Post-Newtonian-accurate regularized SMBH dynamics in galaxy simulations

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From galaxy mergers to GW coalescence

Evolutionary phase	Distance scale (approximate)
Galaxies in group/cluster environment	1 kpc – 1 Mpc
Galaxy mergers	0.1 kpc – 100 kpc
Dynamical friction	10 pc – 1 kpc
Binary hardening by three-body scatterings	0.01 pc – 10 pc
GW emission, SMBH merger	AU scale – 0.01 pc

Tree-gravity/hydro codes

Direct summation codes

Few-body PN codes

Numerical relativity

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- Direct summation codes
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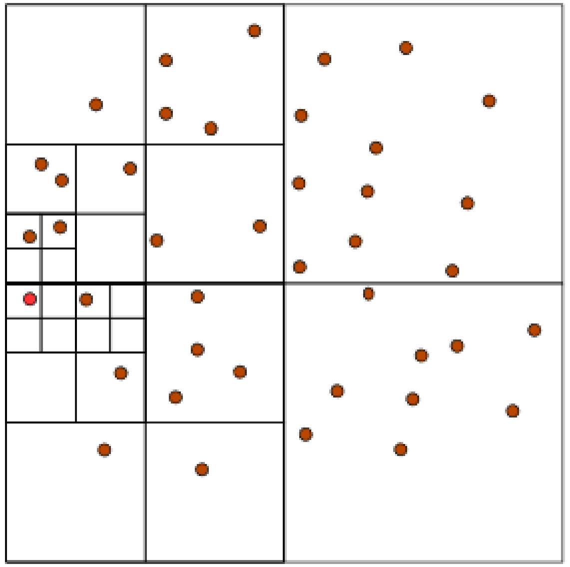
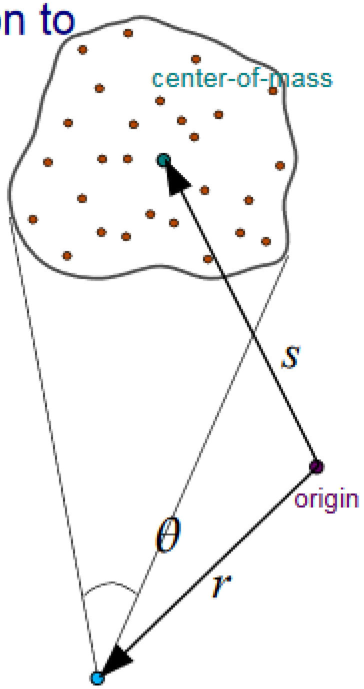
Our focus

Simulating Newtonian gravity: tree algorithms



Idea: Use hierarchical multipole expansion to account for distant particle groups



$$\Phi(\mathbf{r}) = -G \sum_i \frac{m_i}{|\mathbf{r} - \mathbf{x}_i|}$$

We expand:

$$\frac{1}{|\mathbf{r} - \mathbf{x}_i|} = \frac{1}{|(\mathbf{r} - \mathbf{s}) - (\mathbf{x}_i - \mathbf{s})|}$$

for $|\mathbf{x}_i - \mathbf{s}| \ll |\mathbf{r} - \mathbf{s}|$ $\quad \mathbf{y} \equiv \mathbf{r} - \mathbf{s}$

and obtain:

$$\frac{1}{|\mathbf{y} + \mathbf{s} - \mathbf{x}_i|} = \frac{1}{|\mathbf{y}|} - \frac{\mathbf{y} \cdot (\mathbf{s} - \mathbf{x}_i)}{|\mathbf{y}|^3} + \frac{1}{2} \frac{\mathbf{y}^T \left[3(\mathbf{s} - \mathbf{x}_i)(\mathbf{s} - \mathbf{x}_i)^T - \mathbf{I}(\mathbf{s} - \mathbf{x}_i)^2\right] \mathbf{y}}{|\mathbf{y}|^5} + \ldots$$

Springel (2006)

