Errors, chaos and the collisionless limit

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ABSTRACT

We simultaneously study the growth of errors and the question of the faithfulness of simulations of \(N\)-body systems. The errors are quantified through the numerical reversibility of trajectories of small-\(N\) spherical systems integrated to high accuracy. Initially, the errors add randomly, before exponential divergence sets in. Though the exponentiation rate is virtually independent of \(N\), the instability saturates at scales \(1/\sqrt{N}\). This is interpreted by adopting a model due to Goodman, Heggie & Hut (1993). In the third phase, the (diminished) growth is initially driven by multiplicative enhancement of errors as in the exponential stage. It is then qualitatively different for the errors in the phase space variables and the mean field conserved quantities (energy and momentum); the former grow systematically through phase mixing while the latter grow diffusively.

For energy, the \(N\)-variation of the ‘relaxation time’ of error growth follows expectations of two-body relaxation theory. This is not the case for angular momentum, at least up to the particle numbers and timescales considered, and even less so for the velocities. Due to increasingly smaller saturation scales, the information loss associated with the exponential instability decreases with \(N\), especially when viewed in terms of the mean-field conserved quantities. Indeed, the dynamical entropy vanishes at any finite resolution as \(N \to \infty\). In this sense there is convergence to the collisionless limit and confidence that numerical simulations may faithfully represent it, despite the exponential instability and loss of information on phase space trajectories. Nevertheless, the rapid initial growth of errors and the relatively slow \(N\)-variation in its saturation, point to the slowness of the convergence.

Key words: methods: numerical — stellar dynamics — instabilities — chaos — diffusion — gravitation

1 INTRODUCTION

Numerical simulations of Newtonian gravitational systems have long been indispensable to understanding structure formation in the universe and the evolution of galaxies, galaxy clusters and stellar clusters (e.g. Heggie & Hut 2003; Dehnen & Read 2011; Springel 2016). Yet, despite decades of steady increase in sophistication and efficiency, relatively little progress has been made in assessing the accuracy of the \(N\)-body numerical realizations of such systems, or even the qualitative faithfulness of the results obtained to the ‘true’ dynamics. Indeed, increasing efficiency has required larger toleration of errors; in many large simulations, gravitational forces are approximated through methods that are accurate only at the percent level, and low (usually second) order integrators with fixed time-steps are used.

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with the action and angle variables of systems composed of regular trajectories, which will translate to at most polynomial divergence in the phase space coordinates (for a general discussion of regular versus chaotic trajectories in the context of galactic dynamics see, e.g., Binney & Tremaine 2008; hereafter BT). This implies that accurate solutions can in principle be obtained by increasing the order of the integrator and decreasing the time-step. A remedy that does not apply in the presence of the exponential instability, which is invariably displayed by N-body gravitational systems, where it also comes with a timescale that is largely independent of (and may even slowly decrease with) \( N \) (GHH; Hensendorf & Merritt 2002).

Despite this, it is widely believed that N-body simulations do reproduce the correct qualitative behaviour of the modelled systems. In some sense, this is a statistical statement. It embodies the belief that even when the correct trajectories cannot be captured, bulk quantities such as the density and velocity distributions should be more robust and survive numerical errors. This statistical faithfulness may be assessed in terms of the proper rendering of the gross structure of the system, as characterized by the distribution function and the moments derived from it. In this context, confidence in the faithfulness of the simulations stems from the general similarity and stability of gross characteristics (e.g., density and mean velocities and velocity dispersions), when large-N systems are simulated from different initial conditions taken from the same statistical distributions. This stability persists even when different simulation techniques are used, though there is no guarantee that all results are not equally wrong. More rigorous justification of the faithfulness of results may be sought in terms of the existence of shadowing trajectories, though this is generally quite difficult to prove and has only been studied in idealized cases (Quinlan & Tremaine 1992; Hayes 2003). On the other hand, it is known that at least in models where collective instabilities are present, numerical implementation and associated error can play an important role in determining the macroscopic evolution (Sellwood & Debattista 2009; Benhaie et al. 2018). Understanding their role may also be of importance in the context of interpreting the results of cosmological simulations (Thiebaut et. al. 2008; Keller et. al. 2018).

The robustness of the results of simulations can also be viewed in terms of the orbital structure. In general, the phase space of Hamiltonian systems can exhibit a variety of regular and chaotic orbital families (e.g., Lichtenberg & Lieberman 1992; BT), and a numerical method can be said to faithfully represent the dynamics if it qualitatively captures these structures. This again reflects the intimate link between dynamical properties of the system and questions of accuracy and faithfulness of representation via numerical simulation. A N-body trajectory moves in a 6N dimensional phase space; and is, most generally, only constrained by globally conserved quantities, such as the total energy and angular momentum. Nevertheless, in the collisionless limit, as \( N \rightarrow \infty \), the N-body problem should be effectively reduced to that of \( N \) independent systems, as each particle moves in the (self consistent) mean field produced by all the other particles. The relevant phase space structure is six dimensional. If, furthermore, this mean field is time independent and possesses sufficient symmetry, the system is ‘separable’ and the problem is further reduced to that of \( 3N \) independent one dimensional oscillators. In a six dimensional phase space, particles trajectories are confined on tori that can be characterized by conserved quantities, and parametrised for example by action variables describing the amplitudes of the oscillations and angles following the phases. The difference between phases of orbits parametrised by different values of the actions diverge only linearly in time (BT).

A particularly simple and important example is that of a large-N spherical system in a steady state, where each trajectory conserves energy and the components of the angular momentum. The persistence of the exponential instability in this case stands in apparent contradiction to its description in the terms outlined above, proper to the collisionless limit. Nevertheless, as long as the quantities characterising the tori remain reasonably well conserved, the motion will remain qualitatively similar to that in the smooth potential. Indeed, the key feature comes from theoretical arguments and idealized numerical experiments suggesting that the exponential instability is precipitated by relatively close two-body encounters between particles and tends to saturate as the particle number increases, occurring on progressively smaller scales with increasing \( N \) (GHH; Valluri & Merritt 2000; Kandrup & Sideris 2001; Sideris & Kandrup 2002). For example, trajectories moving in a ‘gravitational Lorentz gas’ of fixed particles appear to follow their smooth potential counterparts with increasing precision as the number of fixed particles is increased. The exponential instability timescale itself also increases with \( N \) when softening is introduced (GHH; Huang, Dubinski, & Carlberg 1993; El-Zant 2002).

Although divergence between nearby trajectories implies loss of information concerning integrated trajectories, we will see here that this loss indeed decreases with \( N \) as the instability saturates on progressively smaller scales, even if the exponentiation rate for infinitesimally close trajectories does not decrease with \( N \). Moreover, errors in mean field conserved quantities eventually follow a slow diffusive growth (on timescale comparable to the two body relaxation time in case of energy). The associated total loss of information is thus smaller still. This is the case even if the initial exponential divergence affects these quantities with the same characteristic timescale as the phase space variables. Since, statistically, spherical steady state systems are described by a distribution function composed of the integrals of motion (the energy and angular momentum) of particle trajectories moving in the smooth potential, it is sufficient that the numerical integration of the N-body system preserves the energy and angular momenta of each particle in order to faithfully reproduce the statistical properties described by the distribution function.

In this context, the purpose of the present study was twofold: to examine the divergence of trajectories and its dynamical implications for both the phase space variables and the mean field conserved quantities, and to do this in a way that relates the associated information loss to the accuracy and faithfulness of numerical representations of the dynamics. For this purpose, we examined the time-reversibility of a large number of spherical N-body systems integrated with high precision. In principle, these systems, as all Hamiltonian systems, should be exactly time reversible when the velocities are reversed. Nevertheless, this is not generally the
case with their numerical image; the exponential divergence of trajectories, and associated loss of information, renders them irreversible if a general integrator is used (e.g. Hoover & Hoover 2012). In the context thus set, a simulation can be considered ‘inaccurate’ on timescales on which information loss leads to irreversibility in the phase space variables (positions and velocities), but is only ‘unfaithful’ over timescales on which the mean field conserved quantities in the reversed system differ considerably from the originals. We will use this diagnostic in drawing conclusions concerning the implications, physical and numerical, of ‘chaos’ in N-body gravitational systems.

