Noise-induced instability in self-consistent Monte Carlo calculations

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We identify, analyze, and propose remedies for a numerical instability responsible for the growth or decay of sums that should be conserved in Monte Carlo simulations of stochastically interacting particles. "Noisy" sums with fluctuations proportional to $1/\sqrt{n}$, where n is the number of particles in the simulation, provide feedback that drives the instability. Numerical illustrations of an energy loss or "cooling" instability in an Ornstein-Uhlenbeck process support our analysis.

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I. INTRODUCTION

We consider the computational task of pushing particles in a stochastically interacting system for which system-wide quantities like total energy or momentum are conserved. In general the parameters defining the stochastic process depend self-consistently upon the instantaneous state of the system: for instance, the collision rate might depend upon the system temperature. This dependence can open a numerical feedback channel, which in turn drives an unphysical growth or decay of quantities that should be conserved. The burden of our paper is: (1) to show how such a "heating" or "cooling" instability arises in typical Monte Carlo realizations of a stochastic process described by a Langevin equation, (2) to analytically describe and numerically illustrate the evolution of such an instability, (3) to propose ways of eliminating the instability in Monte Carlo calculations, and (4) to place this work in the context of physical models of plasmas and gases.

A Monte Carlo simulation calculates the time evolution of n computational particles. These n particles constitute a necessarily finite sample of a larger population and each particle has certain associated random variables (e.g., particle velocity). In consequence, sums of a function of individual particle random variables (e.g., total energy or momentum) must themselves be random variables even when meant to represent conserved quantities. Typically, fluctuations in these n-particle sums of random variables are proportional to $1/\sqrt{n}$ and are what could be called "finite sample noise". The presence of finite sample noise in Monte Carlo calculations is not surprising—what is surprising is that finite sample noise can drive a numerical instability which causes quantities that should be conserved not only to fluctuate but also to grow or decay. In this paper we investigate the finite sample, noise induced, instability of self-consistent Monte Carlo simulations.

Our initial motivation was to understand the instability as it occurred in particle-in-cell (PIC) simulations of a plasma to which a stochastic collision operator modeling an Ornstein-Uhlenbeck process had been added [1]. PIC simulations solve field equations on a mesh and advance particle velocities with fields interpolated from nearest mesh points [2]. In this way the number of calculations necessary to advance a system of n particles per time step scales as n rather than as n^2. Because PIC simulations determine the fields only on the mesh, they cannot account for the brief and intense interactions between particles (i.e., collisions) arising when particles approach each other more closely than the distance between adjacent mesh points. For this reason PIC codes have been most frequently used to model systems (e.g., plasmas, neutrons, or galaxies) tenuous enough to be effectively "collisionless".

However, efforts have also been made to incorporate the effect of binary collisions into PIC computer codes with Monte Carlo techniques. As computational time has become more available such "PIC-MCC" (where MCC stands for Monte Carlo calculations) simulations have become more convenient. In Ref. [1], for instance, particles were made to respond not only to electromagnetic fields but also to a stochastic "collision field" described by a Langevin equation but likewise determined only on the mesh. Other PIC-MCC techniques have been used as well [2].

We have organized our paper as follows. Section II introduces the fundamental set of Langevin equations and Sec. III derives conditions under which they conserve a system-wide population average. Section IV recapitulates this material for finite sample averages. Section V analyzes the instability while Sec. VI numerically illustrates the energy decay or "cooling" version of the instability in a Monte Carlo simulation of an Ornstein-Uhlenbeck process. Section VII shows how the instability can be avoided. Finally, Sec. VIII summarizes and discusses applications.

II. FUNDAMENTAL DYNAMICAL EQUATION

Because the Langevin equation is widely applicable (i.e., to all continuous Markov processes), we believe the mathematics of the Langevin equation underlies many, if not all, PIC-MCC simulation codes. Furthermore, because the Langevin equation is mathematically well understood, we believe it is an appropriate tool for code design and analysis.