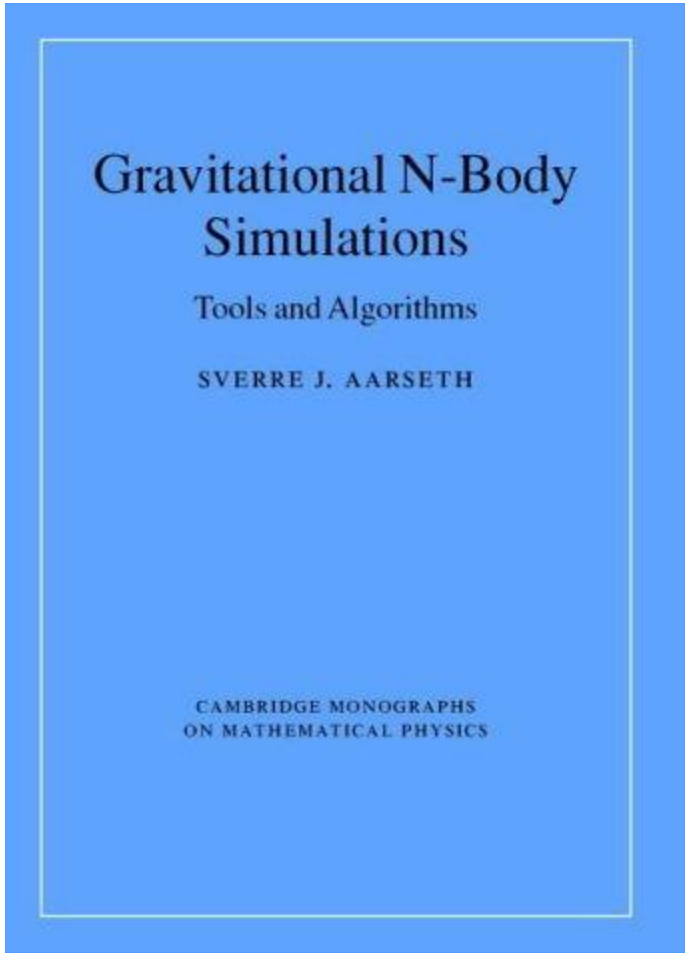
N = particle number

- $\sim\log(N)$ force evaluations per particle
- PM methods also possible for large separations
- Equations of motion integrated with a leapfrog algorithm
- Very large simulations possible
- Example codes: different GADGET versions

Simulating Newtonian gravity: direct summation codes

- N force evaluations per particle
- Typically using very accurate high-order integrators
- Neighbour schemes possible to reduce the number of force computations
- Small softening or special handling of close encounters

- Special computer hardware or GPUs
- Maximum particle number $\sim 10^6$
- Example codes: NBODY 1-7, GRAPE codes



Simulating Newtonian gravity: numerical issues

Point-like simulation particles: $F(r) = -\frac{GMm}{r^2} \rightarrow -\infty \; as \; r \rightarrow 0.$

Also: two-body relaxation timescale boosted by low resolution

Solutions:

1) **Softening:** $F(r) = -\frac{GMm}{(r+\varepsilon)^2} \rightarrow -\frac{GMm}{\varepsilon^2} \; as \; r \rightarrow 0.$

- The softening length ε is the resolution limit of the simulation.

2) **Regularization**: transform the equations of motion so that the problem vanishes.

- Levi-Civita, Kustaanheimo-Stiefel methods, algorithmic chain regularization
- Typically possible only for a small number of particles

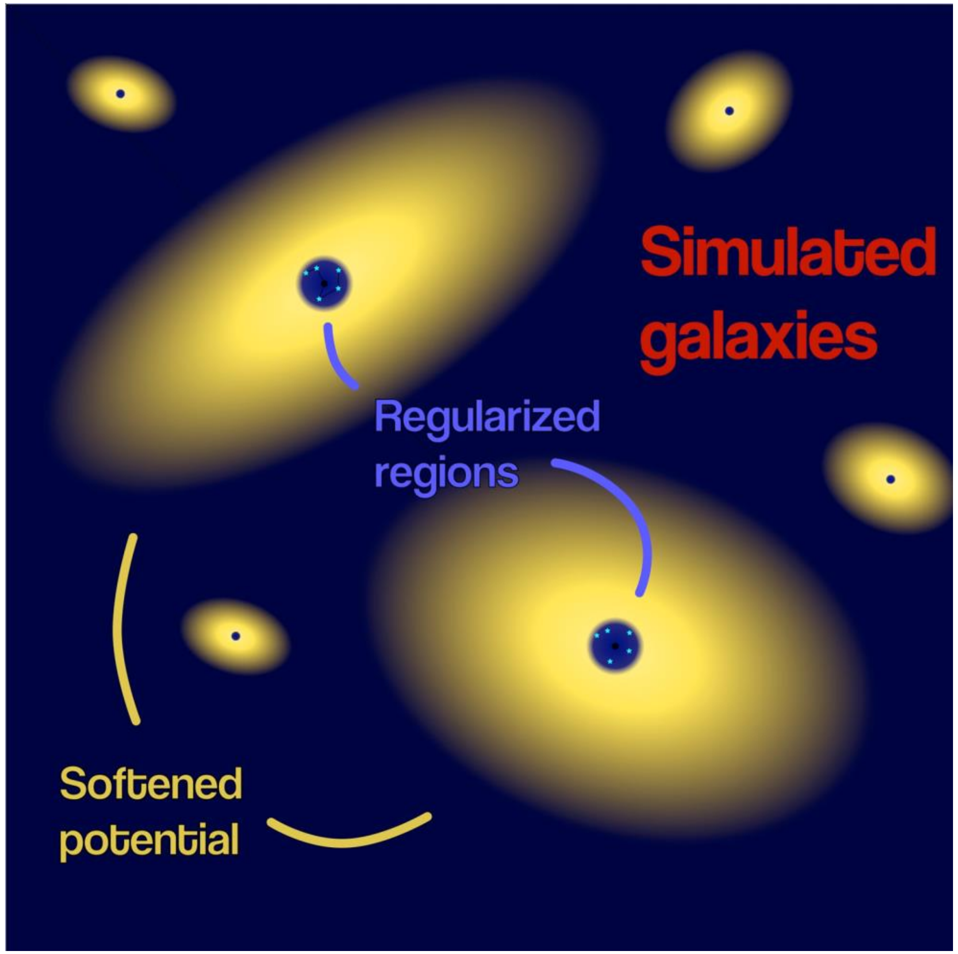
KETJU: regularized SMBH dynamics in Gadget-3

