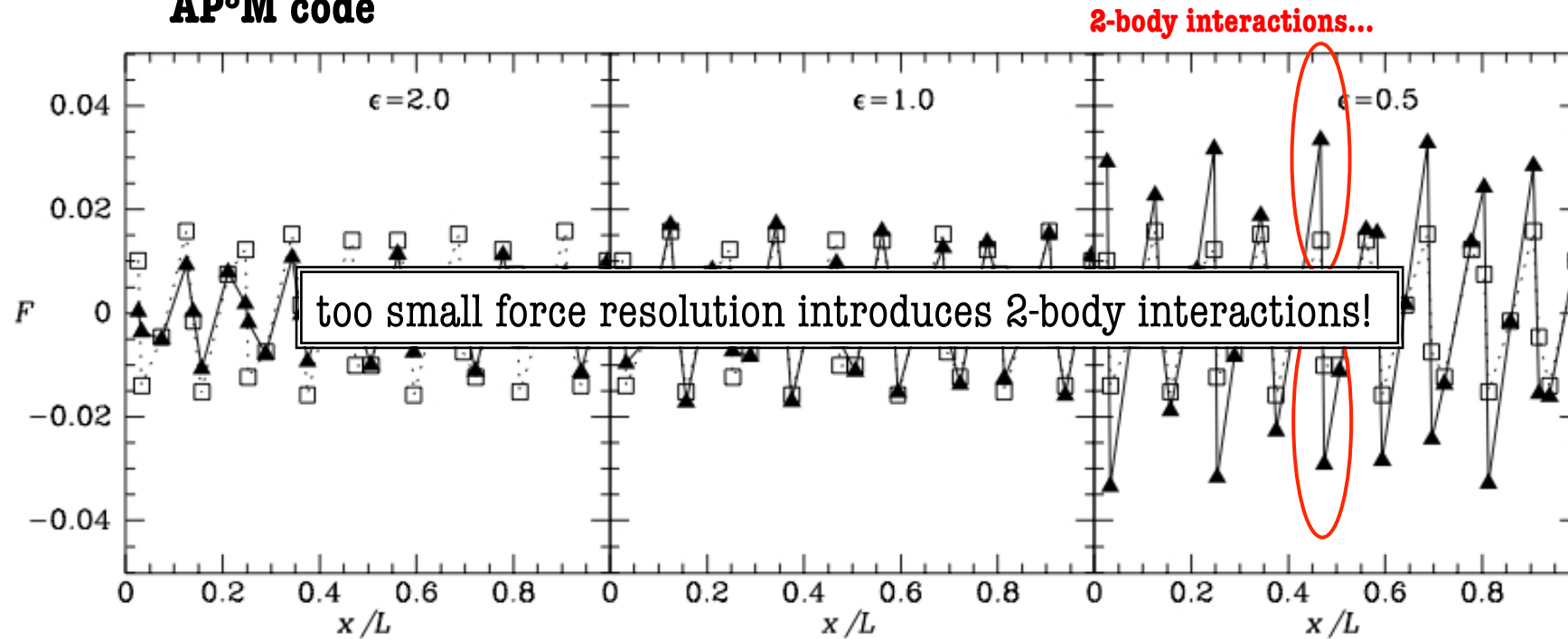
2-body interactions...



- Zel'dovich wave
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AP³M code



CODE TESTING

- the time integration
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 - how accurate is the Poisson solver?

- **evolutionary problems**
 - how do both act together?

- code cross-comparison

- convergence studies

- evolutionary test scenarios
 - check for momentum conservation
 - Layzer-Irvine Energy conservation
 - Zel'dovich wave, again...

- momentum conservation

$$\left| \sum_{i=1}^N \vec{F}_i \right| = 0$$

=> development of net momentum during simulation?

- practical test:

$$\frac{\left| \sum_{i=1}^N \vec{F}_i \right|}{\sum_{i=1}^N |\vec{F}_i|} \approx 10^{-4}$$

- Layzer-Irvine energy conservation
 - Hamiltonian (= total energy)

$$\mathcal{H} = \frac{1}{2ma^2} p^2 + m \frac{\Phi(\vec{x})}{a}$$

... with comoving energies as follows: (remember Hamilton formalism...)

$$T = \frac{1}{2} \sum_{i=1}^N \frac{p_i^2}{m_i a^2}$$

$$U = -\frac{1}{2a} \iiint_{\text{Box}} (\rho(\vec{x}) - \bar{\rho}) \Phi(\vec{x}) d^3x \quad \Delta\Phi = 4\pi G(\rho_x - \bar{\rho}_x)$$

- Layzer-Irvine energy conservation
 - Hamiltonian (= total energy)

$$\begin{aligned} \frac{d\mathcal{H}}{dt} &= \frac{\partial \mathcal{H}}{\partial t} \\ &= -\frac{1}{2} \sum_{i=1}^N \frac{p_i^2}{m_i} \frac{2\dot{a}}{a^3} + \frac{1}{2} \frac{2\dot{a}}{a^2} \iiint_{\text{Box}} (\rho(\vec{x}) - \bar{\rho}) \Phi(\vec{x}) d^3x \\ &= -\frac{\dot{a}}{a} (2T + U) \end{aligned}$$

$$\Rightarrow 0 = \frac{d(T + U)}{dt} + \frac{\dot{a}}{a} (2T + U)$$

$$C = (T + U)_t - (T + U)_{t_{\text{init}}} + \int_{t_{\text{init}}}^t \frac{1}{a} (2T + U) da$$

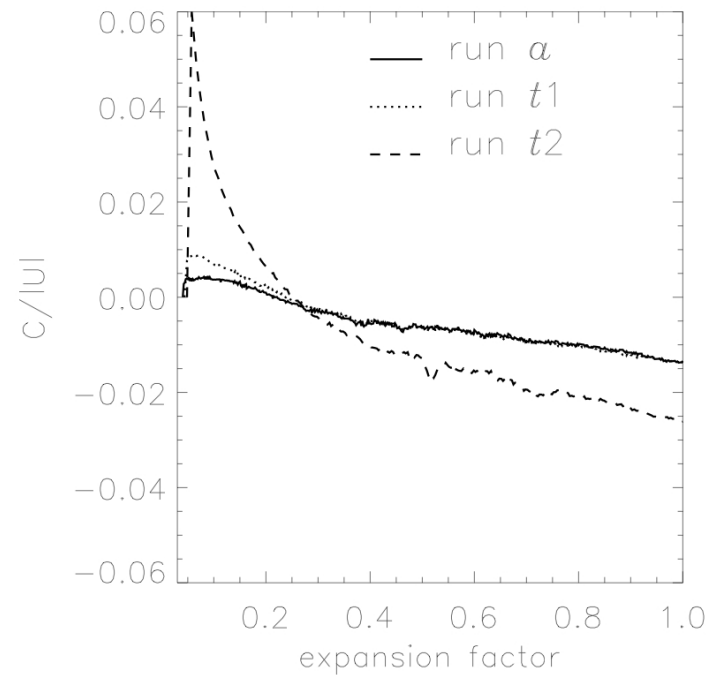
- Layzer-Irvine energy conservation
 - Hamiltonian (= total energy)

$$\begin{aligned} \frac{d\mathcal{H}}{dt} &= \frac{\partial \mathcal{H}}{\partial t} \\ &= -\frac{1}{2} \sum_{i=1}^N \frac{p_i^2}{m_i} \frac{2\dot{a}}{a^3} + \frac{1}{2} \frac{2\dot{a}}{a^2} \iiint_{\text{Box}} (\rho(\vec{x}) - \bar{\rho}) \Phi(\vec{x}) d^3x \\ &= -\frac{\dot{a}}{a} (2T + U) \end{aligned}$$

$$\Rightarrow 0 = \frac{d(T + U)}{dt} + \frac{\dot{a}}{a} \underbrace{(2T + U)}_{= 0 \text{ ?! (virial theorem)}}$$

$$C = (T + U)_t - (T + U)_{t_{\text{init}}} + \int_{t_{\text{init}}}^t \frac{1}{a} (2T + U) da$$

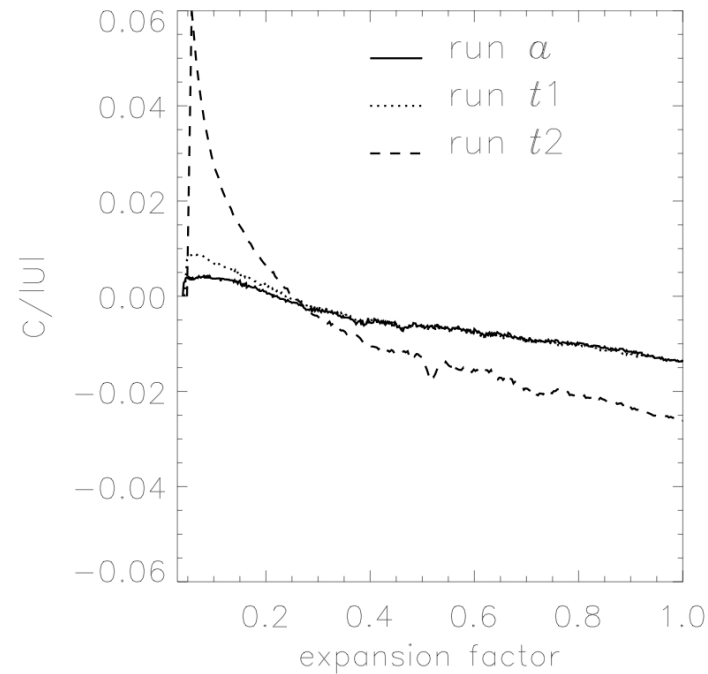
- Layzer-Irvine energy conservation



accuracy at “a few percent” level

$$C = (T + U)_t - (T + U)_{t_{\text{init}}} + \int_{t_{\text{init}}}^t \frac{1}{a} (2T + U) da$$

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accuracy at “a few percent” level

errors due to time integration **and** Poisson solver...

