Monte Carlo methods in stellar dynamics, in application to massive black holes in galactic nuclei

Eugene Vasiliev

Lebedev Physical Institute

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Overview of stellar dynamics and classification of methods

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Overview of stellar dynamical processes

Consider stellar systems composed of a large number of stars ($N_{\star} \gg 1$, for example, a globular cluster with $N_{\star} \simeq 10^5 - 10^6$, or a nuclear star cluster with $N_{\star} \simeq 10^6 - 10^8$).

- Motion in the common gravitational field of the entire system (dynamical timescale $T_{dyn} \sim \frac{R}{V} \sim \frac{R^{3/2}}{\sqrt{GM}}$).
- ▶ Two-body interactions (relaxation timescale $T_{rel} \sim T_{dyn} N_{\star} / \ln N_{\star}$).
- Dynamical friction and mass segregation.
- Gravothermodynamics: negative heat capacity \Rightarrow core collapse.
- Three- and four-body interactions: binary stars as a heat source, soft and hard binaries, ejection of stars from the core, gravothermal oscillations, ...
- External effects (the rest of the galaxy): shocks, tidal truncation and evaporation.

Stellar dynamical methods

 Scale models for the global evolution based on energy flow arguments

(Hénon 1961,1965; Gieles+ 2014)

 Fluid/gaseous models (take moments of the Boltzmann equation, approximate the heat transfer by a closure condition equivalent to a conductive sphere).

(Lynden-Bell&Eggleton 1980; Bettwieser 1983; Louis&Spurzem 1991; Amaro-Seoane+ 2004)

Fokker–Planck models

(Cohn 1979; Quinlan&Shapiro 1990; Takahashi 1995; Einsel&Spurzem 1999)

Particle-based Monte Carlo methods

(Spitzer&Hart 1971; Hénon 1971; Marchant&Shapiro 1979)

Direct N-body simulations

(Aarseth; Heggie; Hut; Makino; McMillan; Portegies Zwart; Spurzem; and many others)

Fokker–Planck methods

- Phase-space description: the one-particle distribution function $f(\mathbf{x}, \mathbf{v}, t)$, and the gravitational potential Φ satisfying the Poisson equation $\nabla^2 \Phi(\mathbf{x}, t) = 4\pi \rho(\mathbf{x}, t) = 4\pi \int d^3 \mathbf{v} f(\mathbf{x}, \mathbf{v}, t)$.
- ► Collisional Boltzmann equation $\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} \Phi \cdot \nabla_{\mathbf{v}} f = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}.$
- ► The collision term uses the approximation of weak scattering ⇒ Fokker-Planck formulation.
- Usually one invokes orbit-averaged approximation (consider the diffusion in the phase space of integrals of motion, such as energy *E* or angular momentum *L*).
- ▶ Discretize the distribution function *f* on a grid in *E* or *E*, *L* and numerically solve the Fokker–Planck PDE to compute the time evolution of *f*.

Fokker–Planck methods

- Can include the effect of a central massive black hole (loss cone processes), mass spectrum (several one-particle distribution functions, one for each stellar mass), tidal boundary, binary heating, rotation (axisymmetric geometry), ...
- (+): Reasonably fast and gives almost noise-free solutions.
- (-): Difficult to include additional physics (such as stellar evolution, binary evolution or realistic three-body interactions); restricted to spherical or at most axisymmetric geometry.

N-body methods

- Provide the most-realistic description of the evolution of stellar system.
- May include all relevant physical processes: direct few-body interactions, stellar evolution, tidal field.
- Special algorithms and hardware are required to cope with enormous dynamical range (especially in the presence of hard binaries – timescales from days to Gyr): adaptive individual timesteps; regularization of two-body motion and few-body encounters, neighbour schemes to split the close(fast) and distant(slow) interactions; hardware acceleration (GRAPE and GPU boards); non-trivial parallelization approaches; ...
- ▶ Most computationally intensive: a $N_{\star} = 5 \cdot 10^5$ simulation of the globular cluster M4 took 3 years...