The generalized Langevin equation is one of two equivalent formulations of a continuous Markov (i.e., memoryless) stochastic process. Here we use it, i.e.,

$$dv = A(v,t)dt + \sqrt{D(v,t)dt}\,N(0,1) , \tag{1}$$

to describe the time evolution of particle velocity v in one dimension. Here $N(0,1)$ stands for a normal random variate with population mean 0 and variance 1. The drift $A(v,t)$ and diffusion $D(v,t)$ coefficients incorporate desired physics including, in our case, conservation of system kinetic energy and linear momentum. The second term on the right hand side of Eq. (1) makes it a stochastic differential equation with v a random variable rather than an ordinary differential equation with v a "sure" variable. When $D(v,t)=0$ for all v and t, Eq. (1) describes a "Liouville" (i.e., deterministic) process; when $A(v,t)=0$ and $D(v,t)=$const, (1) describes a "Wiener" process [3].

Completely equivalent to the generalized Langevin equation (1) is the one-dimensional Fokker-Planck equation

$$\frac{\partial}{\partial t}P(v,t) = -\frac{\partial}{\partial v}[A(v,t)P(v,t)] + \frac{1}{2}\frac{\partial^2}{\partial v^2}[D(v,t)P(v,t)] , \tag{2}$$

where $P(v,t)$ is the time-dependent probability density of v. We will have occasion to use the density $P(v,t)$ and the Fokker-Planck equation (2). However, numerical algorithms for Monte Carlo codes which follow discrete particle behavior are more readily based upon the Langevin equation (1).

Here and throughout the paper we adopt the so-called Ito interpretation [4] of our fundamental stochastic process (1). The integration of stochastic differential equations like (1) cannot, unfortunately, be defined as a Reiman-Steltjes integral. Instead there are a whole set of possible definitions, usually called "interpretations", of an otherwise ill-defined mnemonic form (1). The particular features of the application at hand must be allowed to dictate which definition, i.e., which interpretation, is used. We justify our use of the Ito interpretation in Sec. V. In the meantime we note that the Ito interpretation does not differ from the Stratonovich and other possible interpretations for homogeneous diffusion processes with $D(v,t)=D(t)$.

We also suppress or ignore spatial dependence so that the system of which we write is local (e.g., pertaining to one cell of a PIC code), or, if extended, then homogeneous. We, furthermore, limit our considerations to systems composed of a single species of mass m particles. Then the total linear momentum and kinetic energy of such a system are proportional to $m\langle v\rangle$ and $m\langle v^2\rangle 2$, respectively. Here the bracket notation indicates a system population average

$$\langle f(v)\rangle = \int_{-\infty}^{\infty} dv\, P(v,t)f(v) , \tag{3}$$

where $f(v)$ is an arbitrary function and the probability density $P(v,t)$ is assumed normalized.

III. CONSERVED QUANTITIES

In many applications, total linear momentum and kinetic energy of a species are preserved by intraspecies interactions, i.e., the species mean $\langle v\rangle$ and variance $\langle v^2\rangle - \langle v\rangle^2$ of $P(v,t)$ are constants in the process defined by (1) or, equivalently, (2). These are special cases of the conservation of $\langle f(v)\rangle$ where $f(v)$ is an arbitrary function of v. Conservation of $\langle f(v)\rangle$ is denoted as

$$d\langle f(v)\rangle = 0 . \tag{4}$$

As we shall see, conservation law (4) is consistent with process (1) only when the drift $A(v,t)$ and diffusion $D(v,t)$ coefficients are related in a certain way.

The time evolution of $f(v)$, i.e., an expression for $df(v)$, given the general process (1) is determined by

$$\begin{aligned} df(v) &= f(v+dv)-f(v) , \\ &\approx f'(v)dv + \frac{f''(v)}{2}(dv)^2 , \\ &= f'A\,dt + f'\sqrt{D\,dt}\,N + \frac{f''}{2}D\,dt , \end{aligned} \tag{5}$$

where the prime denotes a derivative with respect to argument, i.e., $f'=df(v)/dv$, $N=N(0,1)$, and function arguments have been and will be suppressed where obvious. Performing the bracket operation on each side of the above we find that

$$d\langle f\rangle = \left[\langle f'A\rangle + \frac{\langle f''D\rangle}{2}\right]dt , \tag{6}$$

since $\langle f'\sqrt{D}N\rangle = \langle f'\sqrt{D}\,\rangle\langle N\rangle = 0$ because the normal variate N is statistically independent of the product $f'\sqrt{D}$. Therefore, if $\langle f\rangle$ is to be conserved, the functions $A(v,t)$ and $D(v,t)$ must be chosen so that