In the next section we describe the numerical setup for our simulations and the method through which the estimates of error growth are evaluated. Section 3 constitutes the bulk of this study. We start by delineating the differences, crucial to the interpretation of our results, between systematic, diffusive and exponential growth of the errors, presenting estimates of the expected numerical errors. We then report the numerical results. The saturation of the instability is explained in terms of a model due to GHH. This predicts the persistence of systematic growth after the saturation of the exponential divergence. In the case of the phase space variables this is followed by evolution by simple phase mixing; in the mean field conserved quantities it is followed by the onset of diffusion, which turns out to be quite different for the case angular momentum as compared with energy. Finally, we evaluate ‘relaxation times’, associated with the growth of errors in the different quantities, contrasting the growth of velocity errors (a standard benchmark in calculations of two-body relaxation) with the that in angular momentum and energy. We summarise these results in Section 3.5. In Section 4 we discuss whether N-body systems can be truly characterised as ‘chaotic’ on any non-infinitesimal scale on the phase space as $N \to \infty$, given the progressively smaller loss of information, particularly as associated with the mean field conserved quantities (a more formal discussion of the relation between chaos, information loss and effective irreversibility is given in the Appendix).

2 NUMERICAL SETUP

2.1 Reversibility as a probe of numerical accuracy and faithfulness

Newtonian N-body systems obey equations where the time variable appears exclusively in second order form. These systems are thus time reversible in principle: an N-body trajectory integrated backwards (after reversing the velocities at the end point) should return exactly to its initial conditions, with all particle positions and (reversed) velocities recovered; an integration, iterated backwards with infinitesimal step size, is the reversed solution, with

\[ f(t) \to f(-t), \]

then reverses velocities and integrates backward for another timespan $t_f$ one should find (for $t > t_f$)

\[ \mathbf{r}(t_f) = \mathbf{r}(2t_f - t) \quad \text{and} \quad \mathbf{v}(t_f) = -\mathbf{v}(2t_f - t). \]

Numerically, however, the situation is different. Even assuming that the forces are calculated to machine precision, there will be roundoff errors in these, as well as in the phase space variables themselves (including the initial conditions). Finite time-stepping also leads to truncation errors. If the errors are sufficiently inflated by intrinsic divergence of trajectories, numerical irreversibility will result, as the accumulating errors in the forward and backward trajectories diverge. It is of course possible to employ formally reversible algorithms; the symplectic mapping embodied in the widely used leapfrog integrator is one such scheme. Nevertheless, what is reversible in this case is a system with a perturbed Hamiltonian, corresponding to the mapping, and truncation errors will persist despite the step-wise reversibility unless the time-step is infinitesimally small. In addition, due to floating point error accumulation, the integration is truly reversible only if integer arithmetic on a lattice is used, as opposed to the usually employed finite precision floating point arithmetic (Hoover & Hoover 2012). Furthermore, limitations associated with implementations of integer arithmetic in practice impose a minimal time-step that is too large to be compatible with acceptable truncation errors (Earn 1994). Finally, even formal reversibility is generally lost when a variable time-step is introduced, even when a reversible integrator is used; and devising a reversible scheme with variable time-stepping is a highly non-trivial task (Dehnen 2017). This makes it difficult, if not impossible, to estimate local truncation errors using conventional methods, which rely on step-size variation, and at the same time maintain numerical reversibility.

In this study, we use a conventional Runge-Kutta integrator with an adaptive time-step determined from a preset tolerance (Press et. al. 2007). The error estimate at each time-step is determined by decreasing the time-step until the tolerance criterion is achieved; namely when the maximum (mixed) error in any one of the phase space variables (any of the positions or velocity coordinates) is smaller than $Tol = 10^{-8}$. This value will be compared with error estimates resulting from comparison of the forward and backward trajectories. As opposed to symplectic integrators, there are no special provisions preventing the loss of information from being equally manifest in both the irreversibility of the of the phase space variables and of the mean-field conserved quantities. This also makes the method convenient for comparing information loss in these quantities, which turns out to be qualitatively different.

2.2 Initial conditions

We start with random realisations of Plummer spheres (e.g., BT). These are simple spherical models that have long formed a benchmark of sorts for theoretical studies of the Newtonian N-body problem. The mass distribution as a function of radius is given by

\[ M(r) = M \frac{r^3}{(r^2 + a^2)^{3/2}}, \tag{1} \]

where $M$ is the total mass of the system and $a$ is a length scale within which the density distribution varies slowly. We take $G = M = a = 1$. We define a mean dynamical time as $t_D = 1/\sqrt{GM(<r)f}$, so that each time unit in our simulations corresponds to about $1/t_D$. The virial radius is at $R_v = a$. The dynamical time there is $t_D(R_v) = 6.4$ time units.
The initial conditions are obtained through the technique of Aarseth, Henon & Wielen (1974). The Newtonian equations of motion, with double precision and direct force evaluation, are integrated using a variable step-size Runge-Kutta method with error tolerance of 10^{-8} per time-step as described above. Direct force calculation and high accuracy requirement naturally limit the number of particles in the systems we probe. In partial compensation for this, we improve the statistics by running a number of random realizations for each N. This enables one to get better statistics with only linear increase (with N) in CPU-time, while the time required for the exact force calculations scales as N^2. We performed 101 runs for systems with N = 128, 256, 512 and 1024, 28 runs with N = 2048, 17 runs with N = 4096 and three runs with N = 8192.

Each random realization is integrated forward in time for a hundred time units. The velocities are then reversed and the system is integrated backwards for another hundred time units. At each point in the reversed trajectory, we measure the differences in the phase space variables (positions and velocities) and the mean field conserved quantities (energies and angular momenta) with corresponding points in the forward trajectory. We thus evaluate the relative and RMS errors, as described below.

### 2.3 Error estimates from simulations

To estimate the errors from the difference in particle positions between the forward and reversed trajectories we calculate

\[
\xi_q^2 = \sum_{N} \left( x_f - x_b \right)^2 + \left( y_f - y_b \right)^2 + \left( z_f - z_b \right)^2 \cdot \frac{1}{\sum_{N} x_f^2 + y_f^2 + z_f^2},
\]

(2)

where \( x_f \) corresponds to a particle's Cartesian \( x \) coordinate in the forward run and \( x_b \) to the value of the corresponding coordinate in the reversed run, when the system is integrated backwards. Errors \( \xi = \xi(t) \) are obtained by subtracting forward-run coordinates at that time \( t \) from the corresponding coordinates in the reversed run identified at \( 2t - t \).

For the simulations studied here, the integration time in either direction \( t_f = 100 \) time units, corresponding to about 29 dynamical times at \( r = 1 \) and 16 dynamical times at the virial radius.

Since when the dynamics is reversed the velocities are also reversed (and their Cartesian components change sign) the corresponding formula in this case is

\[
\xi_q^v = \sum_{N} \left( x_f + x_b \right)^2 + \left( y_f + y_b \right)^2 + \left( z_f + z_b \right)^2 \cdot \frac{1}{\sum_{N} x_f^2 + y_f^2 + z_f^2}.
\]

(3)

Similarly for the angular momenta we have

\[
\xi_L^2 = \sum_{N} \left( L_x f + L_x b \right)^2 + \left( L_y f + L_y b \right)^2 + \left( L_z f + L_z b \right)^2 \cdot \frac{1}{\sum_{N} L_x^2 + L_y^2 + L_z^2}.
\]

(4)

Finally, the errors in energies are calculated from

\[
\xi_E^2 = \sum_{N} \left( E_f - E_b \right)^2 \cdot \frac{1}{\sum_{N} E_f^2}.
\]

(5)

In what follows, we refer to these quantities as the 'relative errors' in the various variables. We will also use the absolute RMS errors, these are obtained by replacing the denominators in the above equations by \( N \).

