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Quiet direct simulation of plasmas

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Abstract

A new approach to particle simulation, called “quiet direct simulation Monte Carlo” (QDSMC), is described that can be applied to many problems of interest, including hydrodynamics, MHD simulation and the modeling of plasmas with arbitrary and arbitrarily varying collisionality. The essence of QDSMC is the use of carefully chosen weights for the particles (e.g., Gauss-Hermite, for Maxwellian distributions), which are destroyed each time step after the particle information is deposited onto the grid and reconstructed at the beginning of the next time step. The method overcomes the limited dynamical range and excessive statistical noise typically found in particle simulations. In this paper QDSMC is applied to hydrodynamics and MHD test problems, and its suitability for modeling semi-collisional plasma dynamics is considered.

I. INTRODUCTION

The dynamics of semi-collisional plasmas, where the mean free path is comparable to length scales of interest in the medium, is germane to a host of plasmas found in nature, e.g., the solar chromosphere, Earth's auroral region, cometary exospheres, and portions of the interstellar medium. Many laboratory plasmas, including those found in boundary regions and divertors of tokamaks and those obtained from laser interactions with target materials, also lie in this regime. The modeling of semi-collisional plasmas poses a challenge both to theory and computation, and the simulation of these plasmas is currently an active area of research [1].

We present in this paper a new simulation technique, which we call “quiet direct simulation Monte Carlo” (QDSMC), that may be applicable the modeling of semi-collisional plasmas. The essence of QDSMC is the use of carefully chosen deterministic samples of the stochastic processes of a system to speed up the convergence of the simulations dramatically over random sampling.

We motivate the idea of QDSMC by considering a simple problem, that of Monte Carlo simulation of diffusion in one dimension

$$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2}. \quad (1)$$

This expression is formally equivalent to the dynamics of Brownian motion [2], and the stochastic differential equation (SDE), i.e., the equation of motion for the diffusing particles' random walks, is

$$dx = \sqrt{2D} dt N(0, 1), \quad (2)$$

with $N(0, 1)$ a normal distribution with zero mean and unit variance. This SDE may be integrated exactly [3], and the result is

$$\begin{aligned} x(t) &= x_0 + \sqrt{2D(t - t_0)} N(0, 1) \\ &= N[x_0, 2D(t - t_0)]. \end{aligned} \quad (3)$$

As is typical for SDEs, the integration results in a distribution of possible random walk paths. Rewriting the normal distribution as a conditional probability for a particle to arrive at position x at time t

$$G(x, t; x_0, t_0) = [2\pi D(t - t_0)]^{1/2} \exp \left[-\frac{(x - x_0)^2}{2D(t - t_0)} \right], \quad (4)$$

we recognize that the normal distribution is merely the Green's function for Equation (1).

The sampling of random walk orbits via integration of the SDEs may thus be interpreted as a Monte Carlo integration of the Green's function for the diffusion equation. While Monte Carlo integration is a very powerful technique for the integration of high-dimensional systems, it is inefficient for low-dimensional integrations, for which deterministic integration techniques converge more rapidly [4]. This motivates the quiet direct simulation Monte Carlo method, where Gaussian-Hermite quadrature [5], a rapidly converging quadrature technique, is used to sample the normal distributions of particle trajectories instead of traditional Monte Carlo. In this way many of the advantages of classical Monte Carlo are retained, but without the statistical noise and finite dynamical range of Monte Carlo. S

The format of this paper is as follows: In Section II we demonstrate the QDSMC method with a formulation of compressible hydrodynamics. In Section III we show how to extend the method to systems with additional physics, e.g. anisotropic pressure tensors, and additional forces, such as the $\mathbf{J} \times \mathbf{B}$ force. A demonstration of this capability is provided in the modeling of MHD. Finally, in Section IV we consider the “worst-case” feasibility of semi-collisional plasma simulation with QDSMC, namely solution of the Fokker-Planck equation of Rosenbluth *et al.* [6]. Unlike hydrodynamics and MHD, where velocity-space structure beyond low-order moments may be neglected, one must resolve velocity space to faithfully capture the kinetic behavior of semi-collisional plasmas. This introduces complications and significant computational overhead to the application of QDSMC.