$$\langle f'A\rangle + \frac{\langle f''D\rangle}{2} = 0 . \tag{7}$$

For example, a Wiener process [$A=0$, $D=$const] conserves momentum ($f=v$) but not kinetic energy ($f=v^2$). The simplest process which conserves both is a time-independent Ornstein-Uhlenbeck process with

$$A(v,t) = A(v) = -\gamma(v-\beta) \tag{8}$$

and

$$D(v,t) = D = \delta^2 , \tag{9}$$

where γ, β, and δ are independent of v and t. Thus an Ornstein-Uhlenbeck process conserves momentum when

$$\beta=\langle v\rangle \ , \tag{10}$$

and kinetic energy when

$$\delta^2=2\gamma(\langle v^2\rangle-\langle v\rangle^2) \ . \tag{11}$$

IV. MONTE CARLO SIMULATIONS

A Monte Carlo simulation determines the time evolution of v for a finite number of particles ($i=1,\ldots,n$) with a time-differenced version of (1):

$$dv_i=A(v_i,t)dt+\sqrt{D(v_i,t)}N_i(0,1) \ . \tag{12}$$

These n particle equations are a sample which must suffice to represent the entire population. How then, in this version of the fundamental equation, are the drift A and diffusion D coefficients chosen so that one or more system quantities are conserved? How, indeed, are these conserved quantities defined?

We replace the population average $\langle f(v)\rangle$ defined by Eq. (3) with a quantity proportional to the finite sample average denoted by $\bar{f}$ and defined by

$$\bar{f}=\frac{1}{n}\sum_{i=1}^{n} f(v_i) \ . \tag{13}$$

The time evolution of $\bar{f}$ is then straightforwardly derived by summing each term in Eq. (5) over the sample and dividing by n. In this way we find

$$d\bar{f}=\left[\overline{f'A}+\frac{\overline{f''D}}{2}\right]dt+\overline{f'\sqrt{D}N}\sqrt{dt} \ . \tag{14}$$

Note that Eq. (14) does not quite take the same form as its population equivalent Eq. (6); (14) contains a third term on the right hand side which is a function of the normal variates $N_i(0,1)$, $i=1,\ldots,n$. If we require the drift A and diffusion D coefficients to satisfy the sample average equivalent of Eq. (7), i.e.,

$$\overline{f'A}+\frac{\overline{f''D}}{2}=0 \ , \tag{15}$$

the sample average $\bar{f}$ is not exactly conserved but evolves according to the stochastic differential equation

$$d\bar{f}=\overline{f'\sqrt{D}N}\sqrt{dt} \ . \tag{16}$$

Equation (16) is cast into more revealing form via the "normal sum theorem"

$$\sum_i a_iN_i(0,1)=N\left[0,\sum_i a_i^2\right]$$

so that

$$d\bar{f}=N\left[0,\frac{\overline{f'^2D}}{n}\right]\sqrt{dt} \ . \tag{17}$$

Thus, as one might expect, the nonvanishing term on the right hand side of (16) or (17) is a finite-sample noise term which vanishes in the limit of indefinitely large sample, i.e.,

$$\lim_{n\to\infty}\overline{f'\sqrt{D}N}=0 \ . \tag{18}$$

Nonvanishing finite-sample noise is never benign. Even when the quantity $f'N\sqrt{D}$ is independent of $\bar{f}$ and constant in time, the resulting Wiener process [i.e., Eq. (17)] causes the supposedly conserved quantity $\bar{f}$ to drift Brownian-motion style within an ever-growing range of magnitude proportional to $\sqrt{t}$. Furthermore, as we shall see, when $f'N\sqrt{D}$ is an increasing (decreasing) function of $\bar{f}$, $\bar{f}$ decreases (increases) systematically. In particular, when $f'N\sqrt{D}$ is linearly proportional to $\bar{f}$ and the application admits of the Ito interpretation, $\bar{f}$ decreases exponentially.

V. NOISE-INDUCED INSTABILITY

Under certain circumstances a sample average $\bar{f}$ with a conserved population average $\langle f\rangle$ can be driven unstable by finite-sample noise even though, according to (17), the increment $d\bar{f}$ is at each time step normally distributed around zero.

