Numerical Convergence in Solving the Vlasov Equation

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Abstract

When the Vlasov equation is investigated numerically using the method of test particles, the particle-particle interactions that inevitably arise in the simulation (but are not present in the Vlasov equation itself) result in an accumulation of errors which eventually drive the collection of test particles toward a state of classical thermal equilibrium. We estimate the rate at which these errors accumulate.

The Vlasov equation plays a central role in classical (and semiclassical) time-dependent mean field theory, and has been used to model a wide variety of many-body processes, from the gravitational $N$-body problem [1], to plasma physics [2], to nuclear dynamics [3]. While the content of the Vlasov equation is conceptually simple — interactions among many particles are replaced by a common mean-field potential — solutions are harder to come by, and must in general be sought numerically. This is often accomplished with the test particle method: a swarm of numerical particles is used to simulate a distribution $f(r,p,t)$ in one-body phase space, and the mean-field potential in which these test particles evolve is obtained from this distribution. Thus, while the Vlasov equation replaces a physical many-body problem with the self-consistent evolution of a one-body phase-space distribution, the test particle method in turn replaces the Vlasov equation with a numerical many-body problem. This raises the issue of convergence: for a given number of test particles, and over a given length of time, how closely can we expect the evolution of $f(r,p,t)$ as obtained
by the test particle method, to resemble the true evolution under the Vlasov equation? In the limit of arbitrarily long evolution time, we can certainly expect the test particle method to fail. In that limit, the unavoidable interactions between individual test particles will drive the swarm of numerical particles toward a Boltzmann distribution of energies, whereas under the Vlasov equation there are no particle-particle interactions, and $f$ typically does not evolve toward classical thermal equilibrium.

A relevant example of this disagreement arises in the application of the Vlasov equation to nuclear dynamics, where the Pauli principle is imposed by insisting that, initially, $f \leq 4/h^3$ everywhere in phase space. Under the Vlasov equation, this condition is preserved exactly with time; with the test particle method, however, classical thermalization occurs, and the Pauli condition is violated. (See Fig. 4 of Ref. [4], I, for an illustration.)

The eventual thermalization of test particles may occur on a time scale longer than that in which one is interested. Nevertheless, it is indicative of a general process, whereby interactions between the test particles introduce errors which drive the numerical solution away from the actual solution of the Vlasov equation. It is thus important to obtain an estimate of the rate at which these errors accumulate. Such an estimate is the goal of the present brief note.

We will restrict ourselves mainly to self-consistent potentials which are local functions of particle density, although a brief discussion of long-range forces will be presented at the end. Working with a simple schematic model, we will argue that errors in the particle energies accumulate diffusively, and we will solve for the functional dependence of the associated diffusion constant $D_E$, in terms of physical and numerical parameters. For the specific case where Gaussian smoothing is used to obtain the particle density $\rho$ from the positions of the test particles, we obtain a more quantitative prediction for $D_E$. Finally, we compare our theoretical predictions with numerical results.

The Vlasov equation is explicitly given by

$$\frac{\partial f}{\partial t} + \{f, H\} = 0,$$

(1)
where \{·,·\} denotes the ordinary Poisson bracket, and the Hamiltonian $H$ is

$$H(r,p) = \frac{p^2}{2m} + U_f(r). \quad (2)$$

The notation $U_f(r)$ is meant to indicate that the mean-field potential $U(r)$ is a functional of the one-body phase space distribution $f$. Often (e.g. when the physical interactions between particles are independent of momentum) the functional dependence of $U$ on $f$ reduces to a dependence only on the density $\rho$ in ordinary space:

$$U_f(r) \rightarrow U_\rho(r) \quad (3)$$

$$\rho(r) = \int dp f(r,p). \quad (4)$$

Throughout this paper, we will assume, for simplicity, that this is the case. Note that if $U$ is linear in $\rho$, then it may be expressed in terms of a two-body physical interaction $V_{12}$:

$$U_\rho(r) = \int d\mathbf{r}' \rho(\mathbf{r}') V_{12}(\mathbf{r}, \mathbf{r'}). \quad (5)$$