Monte Carlo methods

- Stand in between Fokker–Planck and N-body methods in terms of both realism and computational demand.
- May be considered as a way of solving the Fokker-Planck equation by the method of characteristics (discrete tracer particles moving in the phase space) instead of traditional grid-based PDE solution.
- Due to particle-based nature of the model, it is easy to include additional physical effects (as in direct *N*-body simulations), such as stellar evolution, continuous mass spectrum, binary stars, few-body scattering, stellar mergers, etc.
- Designed to study relaxation phenomena, do not resolve processes on dynamical times (assume dynamical equilibrium).
- Existing implementations restricted to spherical geometry (with the exception of the present study).

Monte Carlo methods – classification

Name	Reference	relaxation treatment	timestep	1:1 ¹	BH ²	remarks
Princeton	Spitzer&Hart(1971), Spitzer&Thuan(1972)	local dif.coefs. in velocity, Maxwellian background $f(r, v)$	$\propto T_{dyn}$	-	_	
Cornell	Marchant&Shapiro (1980)	dif.coef. in E , L , self-consistent background $f(E)$	indiv., <i>T_{dyn}</i>	-	+	particle cloning
Hénon	Hénon(1971)	local pairwise interaction, self-consistent bkgr. $f(r, v_{\parallel}, v_{\perp})$	$\propto T_{rel}$	-	-	
	Stodółkiewicz(1982) Stodółkiewicz(1986)	Hénon's	block, $T_{rel}(r)$	-	-	mass spectrum, disc shocks binaries, stellar evolution
	Giersz(1998)	same	same	+	_	3-body scattering (analyt.)
Mocca	Hypki&Giersz(2013)	same	same	+	-	single/binary stellar evol., few-body scattering (num.)
	Joshi+(2000)	same	$\propto T_{rel}(r=0)$	+	_	partially parallelized
Смс	Umbreit+(2012), Pattabiraman+(2013)		(shared)	+	+	fewbody interaction, single/ binary stellar evol., GPU
${\rm Me}({\rm ssy})^2$	Freitag&Benz(2002)	same	indiv. $\propto T_{rel}$	-	+	cloning, SPH physical collis.
Raga	this study (Vasiliev 2014)	local dif.coef. in velocity, self- consistent background $f(E)$	${\rm indiv.} \propto {\rm T_{dyn}}$	-	+	arbitrary geometry

 $^1 \ensuremath{\mathsf{One-to-one}}$ correspondence between particles and stars in the system

 $^2 \, {\rm Massive}$ black hole in the center, loss-cone effects

The Hénon's Monte Carlo approach

- **0.** Assume spherical symmetry and dynamical equilibrium.
- 1. Each particle is characterized by its energy \mathcal{E}_i and angular momentum \mathcal{L}_i .
- 2. To distribute particles in space, use the Monte Carlo sampling: the probability of finding a particle in the interval [r .. r + dr] is proportional to the time spent in this interval

$$dr/v_r = dr/\sqrt{2(\mathcal{E}_i - \Phi(r)) - \mathcal{L}_i^2/r^2}.$$

- 3. Sort particles in radius and compute the potential using recurrence relation $\Phi(r_i) = \sum_{j=1}^{i} \frac{Gm_j}{r_i} + \sum_{j=i+1}^{N} \frac{Gm_j}{r_j}$.
- 4. Simulate the effect of two-body relaxation by pairwise interactions between adjacent stars that change their \mathcal{E} and \mathcal{L} . The timestep for this simulation is $\propto T_{\rm rel}$.
- 5. Model additional effects such as stellar evolution, few-body interactions, collisions or loss-cone captures.
- 6. Repeat.

