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Quiet direct simulation of Eulerian fluids

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The direct simulation Monte Carlo method of modeling fluids requires sampling one or more random variables every time step for each particle. In this paper a ''quiet Monte Carlo'' technique is proposed that eliminates the random sampling and the noise it produces by deterministically generating a small number of computational particles. The technique is applied to particle equations of motion appropriate for modeling an Eulerian fluid. Results indicate that strong one- and two-dimensional shocks with large dynamic ranges are accurately represented with only a few particles per cell.

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The direct simulation Monte Carlo or DSMC method of numerically modeling rarefied gases is said to employ computational particles that free-stream on a fixed grid for a finite interval and then, instantaneously and simultaneously, suffer a random scattering collision. As such, DSMC has been used since 1963 by Bird [1] and others [2] to model high Knudsen number gas flows, in which mean free paths and collision times must be resolved. Pullin [3] adapted the DSMC algorithm to Eulerian fluids by requiring the scattered particle velocities to be drawn from a local Maxwellian. In either application, rarefied gases or ideal fluids, a random number generator is used to advance particle positions and velocities. Although successful, these simulations are computationally expensive because they generate statistical noise that can be controlled only by using many particles or by averaging multiple runs. We propose a method, which we call ''quiet DSMC,'' for doing DSMC dynamics of ideal fluids without calling random numbers—thereby eliminating all statistical noise and the need for averaging.

The formalism underlying the quiet DSMC approach to simulation can be applied to any system that can be described by a Fokker-Planck kinetic equation, including, for example, radiation, neutron, and charged particle transport. Here we focus on fluid dynamics. In this context quiet DSMC is closely related to the lattice Boltzmann method (LBM) [4]. Conventional LBM schemes have two strong limitations that make them unsuitable for modeling transsonic and supersonic flows: They are limited to low Mach numbers, and they are athermal (the models either do not have the correct sound speed/temperature relations or they have unfavorable stability properties). One of the most recently conceived LBM models [5] is able to treat high Mach number dynamics, but at the cost of requiring a large number of particles. In this model the local Maxwellian distributions of particles are represented by choosing the particles' velocities so that each particle travels an integral number of cells in one time step. This eliminates numerical diffusion, but at the cost of requiring a large number of velocities, e.g., 11 velocities per cell per spatial dimension to model low Mach number shocks. As a consequence, properties of the fluid in one cell are distributed over a ''spatial stencil'' of the ten nearest cells (in one dimension), and contact surfaces are ''smeared out'' over a distance of the order of the stencil size. Higher Mach number dynamics would require larger numbers of velocities per cell and thus even larger spatial stencils. We find, and demonstrate below, that quiet DSMC is a possible alternative to compressible LBM that uses fewer particles (typically 2–5 per cell), is not limited in dynamical range, and is straightforward to implement in multidimensions.

In what follows we motivate the quiet DSMC method; a more formal derivation can be found elsewhere [12]. Quiet DSMC uses Gaussian-Hermite quadrature weights and abscissas of the integral $\int_{-\infty}^{\infty}(2\pi)^{-1/2}\exp(-v^2/2)f(v)dv$, where $f(v)$ is an arbitrary function to represent the effect of randomly drawing numbers from the probability density $p(v)=(2\pi)^{-1/2}\exp(-v^2/2)$. According to the theory of Gaussian quadrature [6] the J-point quadrature approximation

$$\int_{-\infty}^{\infty}\frac{e^{-v^2/2}}{\sqrt{2\pi}}f(v)dv\approx\sum_{j=1}^{J}w_j f(q_j) \tag{1}$$

becomes exact when $f(v)$ is a linear combination of the $2J-1$ polynomials $v^0, v^1, \ldots, v^{2J-1}$ if the weights w_j and abscissas q_j are chosen according to standard prescription. Thus, in place of a single random realization of the unit normal random variable $N(0,1)$, i.e., the random number defined by the probability density $p(v)=(2\pi)^{-1/2}\exp(-v^2/2)$, a J-point quiet DSMC calculation would create J deterministic realizations of $N(0,1)$ with weights w_j and abscissa values q_j with $j=1,\ldots,J$. Then the $r=0,1,\ldots,2J-1$ moments of form $\int_{-\infty}^{\infty}(2\pi)^{-1/2}\exp(-v^2/2)v^r dv$ are represented exactly and without fluctuation by $\Sigma_{j=1}^{J}w_j q_j^r$.