An important process in which this instability occurs is the Ornstein-Uhlenbeck process defined by Eqs. (1) and (8)–(11) designed so that the total momentum and kinetic energy is conserved apart from finite sample fluctuations. Then

$$A(v,t)=-\gamma(v-\bar{v}) \tag{19}$$

and

$$D(v,t)=2\gamma(\bar{v}^2-\bar{v}^2) \ . \tag{20}$$

Specifically,

$$dv_i=-\gamma(v_i-\bar{v})dt+[2\gamma(\bar{v}^2-\bar{v}^2)dt]^{1/2}N_i \ , \tag{21}$$

for $i=1,\ldots,n$ [5].

Momentum $[f(v)=mv]$ and kinetic energy $[f(v)=mv^2/2]$ as well as mean $[f(v)=v]$ and variance $\{f(v)=[n/(n-1)](v-\bar{v})^2\}$ functions satisfy supposed conservation laws (15) for this process. However, according to Eq. (17), the time evolution equations for the mean velocity m where here

$$m=\bar{v} \ , \tag{22}$$

and the sample variance s^2 where

$$s^2=\frac{n}{n-1}(\overline{v^2}-\bar{v}^2) \tag{23}$$

for this process are determined by

$$dm=\left[\frac{2\gamma(n-1)dt}{n^2}\right]^{1/2}sN \tag{24}$$

and

$$ds^2=\left[\frac{8\gamma dt(n-1)^2}{n^3}\right]^{1/2}s^2N \ , \tag{25}$$

respectively.

Equation (24) is coupled to (25), and (25) itself has an inhomogeneous diffusion constant depending upon s^2. Equation (25) can be integrated directly but the result depends upon the interpretation of stochastic integration adopted. Given the Ito interpretation and that γ is time

independent, we can invoke the Ito interpretation to arrive at the solution

$$s^2=s_0^2\exp\left\{-\frac{4\gamma(n-1)^2}{n^3}t+2\left[\frac{2\gamma t(n-1)^2}{n^3}\right]^{1/2}N\right\}, \tag{26}$$

where $s_0^2\equiv s^2(t=0)$. s^2 is a so-called log-normal random variable because its logarithm is distributed normally, i.e.,

$$\ln\left\{\frac{s^2}{s_0^2}\right\}=N\left[-\left[\frac{4\gamma(n-1)^2}{n^3}\right]t,\left[\frac{8\gamma t(n-1)^2}{n^3}\right]\right]. \tag{27}$$

This Ito solution of (25), i.e., (26) and (27), is well documented [6].

The other common interpretation of the stochastic differential equation Eq. (25) (i.e., the Stratonovich) results in a log-normal solution of form (27) with zero mean. Since the Ito interpretation leads instead to a very different result, Eq. (27) with nonvanishing mean, our use of the Ito calculus must be justified. The difference between the Ito and Stratonovich interpretations is most succinctly explained in terms of how one would solve an equation like (25) with finite time differencing and summation. A scheme of *explicit* time differencing corresponds to an Ito interpretation while *centered* time differencing corresponds to a Stratonovich interpretation. Explicit time differencing of (25) means determining the increment in s^2 from the old value of s^2. With time centered differencing the increment is determined from the value of s^2 midway into the time increment. Other differencing schemes are, of course, possible and lead to other interpretations. That the final result depends upon the differencing scheme chosen even in the continuum limit is what distinguishes the integration of stochastic differential equations from that of ordinary differential equations.

Our simulations do not solve Eq. (25) directly; rather Eq. (25) is an interpretation of the combined effect of numerically solving many single particle Langevin equations (33) below. However, in numerically integrating each Langevin equation we see no alternative but to assume (and thus do assume) that the system variance is a constant over the time step. Then after each time step the new variance is calculated. For this reason we believe our simulation results are most closely modeled by an explicit differencing, i.e., an Ito interpretation of (25), and the solution (26) or (27) is the relevant one.

Equations (26) and (27) describe a temporal decay in the median of the sample variance s^2 [or, equivalently, temporal decay in the mean of the sample $\ln(s^2)$]. Since s^2 is proportional to the system kinetic energy and thus to its temperature, s^2 decay is equivalent to system cooling. Furthermore, although we cannot analytically solve Eq. (24), general features of its solution are now clear. The sample mean m drifts Brownian-motion fashion and then "freezes" or becomes increasingly fixed as the system cools.

