Simulating black hole dynamics and gravitational wave emission in galactic-scale simulations

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1. Supermassive black holes

• Supermassive black holes (SMBH) are found in the centres of all massive galaxies.

• A strong correlation between the SMBH mass and the stellar mass in galaxies, implying co-evolution.

• Energetic feedback from supermassive black holes might be responsible for setting the maximum mass of galaxies.

• In the standard LCDM model galaxies grow through mergers. Mergers of SMBHs could be detected using gravitational waves in the near future (LISA).
The primary goal of numerical simulations is to calculate the positions, velocities and accelerations of particles in a gravitational field using Newton’s Law of gravity:

\[
\frac{d}{dt}(m_\alpha \mathbf{v}_\alpha) = - \sum_{\beta, \alpha \neq \beta} \frac{G m_\alpha m_\beta}{|\mathbf{x}_\alpha - \mathbf{x}_\beta|^3}(\mathbf{x}_\alpha - \mathbf{x}_\beta)
\]

This is exactly done in collisional direct N-body simulations and hence the calculation scales as \( \propto N^2 \), where \( N \) is the number of particles.

When we want to study large systems with a large number of particles we need to make some approximations.

In the Milky Way there is about 200-400 billion stars, however in a typical simulation there is only some millions of particles.
Numerical simulations II

- In **tree codes** distant particles are grouped together as more massive "particles" for the force calculation.
- In **grid-codes** the particles are distributed on a grid. The gravitational force is calculated from each grid cell, instead of calculating the force from each particle. The grid can also be adaptive.
- In these codes gravity is softened on small scales.

$$\Phi_\alpha = - \sum_{\beta \neq \alpha} \frac{G m_\beta}{\sqrt{r^2 + \epsilon^2}}$$

Tree codes scale as $\propto N \log N$, which is smaller than $N^2$ for large $N$.

Grid-codes scale as $\propto N_g \log N_g$, where $N_g$ is the number of grid points.
The dynamics of black holes have been traditionally studied with global hydrodynamical 10-100 million particle softened simulations (i.e. Gadget-3, RAMSES, AREPO).

An alternative is to use an collisional direct N-body simulation, which are typically restricted to ~1 million particles (i.e. Nbody-7) and typically do not include gas.

In KETJU the best aspects of a global softened code and an accurate N-body code are combined.
The three phases of black hole binary evolution

1. **Dynamical friction** from stars and gas reduces the semi-major axis of the BH binary to ~10 pc.

2. Next, the semi-major axis of the binary will shrink by kicking out stars in complex three-body interactions.

3. The emission of gravitational waves will eventually dominate the loss of orbital energy at very small ~0.01 pc binary separations.

- Current simulation codes are unable to resolve the full BH merging process in a single simulation.

\[
\frac{d}{dt} \left( \frac{F_D}{a} \right) \propto \frac{G \sigma_* M^2}{\sigma_*} \\
\left| \frac{da}{dt} \right| = \frac{64}{5} \frac{G^3 M_1 M_2 (M_1 + M_2)}{c^5 a^3} \frac{1 + \frac{73}{24} e^2 + \frac{37}{96} e^4}{(1 - e^2)^{7/2}}
\]
2. KETJU - Regularized Gadget: Main features

1. KETJU (chain in Finnish): An extension of Gadget-3, which includes an algorithmically regularized chain (Mikkola & Merritt 2008) module that makes two-body collisions integrable by a simple leapfrog integrator.

2. Supports multiple regularized chains, where high-resolution regularized regions can be included around every BH in the simulation.

3. Includes Post-Newtonian corrections up to order 3.5 PN (or $c^{-7}$). Includes an explicit leapfrog that account for the fact that the PN correction terms depend on the particle velocities, and possibly spins, in addition to the particle coordinates. The PN approach is valid up to $\sim 10$ Schwarzschild radii ($R_s$).

\[ \vec{a}_{2\text{-body}} = \vec{a}_{\text{New}} + \sum_{k=2}^{7} c^{-k} \vec{a}_{k/2PN} + \vec{a}_S \]
1. The dynamics in the high-resolution region is regularized through a time transformation that avoids force divergences and allows even for particle collisions (Mikkola & Tanikawa 1999, Preto & Tremaine 1999).