II. QDSMC MODELING OF HYDRODYNAMICS

The “direct simulation” of hydrodynamics got its start from the early work of Bird [7], who presented a model for the simulation of Boltzmann gases, and later Pullin [8], whose equilibrium particle method (EPM) was a direct simulation formulation of Eulerian hydrodynamics. Hydrodynamics direct simulation proceeds by creating at every point on a spatial mesh an ensemble of particles whose velocities are sampled from the local Maxwellian velocity distribution. These particles are then propagated forward in time according to their respective velocities, and the updated fluid quantities are obtained from gathering the particles’ masses, momenta, and energies to the mesh.

Direct simulation of fluids has many advantages, most notably being unconditionally stable and flexible, with complicated boundaries and geometries implemented by simple conditions on particle trajectories. Conserved quantities such as mass and momentum are divided among the simulation particles, so these quantities remain conserved to within numerical roundoff throughout the simulation. Moreover, all the operations needed to advance the particles in direct simulation may be computed from local data, a feature which reduces the need for message passing on massively parallel computers and appears to be requisite for efficient use of these machines. However, the inherent statistical nature of direct simulation introduces statistical noise and limited dynamical range.

QDSMC is a simple modification to Pullin’s algorithm that address these difficulties while retaining the attractive features of direct simulation. In QDSMC we replace the random sampling of $N(0, 1)$ with a deterministic sampling that uses a small number of particles J chosen to preserve the same low-order moments of $N(0, 1)$ and thus preserve the important underlying physics [9]. This sampling uses the weights and abscissa values of Gauss-Hermite quadrature [5]. QDSMC employs no random numbers, so no statistical noise appears in the results.

In essence, in QDSMC every computational particle is split into J particles that perform a weighted sampling of the trajectories accessible to the simulation particle. Left unchecked,

the repeated subdivisions of particles would lead to exponential growth in the total number of particles. We arrest this growth by gathering the masses, momenta, and energies carried by the simulation particles onto the grid every time step and then destroying and remaking the particles. As a side effect, this aggressive creation and destruction of particles allows QDSMC to access arbitrary dynamical range. (Dynamically creating and destroying particles is hardly unique to QDSMC; it has been employed with success in many other contexts [10]).

We consider the following Boltzmann equation

$$\frac{\partial p}{\partial t} + v_x \frac{\partial p}{\partial x} = \tau^{-1} \frac{\partial}{\partial v_x} [(v_x - u)p] + \tau^{-1} \sigma_v^2 \frac{\partial^2}{\partial v_x^2} p. \quad (5)$$

governing the conditional probability density $p = p(x, v_x; x_0, v_{x0})$. Multiplying (5) by m , mv_x , and $m(v_x^2/2 + \epsilon)$ and integrating over v_x recovers the one-dimensional fluid equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0, \quad (6a)$$

$$\rho \frac{\partial u}{\partial t} + \rho u \frac{\partial u}{\partial x} = -\frac{\partial}{\partial x}(\rho \sigma_v^2) \quad (6b)$$

$$\frac{\partial}{\partial t} \left[\frac{\rho(\sigma_v^2 + u^2)}{2} + \rho \epsilon \right] = -\frac{\partial}{\partial x} \left[\frac{3\rho u(\sigma_v^2 + u^2)}{2} + \rho u \epsilon \right] \quad (6c)$$

given that $p \propto (2\pi\sigma_v^2)^{-1/2} \exp[-(v_x - u)^2/(2\sigma_v^2)]$ (i.e., that the relaxation time τ is sufficiently small for the system to be represented everywhere by a local Maxwellian), and given that the parameters of the Boltzmann equation may be associated with the corresponding fluid quantities: $\rho = \rho(x)$ is the mass density, $u = u(x)$ is the x -component of the mean velocity, $\sigma_v^2 = \sigma_v^2(x)$ the variance of v_x , $P = \rho\sigma_v^2$ the pressure, and $\rho(\epsilon + \sigma_v^2/2)$ the internal energy density. The ideal gas equation of state $\rho(\epsilon + \sigma_v^2/2) = Pd/2$ describes particles with d degrees of freedom.