▪ Zel'dovich wave

- analytic representation - 1D

$$x = q + \frac{a(t)}{k} \cos(kq)$$

▪ Zel'dovich wave

- analytic representation - 1D

$$x = q + \frac{a(t)}{k} \cos(kq)$$

$$\dot{x} = \frac{\dot{a}(t)}{k} \cos(kq)$$

▪ Zel'dovich wave

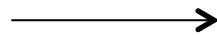
- analytic representation - 1D

$$x = q + \frac{a(t)}{k} \cos(kq)$$

$$\dot{x} = \frac{\dot{a}(t)}{k} \cos(kq)$$

$$\sigma_x^2 = \frac{\sum_i (x^i - x_{true})^2}{\sum_i (x_{true} - q)^2}$$

$$\sigma_v^2 = \frac{\sum_i (\dot{x}^i - \dot{x}_{true})^2}{\sum_i (\dot{x}_{true})^2}$$



check rms errors
as function of k and a

CODE TESTING

- the time integration
 - how to verify the time integration scheme?

- stationary problems
 - how accurate is the Poisson solver?

- evolutionary problems
 - how do both act together?

- **code cross-comparison**

- convergence studies

▪ GADGET-1<http://www.mpa-garching.mpg.de/gadget>

- **fully particle based** force derivation
- combining distant particles into aggregates (i.e. tree code)

▪ AMIGA<http://www.aip.de/People/Aknebe/AMIGA>

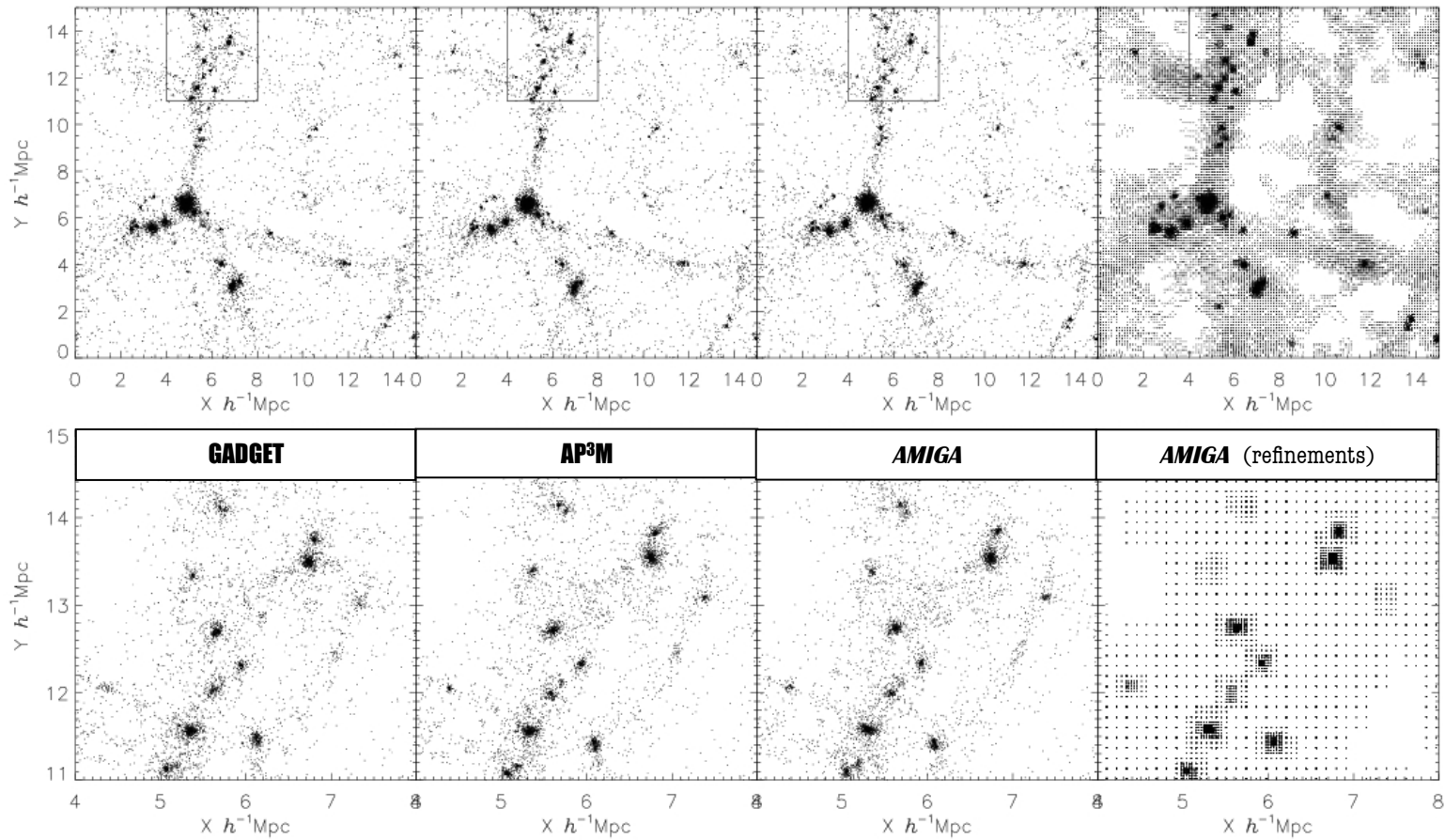
- **fully grid based** force derivation
- places finer and finer grids of arbitrary shape in high density regions (i.e. AMR code)

▪ HYDRA/AP³M<http://hydra.mcmaster.ca/hydra>

- **combination** of particle and grid based force derivation
- no refined grids, no tree structures

- Λ CDM simulation run with various codes
 - identical initial conditions
 - comparable parameter setup

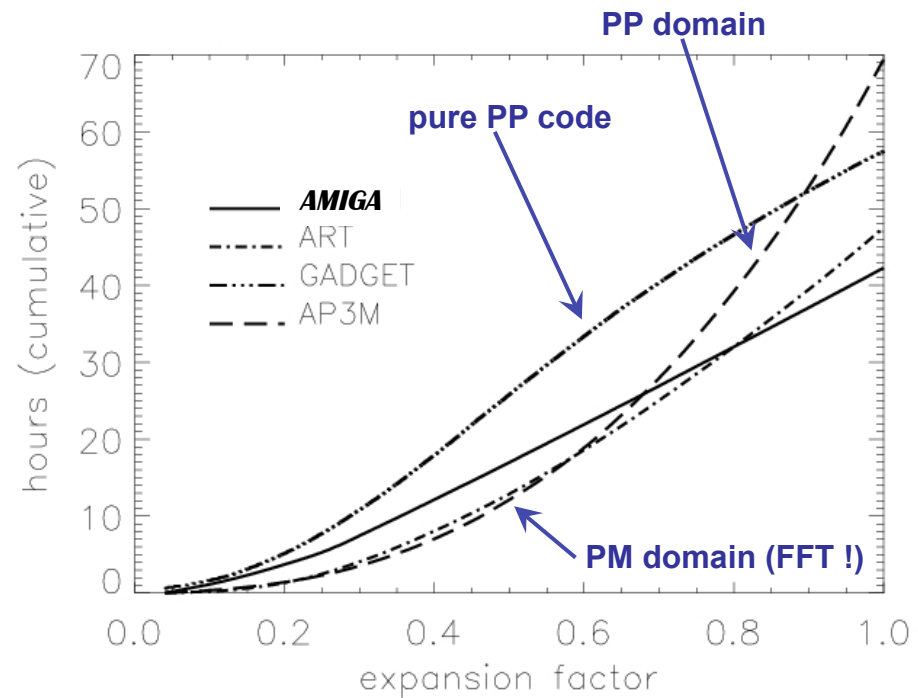
- Λ CDM simulation run with various codes
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Knebe et al. (2000)