The implementation of the test particle method involves two tasks: (1) evolving each of the $N$ test particles in the presence of the time-dependent potential $U$; and (2) constructing $U$ from the positions of the particles at any instant in time. The first is straightforward, involving simply the numerical integration of Hamilton’s equations of motion. The second task requires the particle density $\rho(r,t)$, which is obtained by smearing the position of each point particle with a localized folding function $g$:

$$\rho(r,t) = \frac{A}{N} \sum_{i=1}^{N} g(r-r_i(t)). \quad (5)$$

Here $A$ is the number of physical particles, whereas the sum runs over the test particles, located at positions $r_i(t)$ at time $t$. $g(r)$ is a function localized in a volume $\sigma^3$ around the origin, and normalized to unity: $\int d\mathbf{r} g(\mathbf{r}) = 1$. The parameter $\sigma$ thus measures the distance over which we smear out the particle positions. Gaussian folding functions are commonly used.

To estimate the rate of accumulation of errors introduced by interactions among the test particles, let us consider a simple model in which our many-particle system is confined
within a box of volume $V$. Furthermore, let us take the functional dependence of $U$ on $\rho$ to be local:

$$U_\rho(r) = U(\rho(r)).$$

That is, the potential at $r$ depends only on the density of particles at that point; this corresponds to zero-range interactions among particles, and is commonly used to model short-range interactions such as nuclear forces (see e.g. the Skyrme parametrization [3]). It is important to distinguish here between the mathematical problem one is trying to solve (propagation under the Vlasov equation), and the numerical method used to solve it: even if the potential $U_\rho(r)$ which enters into the Vlasov equation is exactly local — as indeed we are assuming — the interactions between test particles in a numerical implementation will necessarily have finite range, due to the smearing which is employed to extract a smooth density $\rho(r)$ from the positions of a finite number of test particles.

Now, consider an initial phase space distribution $f_0(r,p)$ corresponding to an ensemble of monoenergetic particles distributed uniformly throughout the box, with an isotropic distribution of momenta. Explicitly, this has the form $f_0(r,p) \propto \delta(p-p_0)\Theta_B(r)$, where $p \equiv |p|$, and $\Theta_B(r)$ is equal to 1 (0) if $r$ is inside (outside) the box. As can be seen by inspection, this phase space distribution is a stationary solution of the Vlasov equation, thus under the Vlasov equation the ensemble of particles remains exactly monoenergetic. Our strategy now will be to investigate how such an initial distribution evolves under a numerical simulation using test particles. Specifically, after a time $\Delta t$, what is the amount $\Delta E$ by which the energy of a typical test particle has strayed from its initial value? The growth of $\Delta E$ with $\Delta t$ will then be a measure of the accumulation of error inherent in the test particle method.

Let us take our $N$ test particles — all given the same initial speed $v = p_0/m$ — to be distributed randomly throughout the container, and choose $\sigma$ so that $V/N \ll \sigma^3 \ll V$. This will result in a reasonably smooth numerical density $\rho(r,t)$, without smearing over too large a volume of the box. We can express this density as

$$\rho(r,t) = \rho_0 + \delta \rho(r,t),$$

(7)
where $\rho_0 = A/V$ is the physical density which we are trying to simulate, and $\delta \rho(r, t)$ represents the fluctuations around $\rho_0$ due to the finite number of test particles. To gauge the typical size of $\delta \rho$, note that the value of $\rho$ at a given point is roughly equal to $(A/N)n/\sigma^3$, where $n$ is the number of test particles within a volume $\sigma^3$ of the point in question. (The factor $A/N$ is a conversion factor between the density of test particles and the density of physical particles.) On average, $n$ will be given by $n_0 = N\sigma^3/V$, with fluctuations of size $\sqrt{n_0}$ around this average. These considerations yield the following expression for the typical size of the fluctuations $\delta \rho$:

$$
\delta \rho_{\text{rms}} \sim \frac{A}{N} \frac{\sqrt{n_0}}{\sigma^3} = \frac{\rho_0}{\sqrt{n_0}}.
$$

It should be clear as well that $\delta \rho(r_1, t)$ and $\delta \rho(r_2, t)$ will be correlated only if $r_1$ and $r_2$ are within a distance $\sim \sigma$ of one another. Furthermore, at a given location $r$, the value of $\delta \rho(r, t)$ will be correlated over a time $t_c \sim \sigma/v$, since that is a typical time over which a test particle remains within a volume element $\sigma^3$ of $r$.