Clearly, obtaining a solution to the kinetic equation (5) is equivalent to solving the Euler fluid equations (6a)–(6c). The continuum process (5) is also equivalent to an ensemble of microscopic simulation particles each undergoing an Ornstein-Uhlenbeck process [11]

$$\begin{pmatrix} dx \\ dv_x \end{pmatrix} = \begin{pmatrix} v_x dt \\ 0 \end{pmatrix}_{\text{tr}} + \begin{pmatrix} 0 \\ -\tau^{-1}(v_x - u)dt + \sqrt{2\tau^{-1}\sigma_v^2}dtN(0,1) \end{pmatrix}_{\text{th}}, \quad (7)$$

an Itô process [3] which describe the random dynamics of a particle of mass m relaxing at a rate τ^{-1} to the local fluid velocity u and temperature $kT = m\sigma_v^2$. For what follows, we have intentionally split the differential O-U process into a transport piece, denoted by subscript “tr”, and a thermalization piece, denoted by “th.” The transport differential operator describes particle free-streaming, while the thermalization differential operator drives particle velocities toward $u + \sigma_v N(0, 1)$ without changing their positions. In a fluid (where $\tau^{-1}\Delta t \gg 1$) this thermalization is complete in one time step Δt . Although the transport and thermalization operations are conceptually and computationally distinct, they proceed over the same interval Δt .

The QDSMC algorithm is an operator-splitting approximation to (7) that can be described by three steps that together evolve the fluid forward by a time Δt ; these steps may be repeated as necessary to evolve the fluid further in time.

1. At every point x_i on a spatial mesh where the fluid quantities ρ_i , u_i , σ_{vi}^2 , and ϵ_i are known, we represent the fluid by J particles, each with position x_i and specific internal energy $\epsilon_i = (d-1)\sigma_{vi}^2/2$. The particle masses are $m_{ij} = \Delta x \rho_i w_j \pi^{-1/2}$ and the velocities are $v_{ij} = u_i + \sqrt{2\sigma_{vi}^2} q_j$, with $j = 1 \dots J$ and w_j and q_j the corresponding weights and abscissas of a J -point Gauss-Hermite quadrature [5].
2. Each particle is advanced to a new position $x_{ij}^{\text{new}} = x_i + v_{ij} \Delta t$.
3. Local low-order (≤ 2) velocity moments (i.e. the fluid quantities) are computed by linearly distributing the masses, momenta, and energies carried by the particles onto the mesh.

Steps 1 and 2 perform the “tr” part of (7), and the “th” part, which establishes local thermodynamic equilibrium throughout the fluid, is effected by step 3. For efficiency the Gauss-Hermite weights and abscissas used throughout the simulation in step 1 may be tabulated in advance.

The maximum simulation time step is restricted by the requirement that neighboring

fluid elements cannot stream through one another without interacting. This means that Δt must satisfy

$$\Delta t \lesssim \Delta x / \sqrt{\sigma_v^2 + u^2}. \quad (8)$$

In hot fluids (8) is somewhat more restrictive than the traditional Courant-Friedrichs-Lewy criterion ($\Delta t \leq \Delta x/u$) for hydrodynamics stability [12]. We stress, however, that (8) is a condition for fidelity and not stability since all conserved quantities stay rigorously conserved throughout the simulation irrespective of Δt .

We demonstrate the quiet DSMC method with one- and two-dimensional test problems. The first is the classical Sod problem [13] in which a gas cavity of length unity is filled with an ideal gas having a ratio of specific heats $\gamma = 7/5$, i.e. $d = 5$. A membrane located at the midpoint of the cavity separates two populations of gas: both at rest ($v = 0$), the left with density $\rho_L = 1.0$ and pressure $p_L = 1.0$ and the right with density $\rho_R = 0.125$ and pressure $p_R = 0.1$. At time $t = 0$ the membrane breaks and the gas evolves to a configuration with a leading shock, a contact surface, and a left rarefaction, as shown in Fig. (1). The continuous curves are quiet DSMC solutions to the hydrodynamics equations and the dotted lines are the solutions from an exact Riemann solver [14]. The simulation used 4 particles per cell with 1000 simulation cells and a time step $\Delta t = 4.5 \times 10^{-4}$ for a total of 555 time steps. The quiet DSMC calculation has negligible noise and models the shock and rarefaction well. However, diffusion smears out the contact discontinuity over many (~ 25) simulation cells. The diffusion is a function of the particle weighting algorithm. The effective diffusion coefficient scales like $\Delta x^{1/2}$ [15] and can be reduced by making the lattice spacing Δx smaller (see the dot-dashed line in the inset of Fig. (1) panel (a)).