Gadget-3:

- Softened Newtonian gravity with TreePM algorithm
- Gas dynamics using a modern Smoothed Particle Hydrodynamics
- Sub-resolution star-formation, stellar feedback, SMBH accretion+feedback, metals, metal-dependent cooling...

KETJU:

- A regularized volume around the SMBHs
- Accurate, non-softened dynamics
- Post-Newtonian corrections up to PN3.5, optional spin- dependent terms and their cross terms
- PN approximation accurate down to approximatively 10 Schwarszchild radii of the SMBHs



KETJU (Finnish):
A chain

Algorithmic Chain Regularization (ARCHAIN)

- The equations of motion are time-transformed. Together with a leapfrop integrator, this regularizes the system against Newtonian force divergences.
- Chain: the usage of chained inter-particle vectors significantly reduces the round-off error.
- Bulirsch-Stoer extrapolation method to formally extrapolate $dt \rightarrow 0$. This corresponds to taking a large number of substeps during one Gadget-3 timestep.
- Error in dynamical variables of the chain particles can be pushed down to machine precision.

Define $t \mapsto s$ by

$$\begin{aligned} \mathrm{d}s &= [\alpha(T+B) + \beta\omega + \gamma]\,\mathrm{d}t \\ &= (\alpha U + \beta\Omega + \gamma)\,\mathrm{d}t, \end{aligned}$$

where $\alpha, \beta, \gamma \in \mathbb{R}$, and

$$T = \sum_i \frac{1}{2} m_i \|\vec{v}_i\|^2 \quad \text{kinetic energy,}$$

$$U = \sum_i \sum_{j>i} \frac{G m_i m_j}{\|\vec{r}_{ij}\|} \quad \text{force function,}$$

$$B = -T + U \quad \text{binding energy,}$$

$$\Omega = \text{arbitrary function of } \vec{r}_i,$$

$$\dot{\omega} = \sum_i \nabla_{\vec{r}_i}\Omega \cdot \vec{v}_i.$$

Chain subsystems in Gadget-3

- **Chain particles**

  SMBHs and stars inside the influence radius.

- **Tree particles**

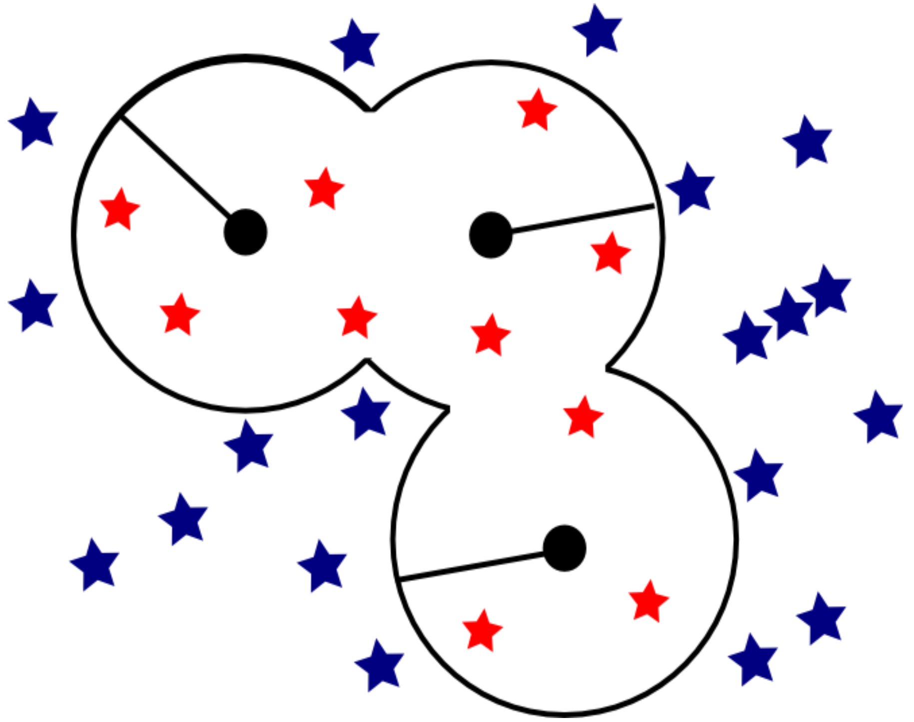
  Ordinary Gadget-3 particles.

- **Perturber particles**

  Tree particles strongly perturbing a chain subsystem.