Thus, our numerical density $\rho(r, t)$ fluctuates in space and time around an average value $\rho_0 = A/V$, where the size of the fluctuations is given by $\delta \rho_{\text{rms}} \sim \rho_0/\sqrt{n_0}$, and these fluctuations are correlated over a distance $\sigma$, and a time $t_c \sim \sigma/v$. Let us now make use of this picture to determine what happens to a given test particle evolving under the potential $U(\rho(r, t))$ computed from this numerical density.

We first expand the potential $U$ around its value at $\rho_0$:

$$
U(\rho(r, t)) = U(\rho_0 + \delta \rho(r, t)) \approx U_0 + U'_0 \delta \rho(r, t),
$$

where $U_0 \equiv U(\rho_0)$ and $U'_0 \equiv \frac{dU}{d\rho}(\rho_0)$. Thus, like the numerical density $\rho$, the potential $U$ fluctuates in space and time around an average value ($U_0$). The typical rate at which $U$ is changing, at a fixed point $r$, is determined by the typical rate of change of $\delta \rho$:

$$
\left| \frac{\partial}{\partial t} U(r, t) \right| \sim U_0 \frac{\delta \rho_{\text{rms}}}{t_c}.
$$

Now consider a single test particle $i$ moving under this time-dependent potential. From
Hamilton’s equations, the rate of change of the total energy $E_i$ of the particle is exactly the value of $\partial U/\partial t$ along its trajectory:

$$\dot{E}_i(t) = \frac{\partial U}{\partial t}(r_i(t), t).$$

(11)

This function $\dot{E}_i(t)$ is autocorrelated over a time scale $t_c \sim \sigma/v$, which is considerably shorter than a characteristic time scale associated with the particle’s motion in the box (e.g. the traversal time across the length of the box). The change in energy $\Delta E_i$ is thus the time integral of a function $\dot{E}_i(t)$ which fluctuates rapidly, with short time correlations; this implies that $\Delta E_i$ evolves diffusively. The associated diffusion constant $D_E$ is then the time integral of the auto-correlation function of $\dot{E}_i(t)$. Approximating this integral by the product of the mean-square value of $\dot{E}_i(t)$ with the correlation time $t_c$, we have, using Eq.10,

$$D_E \sim \left|\dot{E}_i\right|^2 \frac{\sigma}{v} \sim \left(U'_0 \delta \rho_{rms}\right)^2 \frac{v}{\sigma}.$$

(12)

Finally, using $\delta \rho_{rms} \sim \rho_0/\sqrt{n_0}$, and $n_0 = N\sigma^3/V$, we get

$$D_E \sim (U'_0)^2 \rho_0 v \cdot \frac{A}{N} \cdot \frac{1}{\sigma^4}.$$

(13)

Thus after a time $\Delta t \gg t_c$, we can expect the energy of our test particle to have changed by an amount

$$\Delta E \sim (D_E \Delta t)^{1/2},$$

(14)

with $D_E$ given by Eq.13 above. Eqs.13 and 14 together describe the accumulation of error in the energy of a typical test particle, and thus constitute our main result.

Note that we have written $D_E$ as the product of three factors, the first of which contains only physical quantities, while the other two depend on purely numerical parameters: the smearing parameter $\sigma$, and the number of test particles per physical particle, $N/A$. The prediction that the error accumulates more slowly for larger values of $N/A$ is expected; this is the benefit of using more test particles. Eq.13 predicts that one gains even more by increasing the value of the smearing parameter $\sigma$: $D_E \propto \sigma^{-4}$. As pointed out by Reinhard and Suraud
this should not come as a surprise: a larger smearing effectively suppresses the interaction between individual test particles, thus slowing the rate at which energy gets exchanged. Of course, smearing distorts the mean field itself; therefore too much of it, while suppressing errors due to test particle interactions, will result in an inaccurate simulation of the Vlasov equation. Ultimately, one wants $\sigma$ large enough so that $\Delta E$ remains small over the time scale of physical interest, but not so large as to distort the inhomogeneities that are physically present in the mean field.