FIG. 1

The large dynamical range of the quiet DSMC model is evident from a more demanding test problem—the left half of the blast wave problem of Woodward and Colella [16] as described in Ref. [13]. The gas in a closed cavity of length unity is assumed to have $\gamma = 7/5$ and constant initial density $\rho = 1.0$ and velocity $u = 0$ throughout. Initially, the pressure varies by five orders of magnitude from the left of $x = 0.5$, where $p_L = 1000$, and to the right,

where $p_R = 0.01$. Figure (2) shows the propagation of the blast wave, associated contact surface, and rarefaction front after a time $t = 0.012$. The simulation used 1000 simulation cells with 4 particles per cell. The time step was chosen to be $\Delta t = 1.4 \times 10^{-5}$ for a total of 857 time steps. Again, the quiet DSMC simulation shows little noise and the shock and rarefaction regions are captured well.

FIG. 2

Generalization of the method to higher dimensions is straightforward and efficient. For each unit normal random number $N(0, 1)$ appearing in the multi-dimensional O-U equations, one introduces a separate set of Gauss-Hermite weights and abscissas. Two-dimensional fluid models, needing two unit normal random numbers, thus require J^2 particles per grid point, and three-dimensional models require J^3 . Unlike traditional DSMC, where a large number of particles is needed in each dimension for adequate sampling of the random processes, in quiet DSMC J is typically small ($\sim 2-5$). Figure (3) shows density at $t = 1.0$ from a two-dimensional simulation of a blast wave that evolves from initial conditions of uniform density $\rho = 1$ and velocity $\mathbf{u} = 0$ ($\gamma = 5/3$), and with a small, circular region of initially higher pressure: $P_{\text{in}} = 1.0$, $P_{\text{out}} = 0.01$. The Cartesian computational mesh used 200×200 grid cells and 4×4 particles per cell, and the simulation ran for 285 time steps. No asymmetry from grid imprinting is evident.

FIG. 3

III. QDSMC MODELING OF MHD

The QDSMC formulation of hydrodynamics modeling may be extended to include magnetic fields. As with hydrodynamics, we begin with a kinetic equation of Fokker Planck form

$$\frac{\partial p}{\partial t} + \mathbf{u} \cdot \nabla p + \mathbf{a} \cdot \frac{\partial p}{\partial \mathbf{v}} = \tau^{-1} \left(\frac{\partial}{\partial \mathbf{v}} \cdot (\mathbf{u} - \mathbf{v})p + \sigma_v^2 \mathbf{I} : \frac{\partial^2}{\partial \mathbf{v}^2} p \right). \quad (9)$$

Here $\mathbf{I}$ denotes the identity tensor and $\mathbf{a}$ is an arbitrary acceleration provided by extrinsic forces—by “extrinsic” we mean forces like the $\mathbf{J} \times \mathbf{B}$ force that are not contained in the stress tensor $\sigma_v^2 \mathbf{I}$; we refer to forces like pressure gradients which are contained in the stress

tensor as “intrinsic” forces. If we choose $\mathbf{a} = \mathbf{J} \times \mathbf{B}/\rho$, multiply the kinetic equation by m , $m\mathbf{v}$, and $mv^2/2$, and then integrate over velocity space, we recover the MHD equations

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u}) \quad (10)$$

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) = -\nabla \cdot \left[\rho \mathbf{u} \mathbf{u} + \left(P + \frac{B^2}{8\pi} \right) \mathbf{I} - \frac{\mathbf{B} \mathbf{B}}{4\pi} \right] \quad (11)$$

$$\frac{\partial}{\partial t} \left(\frac{\rho u^2}{2} + \frac{3P}{2} + \frac{B^2}{8\pi} \right) = -\nabla \cdot \left[\mathbf{u} \left(\frac{\rho u^2}{2} + \frac{5P}{2} + \frac{B^2}{4\pi} \right) - \frac{\mathbf{u} \cdot \mathbf{B} \mathbf{B}}{4\pi} \right] \quad (12)$$