  User-defined parameter lambda and gamma set the amount of chain and perturber particles.

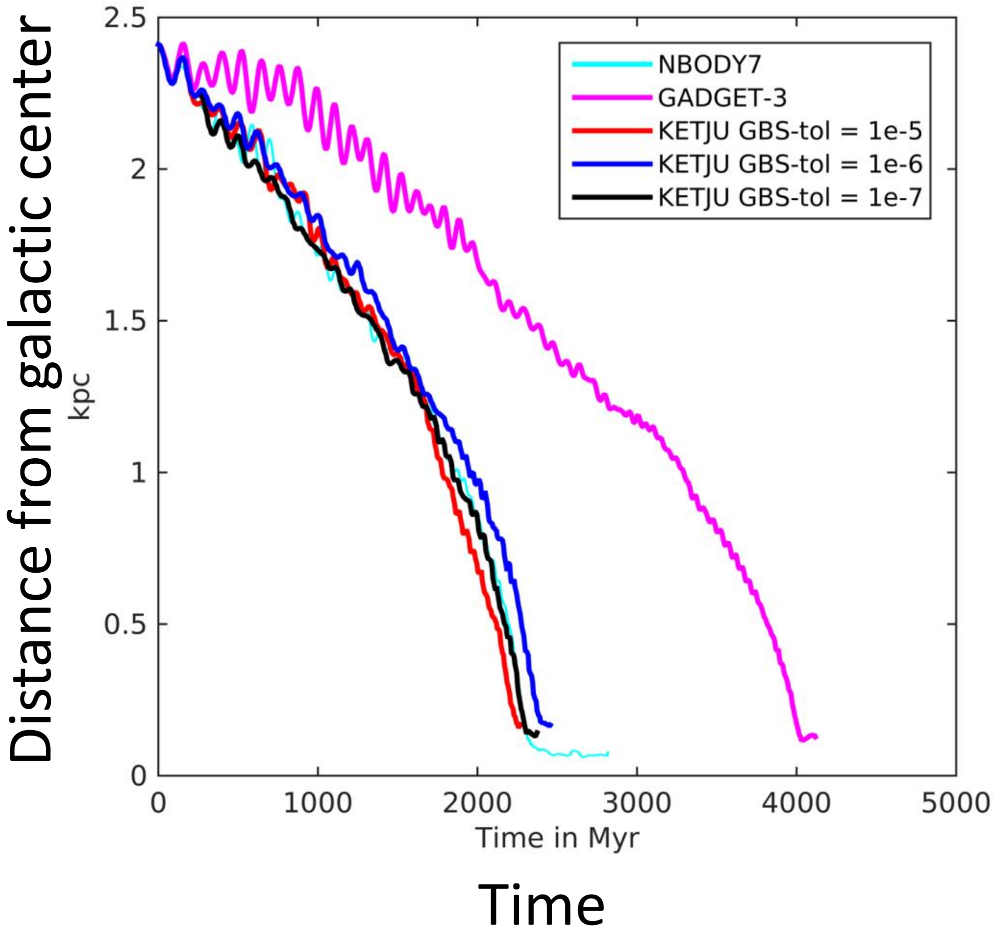
$$r_{\mathrm{infl}} = \lambda \times \frac{M_{\mathrm{BH}}}{10^{10} M_{\odot}} \mathrm{kpc}$$