### 3 PROPAGATION OF ERRORS

#### 3.1 Estimates of Systematic, diffusive and exponential error propagation

#### 3.1.1 Case I: No intrinsic divergence

If there is no intrinsic divergence in time between solutions of initial value problems started with different initial conditions, then the only source of varying phase space separation of solutions in time will be due to numerical errors (e.g., this is the case for two numerical solutions of harmonic oscillators with the same spring constant). If the errors at each step are added, they would generally lie between two extremes; they either add up to zero, so that the RMS error is \( \sim \sqrt{n} \) after \( n \) steps, or are systematic in the sense that the errors scale as \( n \) (e.g., Press et al. 2007).

#### 3.1.2 Case II: Systems with phase mixing

A nonlinear dynamical system, even if it supports only regular trajectories with no exponential divergence, will generally exhibit phase mixing due to the dependence of the characteristic frequencies on the amplitudes of the oscillations. If the system is Hamiltonian its trajectories can always be parametrised in terms of action angle variables \( (J, \Theta) \). When the dynamical evolution is exact (without numerical errors) the actions \( J \) are constant and the angles evolve as \( \Theta = \Theta_0 + \omega t \). Since, given a set of initial condition, \( J \) does not evolve in time, the dynamics does not prompt any intrinsic divergence of nearby solutions in these variables, and the numerical errors can again propagate systematically as \( \delta J \sim n \) (where \( \delta J \) is the magnitude of the typical error per time step), or diffuse as \( \delta J \sim \sqrt{n} \). The angle variables, on the other hand, evolve linearly in time, so we expect the errors in them to propagate as

\[
\delta \Theta = \sum_{i=1}^{n} \delta \Theta_i + \sum_{i=1}^{n} \delta \Theta_i.
\]

(6)

Except for the zeroth term in the second sum, the error is expected to be dominated by truncation error rather than roundoff. As before, the truncation errors in this second sum can add up systematically to \( \sim h \delta \Theta \) or diffusively as \( \sqrt{n} \delta \Theta \). However, in addition to this, the first sum displays a linear intrinsic divergence in time. If the numerical errors in \( h \) add up systematically — that is \( \delta \omega \sim i \delta \omega \) for a typical error of magnitude \( \delta \omega \) associated with typical time-step \( \Delta t \) — the first sum becomes \( \sim \delta \omega \Delta t \sum_{i=1}^{n} \sim n \delta \omega \Delta t \). The associated relative error is then \( \frac{\delta \omega \Delta t}{\omega} \sim n \frac{\delta \omega \Delta t}{\omega} \). Similarly the error scales as \( \frac{\delta \Theta}{\Theta} \sim \sqrt{n} \frac{\delta \Theta}{\Theta} \) if the single step errors are assumed to add up diffusively.

Thus, despite the intrinsic linear divergence, nonlinear systems with regular trajectories subject only to simple phase mixing can, like their linear counterparts, be numerically integrated to arbitrary (machine dependent) precision. For example, the errors Runge-Kutta method used in this study are fifth order in the time step \( \Delta t \approx t_f/n \). They thus scale as \( \Delta t \approx 1/n^5 \). If the errors propagate at most linearly in \( n \), then the total error after \( n \) steps scales as \( \sim 1/n^4 \) or better, which clearly can be made arbitrarily small by decreasing the time-step. This will remain true even if we take into account that the phase space variables (coordinates and
velocities) of regular trajectories do not necessarily diverge linearly in time as the angle variables do (since former are expressed as Fourier series in latter; e.g., BT). It will remain true as long as the divergence can be locally characterised everywhere as a low order power law (as we will see this will be the case once the exponential instability has saturated). Finally, for such systems, the errors in mean field conserved quantities, such as the energy and angular momenta, should propagate as those in the action variables. In particular, if they are primarily driven by independent two-body encounters, the propagation in time should be diffusive (that is, \( \sim \sqrt{t} \)). Due to the weak n scaling, information loss arising from such diffusion is expected to be minimal.

### 3.1.3 Case III: Exponential divergence

In the presence of exponential divergence the situation is quite different from that outlined above. Here, a small error \( \delta X_0 = \delta X_0 \hat{E}_i \) in phase space coordinates \( X = (x, \dot{x}) \), becomes at time \( t_1 \sim \delta X_0 e^{k \Delta t} \hat{E}_1 \), where the unit vector \( \hat{E}_1 \) is in the direction to which \( \delta X_0 \) points after its transformation by the dynamics following one timestep \( \Delta t \). This is not necessarily in the direction \( \hat{E}_0 \); as the dynamical phase space flow, associated with exponential instability, not only stretches but also rotates an error vector. This acts as to align it with the unit vector \( \hat{E}_1 \). Again \( \hat{E}_1 \) is not necessarily the same as \( \hat{E}_1 \). However, since the error unit vectors appearing in such expressions are updated and superseded at each subsequent step, after \( n \) steps we can write

\[
\delta X_n = \sum_{i=0}^{n} \delta X_i e^{k(n-i)\Delta t} \hat{E}_i, \tag{7}
\]

by defining the unit vectors \( \hat{E}_i \) as those in the direction to which the errors \( \delta X_i \) arise at point \( i \), point after being transformed by the dynamics through \( n - i \) timesteps. The exponential inflation implies that, for timesteps large compared to the exponential time \( t_e \), the errors propagate in a manner that makes it impossible to obtain arbitrarily accurate solutions by decreasing the time-step.

Again one may suppose two extremes; the \( \hat{E}_i \) can either be all in the same direction (no rotation), and so the elements of the sum add systematically, or they can be randomly directed. In the latter case they are likely to be normal for large \( N \), as the cosine of the angle between two vectors \( X \) and \( Y \), \( \cos^2(X,Y) = \frac{\sum X_i Y_i}{\sum X_i^2} \sim 1/N \) for large \( N \). In this case one can write

\[
(\delta X)^2 = \sum_{i=0}^{n} (\delta X_i)^2 e^{2k(n-i)\Delta t} \approx \frac{t_e}{2\Delta t} \left( e^{2k(n)/t_e} - 1 \right) (\delta X)^2, \tag{8}
\]

where the last approximate equality assumes a typical numerical error \( \delta X \) per timestep and large \( n \). As we will see below, the exponential instability is driven by increasingly close encounters for sufficiently large \( N \). Closer encounters take place on shorter timescales, thus the direction of the error vector are expected to rapidly fluctuate. Equation (8) should therefore constitute an accurate estimate of the rate growth of errors.

If the differences between the forward and backward trajectories are born of such errors, as long as the exponential divergence persists, one expects this error at time \( t > t_f \)

\[
\xi(t \geq t_f) = |X(t) - X(2t_f - t)|^2 / |X(t)|^2 \tag{9}
\]

to be of the order of the error

\[
(\delta X)^2 (n \geq n_f) = \sum_{i=n_f}^{2n_f} (\delta X_i)^2 e^{2k(2t_f - i)\Delta t}, \tag{10}
\]

where \( n_f \) denotes the typical number of steps in the forward and the reversed runs, and the \( \delta X_i \) represent the relative error per time-step determined by the Runge-Kutta routine tolerance setting (as we discuss in Section 3.2.4).

### 3.2 Propagation of errors in the phase space variables

#### 3.2.1 Coordinates

The left panel of Fig. 1 shows the relative error difference between the forward and reverse evolution in coordinates as defined in (2). The time is measured from the start of the reversed run. On this linear scale the evolution is dominated by what appears to be quasi-linear growth in errors, before flattening as the error becomes of order 1, and all correlation is lost between the coordinates of the forward and reversed systems. This post-exponential growth is characterised by a running power law index as we will see below (Fig. 8).

The details of the early evolution are best examined on the vertical logarithmic scale (right panel in Fig. 1), which shows the growth of coordinate errors for the first 20 time units \( (\sim 6 t_p(r = a)) \). On this scale, linear sections correspond to exponential growth, while the growth during the first few time units corresponds to the quasi-linear addition, implied by equation (7) on timescales smaller than the exponentiation time. The curves then flatten off, indicating a smaller exponentiation rate as the instability saturates. As \( N \) increases it saturates at smaller and smaller scales.