As mentioned earlier, one expects that in the long run the test particles thermalize. This ought to happen on a time scale $\tau$ over which each test particle has had the opportunity to change its energy by an amount comparable to the average particle energy, $mv^2/2$. Thus,

$$(DE \tau)^{1/2} \sim mv^2.$$  \hfill (15)$$

Combining this with Eq.\[13\], we obtain for the thermalization time scale

$$\tau \sim \frac{m^2 v^3}{(U'_0)^2 \rho_0} \cdot \sigma^4 \cdot \frac{N}{A}. \hfill (16)$$

In numerical experiments aimed at studying the relaxation toward thermal equilibrium under the test particle method, Reinhard and Suraud have found that doubling the value of $\sigma$ "gains more than an order of magnitude in the relaxation time" (Ref. [4], p. 227); this is in agreement with our prediction here that $\tau$ scales like $\sigma^4$. Furthermore, these authors have predicted that $\tau \propto N/A$, and have confirmed this numerically.

A few comments are now in order. First, in a realistic test particle simulation, the particles are held together by the mean field itself, rather than being artificially confined within a box. Nevertheless, the mechanism by which the test particles exchange energy with one another remains the same, therefore the result derived within the context of our simple model ought to hold in the more realistic situation as well.

Next, while our main result predicts how the growth of errors scales with the various parameters involved, a more quantitative estimate will depend on the details of how the test particles interact with one another. For instance, the use of a gaussian folding function,
\( g(r) = (2\pi \sigma^2)^{-3/2} \exp(-r^2/2\sigma^2) \), allows for an explicit evaluation of \( \delta \rho_{rms} \). This leads to an expression for \( D_E \) which has the form of Eq.13, but with a numerical factor \( 1/8\pi^{3/2} \) in front. Alternatively, for gaussian folding functions one can evaluate (within the linear approximation) the amount of energy exchanged in a given collision between two test particles, in terms of impact parameter. The further assumption that different particle-particle collisions are uncorrelated leads (after some work) to a diffusion coefficient

\[
D_E = \frac{1}{12\pi} \left( \frac{U'_0}{\rho_0} \right)^2 \rho_0 v \cdot \frac{A}{N} \cdot \frac{1}{\sigma^4}. \tag{17}
\]

It is encouraging that this approach, which differs somewhat from that leading to Eq.13, nevertheless yields the same functional dependence of \( D_E \) on the various quantities involved.

Finally, our assumption that the dependence of \( U \) on \( \rho \) is local (Eq.6) was made both for the sake of simplicity, and because our original motivation to study this problem arose from the application of the Vlasov equation to nuclear dynamics, where short-range physical forces lead to a local \( U_\rho \). However, in many physical applications of the Vlasov equation one deals with long-range forces (e.g. Coulombic and gravitational forces), therefore it may be useful to extend the analysis of the present work, to include non-local mean-field potentials. It is interesting in this context to note that Chandrasekhar [5] has made a detailed calculation of the time scale \( T_E \) required for binary stellar interactions to drive a self-gravitating system of many stars (e.g. a galaxy) toward thermal equilibrium. His result, translated into our notation, is \( T_E \sim m^2 v^3/(Gm^2)^2 \rho \), where we have removed dimensionless factors. Now, the gravitational potential at a given point in the galaxy is roughly \( U \sim -NGm^2/R \), where \( R \) is a distance scale characterizing the size of the galaxy, and \( N \) is the number of stars. If, for purposes of comparison with Eq.16 above, we write \( U' \sim U/\rho \sim U/NR^{-3} \), then we get

\[
T_E \sim \frac{m^2 v^3}{(U')^2 \rho} \cdot R^4. \tag{18}
\]