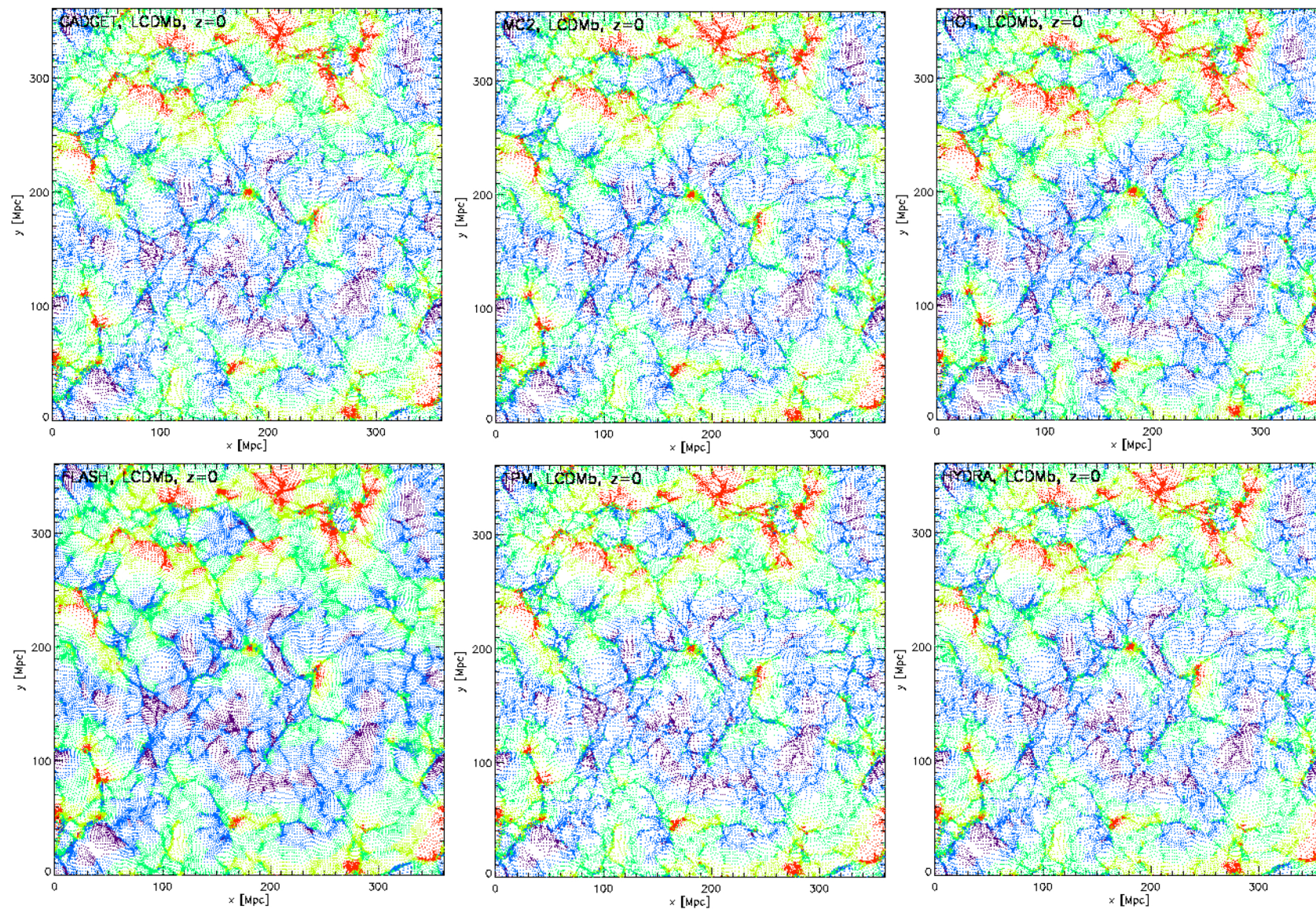
- Λ CDM simulation run with various codes
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<u>code</u>	<u>time</u>
▪ AMIGA	42.3 hours
▪ ART	47.4 hours
▪ GADGET	57.5 hours
▪ AP³M	69.4 hours



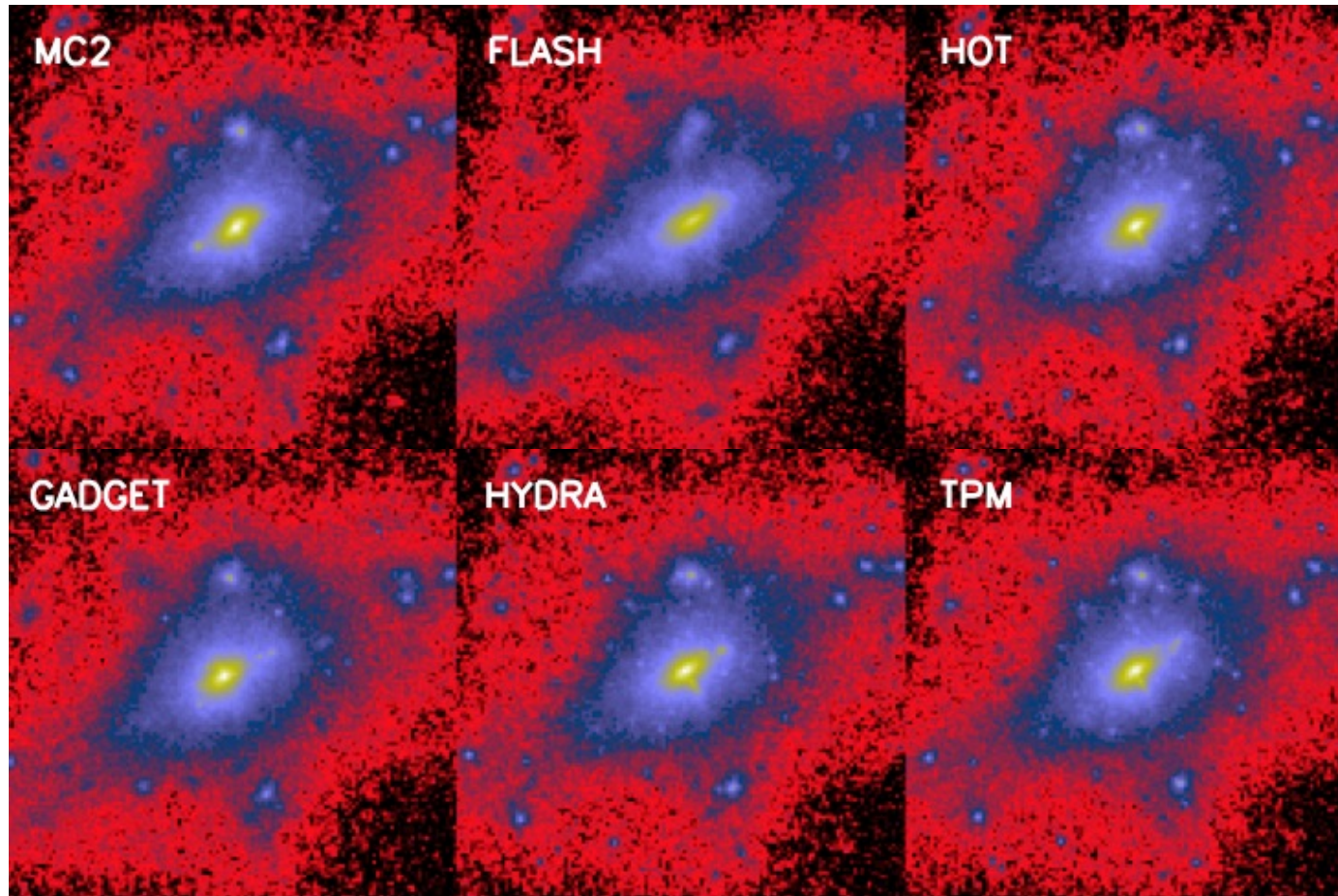
- Λ CDM simulation run with various codes
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more recent comparison by Heitmann et al. (2005)...



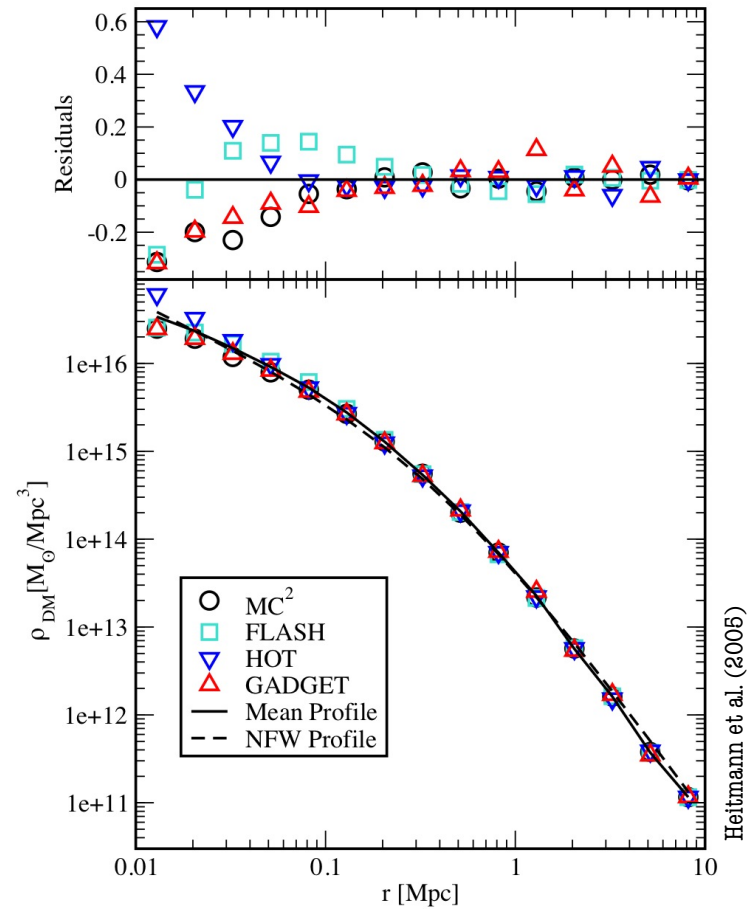
Heitmann et al. (2005)