Chain & Tree memberships updated every timestep

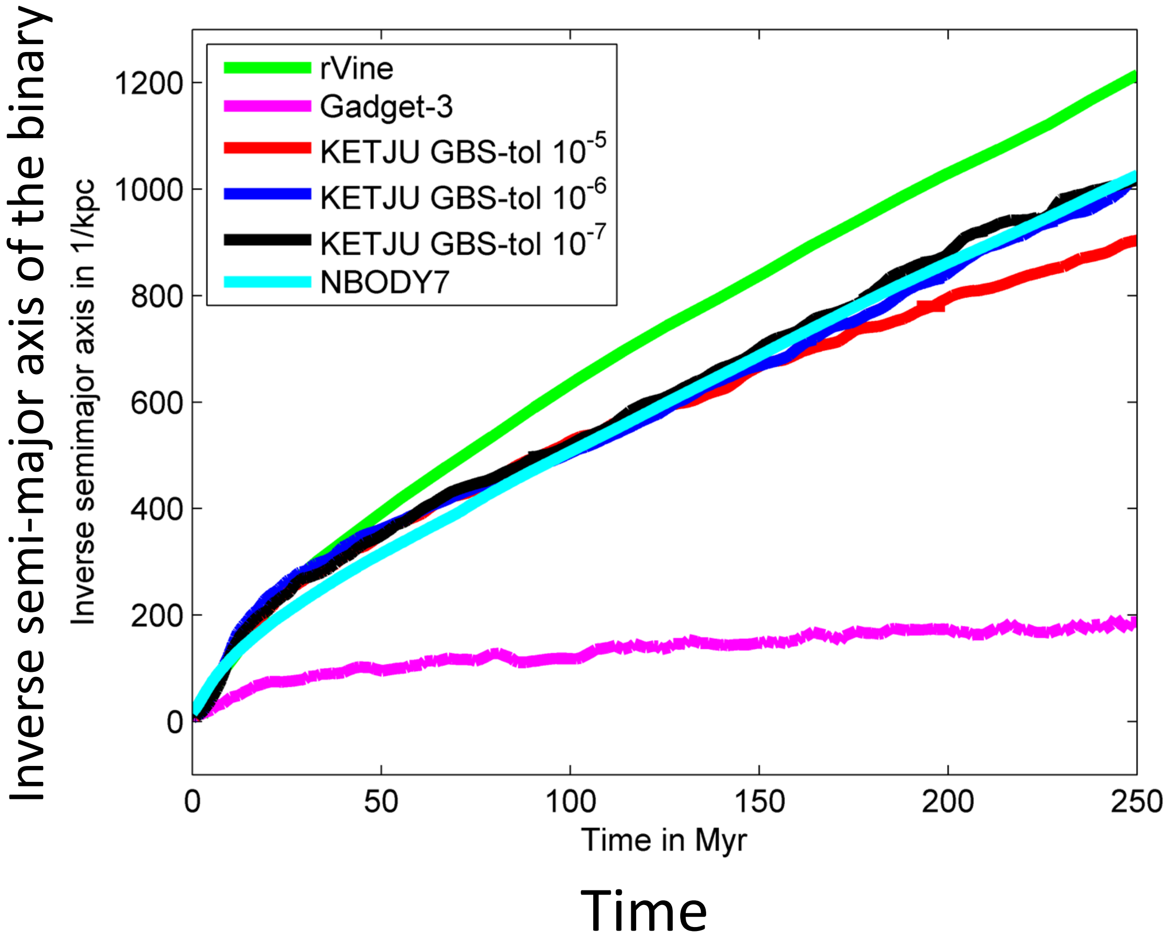
$$r < r_{\mathrm{pert}} = \gamma \times r_{\mathrm{infl}} \left(\frac{m}{M_{\mathrm{BH}}} \right)^{1/3}$$

Comparing KETJU to ordinary Gadget-3 and NBODY7



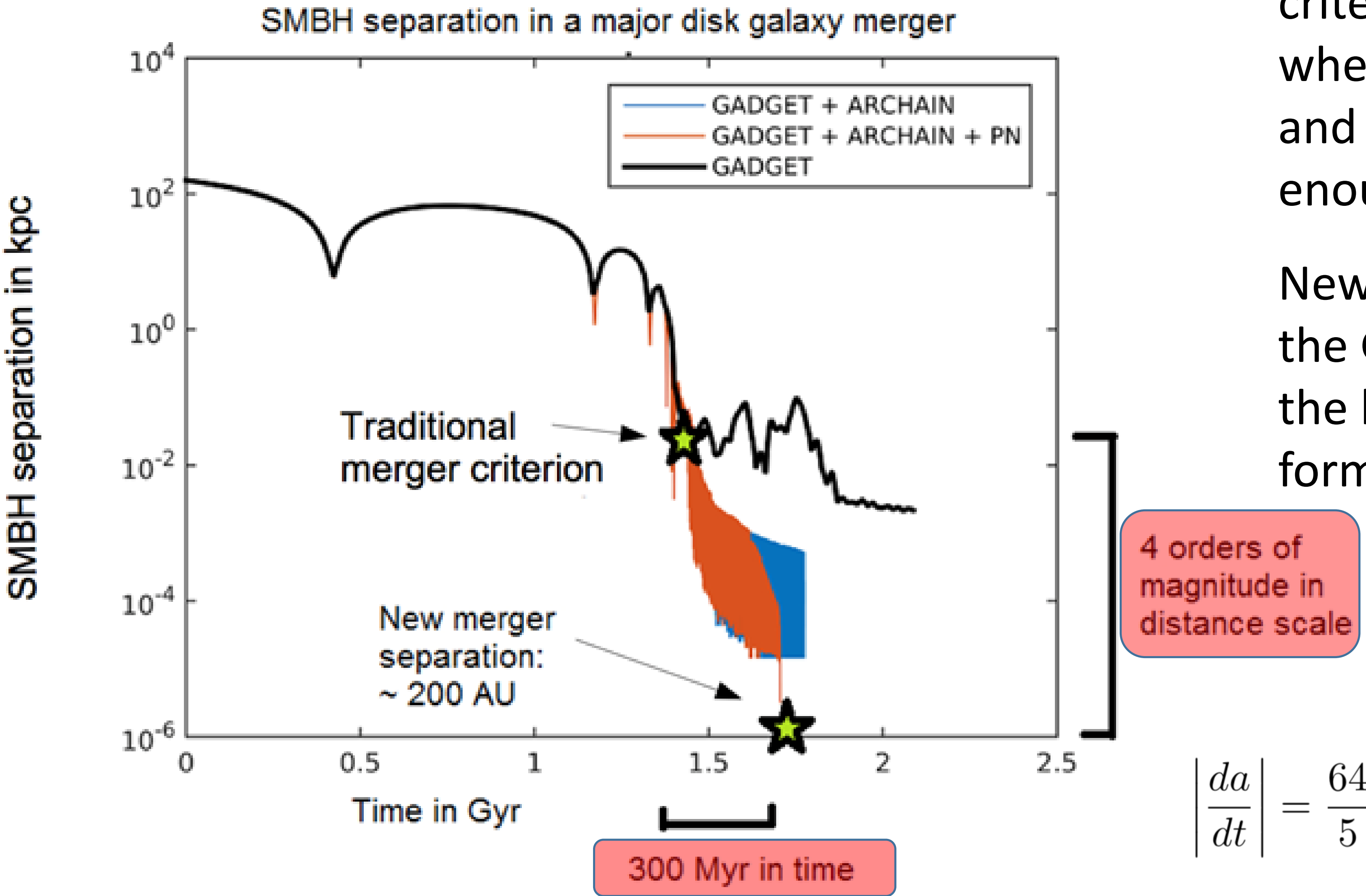
A single SMBH sinking due to dynamical friction in a Hernquist sphere