The presence of the normal variate in the argument of the exponential of (26) insures that the distribution of s^2 is very skew with a long, large-variance, high-temperature tail. However, the negative term proportional to time also suggests that typical values of s^2 decay in time. These interpretations are only apparently contradictory because they refer to different features of Eqs. (26) and (27). It can be shown (see again Refs. [6]) that the expected or mean variance does not change, i.e.,

$$\langle s^2\rangle=s_0^2\ . \tag{28}$$

Evidently, most realizations of the sample cool, modulo fluctuations, while a few become very hot. We call this "noise-induced cooling".

Noise-induced cooling in an Ornstein-Uhlenbeck process is, in the above sense, exponential in time. The exponential decay decrement $(\gamma^{-1}n^3)/[4(n-1)^2]$ is much larger than the time scale for relaxation to equilibrium γ^{-1} when $n\gg 2$. Therefore, in practice (i.e., when $n\gg 2$), exponential noise-induced cooling is significant only for systems which spend much time in thermal equilibrium.

Equations (25)–(27) represent a special case of a larger class of processes exhibiting growth or decay of a sample variable $\bar{f}$ whose population value is conserved. For each member of the class the increment $d\bar{f}$ is a normally distributed random variable with vanishing mean and variance equal to $(f'^2D\sqrt{dt})/n$ as in Eq. (17). Thus the increment $d\bar{f}$ is positive and negative with equal frequency. However, when the size of the increment, i.e., $(f'^2D\sqrt{dt})/n$, increases with $\bar{f}$, the random variable $\bar{f}$ will decay in time; when the increment decreases with $\bar{f}$, the random variable $\bar{f}$ will increase in time. Decay (e.g., cooling) occurs because the system gets "stuck" in a region of phase space where $\bar{f}$ is small much as a Brownian particle gets stuck in the high viscosity region of an inhomogeneous fluid. Likewise $\bar{f}$ grows whenever and because $\bar{f}$ gets "frozen" (i.e., fluctuates weakly), in regions of phase space where $\bar{f}$ is large.

Such dynamics might be more familiar when expressed in terms of a common gambling tactic. Accordingly the gambler decreases his wager by a preselected fraction after every win and similarly increases the wager after every loss. In this way the gambler's wealth can become "frozen" at a high value even though the probability of a loss might be somewhat higher than the probability of a win. The opposite, and possibly more natural, behavior of decreasing the size of the wager after a loss and increasing it after a win leads inevitably to financial ruin.

Heating is also natural in an Ornstein-Uhlenbeck process for which γ is a function of the instantaneous state of the system through the system energy or variance. Suppose, for instance,

$$\gamma=\left[\frac{s^2}{s_0^2}\right]^p\ . \tag{29}$$

Then Eq. (25) would have the form

$$ds^2\propto\sqrt{s^{4+2p}dt}\,N(0,1)\ . \tag{30}$$

We are not aware of exact solutions to Eq. (30) except when $p=0$, i.e., when $\gamma=$const. However, it is straightforward to show that limiting (i.e., $t\to\infty$) stationary solutions to the Fokker-Planck equation (2) corresponding to the Langevin equation (30) have the form

$$P(s^2,t\to\infty)\propto s^{-4-2p}. \tag{31}$$

Therefore, when $p>-2$ the system cools; when $p<-2$ it heats. The marginal case ($p=-2$) leads to a Brownian drift of s^2.

VI. NUMERICAL METHOD

We time difference the set of Eq. (21)

$$dv_i=-\gamma(v_i-\bar{v})dt+[2\gamma(\overline{v^2}-\bar{v}^2)dt]^{1/2}N_i\ , \tag{32}$$

for $i=1,\ldots,n$ by assuming γ, $\bar{v}$ and $(\overline{v^2}-\bar{v}^2)$ are constants independent of the variables v_i and time t over a time step Δt. The nonlinear nature of the square root function make methods based on other assumptions very inconvenient if not impossible to execute. Furthermore, these assumptions make sense because $\bar{v}$ and $(\overline{v^2}-\bar{v}^2)$ are typically weak functions ($\propto v_i/n$) of v_i. Also, the e-folding time of the instability is, according to Eq. (27), $(\gamma^{-1}n^3)/[4(n-1)^2]$, which is, typically (i.e., for $n\gg2$), long compared to the e-folding time for changes in v_i, that is γ^{-1}.