- “Santa Barbara Cluster” (Frenck et al. 1999)

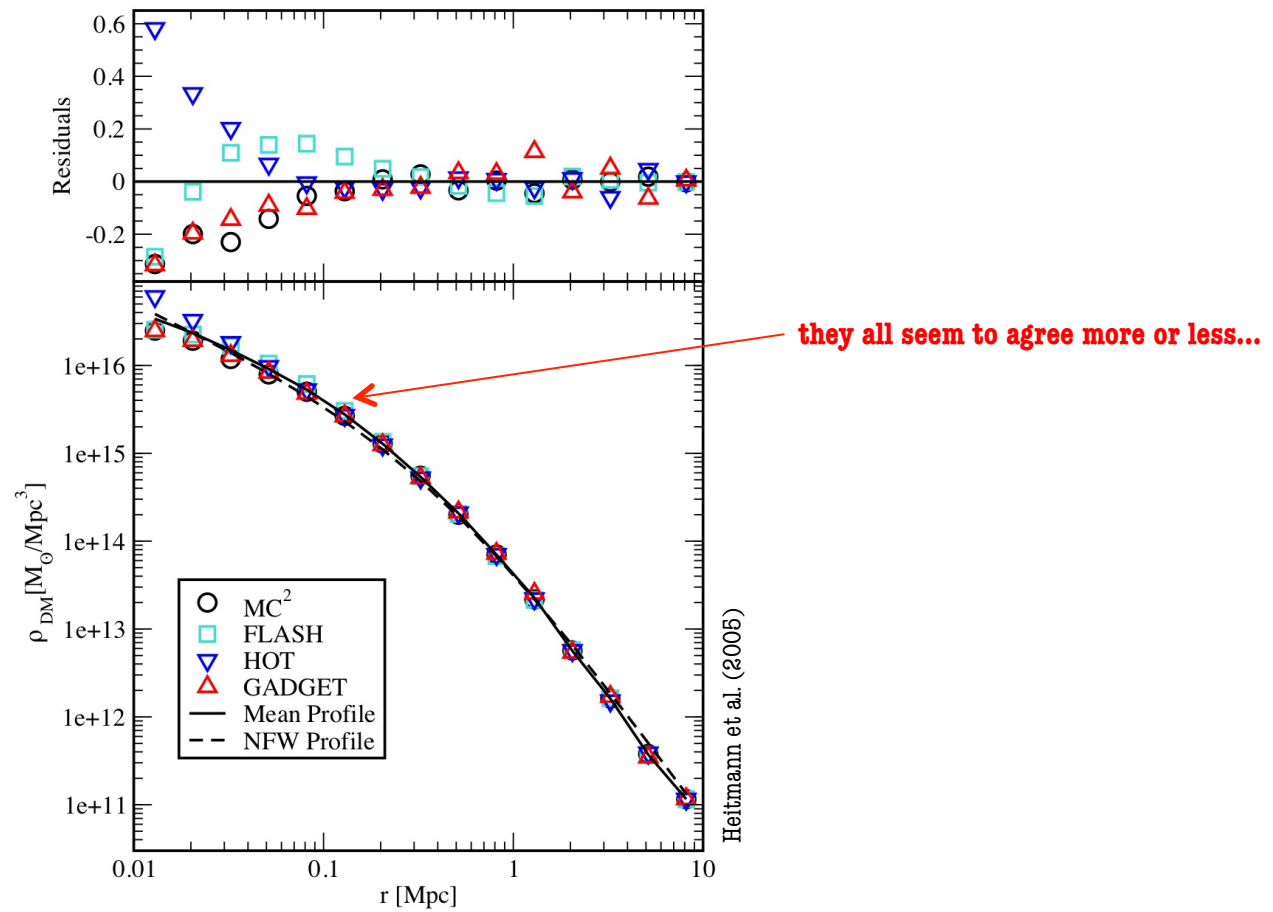


Heitmann et al. (2006)

- “Santa Barbara Cluster” (Frenck et al. 1999)

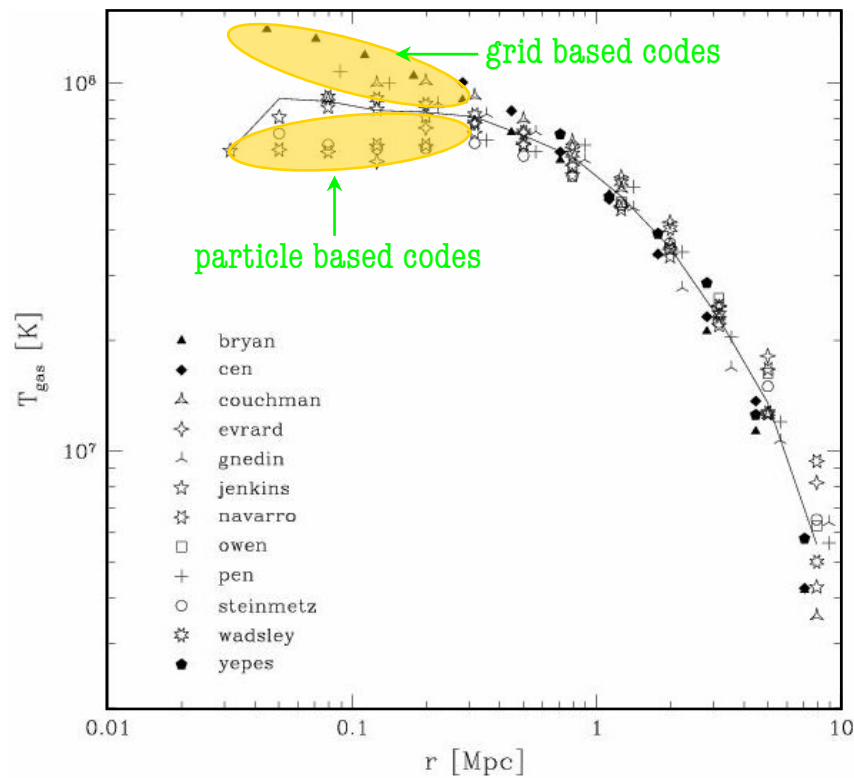


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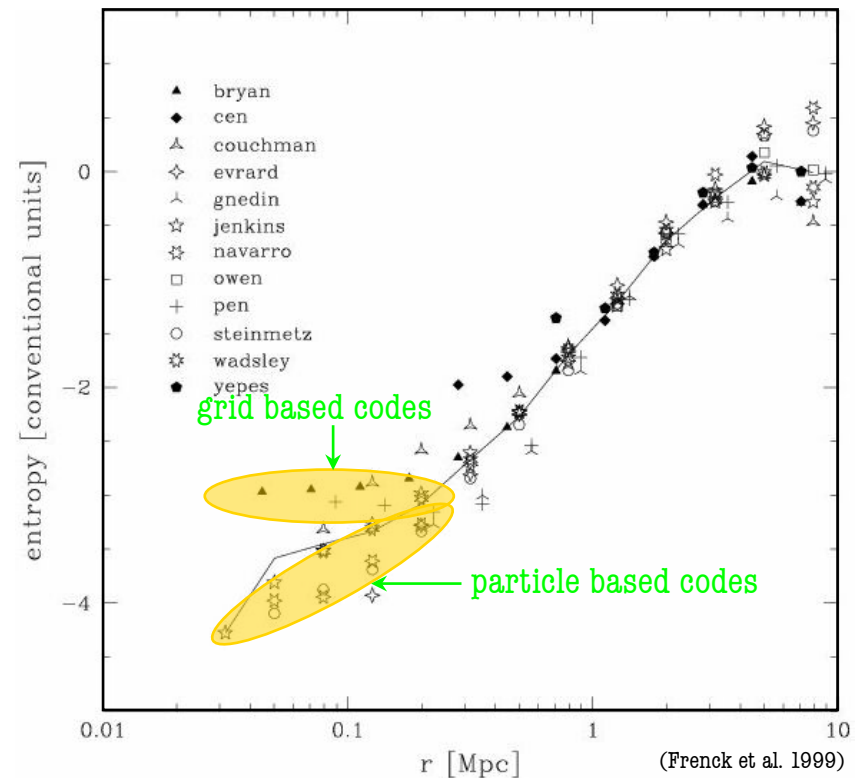


- “Santa Barbara Cluster” (incl. gas physics...)