with $\mathbf{u}$ the local fluid velocity, $\sigma_v^2 = P/\rho$ the velocity variance (proportional to the temperature), ρ the mass density of the fluid, and $\mathbf{J}$ and $\mathbf{B}$ the current density and magnetic field, respectively. The ideal MHD induction equation $\partial \mathbf{B}/\partial t = \nabla \times (\mathbf{u} \times \mathbf{B})$ is assumed. As before with hydrodynamics, we rewrite the Fokker Planck equation (9) in terms of equivalent (Itô) stochastic differential equations of motion for computational particles

$$\begin{pmatrix} d\mathbf{x} \\ d\mathbf{v} \end{pmatrix} = \begin{pmatrix} \mathbf{v} dt \\ \mathbf{a} dt \end{pmatrix}_{\text{tr}} + \begin{pmatrix} 0 \\ -\tau^{-1}(\mathbf{v} - \mathbf{u})dt + \sqrt{2\tau^{-1}\sigma_v^2 dt} \mathbf{N}(0, 1) \end{pmatrix}_{\text{th}}, \quad (13)$$

These equations may be integrated by operator-splitting, and the thermalization step, in the small- τ limit, ensures that the system stays in local thermodynamic equilibrium.

For illustration, we consider a one-dimensional system with physical quantities that vary in the x -direction only and with magnetic field $\mathbf{B} = B_x \hat{x} + B_y(x) \hat{y}$. The induction equation is then

$$\frac{\partial B_y}{\partial t} + \frac{\partial(u_x B_y)}{\partial x} = B_x \frac{\partial u_y}{\partial x} + \eta \frac{\partial^2 B_y}{\partial x^2}, \quad (14)$$

where we have added the effect of a small resistivity η . We can solve this system by staggering the magnetic field advance and the particle push. The following simple updating prescription accomplishes this:

1. At each mesh point X_n we obtain the time-advanced local magnetic field $B_{yn}^{i+1/2}$ by solving the differenced induction equation (14) implicitly using $B_{yn}^{i-1/2}$ and the local velocities u_n^i .

2. At every mesh point X_n , particles are created with positions $x_{nj}^i = X_n$, masses $m_{nj} = \rho_n \Delta x w_j$ and velocities $v_{nj} = u_n^i + \sqrt{\pi} \sigma_{vn} a_j$, where w_j and a_j are the weights and abscissas of J -point Gauss Hermite quadrature.
3. The particle positions are advanced by $\Delta t/2$ according to $x_{nj}^{i+1/2} = x_{nj}^i + (v_x)_{nj}^i \Delta t/2$.
4. Particle densities are extrapolated from the previous values of density on the mesh, i.e. $\rho_n^{i+1/2} = (3\rho_n^i - \rho_n^{i-1})/2$. The density and magnetic field at time $t^{i+1/2}$ are used to compute the acceleration $a_n^{i+1/2}$ on the mesh, and the acceleration values are (linearly) interpolated to the particles to advance the particle velocities: $v_{nj}^{i+1} = v_{nj}^i + a_{nj}^{i+1/2} \Delta t$.
5. The particle positions are advanced by $\Delta t/2$ using the updated particle velocities to get the final particle positions, viz. $x_{nj}^{i+1} = x_{nj}^{i+1/2} + (v_x)_{nj}^{i+1} \Delta t/2$.
6. The mass, momentum, and energy carried by the particles are accumulated onto the mesh via linear weighting to obtain the fluid quantities ρ_n^{i+1} , u_n^{i+1} , and $(\sigma_v^2)_n^{i+1}$. Retention of only these low-order moments of the particle information is equivalent to the “thermalization” step in the $\tau \rightarrow 0$ limit.

This advancement scheme is time-centered. However, the the inverse fluid density arising in the acceleration is obtained by extrapolation, so it can be problematic, particularly when the density changes rapidly over a time step—near a shock interface, for example. Of course, many improvements to the simple time-stepping presented here can be envisioned (e.g. iteration to correct the density near shock interfaces), and these possibilities are currently being investigated by the authors.