Relaxation in the Hénon's approach

- The relaxation process is a cumulative effect of a multitude of two-body encounters, each one changes the velocity of the star only slightly.
- ▶ In a single encounter with a field star 2, the velocity of test star 1 is changed by $\Delta v_1 = \frac{m_2}{m_1+m_2} v_{rel} 2 \sin(\beta/2)$, where β is the deflection angle: $\sin \beta/2 = \frac{G(m_1+m_2)}{v_{rel}^2 \rho}$, v_{rel} is the relative velocity, and p is the impact parameter.
- ► The cumulative effect of many encounters with all possible impact parameters during a time interval Δt is given by $\langle \Delta v_1^2 \rangle = 8\pi G^2 \ln \Lambda \langle \nu_2 m_2^2 v_{\text{rel}}^{-1} \rangle \Delta t$, where ν_2 is the local number density of field stars.
- ▶ Instead of simulating all these independent encounters, one replaces them with one representative interaction with deflection angle β_{eff} whose statistical properties are the same: equating the mean values of $\langle \Delta v_1^2 \rangle$ gives $\sin^2(\beta_{eff}/2) = 2\pi G^2 (m_1 + m_2)^2 v_{rel}^{-3} \nu_2 \Delta t \ln \Lambda$, and equating the dispersion additionally requires $2 \sin^2(\beta_{eff}/2) = 1/\ln \Lambda$.

Relaxation in the Hénon's approach

- Simulate the effect of two-body relaxation in a statistical sense by following a single scattering event for each particle (encounter with another particle, adjacent in radius).
- Pick up two stars that are neighbours in radius (to sample the local velocity distribution properly).
- From the energy *E_i*, angular momentum *L_i* and radius *r_i*, compute the radial and tangential components of velocity *v_{||}*, *v_⊥* of each particle and their relative velocity *v_{rel}* (assuming random orientation of tangential components).
- ► Assign the effective deflection angle β_{eff} of the single encounter using the above definition; it should not be too large, since we are simulating slow diffusion and not strong scattering, which imposes an upper limit on the timestep Δt.
- ► Compute new values of *E_i*, *L_i* after the encounter; repeat for all particles.

Hénon's Monte Carlo approach in practice

- This formulation of Monte Carlo method was proposed by Michel Hénon in 1971.
- Further improved by Stodółkiewicz(1982,1986), who introduced individual timesteps and developed probably the first "all-in-one" simulation code that included tidal field and shocks, primordial and dynamically formed binaries, stellar evolution.
- Starting in late 1990s, three independent implementations have been put forward by Giersz (Copernicus astronomical center in Warsaw), Rasio et al. (Northwestern University, Illinois), and Freitag (Bern). The first two are being actively developed at present, include a wide range of additional physical effects and are used for studies of globular clusters in our Galaxy. The third implementation was more specifically targeting galactic nuclei, included a detailed treatment of stellar collisions and loss cone effects.

Other Monte Carlo approaches

Spitzer&Hart(1971) proposed a different way of simulating the relaxation: instead of pairwise interactions, one applies a perturbation to velocity based on local (position-dependent) firstand second-order diffusion coefficients:

$$\begin{split} \Delta v_{||} &= \langle \Delta v_{||} \rangle \Delta t + \zeta_1 \sqrt{\langle \Delta v_{||}^2 \rangle \Delta t} \,, \quad \Delta v_{\perp} &= \zeta_2 \sqrt{\langle \Delta v_{\perp}^2 \rangle \Delta t} \,, \\ \text{where } \zeta_1, \zeta_2 \text{ are two independent normally distributed random } \\ \text{numbers, } \Delta t \text{ is the timestep, and the coefficients} \\ \langle \Delta v_{||} \rangle, \langle \Delta v_{||}^2 \rangle, \langle \Delta v_{\perp}^2 \rangle \text{ are computed from the two-body relaxation} \\ \text{the ory, averaging the deflection in a single encounter not only over } \\ \text{the impact parameter (as in Hénon's method), but also over the magnitude and orientation of \mathbf{v}_{rel}. } \end{split}$$

Thus instead of individual pairwise encounters all stars independently diffuse in the phase space.

In the original Spitzer's formulation, orbits of stars are integrated numerically with timestep $\Delta t \ll T_{\rm dyn}$, but he used a simplifying assumption of spherical symmetry.