2. The particles are organized into a chain and in the calculation inter-particle vectors are used which significantly reduces round-off errors.

3. Particles in the chain are integrated using the Bulirsch-Stoer extrapolation method, in which a large number (~100) substeps are taken during a full Gadget timestep resulting in good convergence.

Define $t \mapsto s$ by

$$ds = [\alpha(T + B) + \beta \omega + \gamma] \, dt$$

$$= (\alpha U + \beta \Omega + \gamma) \, dt,$$

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

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

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

$B = -T + U$ binding energy,

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

$\dot{\omega} = \sum \nabla_{\vec{r}_i} \Omega \cdot \vec{v}_i.$
1. **Chain particles:** All the SMBH particles and stellar particles that lie within the influence radius of the SMBHs. Typically $r_{\text{infl}} \sim 5$-10 pc.

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

2. **Perturber particles:** Simulation particles, which induce strong tidal perturbations on a chain system. Typically $r_{\text{pert}} = 2r_{\text{infl}}$

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

3. **Tree particles:** Other particles that do not reside near any of the SMBHs act as ordinary GADGET-3 particles.
Test Simulation with a total of 5 SMBHs. Four SMBHs are situated at the corners of tetrahedron and one is found in the centre. Each SMBH is initially surrounded by 1000 particles.
• Typically in softened simulations BHs merge instantly when they are within the softening length. We use instead a physically motivated merger criterion from the gravitational wave dominated coalescence time (Peters’ 1963 formula):

\[
t_c \sim \frac{a}{4\dot{a}} \quad \left| \frac{da}{dt} \right| = \frac{64}{5} \frac{G^3 M_1 M_2 (M_1 + M_2)}{c^5 a^3} \left(1 + \frac{73}{24} e^2 + \frac{37}{96} e^4 \right) (1 - e^2)^{7/2}
\]
Gravitational wave background

Example evolution: $m_1 = m_2 = 10^9 M_\odot$, $d_c \approx 1$ Gpc, $z = 0.25$

- A circular binary (e=0) emits GWs only at $n=2$ harmonic (2xorbital frequency).
- With higher eccentricity, the GW signal comes over many harmonics.

- Many SMBH binaries in different stages of evolution emitting GWs. GW signals sum to an unresolved background.
- Amplitude and shape affected by: 1) Density of binary mergers, 2) Masses, eccentricities and 3) Environment (stellar scattering etc.)
Large cosmological simulations, such as the 106.5 Mpc box Illustris simulation can be used to predict the GWB.

The softening length of baryons is ~0.7 kpc, black holes thus merge at ~1 kpc separation in the simulation.

Use Analytic subgrid models and eccentricity as an input:
1. Dynamical friction (~kpc scales)
2. Stellar loss-cone scattering (~1- 10 pc scales)
3. Gas drag from a circumbinary, viscous disc (~10^{-3}-5 pc)
4. GW emission (~10^{-5}-5 pc)

The $f^{-2/3}$ powerlaw assumes purely GW driven coalescence.

More realistic models that include environmental interactions result in a spectral turnover, which for high eccentricities could be in the Pulsar timing array window.

4. KETJU initial conditions and simulations

<table>
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<th>Run</th>
<th>(m_{\bullet 1}(10^9 M_\odot))</th>
<th>(m_{\bullet 2}(10^9 M_\odot))</th>
<th>(M_\star(10^{10} M_\odot))</th>
<th>(N_\star(\times 10^6))</th>
<th>(q)</th>
<th>(a_0) (pc)</th>
<th>(e_0)</th>
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<td>1.7</td>
<td>49.8</td>
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<td>0.958</td>
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<tr>
<td>B</td>
<td>10.2</td>
<td>1.7</td>
<td>58.1</td>
<td>5.81</td>
<td>6:1</td>
<td>5.45</td>
<td>0.971</td>
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<tr>
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<td>11.9</td>
<td>1.7</td>
<td>66.4</td>
<td>6.64</td>
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<tr>
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<td>1:1</td>
<td>0.520</td>
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</tr>
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</table>

- Our collisionless (no gas) initial conditions are modelled using isotropic Dehnen profiles (\(\gamma=1.5\) or \(\gamma=1.0\)) for the stars and \(\gamma=1.0\) for the dark matter, including a central SMBH.

\[
\rho(r) = \frac{(3 - \gamma)M}{4\pi} \frac{a}{r^{\gamma}(r + a)^{4-\gamma}}
\]

- We simulate unequal-mass mergers of very massive core galaxies (runs A-D) and one lower mass equal-mass merger (run X).