Normal random variables arise naturally in particle simulations of fluid behavior because the fluid particle coordinates are governed by stochastic differential equations of motion. For instance, the one-dimensional Ornstein-Uhlenbeck (OU) process equations

$$dx=v_x dt, \tag{2a}$$

$$dv_x=-\gamma(v_x-u)dt+\sqrt{2\gamma\sigma_v^2 dt}N(0,1) \tag{2b}$$

describe the random dynamics of a particle of mass m relaxing at a rate γ to the local fluid velocity u and temperature

$kT=m\sigma_v^2$. The velocity equation (2b) is solved [7] by $v_x(\Delta t)=u+e^{-\gamma\Delta t}(v_{x0}-u)+\sigma_v(1-e^{-\gamma\Delta t})^{1/2}N(0,1)$ given initial condition $v_x(0)=v_{x0}$. In the thermalization limit, $\gamma\Delta t\gg 1, v_x(\Delta t)$ becomes the random variable $u+\sigma_v N(0,1)$ drawn from a local Maxwellian. The OU process equations of motion (2) are equivalently described by a Fokker-Planck kinetic equation

$$\frac{\partial p}{\partial t}+v_x\frac{\partial p}{\partial x}=\gamma\frac{\partial}{\partial v_x}[(v_x-u)p]+\gamma\sigma_v^2\frac{\partial^2}{\partial v_x^2}p \tag{3}$$

governing the conditional probability density $p=p(x,v_x;x_0,v_{x0})$ where $v_x^2/2+\epsilon$ is proportional to the total particle energy and ϵ, the specific internal energy (ignoring translational kinetic energy in the x direction), is the same for all particles at each locale. Multiplying Eq. (3) by $1, v_x$, and $v_x^2/2+\epsilon$ and integrating over v_x recovers the one-dimensional fluid equations

$$\frac{\partial\rho}{\partial t}+\frac{\partial}{\partial x}(\rho u)=0, \tag{4a}$$

$$\rho\frac{\partial u}{\partial t}+\rho u\frac{\partial u}{\partial x}=-\frac{\partial}{\partial x}(\rho\sigma_v^2), \tag{4b}$$

$$\frac{\partial}{\partial t}\left[\frac{\rho(\sigma_v^2+u^2)}{2}+\rho\epsilon\right]=-\frac{\partial}{\partial x}\left[\frac{3\rho u(\sigma_v^2+u^2)}{2}+\rho u\epsilon\right], \tag{4c}$$

given that $p\propto(2\pi\sigma_v^2)^{-1/2}\exp[-(v_x-u)^2/(2\sigma_v^2)]$. Here $\rho=\rho(x)$ is the local 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 equation of state $\rho(\epsilon+\sigma_v^2/2)=Pd/2$ describes particles with d degrees of freedom. A particle simulation with particle coordinates advanced each time step Δt by an OU process with a collision rate large enough so that $\gamma\Delta t\gg 1$ ought to reproduce the fluid dynamics of Eq. (4). We adopt this approach here.

Traditionally, DSMC calculations split particle transport and particle thermalization into two distinct operations; we do the same. This is possible only if the computational splitting corresponds to a formal operator splitting [8] of the appropriate process. In fact, we split the differential OU process (2) into a transport piece, denoted by subscript ''tr'' and a thermalization piece, denoted by ''th,'' as follows:

$$\begin{pmatrix} dx \\ dv_x \end{pmatrix}=\begin{pmatrix} v_x dt \\ 0 \end{pmatrix}_{\rm tr}+\begin{pmatrix} 0 \\ -\gamma(v_x-u)dt+\sqrt{2\gamma\sigma_v^2 dt}N(0,1) \end{pmatrix}_{\rm th}. \tag{5}$$

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 $\gamma\Delta t\gg 1$) 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 quiet DSMC algorithm proposed can be described with three steps that together evolve the fluid forward by a time Δt. To evolve the fluid to a time t we repeat these steps $t/\Delta t$ times.

(1) At every point x_i on a spatial mesh where the fluid quantities $\rho_i, u_i, \sigma_{vi}^2$, and ϵ_i are known, we represent the fluid by J particles, each with position x_i and specific internal energy $\varepsilon_i=(d-1)\sigma_{vi}^2/2$. 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 $j=1,\ldots,J$ and w_j and q_j the corresponding weights and abscissas of a J-point Gauss-Hermite quadrature [6].

(2) Each particle is advanced to a new position $x_{ij}^{\rm new}=x_i+v_{ij}\Delta t$.

(3) Local low-order ($\leqslant 2$) 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 Eq. (5), and the ''th'' part, which establishes local thermodynamic equilibrium throughout the fluid, is effected by step 3. The $2J$ Gauss-Hermite weights and abscissas used throughout the simulation in step 1 may be tabulated in advance.

Distributing the particle quantities m_p, v_p, and ϵ_p follows from

$$m_i=\sum_p m_p W_{pi}, \tag{6}$$

$$p_i=\sum_p m_p v_p W_{pi}, \tag{7}$$

$$E_i=\sum_p m_p\left(\frac{1}{2}v_p^2+\epsilon_p\right)W_{pi}, \tag{8}$$

where m_i, p_i, and E_i are the mass, momentum, and energy of the fluid contained in computational cell i, and the linear weights W_{pi} are defined by

$$W_{pi}=\begin{cases}(x_p-x_{i-1})/(x_i-x_{i-1}) & \text{if } x_{i-1}<x_p\leqslant x_i\\ (x_{i+1}-x_p)/(x_{i+1}-x_i) & \text{if } x_i<x_p\leqslant x_{i+1}\\ 0 & \text{otherwise.}\end{cases} \tag{9}$$

From these quantities the fluid density $[\rho_i=2m_i/(x_{i+1}-x_{i-1})]$, velocity $(u_i=p_i/m_i)$, and velocity variance $[\sigma_{vi}^2=(2E_i-u_i^2)/m_i d]$ may be obtained. Linear weighting introduces a small amount of numerical diffusion into the model, which has the effect of artificially smoothing the profiles of fluid quantities. We have found that less diffusive weighting schemes, such as ''nearest grid point'' weighting, are noisy.