We demonstrate the MHD method with two test problems. The first is a test of the dispersion of shear Alfvén waves and is shown in Fig. 4. Good agreement is observed between the theoretical and observed dispersion relations. The second MHD test problem is a simple MHD shock tube. This shock tube problem is, in essence, the Sod problem with the addition of a parallel magnetic field and a current sheet at the interface; it resembles

FIG. 4

the construction of Brio and Wu [17], but with a weaker initial magnetic field. The initial conditions are

$$\begin{aligned} \rho_L = 1.0, \quad \rho_R = 0.125, \quad P_L = 1.0 \quad P_R = 0.1 \\ B_{yL} = 1.0, \quad B_{yR} = -1.0, \quad B_x = 0.75, \quad u = 0 \end{aligned} \tag{15}$$

with a ratio of specific heats $\gamma = 5/3$ and with the magnetic field normalized as in (10)–(12). In Fig. 5 we show the results at $t = 150$ for the breakup of the discontinuity into a sequence of structures, including a fast rarefaction (FR), a slow compound wave (SM), a contact discontinuity (CD), and a slow shock (SS). The simulation had 800 cells with 4 particles/cell (3200 particles total).

FIG. 5

Some remarks are in order regarding this formulation of MHD. First, our construction resembles the distribution function method (DFM) of Huba and Lyon [18], except that we reconstruct the particle distributions directly from distribution functions (of considerably simpler form) instead of working with fluxes computed from distribution functions. One cannot use the DFM distribution functions in QDSMC, incidentally, because the DFM distribution functions are negative-valued for some v . The extra cost in QDSMC is the need to compute the acceleration from extrinsic forces on the particle orbits. (It is possible for some systems to include magnetic pressure and tension as intrinsic forces—see Appendix A). Finally, we note that arbitrary extrinsic forces such as gravity may be applied to the fluid through a suitable choice of $\mathbf{a}$ in (9). Intrinsic forces, e.g. those arising from an anisotropic pressure tensor, may be included by suitable definition of the stress tensor σ_v^2 . Such a model would be appropriate for adding finite Larmour radius effects or material stresses and elastic/plastic flow. The downside of using an anisotropic pressure tensor is that particle creation would entail solving at every time step a three-dimensional eigenvalue problem at each mesh point. Except for simple pressure tensors, the computational overhead of this step would be considerable and, e.g. when the pressure matrix is nearly singular, could potentially dominate that of pushing the particles.

IV. QDSMC MODELING OF SEMI-COLLISIONAL PLASMAS

The applicability of QDSMC to systems described by a Fokker-Planck kinetic equation suggests that it may be used to model collisions among plasma particles. We examine this possibility here. Let us consider the feasibility of modeling with QDSMC the full Fokker-Planck dynamics of scattering among particles in three velocity dimensions; this problem represents the “worst case” scenario, one where the highest level of description of the scattering process is needed.

We start with the Fokker-Planck model of Rosenbluth *et al.* [6] for small-angle Coulomb collisions. The distribution function f_T of test species T obeys

$$\frac{\partial f_T}{\partial t} = \sum_{\alpha} \left[-\frac{\partial}{\partial v_i} \left(f_T \frac{\partial h_{\alpha}}{\partial v_i} \right) + \frac{1}{2} \frac{\partial^2}{\partial v_i \partial v_j} \left(f_T \frac{\partial^2 g_{\alpha}}{\partial v_i \partial v_j} \right) \right] \frac{4\pi n_{\alpha} q_T^2 q_{\alpha}^2}{m_T^2} \log \Lambda, \quad (16)$$

where g_{α} and h_{α} are the Rosenbluth potentials. If we assume that g_{α} and h_{α} do not vary significantly over a time step, then (16) may be written as a stochastic differential equation

$$dv = \mathbf{A}dt + \mathbf{B} \cdot (dt^{1/2} \mathbf{N}(0, 1)) \quad (17)$$

where the velocity-space “drag” and “diffusion” terms $\mathbf{A}$ and $\mathbf{B}$ have the form

$$A_i = \frac{\partial}{\partial v_i} \sum_{\alpha} h_{\alpha} \frac{4\pi n_{\alpha} q_T^2 q_{\alpha}^2}{m_T^2} \log \Lambda \quad (18)$$

$$B_{ij} = \frac{\partial^2}{\partial v_i \partial v_j} \sum_{\alpha} g_{\alpha} \frac{4\pi n_{\alpha} q_T^2 q_{\alpha}^2}{m_T^2} \log \Lambda. \quad (19)$$