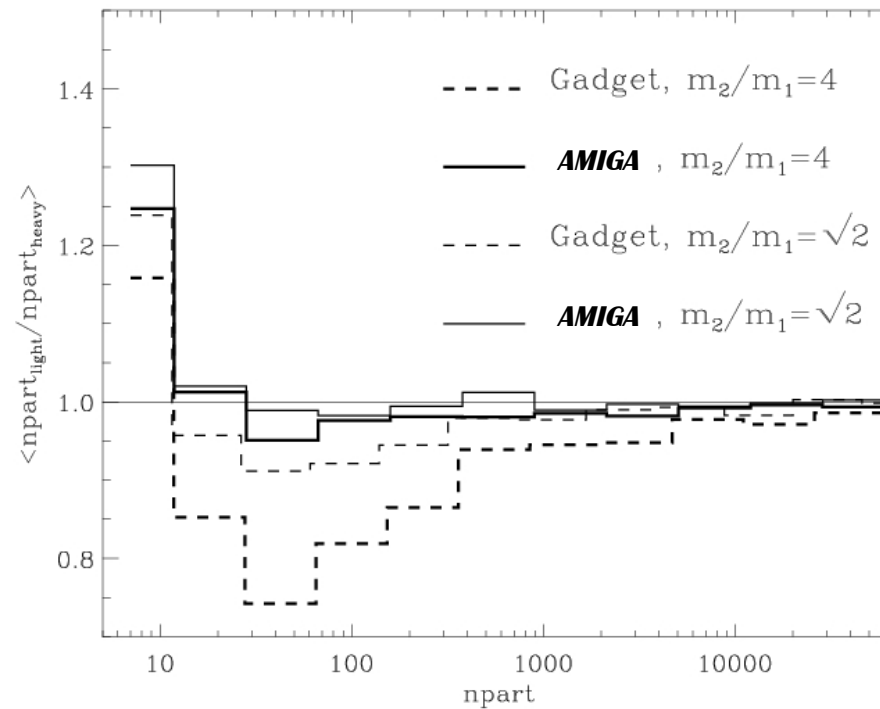
temperature profile



entropy profile



- mass segregation
 - run simulation with 2 mass species and check for segregation



- ✘ **GADGET** (tree code) \Rightarrow expels lighter particles from halos
- ✓ **AMIGA** (AMR code) \Rightarrow ratio always about unity

- major differences

- tree codes: spatially fixed force resolution
- AMR codes spatially adaptive force resolution

- ✓ resolve the local inter-particle separation at all times and at all places
... nor more, no less!
- ✓ particles are “phase-space” markers rather than interacting “billiard balls”

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CODE TESTING

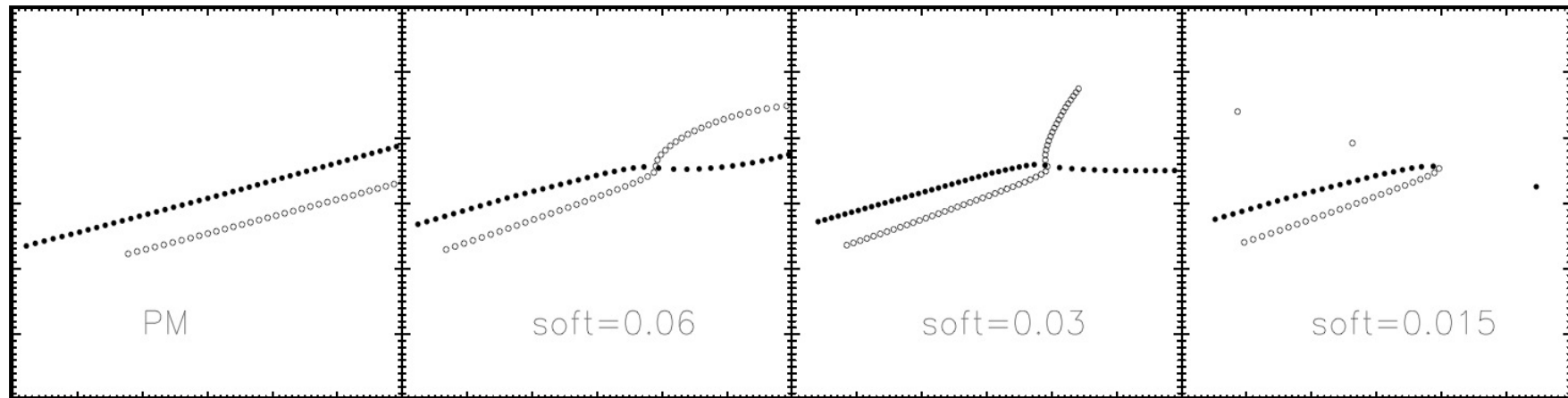
stability and credibility of (scientific) results...

- the relation between...

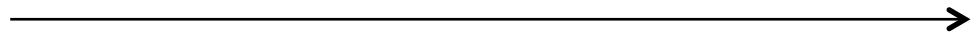
→ *particle number, time step and softening?*

in-depth study by Power et al., MNRAS 338, 14 (2003)

- time step and softening

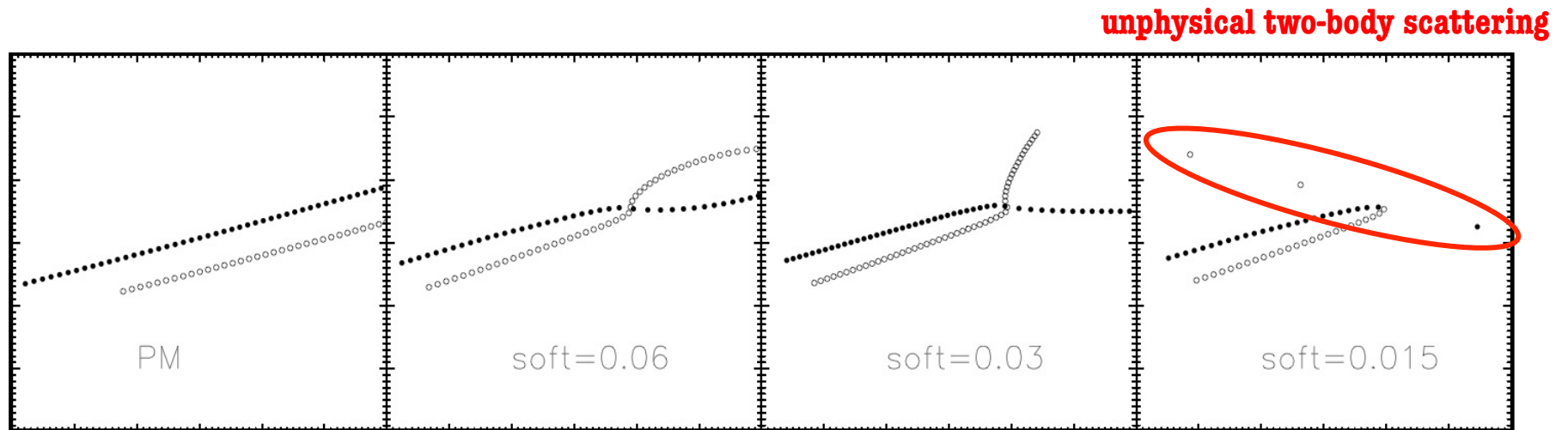


(Knebe et al. 2000)

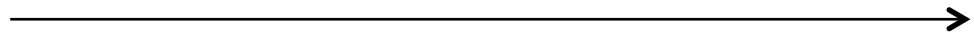


increasing the force resolution
(without adjusting the time step...)