An important point to note is this flattening takes place while the errors are orders of magnitudes smaller than one (compare with the flattening on the linear y-scale plot). This need not be the case, as in many systems where chaos leads to global evolution, saturation of the exponential separation of initially nearby trajectories (and associated error) occurs only when the separation is of the order of the characteristic system scale. A case in point pertains to chaos in smooth gravitational potentials, which can stem from global asymmetries (such as triaxiality) in the smoothed out matter distribution. It can be distinguished from ‘N-body chaos’ by precisely this feature (e.g., Kandrup & Sideris 2003). The relatively small saturation scale can be explained by a simple model due to GHH, which explains fits our results well, and which we now briefly describe while adopting it to our
2.2 A simple model

Consider two particles on nearby trajectories. When they undergo a gravitational encounter with a third particle, the (small) difference in impact parameter is \( \delta p \). During the encounter, one 'test' particle, which we call the 'first', is deflected more. At time \( \tau \) following this encounter, the difference in impact parameters for particles with typical speeds \( v \) and mass \( m \) is \( \delta p \sim (1 + Gm/r^2v^2)\delta p \) (assuming deflection angles are small relative to right angles). If the particles all move in a plane, it is clear that a second encounter will increase the impact parameter such that \( \delta p'' \sim (1 + Gm/r'v'^2)\delta p \), even if the situation is reversed; that is, even if the second test particle is closer this time to the perturbing particle. But even in general, if the encounters are strong enough, the errors arising from successive encounters can be multiplied such that \( \delta p(l) \sim (1 + Gm/r^2v^2)^l\delta p \). The associated exponentiation rate is then

\[
k = \frac{1}{\tau} \ln \left(1 + \frac{Gm}{r^2v^2}\right),
\]

which is valid as long as \( \delta p \) remains small. This simple picture is elaborated upon in GHH. In particular, by combining the perturbations statistically, using the second moment equations, it is shown in their Section 3.2 that the exponential growth persists even when considering weaker encounters.
errors, when the idea of simply multiplying the errors as above is not strictly valid.

Now we note that if the separation $\delta p$ is large, then during the encounter one has $\delta p' = p_1' - p_2' = (1 + Gm/v(p_1p_2)(p_1 - p_2)$, so that for $p_2 \gg p_1, p_2 = p_2$ (the particle much further away remains unaffected by the encounter). In this case, we have $p_1 \sim p_1 + G\eta v p_1 v$, and the are deflections add up to zero. (Though adding the squares of the velocity deflections, as appropriate for a diffusive process, would lead to the standard two body relaxation time). The exponential instability is thus intricately linked to the proximity of the two test particles relative to the impact parameter of encounter with the perturbing third particle.

In the context, saturation of the exponential growth should then occur when $\delta p$ can no longer be considered small relative to the characteristic impact parameter $p$ of encounters that drive the exponential growth, as opposed to the system size. This is the major difference between the exponential instability in $N$-body systems and exponential instability that implies global chaos’ and relaxation leading evolution in the system properties on the exponentiation scale.

This characteristic, maximal impact parameter can be estimated by observing that the exponentiation rate is found to be virtually $N$-independent (as can be deduced from Fig. 1 for larger $N$, and more precisely by solving the linearised variational equations, as in, e.g., GHH). From equation (11), this will be the case if both $\tau$ and $Gm/\eta v$ are $N$-independent. The timescale $\tau$ will be so if the number of encounters $\eta$ per crossing time is $N$-independent. For impact parameters $p$ and smaller, this number can be estimated, in terms of the characteristic system size $R$ as $\eta = t_D/\tau \sim N/R^2 \times p^2 R \sim N p^2 / R^2$. The second condition requires that $p^2 = C G \eta v$, where $C$ is some constant of proportionality. If, as in our simulations, $m = M/N$, the characteristic speed is $N$-independent and of the order of $v \sim R/t_D \sim \sqrt{GM/R}$. Therefore $k$ is independent of $N$ if $p^2 = C F / t_D$, where $F = \eta^{-1} \equiv \frac{v}{M}$. Thus the second condition for $N$-independence of the exponentiation rate is automatically fulfilled if the first one is.

Furthermore, if $\eta \ll 1$ encounters are too rare to be important. On the other hand, $\eta \gg 1$ corresponds to relatively large impact parameters and the statistical combination of such weak encounters lead to progressively smaller contributions to the exponential timescale (as shown in GHH). Therefore the main contribution to the exponential instability comes from impact parameters with $\eta \sim F \sim 1$. That is, for encounters that occur about once per crossing time, and are of strength $C^{-1} \sim \eta^2$.

The above implies that for larger $N$ the exponential instability, and associated error growth, saturates at scales $\sim R/\sqrt{N}$ as the number of particles increases. Which means that if we plot the exponentiation rate as a function of coordinate separation $\delta x$, it should be flat up to $\delta x \sim R/\sqrt{N}$, before falling off for larger $\delta x$. To describe this pattern quantitatively, we suppose that the errors remain multiplicative despite the relatively large separation. In this case, we can replace $p^2$ in with $p_1$ and $p_2$ in (11), as these begin to differ significantly, so that $k \sim \frac{1}{2} \ln (1 + Gm/\eta v p_1 p_2)$. Furthermore we can set $p_1 = FR/\sqrt{N}$ and $p_2 = p_1 + \delta x$ to get

$$k = \frac{1}{\tau} \ln \left(1 + \frac{Gm v}{F R / \sqrt{N} (F R / \sqrt{N} + \delta x)}\right) \quad (12)$$

Fig. 2 shows the fits to the numerically derived exponentiation scale for different $N$, using this formula (with $\delta x$ derived from the numerically calculated RMS variation). For exponentiation rate $k \geq 0.1$ these fits are good for relatively large $N$ (we briefly discuss below why the fits get progressively worse for smaller $N$).

The results are straightforward to explain. Since, while keeping the total mass of the system fixed, $m = M/N$ and $Gm/\eta v$ is constant (and all quantities are of order one in our units) then

$$k \approx \frac{1}{\tau} \ln \left(1 + \frac{N^{-1/2}}{(R N^{-1/2} + \delta x)}\right) \quad (13)$$

As long as $\delta x \ll R N^{-1/2}$, $k$ is constant. As $\delta x$ increases, however, $k \rightarrow \frac{1}{2} \ln (1 + R N^{-1/2} \delta x^{-1})$. And since, for large enough $N$ and non-infinitesimal $\delta x$, $R N^{-1/2} \delta x^{-1}$ is small, then $k \approx \frac{1}{2} R N^{-1/2} \delta x^{-1}$. Therefore, although the exponential timescale for the divergence of infinitesimally close trajectories does not depend on $N$, growth during the subsequent saturation stage does, and so does of course the total error after the exponential instability has saturated entirely. As we will see in subsequent sections, this implies that the information loss on the dynamics, as measured by ‘relaxation times’ and more formal measures as the Kolmogorov entropy, will be $N$-dependent on any scale beyond the linear regime of infinitesimally nearby trajectories.

The fact that the fits remain good, even after the exponentiation rate $k$ has decreased by an order of magnitude, means that coherent scattering, leading to the multiplicative enhancement of errors in the manner assumed in (12), remains effective even after the exponential growth stage proper has ended. This reflects a phase of systematic growth of errors in the phase space variables intermediate between the exponential (constant $k \sim 1$) stage and the regime where simple phase mixing finally dominates the growth. In this
context one also expects this systematic error growth phase to separate an eventual diffusive evolution of the errors in the mean field conserved quantities from the exponential growth stage. We will see that this is indeed the case.

The worsening quality of the fits using equation (12) as \( N \) decreases is related the fact that, for smaller \( N \), the exponential region of the growth of errors is small; early evolution is dominated by the initial rapid growth, taking place on timescale smaller than the e-folding time, then saturation starts to set in. This can be seen from the right hand panel of Fig. 1 and also, more clearly, in the evolution of velocity errors, which we look at next.

### 3.2.3 Velocities

The velocity errors (Fig. 4) saturate at the same time as the coordinates, but with larger values, due to the steeper pre-exponential growth that sets the initial conditions for the exponential stage. This can also be explained in the context of the model described above; in its context (as in standard two-body relaxation theory), the velocity kicks are local, reflecting discontinuous jumps, while the errors in positions subsequently grow as a result of these velocity changes (cf. Equations 11 of GHH).