Such an SDE may be solved in each velocity-space cell to determine how the “mass” contained in the cell propagates to neighboring cells. The matrix $\mathbf{B}$ is symmetric, so the evolution of velocity component v_i (velocity projected along the i th eigenvector of $\mathbf{B}$) obeys $v_i(t + \Delta t) = N_i[v_i(t) + A_i \Delta t, \lambda_i^2 \Delta t]$, where λ_i is the i th eigenvalue of $\mathbf{B}$ and A_i is the projection of $\mathbf{A}$ along the i th eigenvector. The three normal distributions N_i may be sampled with the Gauss-Hermite prescription and require, nominally, the creation of eight particles for each mass point in a cell to reproduce the three-dimensional velocity-space drift and diffusion.

Care must be taken when creating and weighting the particles to prevent numerical heating. Area weighting with particle creation at cell centers, for example, preserves mass and momentum, but not energy. Energy conservation requires that the mass distributions be created such that the variances and covariances of the mass distributions in each cell are preserved. This may be accomplished by: (a) During the gather step of QDSMC the covariance matrix $\underline{\sigma}_v^2 = \sum_p w_p (\mathbf{v}_p - \bar{\mathbf{v}})(\mathbf{v}_p - \bar{\mathbf{v}}) / \sum_p w_p$ of the mass distribution in the cell is computed (w_p is the component of the particle mass weighted to the cell, and $\bar{\mathbf{v}}$ is the mean velocity in the cell), and (b) during the particle creation step, eight masses are placed at positions $\bar{\mathbf{v}} \pm \Sigma_{v1} \boldsymbol{\xi}_1 \pm \Sigma_{v2} \boldsymbol{\xi}_2 \pm \Sigma_{v3} \boldsymbol{\xi}_3$, with $\boldsymbol{\xi}_i$ the normalized eigenvectors of $\underline{\sigma}_v^2$ and Σ_{vi}^2 the corresponding eigenvalues. This entails the use of eight mass points per velocity space cell.

Thus, QDSMC simulation of the Rosenbluth collision model would require 8×8 particles of each species in each velocity-space cell. A modest resolution of velocity space, say $10 \times 10 \times 10$, would need 64000 particles/species per spatial cell, or a total of 64 million particles of each species for a PIC simulation with a 1000 spatial cells. This is feasible with present-day computers, though costly. The use of approximate, simpler collision models to capture the salient physics would clearly be desirable.

V. CONCLUSIONS

We have presented a flexible simulation method, the “quiet direct simulation Monte Carlo” method, which may be used to simulate kinetic systems efficiently, accurately, and with a small number of computational particles. The QDSMC method represents a fruitful line of thinking that, we believe, complements the current, continuing trend in plasma physics computation, i.e., towards the use of simulation algorithms that run efficiently and with minimal message passing on massively parallel computers. QDSMC exploits how Fokker-Planck kinetic equations may be written in terms of microscopic equations of motion which are of the form of Itô stochastic differential equations, and it is a prescription for sampling deterministically the unit normal random numbers $N(0, 1)$ that appear in

the SDEs and for aggressively destroying and remaking the particles every time step. This sampling and creation/destruction of particles leads to accurate, low noise representations that use only a small number of particles (typically 2–4 particles/cell/dimension) and which have arbitrary dynamical range. In hydrodynamics simulation, the computational cost of a single QDSMC time step is the same, to within a constant factor proportional to the number of particles per cell, as that of explicit finite differencing; the Courant-Fredrichs-Lewy condition on the time step—a condition for fidelity of the simulation and not stability, as the hydrodynamics method is unconditionally stable—is slightly more restrictive than that of an explicit differencing scheme.

For illustration, we have applied QDSMC to three physical systems: hydrodynamics, magnetohydrodynamics, and kinetic plasmas. We have demonstrated QDSMC on a variety of one- and two-dimensional hydrodynamics test problems, and good agreement with analytic solutions was obtained with no added flux-limiting or artificial viscosity. The method as presented has a small amount of numerical diffusion, however, arising both from the area weighting used to gather particles to the computational mesh and from operator-splitting the transport and thermalization steps. This numerical diffusion could, in principle, be controlled by use of flux limiting techniques, however for clarity of presentation we have ignored these complications here.