- time step and softening

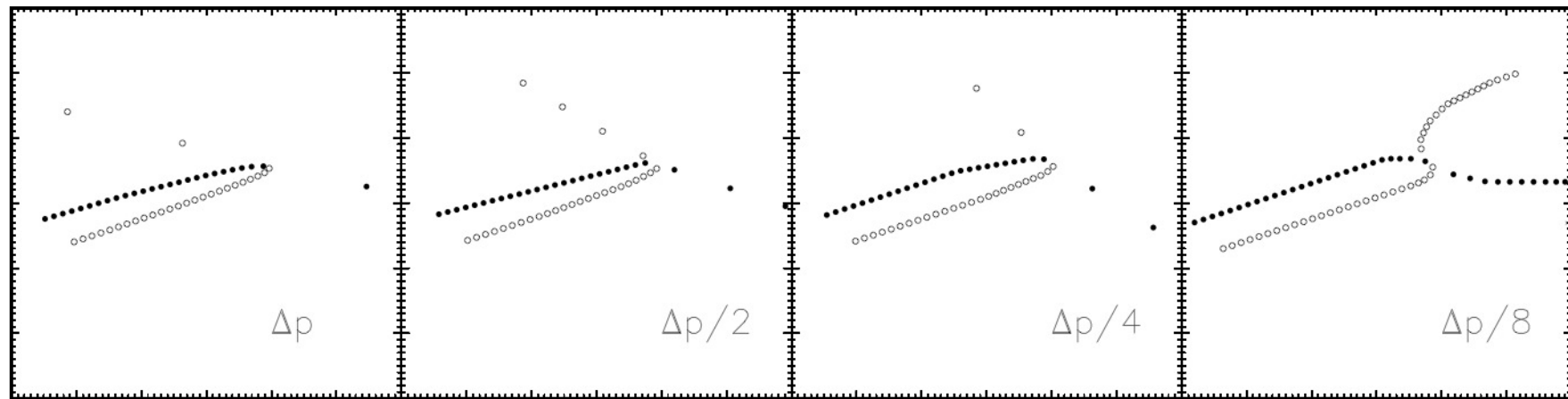


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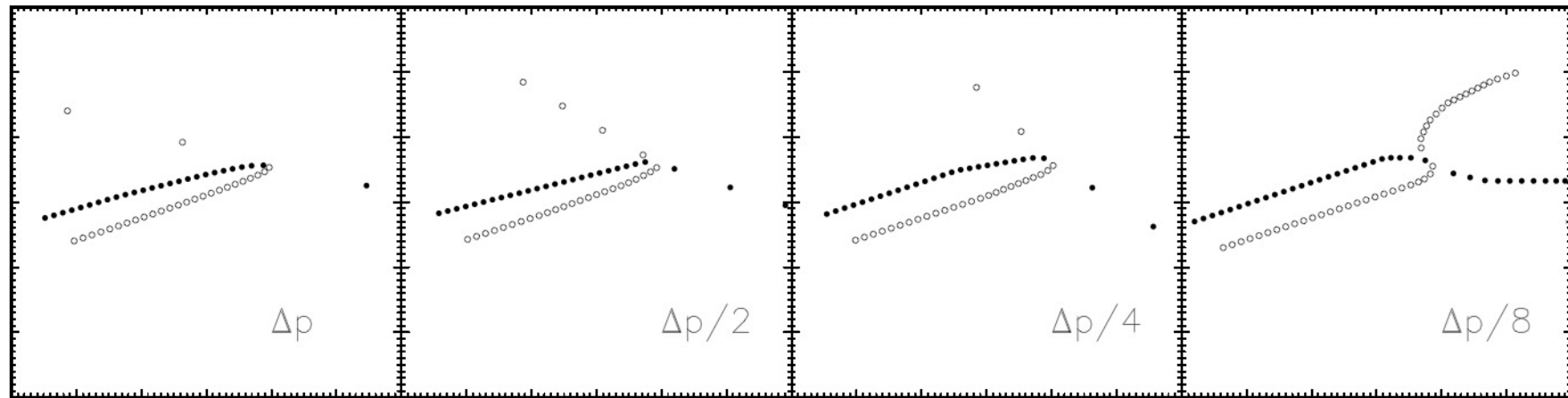
- time step and softening



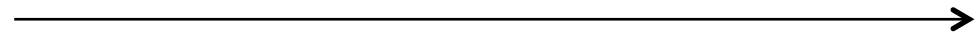
(Knebe et al. 2000)

simultaneously decreasing the time step
remedies the problem

- time step and softening



(Knebe et al. 2000)



simultaneously decreasing the time step
remedies the problem

choose time step and softening wisely...

- the relation between...

→ *particle number, time step and softening?*

- convergence study:

run the same simulation again and again
gradually varying one of the technical parameters...

in-depth study by Power et al., MNRAS 338, 14 (2003)

- particle number

we aim at solving the collisionless Boltzmann equation
using particles as phase-space markers¹...

...and hence their dynamics should be determined
by the mean field and not two-body interactions!

¹cf. "The N-Body Approach" lecture...

- particle number

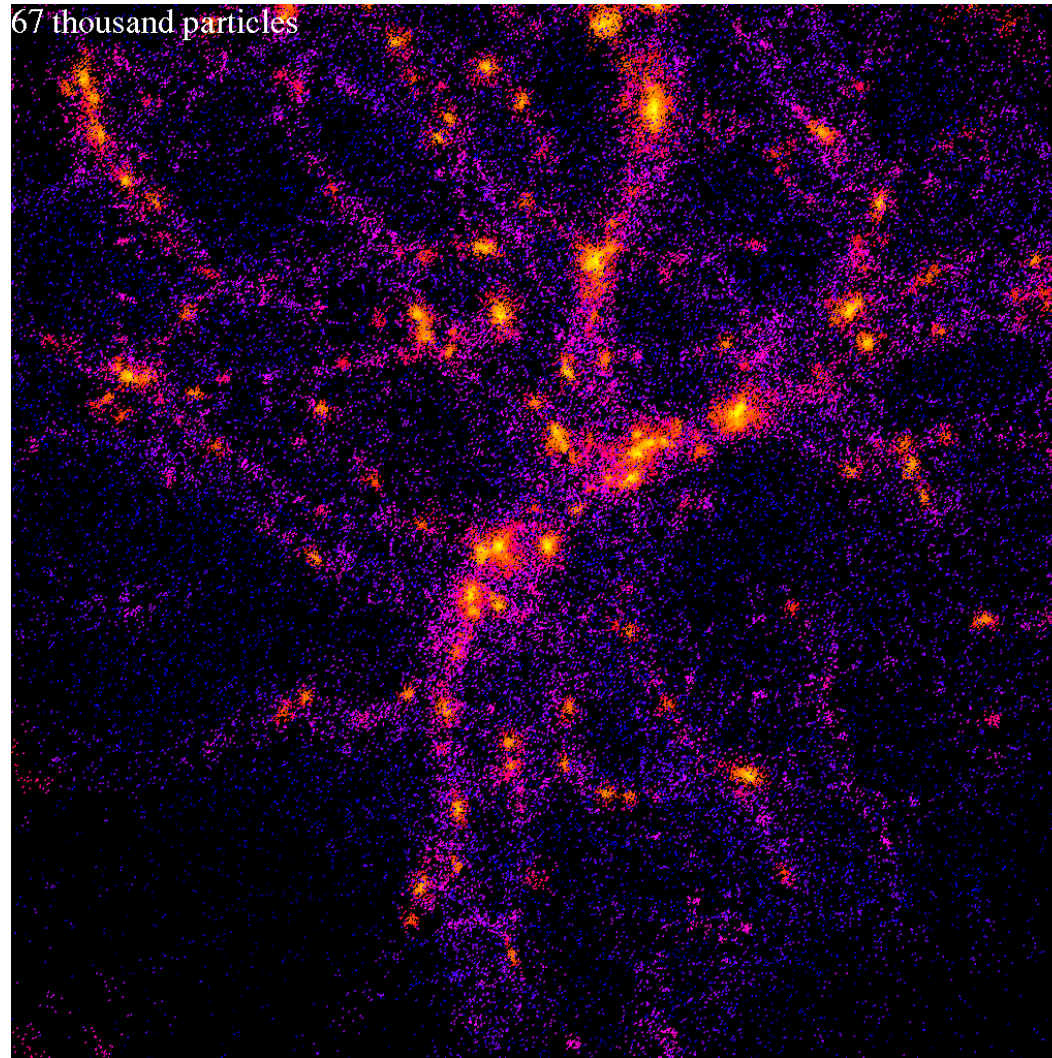
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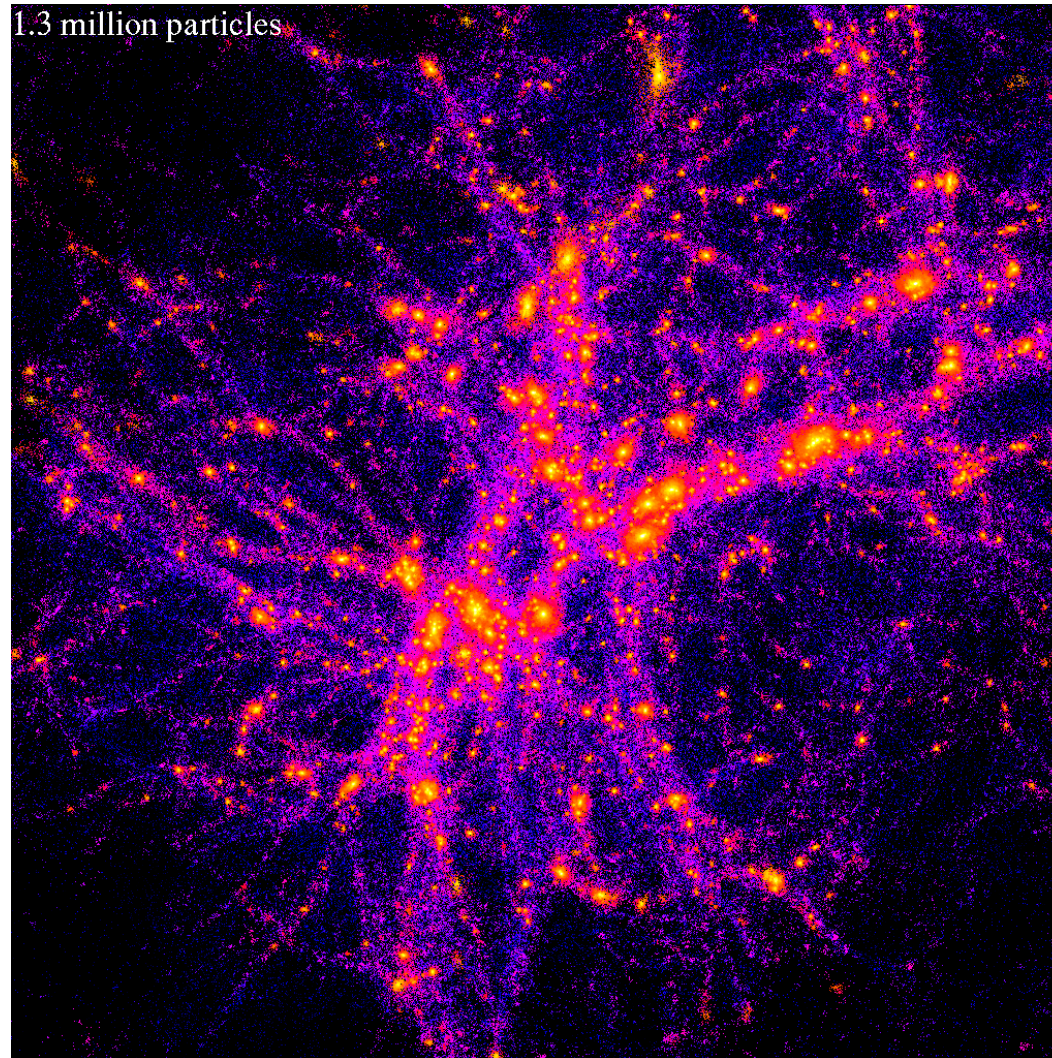
how can we be sure to use enough particles in this approach?