Separating variables and integrating (32) we find [7] the difference equations

$$v_i(t+\Delta t)=v_i(t)e^{-\gamma\Delta t}+\bar{v}(t)(1-e^{-\gamma\Delta t})+s\sqrt{1-e^{-2\gamma\Delta t}}N_i \tag{33}$$

for $i=1,\ldots,n$. These are used in all subsequent calculations. Equation (33) is also an alternative starting point for derivations of Eqs. (24) and (25).

In computations particle velocities were chosen initially from a normalized Maxwellian distribution (i.e., a Gaussian probability density) with unit temperature (i.e., initial variance $s_0^2=1$). Each time step the n particle velocities were advanced with the n equations (33) and quantities m and s^2 were updated and stored. Calculations were done on the Amherst College Open VMS VAX Version 6.0 computer operating system running VAX PASCAL.

Figures 1(a) and 1(b) show typical time histories of the mean [Fig. 1(a)] and variance [Fig. 1(b)] when $\gamma=1.0$. The time step size is small enough, $\Delta t=0.001$, to eliminate finite time step effects. Note that in both runs the trend in s^2 [Figs. 1(b)] is down although occasionally s^2 fluctuates upward as well. As expected the mean m [Fig. 1(a)] fluctuates then "freezes", i.e., becomes fixed, as s^2 decays. Increasing the number of particles in the simulation from $n=35$ to $n=350$ weakens the noise-induced

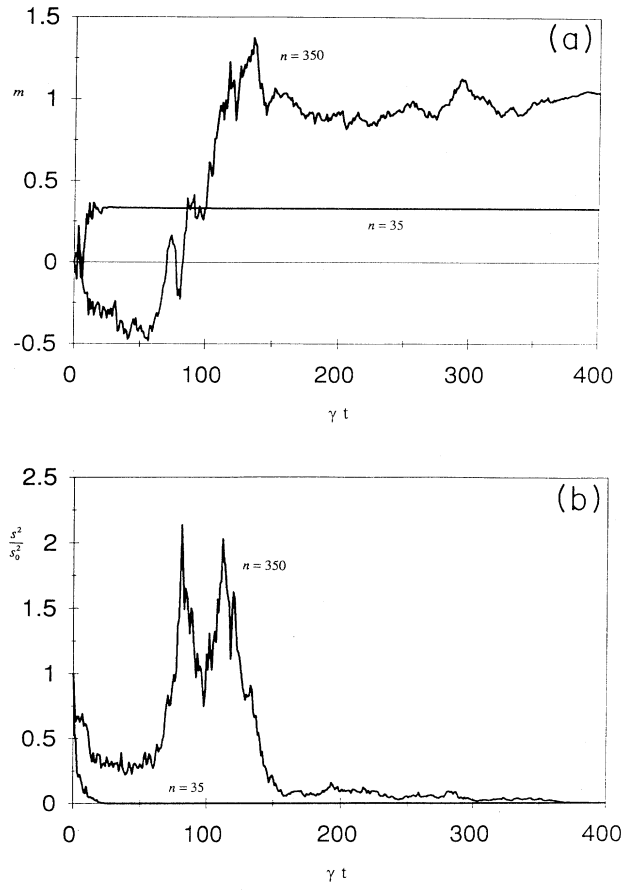

FIG. 1. Time evolution of the velocity mean m [Fig. 1(a)] and variance s^2 [Fig. 1(b)] for two runs of different sample sizes ($n=35$ and 350). The process is Ornstein-Uhlenbeck with constant γ, i.e., the process is determined by Eq. (33) with $\gamma\Delta t=0.001$. The mean velocity m fluctuates randomly then "freezes" as the variance "cools". Increasing the sample size from $n=35$ to 350 weakens but does not eliminate the instability.