Indeed, for smaller \( N \), the initial growth is dominated by strong encounters. From the right hand panel of Fig. 4, we observe that there is hardly a well defined region of exponential growth in this case; e.g., in the case of \( N = 128 \), where there is very rapid growth to the 10% level, followed by saturation. This is due to the large contribution of large jumps in the velocities, caused by strong encounters. For such encounters one also expects the errors calculated by the Runge-Kutta regime to exceed those inferred from comparing forward and backward trajectories. This is to be expected because the former method considers at each time-step the same initial conditions (up to roundoff error), and estimates the local error through this time-step. In the latter case, on the other hand, there is already a difference between the forward and backward initial conditions at the start of the encounter, due to differences accumulated through the previous evolution of each system. A strong encounter strongly amplifies this difference.

3.2.4 Comparison with estimate of Section 3.1.3

In Fig. 5 we plot the initial rise of the relative error in phase space coordinates (Euclidean norm of positions plus velocities). For relatively large \( N \) this can be fit (before saturation sets in) with the model of equation (10) with an assumed typical time-step of \( 10^{-2} T_{D}(r = a) \) and a truncation error of \( 0.5 \times 10^{-9} \), (shown by the dashed line). This is smaller than the truncation error set by the tolerance used in the Runge-Kutta routine \( (Tol = 10^{-8}) \). But as this tolerance constrains the maximal error in any one of the phase space coordinates, while the estimate from the simulation is an RMS estimate, the two are consistent. This is not the case however with the low-\( N \) runs, where a similar fit requires assuming a tolerance level orders of magnitude above \( 10^{-8} \). Thus, for relatively small \( N \), when contributions of strong encounters are non-negligible, the Runge-Kutta error estimate underestimates the error growth inferred from comparing the backward and forward trajectories, while for larger \( N \) the two estimates are consistent.
3.3 Errors in mean field conserved quantities

The growth of errors described above can be characterised by three stages; an early quasi-linear addition of errors, a period of exponential growth, and an extended period of slower increase. The first two stages in the growth of errors of the energy and angular momentum, which are conserved integrals of motion in mean field equilibrium systems, are similar to the phase space variables (as can be seen from Fig. 6).

The third phase of evolution is quite different however. This is expected of course if the post-exponential error growth in the phase space variables is dominated by phase mixing, characteristic of the divergence in phases between different regular trajectories with different characteristic frequencies and action variables, as conserved quantities are not subject to phase mixing. However the evolution of errors in angular momenta shows that this is not the whole story, as the growth of errors follows that of the velocities well into the post-exponential regime before it saturates. This is especially true for relatively small $N$, as can be seen from Fig. 7. It suggests that the effect of coherent, multiplicative, scattering persists well beyond the exponential stage with constant exponentiation time, as already suggested by the fits in Fig 2. This causes systematic growth, as opposed to diffusive growth, in errors. For angular momenta, a proper diffusive limit in fact is only clearly apparent for the case with $N = 8192$, when the systematic growth saturates at small enough values as to allow for the subsequent diffusive evolution in errors to become apparent over the timescale considered here.

The panels of Fig. 7 show that the error growth rate in energy, which is the usual benchmark employed for the presence of relaxation and validity of the collisionless limit, is far slower than in the angular momenta. The precise mechanism behind this phenomenon may well be worth studying in detail, but is beyond our present scope. We mention however that error growth in energy may be heuristically understood in terms of it being a scalar. Consider for instance the following simple example: two particles deflected by a third one (sharing the same plane), such that the respective deflections lead to normal velocity perturbations $v_1$ and $v_2$. Next consider another encounter with the same magnitude of impact parameters and relative velocity but where the perturbing particle is on the opposite side of the two particles; if particle 1 and 2 were at impact parameters $p_1 < p_2$ from perturbing particle in first encounter, they are at distances $-p_2$ and $-p_1$ respectively, for the second one. The perturbations to the velocities of the first particle is now $v_1 - v_2$ and that of the second particle is $v_2 - v_1$. The vector difference is $2(v_1 - v_2)$, which will affect the difference in angular momenta. The kinetic energy of each particle also changes due to the two perturbations, but the net difference after the two encounters is zero. In terms of the GHH model, it would appear that mainly the weaker encounters that add up statistically would contribute in the case of energy divergence. Due to the slower systematic growth that results, the diffusion stage can be clearly observed in the case of energy for particle numbers considered here.

To further quantify our statements concerning the stages of evolution of errors we have calculated the evolution of the logarithmic derivatives of the errors. These are presented in Fig. 8, where a vertical value of 0.5 corresponds to $\sim 1/2$ diffusive growth of errors. As can be seen, this is reached for the energy, but only after significant post-exponential evolution evolution. (In these plots, the early rise corresponds to exponential stage, while the subsequent rapid fall and flattening up to $t \sim 20$, corresponds to the timescale for the exponential timescale to decline to $\sim 0.1$; cf. Fig. 2). The post-exponential evolution of errors is characterised by a running power law index; for velocities this is $\sim 2$ at $t \sim 20$, saturating towards smaller values (reflecting errors reaching order one) more slowly as $N$ increases. The behaviour of the logarithmic derivative of the growth of errors in coordinates is qualitatively similar; also faster than the corresponding one for angular momentum and (especially) energy. This difference will determine the different rates of relaxation associated with these quantities, which we will examine next.

3.4 Relaxation times

We would like to estimate the timescale over which the error in a given variable $V$ reaches a threshold $h$ ($V$ can either be a phase space variable or a mean field conserved quantity). During the exponential phase, the growth in $V$ is $\delta V \sim e^{t/c} \delta V_0$, where $\delta V_0$ is determined by the value of the error at the start of exponential growth stage. The timescale to reach $h$ is thus $\ln \delta V_0 / c$. According to the picture presented above (Section 3.2), exponential growth persists until saturation time $t_c$, when $e^{t_c/c} \delta V_0 \sim R/\sqrt{N}$ (where as before $x$ is a spatial Cartesian coordinate). Assuming this characteristic exponentiation rate for both $V$ and $x$, (as we already found), and that for $t \gg t_c$ the divergence can be approximated by a power law in time, one may write (for $t \geq t_c$)

$$\delta V \sim \frac{R}{\sqrt{N}} \left(1 + \frac{t - t_c}{t_c}\right)^{3/2} \frac{\delta V_0}{\delta x_0}.$$  \hspace{1cm} (14)

From Fig. 8, $1 \leq s \leq 2$ for $t > 20$, before either diffusion ($s = 1/2$) or saturation ($s \to 0$) sets in (depending on the variable considered. For $t \gg t_c$ one expects a threshold $\delta V = h$ to be reached on timescale $t_{\text{relax}} \sim t_c N^{1/2}$. Thus, when a diffusion process is eventually dominant one expects, for a large enough threshold, an error growth that is roughly linear in $N$, akin to that deduced from two-body relaxation estimates. On the other hand, for the systematic evolution — characteristic of the error growth in the phase space variables before saturation sets in — one expects the threshold to be reached on times scales scaling as $\sim N^{1/4}$ to $N^{1/2}$.

Fig. 9 shows the ‘relaxation times’, taken to reach thresholds $h = 5\%$ and $h = 33\%$. The timescales to reach the 5% threshold are dominated by the early exponential evolution. The exponentiation rates do not vary much with $N$ or variable type, the error $\delta V_0$ at the start of the exponential period however does, particularly to due to the role of strong encounters as described in the previous subsection — hence the dependence on $N$ and variable type. In the case of energy error growth, which as was seen is relatively slow, the associated relaxation time at $h = 5\%$ is large enough for the effect of the post-exponential power law evolution to be dominant for larger $N$. It is consistent with $h \sim N^{1/4}$ for $N = 512$ and larger.

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Figure 6. Early growth of the relative error in the mean field conserved quantities; the energy (left) and angular momenta (right), calculated using equations (5) and (4) respectively. This early evolution is similar to that of the phase space variables (especially velocities), with the same exponential growth rate; the exponential instability stage does not distinguish between the phase space variables and the quantities conserved in the mean field, collisionless, limit. The flattening that follows the exponential stage is sharper in the case of energy.