¹cf. "The N-Body Approach" lecture...

- particle number

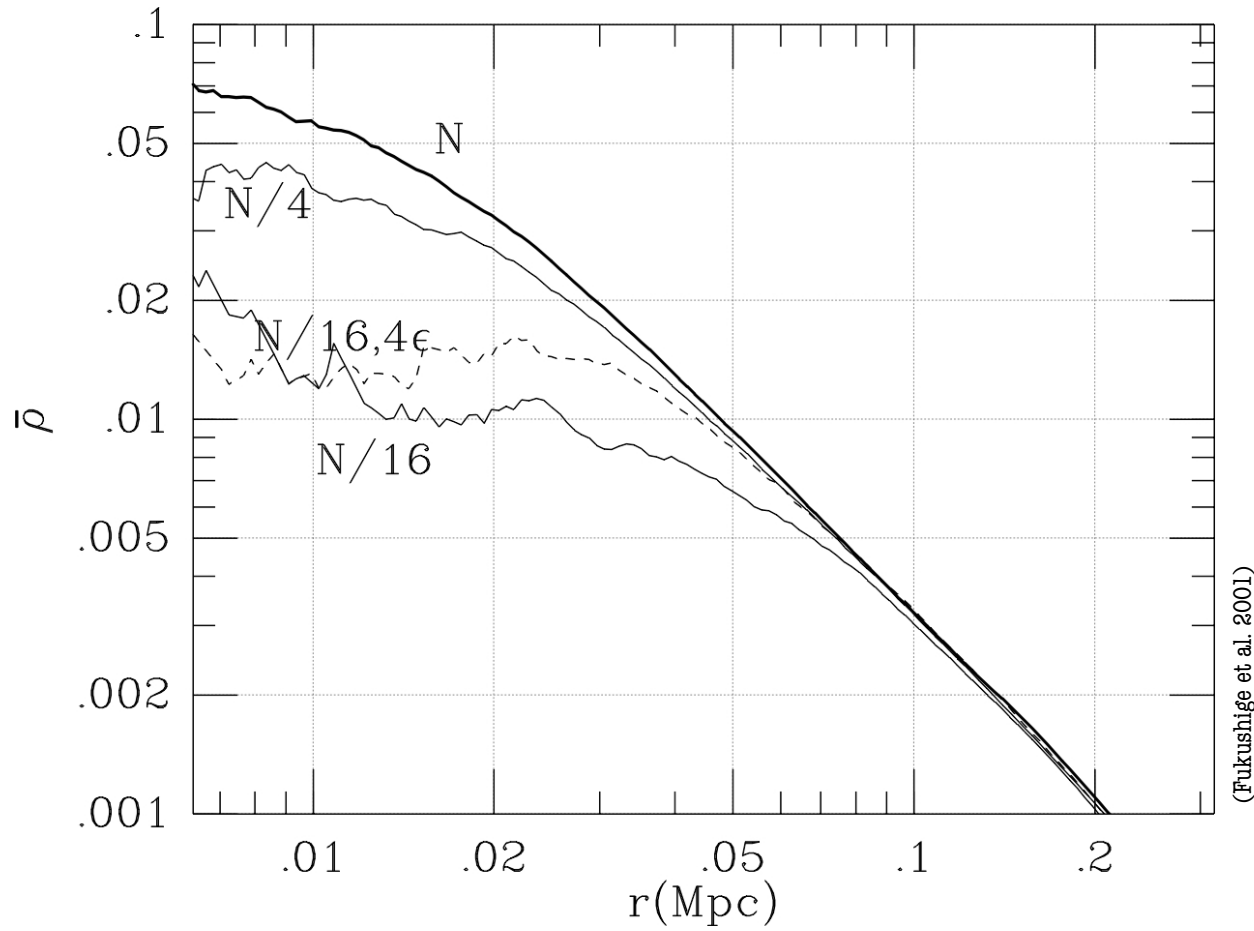


- particle number



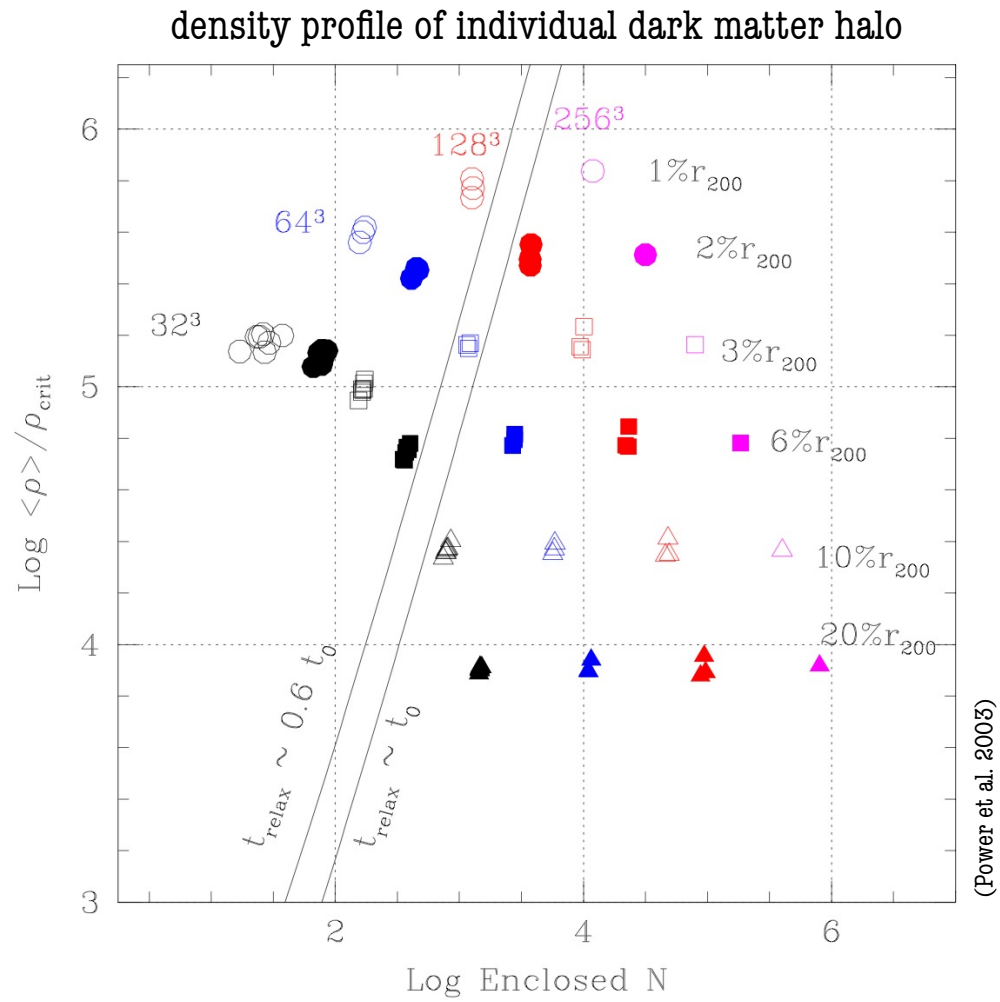
- particle number

density profile of individual dark matter halo



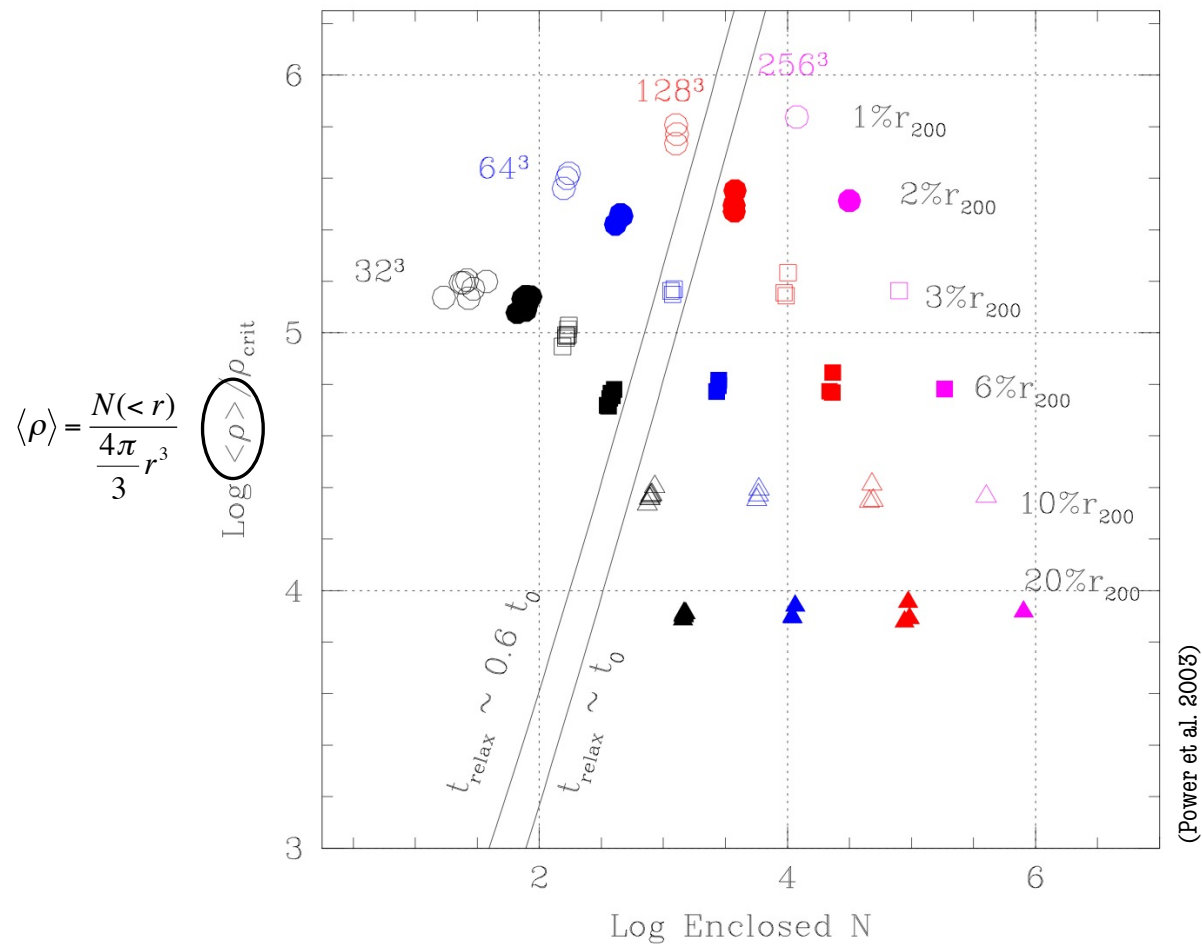
(Fukushige et al. 2001)

- particle number



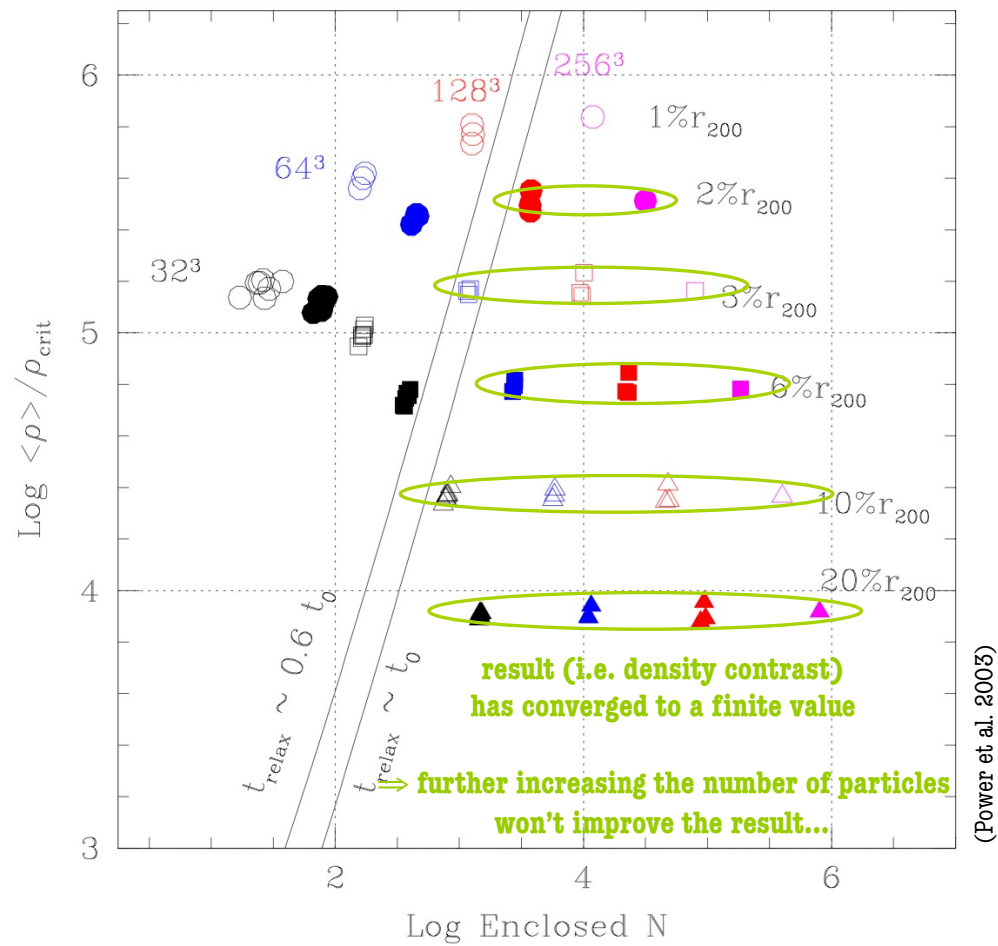
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- particle number

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- collisional relaxation

- relaxation time

“When a finite number of particles is used to represent a system, individual particle accelerations will inevitably deviate from the mean-field value when particles pass close each other.”

(Power et al. 2003)

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$$\frac{t_{relax}}{t_{cross}} \approx \frac{N(< r)}{8 \ln(r/\varepsilon)} \approx \frac{N}{8 \ln N}$$

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$$\frac{t_{relax}}{t_{cross}} \approx \frac{N(< r)}{8 \ln(r/\epsilon)} \approx \frac{N}{8 \ln N}$$

$t_{cross} = r/v$

**number of encounters required to change
a particle's velocity by of order itself...**

(cf. Binney & Tremaine 1987)

- collisional relaxation

- relaxation time

“When a finite number of particles is used to represent a system, individual particle accelerations will inevitably deviate from the mean-field value when particles pass close each other.”