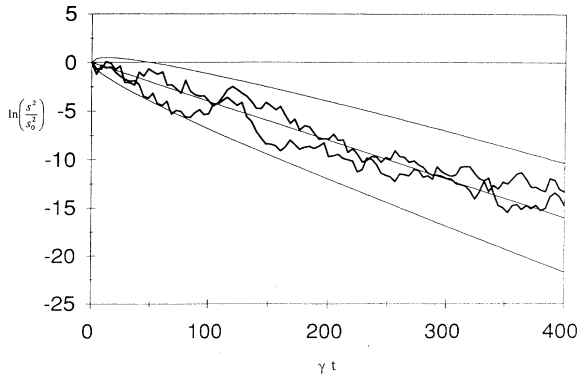

FIG. 2. Time evolution of the velocity variance s^2 on a semilog plot for two stochastically distinct realizations of an Ornstein-Uhlenbeck process with constant γ (dark lines). The number of particles $n=100$ and $\gamma\Delta t=0.001$. Light lines represent the theoretical mean of $\ln(s^2/s_0^2)$ and the envelope formed by the mean $\pm$ one standard deviation of $\ln(s^2/s_0^2)$ as predicted by Eq. (27).

numerical instability but does not eliminate it. These observations are consistent with Eqs. (24) and (25) and solution (26).

Figure 2 more positively identifies the instability as that analyzed in Sec. V. Here are time histories of the variance s^2 for two, typical, process-wise identical (i.e., in Eq. 33 $\gamma=1$ and $\Delta t=0.001$) but stochastically distinct realizations on a semilog plot. Individual histories of $\ln(s^2/s_0^2)$ fall within a standard deviation of the mean of the log-normal solution (27). Light lines show the theoretical mean and standard deviation envelope, $-4\gamma t[(n-1)^2/n^3]$ and $-4\gamma t[(n-1)^2/n^3] \pm\sqrt{8\gamma t[(n-1)^2/n^3]}$, respectively, of the log-normal solution (27). Recall that the mean of the log-normal solution (27) corresponds to the median of exponential solution (26) and that the mean or expected value of the exponential solution (26) is constant in time.

VII. REMEDIES

We've noted (see Fig. 1) that as the sample size increases the instability weakens. In particular, when γ is time independent, the time dependence of $s^2 \propto \exp\{4\gamma[(n-1)^2/n^3]t\}$. Therefore, while this instability can be rendered inconsequential either by increasing the sample size n or limiting the run time T so that

$$\frac{4\gamma T}{n} \ll 1 , \tag{34}$$

this remedy is not always practicable. In PIC simulations, for instance, finite sample noise within a cell may be large because the number of particles per cell n often averages less than 10.

Recall that we could not solve the instability Eqs. (17) or (30) for any but an Ornstein-Uhlenbeck process with time independent γ. Therefore, when $\gamma \propto s^{2p}$ with $p \neq 0$ and for processes other than Ornstein-Uhlenbeck, the instability growth may be even more robust than for Ornstein-Uhlenbeck with $p=0$. Certainly, since $p=0$ leads to exponential damping and $p=-2$ is the marginal Brownian drift case, we expect that $p>0$ leads to faster than exponential damping. Therefore, it is imprudent to depend in all cases on the criterion (34).

For these reasons, methods for defeating the noise-induced instability in Monte Carlo calculations are required which do not depend upon either sample size n or run time T or upon understanding the detailed dynamics of the instability. We propose two such methods both of which completely eliminate the instability by eliminating all fluctuations in samples $\bar{f}$ of conserved quantities $\langle f(v)\rangle$.

The simplest method is, after each velocity advance by the appropriate Langevin equation [e.g., via Eq. (33)], to linearly transform the particle velocities so that their mean and variance recover the desired values. Suppose, for instance, the velocities have been advanced to the values $\{v_i', i=1,\ldots,n\}$ and that this set has a mean m' and variance $s^{2'}$. Suppose also, as is likely, m' and $s^{2'}$ deviate from the previous (desired) values m and s^2. The renormalization

$$v_{i'} \rightarrow v_i ,$$

where

$$v_i = m + (v_{i'} - m')\sqrt{s^2/s^{2'}} , \tag{35}$$

for $i=1,\ldots,n$ returns the mean and variance to m and s^2. Since the transformation is linear in the velocities, it also maps an initially Maxwellian velocity distribution into the same Maxwellian. We have implemented transformation (35) and found that, indeed, it allows the system to evolve stochastically while preserving constant velocity mean and variance.