Other Monte Carlo approaches

 Spitzer&Shapiro(1972) went one step further and switched from local diffusion coefficients in velocity to the coefficients in energy *E* and angular momentum *L*, averaged over radial motion (assuming spherical symmetry):

$$\begin{split} \langle \Delta E \rangle &= v \langle \Delta v_{\parallel} \rangle + \frac{1}{2} \langle \Delta v_{\parallel}^2 \rangle + \frac{1}{2} \langle \Delta v_{\perp}^2 \rangle , \quad \langle \Delta E^2 \rangle = v^2 \langle \Delta v_{\parallel}^2 \rangle , \quad \dots, \\ \langle X \rangle_{\mathsf{avg}} &\equiv \left[\int_{r_{\mathsf{peri}}}^{r_{\mathsf{apo}}} \frac{dr \langle X \rangle}{v_{\mathsf{rad}}} \right] \middle/ \left[\int_{r_{\mathsf{peri}}}^{r_{\mathsf{apo}}} \frac{dr}{v_{\mathsf{rad}}} \right]. \end{split}$$

In this orbit-averaged approach, one does not need to integrate the orbits explicitly, just follow the changes in particle's integrals of motion $\mathcal{E}_i, \mathcal{L}_i$ which occur on the relaxation timescale.

Shapiro et al. further developed this approach to include the effect of a central massive black hole (capture of particles with low L), stellar collisions, adaptive refinement of particles in central region of the model, and other sophistications.

Interlude: simulations of collisionless systems

A stellar system in which the relaxation time $T_{rel} \gg T_{Hubble}$ is called collisionless. Example: massive galaxies, but not necessarily ultracompact dwarf galaxies or nuclear star clusters. The evolution of such systems is governed by the collisionless Boltzmann equation (CBE) for the distribution function $f(\mathbf{x}, \mathbf{v}, t)$, which may be solved by

- direct integration of CBE on a grid in phase space;
- method of characteristics: sample the distribution function by N particles and allow them to move in the mean gravitational field. The key difference between methods is the way of solving the Poisson equation:
 - Grid-based methods (including adaptive mesh refinement) employ
 Fourier transform to find the potential discretized on a grid in space;
 - Direct summation over all particles (impractical) or an approximation based on a hierarchical spatial tree or the fast multipole method;
 - For systems with well-defined center expansion of potential/density pair over a suitable basis set, usually involving spherical harmonics.

Self-consistent field method

The idea is to expand both density and potential of the system using a suitable (usually orthogonal) set of basis functions which are themselves solutions of Poisson equation (Hernquist&Ostriker 1992):

$$ho(\mathbf{x}) = \sum_{\mathbf{n}} \mathcal{C}_{\mathbf{n}}
ho_{\mathbf{n}}(\mathbf{x}) \ , \ \ \Phi(\mathbf{x}) = \sum_{\mathbf{n}} \mathcal{C}_{\mathbf{n}} \Phi_{\mathbf{n}}(\mathbf{x}) \ , \ \
abla^2 \Phi_{\mathbf{n}}(\mathbf{x}) = 4 \pi
ho_{\mathbf{n}}(\mathbf{x}) \ ext{for } orall \mathbf{n}.$$

Usually one takes the basis functions to be products of some function in radius and spherical harmonics:

$$\begin{split} \Phi_{\mathbf{n}}(\mathbf{r}) &= \Phi_{n,l}(\mathbf{r}) \ Y_{l}^{m}(\theta,\phi); \ \mathbf{n} \equiv \{n,l,m\}. \\ \text{The coefficients of expansion } C_{\mathbf{n}} \text{ are computed from the positions} \\ \text{of all } N \text{ particles as } C_{\mathbf{n}} &= \int d^{3}\mathbf{x} \ \Phi_{\mathbf{n}}(\mathbf{x}) \ \rho(\mathbf{x}) = \sum_{i=1}^{N} \Phi_{\mathbf{n}}(\mathbf{x}_{i}) \ m_{i}. \end{split}$$

The simulation workflow is:

- 1. Compute the coefficients of potential from particle positions;
- 2. Move particles according to forces obtained by differentiating the potential, with a timestep $\Delta t \ll T_{\rm dyn}$.