GBS-tol = Bulirsch-Stoer integrator accuracy



A SMBH binary hardening via 3-body interactions of stars

Realistic SMBH merger timescales Gadget-3 – like codes



The original Gadget-3 merger criterion: merge SMBHs instantly when their softening lengths overlap and the relative velocity is small enough

New KETJU criterion is based on the GW coalescence timescale of the binary obtained from Peter's formula (1964)

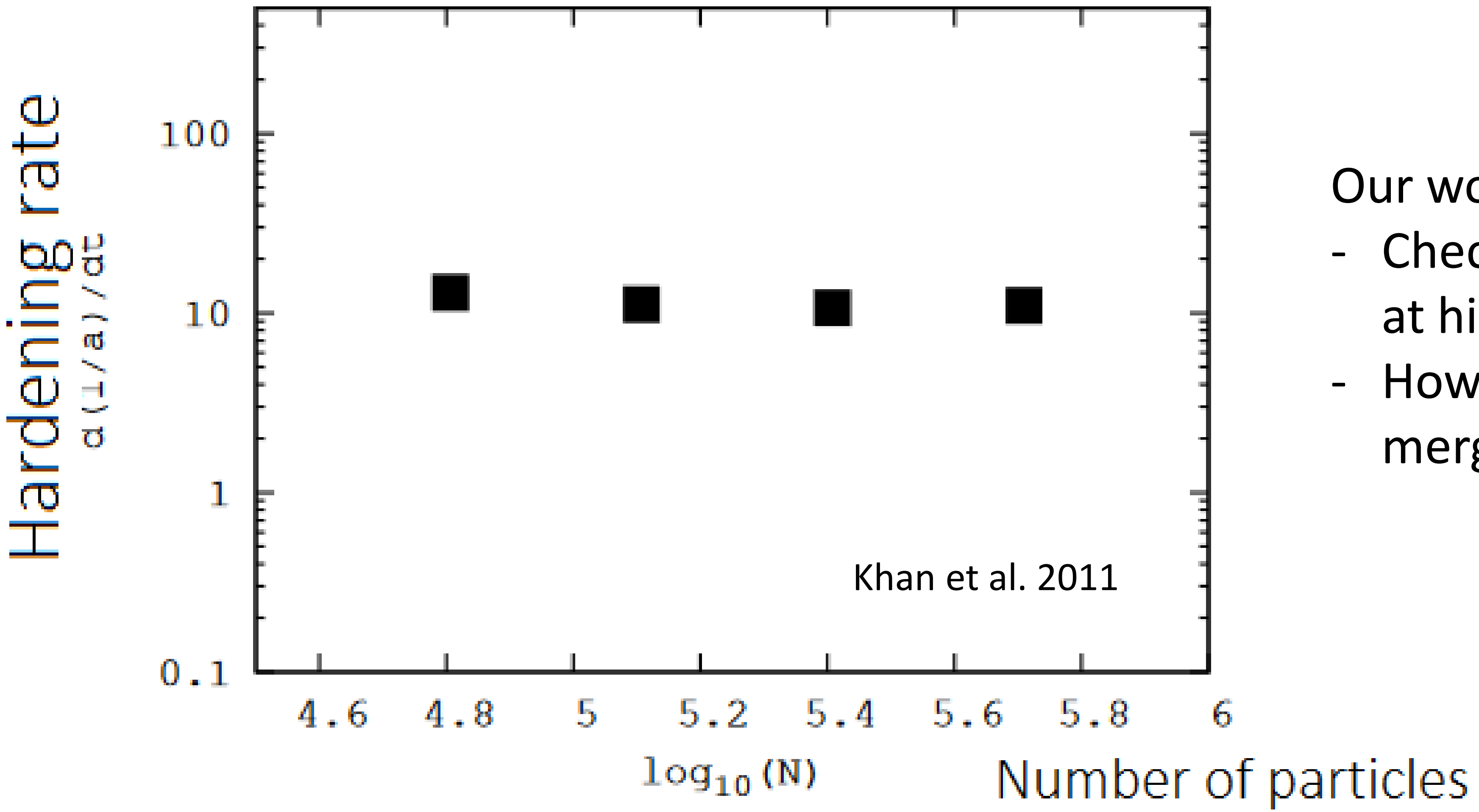
$$t_c \sim \frac{a}{4\dot{a}}$$ < Gadget timestep