Another option is to advance the velocities with "quasinormal" $\{Y_i(0,1), i=1,\ldots,n\}$ rather than normal $\{N_i(0,1), i=1,\ldots,n\}$ variates. The purpose of the quasinormal variates Y_i is to zero the term on the right hand side of Eq. (16) that drives the noise-induced instability. Thus the Y_i are a function of the N_i chosen so that

$$\overline{f' Y\sqrt{D}} = 0 , \tag{36}$$

for each function $f(v)$ corresponding to a conserved quantity. When $f(v)$ corresponds to the sample mean, $f(v)=v$, and the sample variance, $f(v)=[n/(n-1)](v-\bar{v})^2$, and when the process is Ornstein-Uhlenbeck with $D(v,t)=2\gamma(\overline{v^2}-\bar{v}^2)$, the conditions (36) become

$$\bar{Y}=0 , \tag{37}$$

and

$$\mathrm{Cov}_S\{v,Y\}=0 , \tag{38}$$

respectively, where $\mathrm{Cov}_S\{v,Y\}$ denotes the sample covariance of v and Y,

$$\mathrm{Cov}_S\{v,Y\}=\overline{vY}-\bar{v}\,\bar{Y} . \tag{39}$$

We also require that the Y_i have unit variance,

$$\overline{Y^2}=1 . \tag{40}$$

The three-parameter linear transformation

$$Y_i = a + bN_i + cv_i , \tag{41}$$

which satisfies these three requirements (37), (38), and (40) is $N_i \rightarrow Y_i$, where

$$Y_i = \left[\frac{n-1}{n}\right]^{1/2} \frac{[(N_i-\bar{N})s^2-(v_i-m)\mathrm{Cov}_S\{Nv\}]}{s\sqrt{s^2\mathrm{Cov}_S\{N^2\}-\mathrm{Cov}_S^2\{Nv\}}} . \tag{42}$$

Sample Monte Carlo simulations of the Ornstein-Uhlenbeck process (33) with quasinormal variates Y_i, defined by transformation (42), replacing the normal variates N_i successfully conserve mean m and variance s^2 without distorting an initially Maxwellian velocity distribution.

Replacing normal variates with quasinormal ones is, possibly, more conceptually direct than renormalizing velocities. The former method does not allow the sample

mean and variance to fluctuate at all while the latter corrects for fluctuations once they have occurred. However, the simplicity of the velocity shift, Eq. (35), is an important advantage.

These remedies employ transformations which satisfy either two (velocity shift) or three (normal variate shift) constraints. Therefore when applied to very small samples, i.e., $n \leq 2$ or $n \leq 3$, respectively, their effect is merely to return velocities or normal variates to their values before the stochastic advance.

VIII. CONCLUSION

The initial motivation for this work was to understand the unphysical cooling of plasma particles in a PIC simulation that modeled intraspecies particle collisions with a $\gamma = \text{const}$, Ornstein-Uhlenbeck process. When the effect of temperature $T[\propto s^2]$ on the plasma particle collision cross section [8] is incorporated into this model so that

$$\gamma = \langle nv\sigma \rangle \propto T^{-3/2} \tag{43}$$

the plasma should heat instead. Likewise, a simulation of a collisional gas of hard spheres will have

$$\gamma = \langle nv\sigma \rangle \propto T^{1/2} . \tag{44}$$

Therefore, the hard sphere gas will cool. We suspect this finite sample, noise induced, instability inhabits other Monte Carlo simulations as well. All the instability requires is: (1) a Monte Carlo calculation of a (multiparticle) set of Langevin equations or their equivalent, (2) sums which should be conserved, and (3) a diffusion coefficient D that is a function of the "conserved" sum $\bar{f}$.

Ornstein-Uhlenbeck processes, because of their simplicity, are widely used to model nonequilibrium processes. We analyzed in detail and numerically illustrated the instability of an Ornstein-Uhlenbeck process. In our analysis, the increment in the size of the supposed conserved kinetic energy is directly proportional to the current size of the kinetic energy and so, according to a straightforward but possibly counter-intuitive deduction via the Ito calculus, the system cools.

Fortunately, there are simple remedies which do not depend upon increasing the sample size or limiting the run time of the simulation. The simplest is to linearly shift the particle random-variables so as to return the "conserved" quantities back to their desired values.

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