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$$\frac{t_{relax}}{t_{cross}} \approx \frac{N(< r)}{8 \ln(r/\epsilon)} \approx \frac{N}{8 \ln N}$$

$$\frac{r}{\epsilon} \approx \frac{rv^2}{Gm} \approx \frac{r \frac{GNm}{r}}{Gm} \approx N$$

a close encounter ϵ entails $\Delta v \approx v$

- collisional relaxation

- relaxation time

“When a finite number of particles is used to represent a system, individual particle accelerations will inevitably deviate from the mean-field value when particles pass close each other.”

(Power et al. 2003)

$$\frac{t_{relax}}{t_{cross}} \approx \frac{N(< r)}{8 \ln(r/\varepsilon)} \approx \frac{N}{8 \ln N}$$

⇒ the relaxation time t_{relax} should exceed the age of the Universe t_0 :

$$t_{relax}(r, N, \varepsilon) \geq 0.6 t_0$$

- empirically derived relations meeting this requirement:

- choose gravitational softening to ensure $a_{2\text{body}} < a_{\text{meanfield}}$

$$\varepsilon \approx 4 \times \frac{R_{\text{vir}}}{\sqrt{N_{\text{vir}}}}$$

- regard those regions as converged where the circular orbit time-scales exceeds

$$t_{\text{circ}}(r_{\text{converged}}) > 15 \times \left(\frac{\Delta t}{t_0} \right)^{5/6} t_{\text{circ}}(R_{\text{vir}})$$

\swarrow

$$\frac{\Delta t}{t_0} = \frac{1}{N_{\text{steps}}}$$

- do trustworthy science...