$$\left|\frac{da}{dt}\right| = \frac{64}{5}\frac{G^3 M_1 M_2 (M_1 + M_2)}{c^5 a^3}\frac{1 + \frac{73}{24}e^2 + \frac{37}{96}e^4}{(1-e^2)^{7/2}}$$

Ongoing work: dry mergers and resolution effects in hardening rates

Khan et al. 2011: SMBH binary hardening rate independent of particle mass as torques from the merger fill the loss cone faster than 2-body relaxation does → low-res results generally valid?

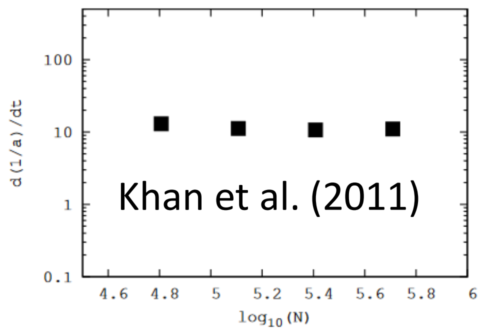
Hardening rate $= \frac{d}{dt}\frac{1}{a}$



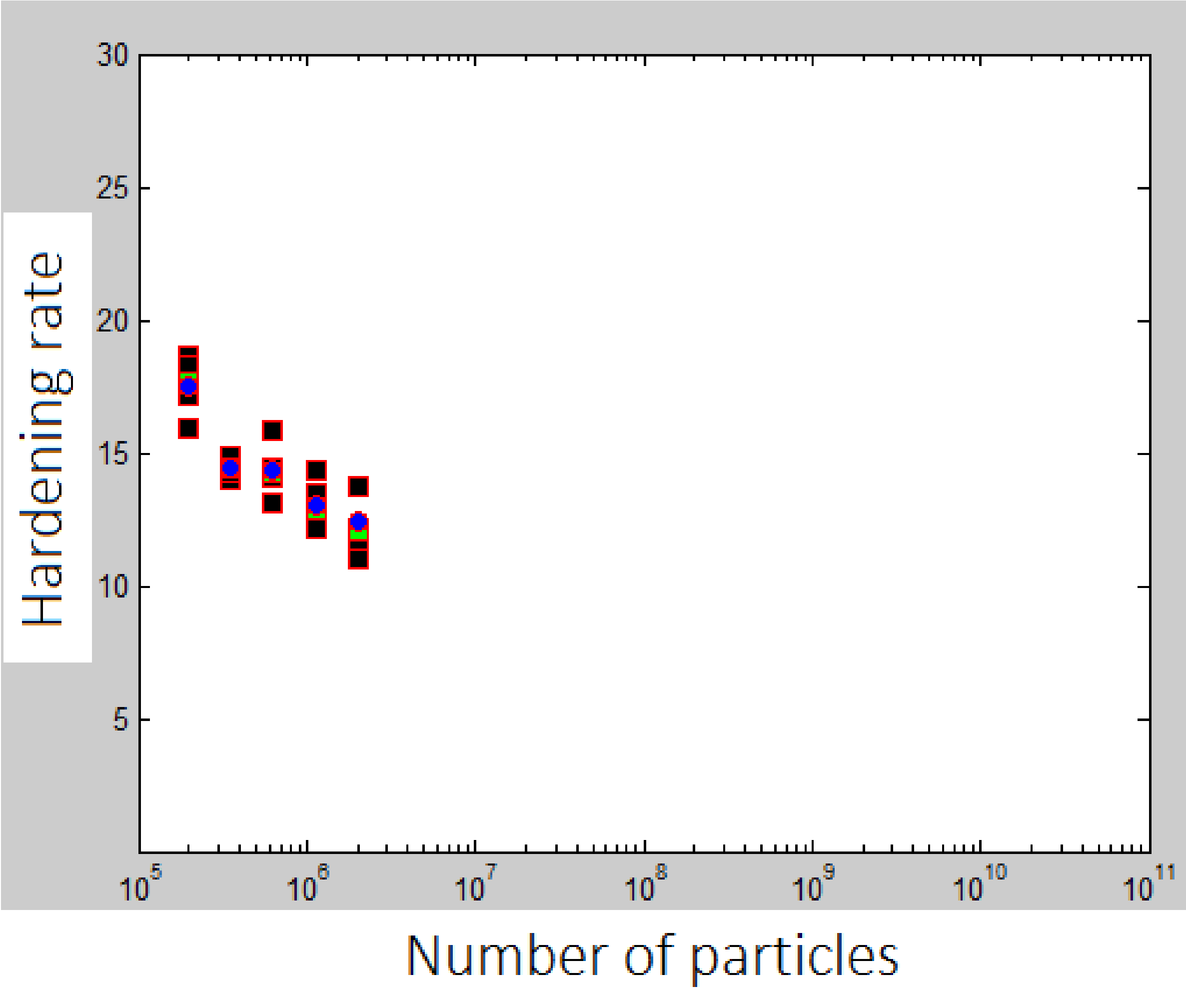
Our work:

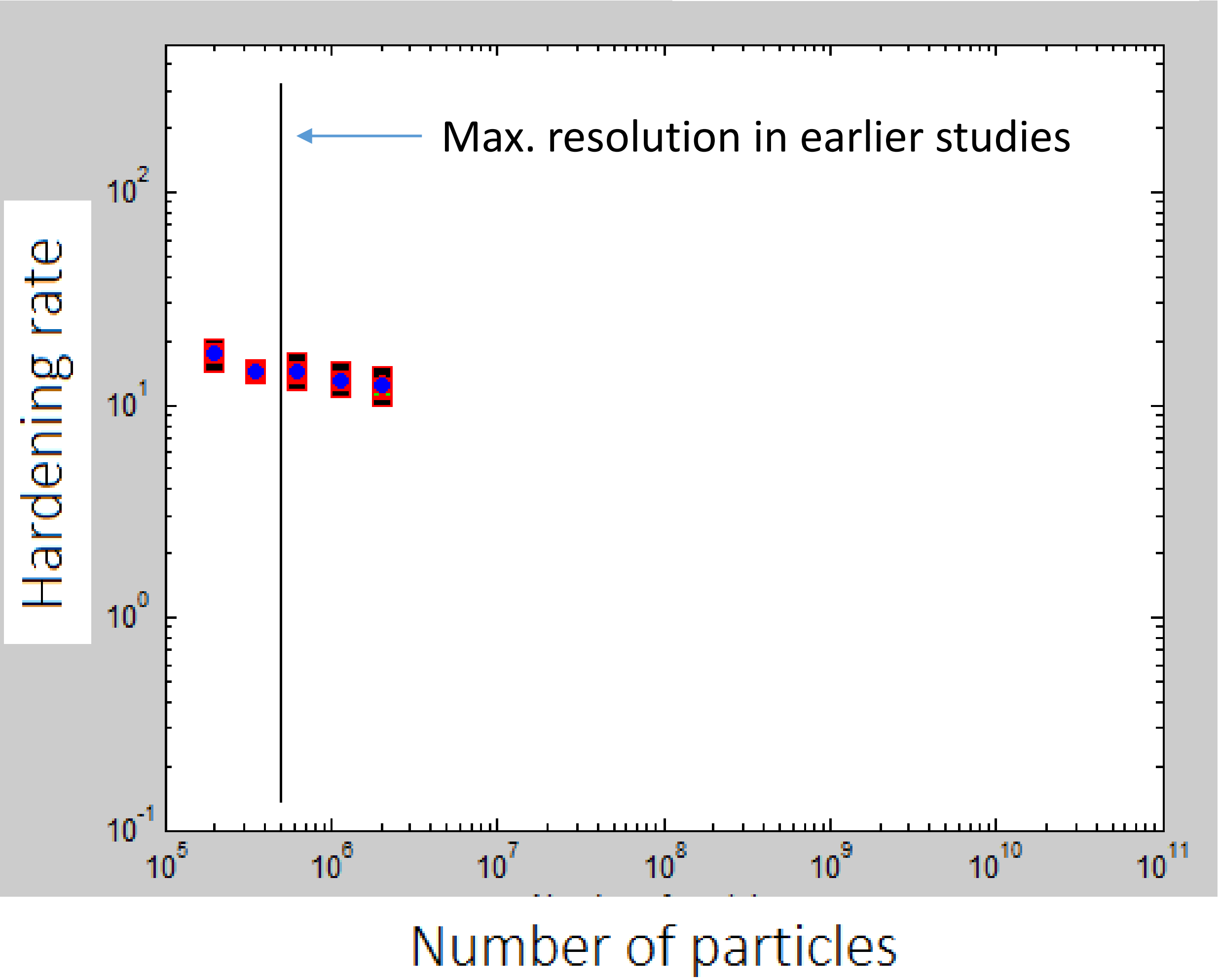
- Check the validity of this claim at higher resolutions
- How about the DM halo or merger geometry etc...?

Hardening rates continued...



Same plot with different y-axis





Summary

- We have developed KETJU, a regularized dynamics module for Gadget-3.
- Resolution effects properly studied.
- More accurate SMBH merger timescale estimates.
- Next step: regularized simulations with full Gadget hydrodynamics + feedback