- The final phases of the SMBH inspirals are simulated at very high resolution starting at a separation of \(a_0\), with initial eccentricities of \(e_0\).
We compare the resolved KETJU SMBH binary evolution to two semi-analytic models. 1) “Peters model”: Keplerian binary with orbit averaged leading GW emission (PN 2.5) term (Peters 1964):

\[
\frac{da}{dt} = -\frac{64}{5} \frac{G^3 m_1 m_2 M}{c^5 a^3 (1 - e^2)^{7/2}} \left(1 + \frac{73}{24} e^2 + \frac{37}{96} e^4\right)
\]

\[
\frac{de}{dt} = -\frac{304}{15} \frac{G^3 m_1 m_2 M}{c^5 a^4 (1 - e^2)^{5/2}} e \left(1 + \frac{121}{304} e^2\right)
\]

2) “Peters-Quinlan model”: Peters model + Quinlan (1996) scattering from a stellar background (H & K are fitted constants):

\[
\frac{d}{dt} \left(\frac{1}{a}\right) = -\frac{2}{GM_\mu} \frac{dE}{dt} = \frac{G \rho}{\sigma} H
\]

\[
\frac{de}{dt} = -Ka^{-1} \frac{da}{dt} = K \frac{G \rho}{\sigma} H a,
\]
• **Left:** Evolution of the semi-major axis as a function of time, the Peters models typically overpredict, whereas the Peters+Quinlan models underpredict the coalescence times. **The environment is important.**

• **Right:** The relative difference in eccentricity with respect to the resolved KETJU calculations as a function orbital frequency.
We calculate the total energy spectrum emitted over the binary lifetime \( \frac{dE_{GW}}{df} \).

A good indicator for the GWB, several sources in different phases \( \sim \) integrated emission of a single source.

Two options for calculating the spectrum:

1. **Semi-analytic (Keplerian) orbit averaged formulae**: fast and fairly accurate for \( a>100 \, R_S \).

2. **Direct discrete Fourier transform of the waveform**: allows including waveform PN corrections, significant at very small \( a<100 \, R_S \).

The two GW calculation methods are in good agreement, but since the semi-analytic method is significantly faster, we use it for large separations.
GW calculations comparisons

- The GW spectra are all fairly similar and show the characteristic peaked shape of an initially eccentric binary.

- Differences to commonly used semi-analytic models can be in excess of 10% in the Pulsar timing array bands (see insets).
• Since KETJU interfaces with GADGET, SPH can be used to resolve the large-scale hydrodynamics of the gas.
• The circumbinary disc is directly resolvable, but the individual accretion discs must be treated with a subresolution model.
• The prolonged binary phase will require improved accretion models compared to the standard Bondi-Hoyle prescription.
• Accurate dynamics combined with detailed hydrodynamics will be important for making accurate model predictions for LISA.
The KETJU code is a version of Gadget includes an algorithmically regularized chain module that makes two-body collisions integrable by a simple leapfrog integrator.

Semi-analytic models commonly used in unresolved cosmological simulations appear to give accurate enough GW emission (~10%) for PTA predictions, especially if the stellar population is modelled properly.

LISA will be most sensitive to GW signals from SMBHs with masses in range $10^6$-$10^7 \ M_\odot$, thus modelling the accurate small-scale dynamics simultaneously with the gas physics will be important.

In Helsinki the ERC KETJU project has started in July, 2019 and we are now in the process of hiring a number of dynamics/GW experts (2 postdocs (deadline 15\textsuperscript{th} November) and PhD students).