Figure 7. Comparison of the error growth in the different variables for $N = 128$ (upper left), $N = 512$ (upper right), $N = 2048$ (lower left) and $N = 8192$ (lower right). Note that the growth in angular momentum mimics that of the velocities early on, before the former saturates. Beyond this point, the velocity errors grow through phase mixing, while momentum errors grow diffusively. This diffusive growth is only clearly seen for relatively large $N$ and large times; for lower $N$, the errors from the previous stages are large and the diffusive error growth is drowned out by this background. For energy, beyond $t > 30$, diffusive growth of errors is always apparent (see also Fig. 8 and associated discussion of the approach to the diffusion limit).
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For the threshold of 33%, there is clear separation between the relaxation times associated with the different variables. For the energy, a diffusion process is dominant at all $N$, and the relaxation time for error growth to reach $h = 33\%$ is roughly linear as expected. Indeed, it is fit quite well by a two-body relaxation estimate with Coulomb logarithm $\gamma = 0.11$, as suggested by Giersz & Heggie (1994). (Note that the last two points, $N = 4096$ and $N = 8192$, are missing because the energy error does not reach 33% over the timescales considered). In contrast, the timescales associated with velocity and angular momentum error growth are still dominated by the initial two phases, of early and exponential evolution, for relatively small $N$, namely up to $N = 512$. For larger $N$, the timescale associated with the velocity grows as $\sim N^{1/4}$ (corresponding to $s \sim 2$ in (14)). The angular momentum relaxation to the 33% level, on the other hand, follows roughly a $N^{1/2}$. Except for the last point, when it steepens significantly as diffusion becomes important for $N = 8192$.

3.5 Summary and discussion

There are three qualitatively different ways through which errors in the trajectories of $N$-body systems can grow. They can grow systematically as linear or polynomial functions in the number of time-steps $n$, or they can undergo a random walk and grow diffusively as $n^{1/2}$, or they can grow exponentially. Through examining the numerical reversibility of spherical $N$-body systems, we have observed three stages of error growth incorporating these different aspects. Through the first two stages, the error growth is similar for the phase space variables (coordinates and velocities) and the mean field conserved quantities (energies and angular momenta), while the third stage is characterized by different modes of errors growth for the two types of variables. The difference becomes apparent once the ‘chaos’ of the exponential instability has saturated; and also the subsequent systematic growth, associated with the same sort of coherent scattering that lead to the exponential instability, has subsisted. The error in the phase space variables can then grow by phase mixing, while that of the mean field conserved quantities grows via a diffusion process.

An initial stage of evolution occurs over timescales smaller than the exponential divergence timescale. In this case the errors involved are principally truncation errors enhanced by strong encounters, significant especially for relatively low $N$ systems. Such errors can in principle add up systematically or diffusively. Given that they are driven by encounters that last a small fraction (< $1/\sqrt{N}$) of a dynamical time — which determines the timescale over which the error vectors randomly change their orientation in a high ($6N$) dimensional space — the latter seems more plausible. This initial stage is followed by the exponential stage, with associated exponentiation time that is a fraction of a dynamical time for all variables. A fit that assumes that errors add up diffusively in the initial stage, and that the subsequently exponentially inflated errors also add up diffusively, is shown in Fig. 5. The characteristic exponentiation timescale of this fit is 0.55 time units, corresponding to 0.16 $t_{p}(r = a)$ and 0.09 $t_{p}(R_{v})$. The error inferred from comparison of the forward and reverse dynamics is compatible to those estimated by the Runge-Kutta routine for relatively large $N$ but are
much larger than these for smaller $N$. We interpret this in terms of the effect of strong encounters, which diminishes as $N$ increases.

The exponential growth in coordinate errors does not saturate at dimensions comparable to the system size; in fact, it already effectively ceases as the distance between two initially nearby trajectories (in our case the forward and reverse trajectory) becomes of order $1/\sqrt{N}$ the characteristic system size. We use a model due to GHH to interpret this phenomenon. In its context, the fits of Fig. 2 show that the coherent, multiplicative enhancement of errors due to encounters, that leads to exponential divergence, persists even after the saturation of the exponential growth. In fact up to when the effective exponential rate is $\leq 10\%$ its initial flat value. This implies that the systematic post-exponential evolution of the errors in the phase space variables is not simply dominated by phase mixing, and neither is the post-exponential growth of errors in the mean field conserved quantities immediately diffusively. For angular momentum, diffusive evolution in fact only becomes apparent at larger $N$ and late times (cf. Fig. 7). Nevertheless, though post-exponential growth of errors in angular momentum initially mimics that in velocities, it saturates at smaller and smaller values as $N$ increases. This marks a split between further evolution via phase mixing in the phase space variables, and slower diffusive growth for the mean field conserved quantities. In the case of angular momentum the saturation level is large, and the effect of diffusive growth less clear. The growth of energy errors, on the other hand, starkly illustrates the effect; it clearly displays diffusive behaviour, with growth rate $\sim t^{1/2}$, after $\sim 10D(r = a)$. The post-exponential evolution of the errors in the phase space variables on the other hand can be locally characterised by a power law time evolution with index $1 \leq s \leq 2$.

The different modes of error growth lead to different estimates of the associated ‘relaxation times’ — that is, the time the errors in a given variable reach a certain fixed relative error level. For small threshold levels (e.g., $5\%$), the errors are dominated by the early growth. Here, the $N$ variation is due to the initial errors imposed by the first stage of evolution providing the initial conditions for the exponential stage. The relaxation times are very similar for the velocity and angular momentum, and also for the energy at lower $N$. At higher $N$ (e.g. $33\%$ level) the energy error growth is already fully diffusive, its $N$ variation is nearly linear and well explained by a two-body relaxation law with Coulomb logarithm $\gamma = 0.11$, a value suggested by Giersz & Heggie (1994). Assuming that error growth continues diffusively to the $100\%$ level, and noting that the dynamical time at the virial radius $tD(R_v) = 6.4$ in our units, translates to $t_{relax} = 0.26 N^{26/117} tD(R_v)$. This is quite similar to standard estimates of the two-body relaxation time.

On the other hand, the velocity perturbations — which are often considered in calculations of the two-body relaxation times, where mean field dynamics are assumed to be additively separable from the fluctuations due to discreteness noise — do not grow diffusively; even following the stage of systematic growth entailed with the persistence of coherent multiplication of errors, phase mixing dominates. The angular momentum error growth initially follows that of the velocities, but is gradually influenced by diffusive growth at late times, an effect that becomes more apparent as $N$ increases. It is quite plausible that for larger $N$, and longer timescales, its growth with $N$ could converge to the two-body relaxation time, but the significant difference found here with energy relaxation appears worth studying in detail. It seems intimately connected to momentum being a vector quantity, and may well affect for example the the structure of simulated objects, particularly velocity anisotropies and spatial symmetry if the strong evolution in angular momentum extends to axion variables in triaxial potentials, where their non-conservation evolution towards axisymmetry, Such
effects may be particularly important in small haloes and subhaloes identified in cosmological simulations with relatively small number of particles and far larger errors in forces calculations and time integrations than in the simulations presented here. In such situations, conventional estimates of the effect of discreteness noise, through standard two-body relaxation prescriptions, may not capture the full complexity of its effects. Finally, even in the case of energy, the diffusion limit is only reached for relatively large error threshold. This is the case even if the convergence to the collisionless limit is indeed present in a formal sense, as discussed below.

4 CHAOS AND COLLISIONLESS EQUILIBRIA

In what sense are $N$-body gravitational systems ‘chaotic’? Generally one can identify chaos with the presence of a positive Lyapunov exponent. The exponential divergence between nearby trajectories does imply the existence of at least one 'finite time' positive exponent (strictly speaking, the exponents involve an infinite time limit, which is not well defined for systems with non-compact phase space as $N$-body systems). But the results of the previous section confirm that this instability does not imply global structural evolution on the associated timescale, as it saturates on progressively smaller scales as $N$ increases. Mean field conserved quantities, such as energy and angular momentum, eventually evolve via a standard diffusive process. So in what formal sense are these systems chaotic; and does it matter, from a physical point of view?