A simple QDSMC formulation of MHD was presented as well. Results were shown for a one-dimensional shock tube with a weak magnetic field. Current work by the authors is focussed on improving the simulation method, particularly the treatment of the extrapolated density appearing in the $\mathbf{J} \times \mathbf{B}$ force.

Finally, it was demonstrated how the Fokker-Planck description of collisions among plasma particles might be simulated with QDSMC. Such a collision model could potentially be added to a traditional particle-in-cell plasma simulation. Unlike hydrodynamics and MHD modeling, full kinetic plasma modeling requires resolving the velocity-space structure of the particle distribution functions. This can be accomplished to an arbitrarily fine level of detail by using a velocity-space grid, however the QDSMC method, when applied to

the full Fokker-Planck collision operator, is expensive, requiring a minimum of 64 particles per velocity space cell to both resolve the 3D velocity-space drift and diffusion and conserve energy. Simplified Langevin collision models, may be more practical for the application of QDSMC to this problem.

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APPENDIX A: AN ALTERNATIVE KINETIC FORMULATION OF MHD

For completeness we describe an alternative kinetic formulation of MHD with the curious feature that the total momentum and energy, including Poynting flux and energy of the magnetic field, is carried by the particles. If we use in place of $\sigma_v^2 \mathbf{I}$ in (5) a stress tensor $\underline{\underline{\sigma}}_v^2$ of the form

$$\underline{\underline{\sigma}}_v^2 = \rho^{-1} \left[\left(P + \frac{B^2}{8\pi} \right) \mathbf{I} - \frac{\mathbf{B}\mathbf{B}}{4\pi} \right], \quad (\text{A1})$$

then multiplication of the ensuing kinetic equation by m , $m\mathbf{v}$ and $mv^2/2$ and integration over velocity yields the MHD equations to within a spurious source term $(\partial/\partial t + \nabla \cdot \mathbf{u})(B^2/16\pi)$ in the energy equation. (Computationally, this term could be corrected for easily, or it could be eliminated altogether by adding to $\underline{\underline{\sigma}}_v^2$ an additional tensor $\mathbf{T}$ satisfying $\nabla \cdot \mathbf{T} = 0$, $\mathbf{T} \cdot \mathbf{u} = 0$ and $\text{Tr } \mathbf{T} = B^2/8\pi\rho$). This kinetic MHD formulation is unsatisfactory, however, for many applications—equation (A1) has as one of its eigenvectors the vector $\mathbf{B}$ with corresponding eigenvalue $P - B^2/8\pi$. For sufficiently small β this eigenvalue is negative and corresponds

to a nonsensical, imaginary “width” of the Maxwellian particle distribution in the parallel direction.

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APPENDIX: FIGURE CAPTIONS

FIG. 1. Continuous line: quiet DSMC simulation with 4 particles per cell of the Sod test problem at time $t = 0.25$. Broken line: exact solution. The inset in panel (a) shows a blow-up of the region near the contact discontinuity for two different simulation runs: with 1000 simulation cells (continuous line) and with 4000 simulation cells (dot-dashed line).

FIG. 2. Continuous line: quiet DSMC simulation with 4 particles per cell of the blast wave test problem of Woodward and Colella [16]. Broken line: exact solution.

FIG. 3. Panel (a): two-dimensional quiet DSMC simulation of a blast wave from an azimuthally symmetric initial pressure profile (dashed curve). Panel (b): density v. radius for horizontal (circles) and 45° diagonal (squares) cuts across the evolved density profile. The profiles are essentially identical and in good comparison with density from a one-dimensional, first-order Godunov, Roe approximate Riemann solver (solid line).

FIG. 4. Test of the shear-Alfvén dispersion relation for $\Delta B/B_0 = 0.005$. The solid curve is the analytic dispersion relation, and the points are the simulation results. 256 cells were used, with 4 particles/cell.

FIG. 5. Sod test problem with the addition of a magnetic field. The initial configuration has a jump in B_y (i.e. a thin current sheet in the $\hat{z}$ -direction) at the location of the original discontinuities in pressure and density. Initial profiles are shown in the dashed curves. The solid curves are the evolved density, v_x , T , and B_y after a time $t = 150$. The simulation used 800 cells and 4 particles per cell (3200 particles total).

FIGURES

FIG. 1.

FIG. 2.

FIG. 3.

FIG. 4.

FIG. 5.