Self-consistent field method

- This method works rather accurately for systems that have a well-defined center and are well approximated by a moderate number (~ few dozen) of expansion terms.
- Since particles do not interact with each other explicitly, but their motion is mediated by a smooth potential which represents the mean field, this method is well suited for collisionless simulations.
- However, it is not entirely free of numerical relaxation, since the discreteness noise in the expansion coefficients lead to time-dependent fluctuations in the potential. In fact, the magnitude of numerical relaxation is only a factor of few lower that for other methods with the same N.
- A possible way to reduce fluctuations:
 - 1. use longer time intervals between updating the potential expansion coefficients (but keep short enough timesteps for integrating the orbits);
 - 2. during each update interval, store several sampling points for each particle, to increase the effective number of points used in computing coefficients and hence to reduce discreteness noise.

Temporal smoothing in the SCF method

Using a longer interval between potential recomputation and increasing the number of sampling points per particle does help to reduce the artificial relaxation rate by 1-2 orders of magnitude.



The novel Monte Carlo method for arbitrary geometry

The combination of the temporally-smoothed SCF approach for representing arbitrary non-spherical potential with the Spitzer's formulation of two-body relaxation using local velocity diffusion coefficients leads to a new implementation of the Monte Carlo method suitable for arbitrary geometry.

Gravitational potential:

particles move in a smooth potential represented by a basis-set expansion.

Orbit integration:

variable timestep Runge-Kutta; orbits are computed in parallel, independently from each other, during each update interval.

Two-body relaxation:

apply perturbation to particle velocity using local diffusion coefficients.

Potential and distribution function update:

update interval \gg dynamical time \Rightarrow temporal smoothing; use many sampling points per particle during each update interval \Rightarrow reduce discreteness noise.

The treatment of two-body relaxation

Local (position-dependent) velocity diffusion coefficients:

$$egin{aligned} & \mathbf{v}\langle\Delta\mathbf{v}_{\parallel}
angle = -\left(1+rac{m}{m_{\star}}
ight)I_{1/2}\;, \ & \langle\Delta\mathbf{v}_{\parallel}^{2}
angle = rac{2}{3}\left(I_{0}+I_{3/2}
ight), \ & \langle\Delta\mathbf{v}_{\perp}^{2}
angle = rac{2}{3}\left(2I_{0}+3I_{1/2}-I_{3/2}
ight), \end{aligned}$$

here m and m_{\star} are masses of the test and field stars, and



After each timestep, the perturbations to the velocity are computed as

$$egin{aligned} \Delta m{v}_{\parallel} &= \langle \Delta m{v}_{\parallel}
angle \Delta t + \zeta_1 \sqrt{\langle \Delta m{v}_{\parallel}^2
angle \Delta t} \,, \ \Delta m{v}_{\perp} &= \zeta_2 \sqrt{\langle \Delta m{v}_{\perp}^2
angle \Delta t} \,, \end{aligned}$$

where ζ_1, ζ_2 are two independent normally distributed random numbers.

Application to massive black holes in galactic nuclei

The primary motivation for the development of the new Monte Carlo method is to study the dynamical evolution of galactic nuclei with single/binary massive black holes (MBH).

- Stars with low angular momentum interact with the central MBH(s): are captured, tidally disrupted, or scattered away by the binary.
- These processes depend on the efficiency of angular momentum variation of stars, which changes both due to two-body relaxation (collisional) and because of torques in a non-spherical potential (collisionless).
- ► The number of stars in a realistic galactic nucleus (10⁶ 10⁹) far exceeds the presently accessible range for collisional N-body simulations.
- Scaling to a different number of particles would distort the interplay between collisional and collisionless effects.
- Need to adjust the relaxation rate independently from the particle number.

The new Monte Carlo method is ideally suited for this task.

Loss cone in non-spherical stellar systems

The loss cone is the low angular momentum region of phase space, where stars are interacting with the single or binary black hole and are eliminated from the system (captured or ejected).

In a non-spherical potential, the angular momentum ${\cal L}$ of any star is not conserved, but experiences oscillations.

Therefore, much larger number of stars can attain low values of \mathcal{L} and enter the loss cone at some point in their (collisionless) evolution, regardless of two-body relaxation.



An example of orbit in a triaxial potential



Feeding rates of a single MBH

The Monte Carlo method has been applied to the problem of massive black hole by star captures. We computed the capture rates for a family of models of galactic nuclei (the black hole mass M_{\bullet} ranging from 10^7 to $10^9 M_{\odot}$ and the radius of influence given by $r_{\rm infl} = 45 \left(M_{\bullet}/10^8 M_{\odot}\right)^{0.56}$ pc), in three geometries.