A key issue concerns information loss, reflected in the numerical irreversibility observed in the previous section, and whether it actually affects macroscopic parameters (spatial density, velocity dispersion etc.) describing the gross statistical properties of the system (represented by moments of the one particle distribution function in case of collisionless systems). As discussed in the introduction, such loss would affect the 'faithfulness' of our numerical representations as well as their accuracy. It also entails intrinsic dynamics that are qualitatively different from the corresponding collisionless case. To reconcile the fact of positive Lyapunov exponent with apparent lack of macroscopic evolution on the characteristic timescale, one should show that the associated loss of information decreases with $N$ at any macroscopic scale and that it leaves the statistical quantities characterising macroscopic structure largely unaffected. We attempt this here.

The concept of dynamical information loss can be made precise through the Kolmogorov entropy, which essentially measures the rate of increase in the information needed to follow a phase space trajectory in time (e.g. Lichtenberg & Lieberman 1992). A formal definition is technically involved, and a discussion as how it can be applied to $N$-body systems, showing its close connection to effective reversibility, is relegated to the Appendix. Here we use a simpler definition based on the growth of coarse grained phase space volume $1$.

First, assume that our dynamical system, the $N$-body system, can be considered collisionless in the conventional sense. In astrophysical studies this is usually taken to be true for timescales considerably smaller than the energy relaxation time. We will assume this to be the case. In this case, the system is completely characterised by the six dimensional phase space distribution function $f$. In a steady state spherical system, this is a function of particle energy $E$ and angular momentum (BT). We will assume here that $f = f(E)$. This form of the can either arise due to initial conditions (with isotropic velocities), or because, as we saw in the previous section, the growth of errors in energy is significantly slower than in angular momentum, and thus the associated ‘relaxation time’ considerably longer. (It is straightforward to extend the following discussion for the case in which $f = f(E, J)$).

Let $\Omega(0)$ be the coarse grained volume, occupied by a distribution of phase points at time $t_0$, in a phase space discretised into cells of volume $\Delta \Omega$. This volume is obtained by counting the number of cells that the phase points occupy. Liouville’s theorem notwithstanding, after $n$ time steps, the volume on the coarse grid will evolve such that $\Omega(n) \geq \Omega(0)$, as trajectories initially confined to a cell $c_j$ at time $t_0$ can spread over many cells at later times. The Kolmogorov entropy over the partition determined by $\Omega(0)$ is then defined as

$$K(\Delta \Omega) = \lim_{n \to \infty} \frac{1}{n} \log \frac{\log \Omega(n)}{\Omega(0)}.$$  \hspace{1cm} (15)

The Kolmogorov entropy proper is the limit of $K(\Delta \Omega)$ as $\Delta \Omega \to 0$. A nonzero value results from exponential divergence associated with the presence of a positive Lyapunov exponent. It is often the case that the associated ‘chaotic mixing’ can lead in such cases to important consequences concerning the gross structure of a system and its statistical properties.

Due to the exponential divergence at infinitesimal scales, $N$-body systems have positive Kolmogorov entropy in the formal sense. However, as found in Section 3.2, the exponential divergence of nearby trajectories of $N$-body systems dies off at progressively smaller scales. This means that, at any finite volume resolution $\Delta \Omega$, $K = 0$ as $N \to \infty$. For, given any two initially infinitesimally nearby trajectories, there is a maximal spatial distance $\sim R/\sqrt{N}$ (with corresponding maximal difference in velocities) beyond which they cannot separate by means of the exponential divergence. This inference is consistent with the fact that the exponentiation rate itself decreases with $N$ if the effective resolution scale, determined by a softening length, is larger than $\sim R/\sqrt{N}$ (GHH; El-Zant 2002).

In general, the total volume through which a phase space point is uncertain following the end of the exponential stage decreases as $1/N^3$, which limits the associated information loss, which for and initial error $\Delta x$ goes as $\log \left( \frac{R}{\Delta x \sqrt{N}} \right)$.

Eventually, in any numerical implementations there is a maximal resolution imposed by machine precision. Thus, in principle, beyond $1/\sqrt{N} \sim 10^{-14}$ there would be no meaning for ‘chaos’ due to the exponential instability, as far as double precision numerical implementation is concerned.

The second point to note is that, beyond the exponential regime, the loss of information is limited by the transition to a slow diffusive growth. Suppose for example that our

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1 A physically motivated discussion for this definition is given in Sagdeev, Usikov, & Zaslavsky (1988). A mathematical proof of its equivalence to the general definition in the case of ergodic systems (where trajectories can visit every point of the available phase space; e.g. BT) is given in Young (2003).
set of trajectories are started on the same energy surface of phase space, they will remain confined to volumes of the phase space of relatively narrow thickness $\Delta E(t)$ that eventually grows only on the two body relaxation timescale (as we saw in the previous section). To quantify this limitation on information loss, consider a set of initial conditions initially known to be confined to a cell of phase space $\Delta \Omega(0)$, and after $n$ timesteps have completely uncertain location within the phase space volume

$$\Omega(\Delta E) = \frac{\partial \Omega(E)}{\partial E} \Delta E = (4\pi)^2 \Delta E \int_0^{r_{\text{max}}} v(E, r)^2 dr,$$  \hspace{1cm} (16)

where $\Omega(E)$ is the phase space volume enclosed by energy surface $E$ (and $r$ and $v$ are radial particle coordinates and speeds). As $N$ increases, rate of information loss on the phase space position over the energy shell decreases (as we saw in the previous section). But even with total uncertainty over the energy shell, the information loss is smaller by a factor $\sim \Delta E/E$ compared to when energy is not well conserved.

The ratio $\Omega(\Delta E)/\Delta \Omega(0)$ scales as $\sim \Delta E/\delta v(\delta r)$, where $r$ and $v$ are understood to represent characteristic positions and speeds at energy $E$, and $\delta r$ and $\delta v$ the initial uncertainties in these. Suppose that during the evolution the energy errors remain of the order of the initial uncertainty, so that $\Delta E \sim (\delta v)^2$ and $\Omega(\Delta E)/\Delta \Omega(0) \sim (\delta r/\delta v)^2$. Thus, with initial relative uncertainties $\delta v/v$, $\delta r/r \sim 10^{-14}$, say, and even if energy errors remain of order of their initial uncertainty throughout the evolution, the final volume $\Omega(\Delta E)$, within which the phase points are equally likely to have wandered after $n$ steps, is $\sim 10^{28}$ the original volume $\Omega(0)$. This is huge, but it is still tiny relative to the loss of information if the uncertainty in particle energy was of order one. In this case an additional factor of $10^{28}$ (28 in terms of logarithmic information loss) is involved.

Furthermore, as long as the timescales involved are much smaller than the energy relaxation time, the loss of information due to uncertainties in phase space position does not significantly reflect on the distribution function $f = f(E)$, and hence should hardly affect the macroscopic state of the self gravitating configuration described by $f$ and its moments (density distribution and velocity dispersions). Indeed, if particles are labelled by their energies and the phase space partitioned into energy cells $\Delta E$, instead of $\Delta x, \Delta v$, then the coarse grained $\Omega(\Delta E(t))$ does not change significantly over timescales smaller than the energy relaxation time. The entropy given by equation (15) would still be non-zero over infinitesimal scales, as on these scales the exponential divergence affects the mean field conserved quantities in the same manner as the phase space variable. But after it saturates the information loss is minimal. A similar situation would arise if $f = f(E, J)$, or a function of action variables in general integrable potentials.

To sum up. For any finite phase space resolution the Kolmogorov entropy tends to zero as $N \rightarrow \infty$. In particular, for a given $N$, for any spatial resolution $\sim R/\sqrt{N}$ it tends to zero. From this perspective, the exponential instability in $N$-body systems does not imply that they display ‘chaotic mixing’, which explains why they do not generally display relaxation and evolution of macroscopic on the exponential timescale, a characteristic of systems where the exponential instability saturates on larger scales (Kandrup \\& Sideris 2003). Second, although dynamical evolution leads to large loss in information regarding the phase space positions of trajectories, this is still very small compared to the significant loss of information associated with the error growth in the mean field conserved quantities, which at least in the case of energy happens occurs over the standard two body relaxation time. On timescales shorter than this, the macroscopic structure of $N$-body systems, at least for those described by distribution functions that are expressed in terms of the mean field conserved quantities, are largely unaffected by the exponential instability. This gives some credence to the faithfulnes of $N$-body simulations, despite the loss of information inherent in numerical integration. It also gives credence to the modelling of gravitation systems through orbital integration in smooth potentials.