\(^1\) including the logarithm of a quantity which is essentially the ratio of kinetic to potential energy for a typical star in the system.
This has the form of our Eq.16, only with \( \sigma \) replaced by \( R \), and without the factor \( N/A \) (since there are no “test particles”). The fact that the size of the entire galaxy, \( R \), appears in place of our smoothing parameter \( \sigma \), suggests that — in comparison with short-range forces — long-range forces such as gravity strongly suppress the collisional relaxation toward thermal equilibrium. This is consistent with numerical findings: in semiclassical simulations of nuclear dynamics, the (undesirable) approach to classical Boltzmann equilibrium often takes place on a time scale comparable with the mean-field dynamics in which one is interested \[6\]. In contrast, simulations of the many-body gravitational problem evolve rapidly to a near-static “collisionless equilibrium”, which differs from a microcanonical distribution \[7\].

We now present the results of numerical experiments which we have performed to test our predictions. We simulated the schematic model discussed above — a gas of particles confined to a box — where the box was taken to be a cube of volume 1000 (in arbitrary units) with periodic boundary conditions, and the mean field potential was taken as \( U(\rho) = -0.6\rho + 4\rho^2 \). \( A = 200 \) physical particles of mass \( m = 1 \) were assumed, the initial speed of each particle was set to \( v = 1 \), and a gaussian folding function was used. In each simulation, we allowed the gas of particles to evolve for a time \( \Delta t = 2.5 \), and we followed the growth of the mean square change in test particle energy, \( \langle (\Delta E)^2 \rangle \equiv \frac{1}{N} \sum_{i=1}^{N} (\Delta E_i)^2 \), over this time. For each simulation, we found \( \langle (\Delta E)^2 \rangle \) to grow linearly with time\[4\], in agreement with Eq.14. To extract a numerical energy diffusion coefficient \( D_E \), we divided the final value of \( \langle (\Delta E)^2 \rangle \) by \( \Delta t \).

We ran two sets of simulations. In the first set, the smearing parameter was held fixed at \( \sigma = 1 \), and the number of test particles was varied from \( N = 2000 \) to \( N = 10000 \). In Fig.1 we plot the resulting values of \( D_E \) as a function of \( N/A \) on a log-log plot. From Eq.13, we expect the data to fall along a straight line of slope -1; the solid line gives the best fit of the data to a line of this slope. In the second set of simulations, the number of test particles

\[2\] aside from the inevitable short quadratic growth at the start
was held fixed at 4000, and the smearing parameter was varied from $\sigma = .5$ to $\sigma = 1$. Fig.2 plots the resulting values of $D_E$ as a function of $\sigma$ on a log-log plot, and the solid line gives the best fit of the data to a line of slope -4. In both figures we find good agreement between the prediction of Eq.13 and the numerical results. If we allow the slope of the lines to vary as well, then a best fit of straight lines to the two sets of data yields slopes of $-1.08$ and $-4.54$, instead of $-1$ and $-4$. Thus, the discrepancy between the predicted slope and the best fit to numerical data is on the order of 10% in each case.

Since we used a gaussian folding function in our numerical simulations, it is interesting to compare the results directly to the quantitative prediction of Eq.17. That prediction is depicted by the dotted line in each of the figures. We see that Eq.17 overestimates the value of $D_E$ by a factor of nearly 2. We believe that this discrepancy is due to our neglect of correlations between different collisions. (Since motion in our mean field is highly regular, we can expect that the energy exchanged in a given collision between two test particles will be somewhat correlated with the energy exchanged at the next collision of those two particles.)

To conclude, we have argued in this paper that when the Vlasov equation is studied numerically using the method of test particles, the inevitable interactions between test particles introduce errors which accumulated diffusively. Our main result — a prediction of how the associated diffusion constant scales with the available numerical parameters — was shown to agree well with the results of computer simulations.

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FIGURES

FIG. 1. The energy diffusion constant $D_E$ as a function of $N/A$, the number of test particles per physical particle. The heavy dots show the values of $D_E$ extracted from numerical experiments, the solid line shows the best fit of these points to a straight line of slope -1, and the dotted line shows the quantitative prediction of Eq.17.

FIG. 2. $D_E$ as a function of smearing parameter $\sigma$. The solid line is a best fit of the data to a straight line of slope -4; the dotted line represents Eq.17.