These models are far beyond the reach of conventional *N*-body simulations, although we have calibrated the Monte Carlo code against a direct *N*-body simulation in the low *N* regime $(\leq 10^6)$.

Black holes with $M_{\bullet} \gtrsim 10^7 M_{\odot}$ are deep in the empty loss cone regime, and the inclusion of non-spherical torques greatly increases the capture rate.

This study confirmed our earlier analysis based on the Fokker–Planck formalism, and extended it to triaxial systems.



Evolution of binary MBH and the final-parsec problem

- Galaxy mergers result in formation of binary MBH.
- A star passing near the orbit of a binary MBH experiences a complex 3-body interaction, which typically results in the ejection of the star with a higher energy than it had before the encounter. Thus a star carries away the energy and angular momentum from the binary, so that its semimajor axis *a* decreases.
- ▶ If the density of incoming stars is kept constant, the binary shrinks at a constant rate: $\frac{d}{dt}\left(\frac{1}{a}\right) \approx 16\frac{G\rho}{\sigma} \equiv H_{\text{full}}$ [Quinlan 1996].
- ► However, the reservoir of low-L stars (the loss cone) is quickly depleted, so in the absense of efficient repopulation mechanisms the binary stalls at a separation a ~ 1 pc.
- ► This has been called the final-parsec problem [Milosavljevic&Merritt 2002].
- ► If, however, the loss cone is refilled efficiently enough, the binary continues to shrink, and below a ~ 10⁻² pc the emission of gravitational waves leads to a quick coalescence.

Evolution of binary MBH and the final-parsec problem



[[]from Khan+ 2012]

Evolution of binary MBH with the Monte Carlo method

Follow the evolution of binary MBH in a series of short "episodes":

- during each episode, evolve particles in a time-dependent potential of binary MBH moving on a Keplerian orbit with fixed parameters;
- at the end of episode, record the changes of energy and angular momentum of each particle during each close encounter with the binary, sum them up and adjust the orbit of the binary using conservation laws [e.g. Sesana+ 2007, Meiron&Laor 2012];
- this automatically provides the correct rate of the loss cone repopulation (due to both non-spherical torques and two-body relaxation) and change of shape of the gravitational potential.

Preliminary results of Monte Carlo simulations

- ► Monte Carlo simulations are in qualitative agreement with direct N-body simulations, performed with N ≤ 10⁶ (verification of the method).
- The rate of binary shrinking does not stay constant, but decreases with time; it is never even close to the full loss cone rate H_{full}.



Preliminary results of Monte Carlo simulations

- ► Monte Carlo simulations are in qualitative agreement with direct N-body simulations, performed with N ≤ 10⁶ (verification of the method).
- The rate of binary shrinking does not stay constant, but decreases with time; it is never even close to the full loss cone rate H_{full}.
- Long-term evolution of both spherical and axisymmetric systems leads to the stalling of the binary in the absense of relaxation.
- In the triaxial case there is no stalling, and little additional "benefit" from relaxation (loss cone repopulation is mainly due to collisionless torques).



Summary

- The Monte Carlo method for dynamical evolution of stellar systems offers an efficient and rather accurate alternative to direct *N*-body simulations, and can be applied in the regime of high *N* which is presently infeasible for direct simulations.
- An extension of the method to non-spherical geometry is rather straightforward and is based on the self-consistent field method with temporal smoothing.
- This method is very well suited to simulations of galactic nuclei with massive black holes, due to its ability to properly represent the balance between collisionless and collisional effects by adjusting the relaxation rate.
- ▶ Its application to the feeding of MBH by stellar captures shows that in axisymmetric and triaxial systems this feeding rate is much higher than in the spherical case, especially for $M_{\bullet} \gtrsim 10^8 M_{\odot}$.
- Another application to the evolution of binary MBH demonstrates that the final-parsec problem in the collisionless limit still exists in spherical and axisymmetric cases, but not in the triaxial one.