5 CONCLUSION

We have examined two related aspects of $N$-body gravitational systems; the temporal growth of errors in the solutions and the faithfulnes of numerical simulations of such systems. We did this by considering the simple case of spherical systems in dynamical equilibrium, and quantifying a direct consequence of the growth of errors, namely the numerical irreversibility of the solutions. For this purpose, we ran a suite of small $N$ but high accuracy simulations, in the range of $N = 128$ to $N = 8192$. The simulations were conducted using a Runge-Kutta method, which does not incorporate any time reversal symmetries, does not distinguish between phase space variables and mean field conserved quantities (such as energy and angular momentum), and where the accuracy can be estimated via a predetermined tolerance (set at $10^{-8}$).

Three phases of error growth can be distinguished. A simple calculation and numerical results show that the errors add up randomly before the well known local exponential instability of $N$-body systems sets in. As have been found in other studies, the exponential growth time is virtually independent of $N$. However the initial pre-exponential growth is sensitive to $N$; as measured by the irreversibility of the computed dynamics, it is larger than the estimated truncation error for relatively small $N$ but significantly smaller than that error for larger $N$. Moreover, the exponential instability saturates at smaller timescales as $N$ increases. A simple model of the exponential divergence, originally due to Goodman, Heggie \\& Hut (1993), is used to quantitatively interpret this phenomenon.

These first two phases of the error growth, along with the $N$ dependence of the resulting error, set the stage for the third phase, by providing its initial conditions. This third stage starts dominated by systematic growth driven by the same mechanism of coherent, multiplicatively reinforcing deflections, born of encounters of the same sort that lead to the exponential instability. Subsequent to this, the growth of errors is qualitatively different in the case of the phase space variables (coordinates and velocities) and the conserved quantities of the mean field dynamics (energies and angular momenta); the former grow through phase mixing, while the latter grow according to a diffusion ($\sim t^{1/2}$) law. This implies different timescales for error growth and their variation with $N$.  

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The convergence towards the diffusion limit is particularly clear in the case of energy error growth, where the inferred ‘relaxation time’ is of the form of that obtained from standard two-body relaxation theory. The convergence rate towards that limit is much slower in the case of the angular momenta. The associated short error growth times may have significant consequences for estimating the effect of discreteness effects in simulations. Velocity anisotropies may be particularly affected by the larger growth rate of angular momentum errors, and if the phenomenon applies to general action variables in non-spherical potentials, associated errors can affect the shapes of the corresponding objects (presumably rendering them more spherical).

While the exponential instability persists in the linear regime of infinitesimally nearby trajectories, and thus in this sense even large-N softened gravitational systems are ‘chaotic’, when viewed from a dynamical entropy viewpoint a somewhat different picture emerges. Because the exponential instability saturates at increasingly smaller scales, the Kolmogorov entropy, which must be positive for a chaotic system, tends to zero at any finite phase space resolution level as $N \to \infty$. Indeed the volume in which a phase space trajectory can be localised following the completion of the exponential divergence stage decreases as $1/N^3$. A finite resolution level is inherent in any numerical representation, which is ultimately limited by machine precision (or by softening, which has been shown to increase the exponential timescale as $N$ increases: e.g. GHH; El-Zant 2002) . This necessarily limits the sense in which $N$-body systems can be termed ‘chaotic’. The loss of information is especially minimal if it is viewed in terms of mean field conserved quantities. As measured by the energy errors at least, for the equilibrium systems studied here, the timescale for energy growth in fact simply mimics the classical two body relaxation time as the diffusion limit is reached. In this sense, the dynamics thus tends to its mean field counterpart as $N$ increases, despite the persistence of the exponential instability on infinitesimal scales.

This gives credence to the standard assumptions of stellar dynamics, based on the collisionless limit. Nevertheless, the rapid initial (exponential and systematic) error growth, implies that the convergence to the collisionless limit to high precision (at the 10% error levels say) is slow, even when measured in terms of energy errors. For, even though the exponential instability saturates at progressively smaller scales, the corresponding reduction in errors at the completion of the exponential stage follows a less steep scaling $1/\sqrt{N}$ relative to that of the standard relaxation time. This weak scaling will be dominant before the diffusion limit is reached. The errors in the phase space variables never reach a diffusive stage; they continue to propagate systematically through phase mixing, and retain a weak $N$ scaling even for relative error thresholds of order one.

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APPENDIX A: KOLMOGOROV ENTROPY AND EFFECTIVE IREVERSIBILITY
Assume we are dealing with timescales that are small compared to the energy relaxation time, and that the system is described by a 6-d probability phase space distribution function $f = f(E)$ obeying the collisionless Boltzmann equation (and so $f$ is constant along particle trajectories). Discretise the phase space into cubic cells, each with volume $\Delta \Omega$, and follow the evolution of a particle trajectory from specified initial conditions. Then record the cell number $c_i$ at which a trajectory is located at time times $t_i$ with $i = 1, \ldots, n$. The Shannon information entropy of this partition of cells under the action of the trajectory is

$$S = - \sum_{i=1}^{n} p_i \log p_i.$$

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where probabilities $p_i$ are proportional to the time the trajectory spends in cell $i$.

Now consider a group of trajectories initially localised in one of the phase space cells. The Shannon entropy for this system of trajectories generally increases as the system evolves, and is maximized as the probabilities $p_i$ equate, so that $p_i \rightarrow f(E)$ on all cells. The Kolmogorov entropy distinguishes between any general increase in Shannon entropy (e.g. due to phase mixing) and that associated with exponential instability. For our purposes the concept can be developed as follows.

Suppose that after at time $t_1$ we take a distribution $f$ of points over the cubic phase space cell $c_1$ where our integrated trajectory resides. If we reverse back the trajectories in this cell to time $t_0$, the collisionless evolution ensures that the fine grained density $f$ is conserved and the distribution will end up under the reversed dynamics in cell $c_{0,1}$ of same volume as $c_1$. If there is no divergence between neighbouring trajectories the shape of the cell is conserved during the evolution, and volume conservation implies that cell $c_{0,1}$ will coincide with $c_0$ where they all started. In the presence of divergence however, trajectories reversed from $c_1$ may fall in cells other than $c_0$. In fact the cell $c_{0,1}$ containing the reversed trajectories will be distorted by the evolution and will in general not be cubic anymore. The intersection of $c_{0,1}$ with $c_0$ will generally define a cell of smaller volume. The continuation of this procedure for times $t_2, t_3,..., t_n$ defines progressively smaller cells, determined by the intersections of $c_{0,1}, c_{0,2},..., c_{0,n}$ with $c_0$. Now if we label the cells defined by these intersections as $d_j$ (with $j = 1,...,n$), and repeat the process for different trajectories of the system (with initial conditions sampled from the distribution function $f(E)$), we can define a finer partition of the phase space. The associated probabilities $p_{d_j}$ (which are proportional to $f(E)$ integrated over smaller and smaller volumes of the intersection cells), decrease with increasing maximal time step $n$.

The Kolmogorov entropy measures the increase per time-step of the Shannon information entropy of this increasingly finer partition as volume $\Delta \Omega$ and the time-step $\Delta t$ both go to zero. This corresponds to the loss of information per time-step, which leads in practice to the inability to numerically track and reverse a trajectory. The reason we obtain finer partitions from the reversed dynamics — and corresponding increase in Shannon entropy — was that trajectories that were initially confined to a cell $c_i$ at time $t_i$ could be dynamically evolved into occupying many cells (hence the increased in coarse grained volume). This formally relates the phenomenon of effective irreversibility, due to information loss, to the local exponential divergence between nearby trajectories. It also relates the definition here to the more intuitive one given in the body of the paper.

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