The maximum simulation time step is restricted by the requirement that neighboring fluid elements cannot stream through one another without interacting. Alternatively stated, because Eq. (2) describes an Itô process [7] having constant

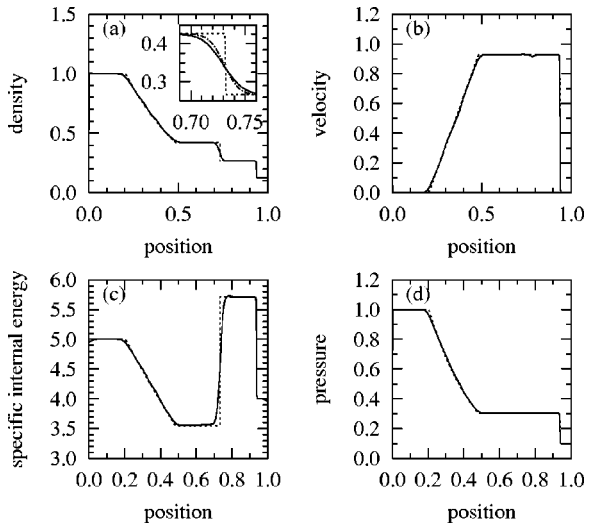

FIG. 1. Continuous line: quiet DSMC simulation with four particles per cell of the Sod test problem at time $t=0.25$. Broken line: exact solution. The simulation used four particles per cell with 1000 simulation cells and a time step $\Delta t=4.5\times10^{-4}$ for a total of 555 time steps. The inset in panel (a) shows a zoom 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).

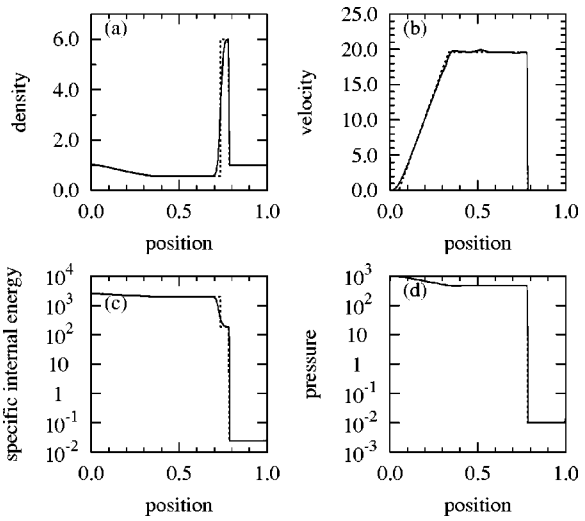

FIG. 2. Continuous line: quiet DSMC simulation with four particles per cell of the blast wave test problem of Woodward and Colella [14]. Broken line: exact solution. The simulation used 1000 simulation cells with four particles per cell. The time step was chosen to be $\Delta t=1.4\times10^{-5}$ for a total of 857 time steps.

parameters u and σ_v^2, the simulation particles may not, in one time step, move so far that u or σ_v^2 changes appreciably. Thus, Δt must obey

$$\Delta t \lesssim \Delta x/\sqrt{\sigma_v^2+u^2}. \tag{10}$$

In hot fluids Eq. (10) is somewhat more restrictive than the traditional Courant-Friedrichs-Lewy criterion ($\Delta t \leqslant \Delta x/u$) for hydrodynamics stability [13]. We stress, however, that Eq. (10) establishes conditions for fidelity and not stability. Since conserved quantities stay rigorously conserved throughout the simulation, quiet DSMC is stable regardless of the size of Δt.

We demonstrate the quiet DSMC method with one- and two-dimensional test problems. The first is the classical Sod problem [9] 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 $p_L=0.1$. 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 [10]. The quiet DSMC calculation has negligible noise and models the shock and rarefaction well. However, diffusion smears out the contact discontinuity over many ($\sim$25) simulation cells. The diffusion is a function of the particle weighting algorithm. The effective diffusion coefficient scales like $\Delta x^{1/2}$ [11,12] and can be reduced by making the lattice spacing Δx smaller [see the dot-dashed line in the inset of Fig. 1 panel (a)].

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 [14] as described in Ref. [9]. 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 $t=0.012$. Again, the quiet DSMC simulation shows little noise and the shock and rarefaction regions are captured well.

Generalization of the method to higher dimensions is straightforward and efficient. For each unit normal random number $N(0,1)$ appearing in the multidimensional OU 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 are 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 $\boldsymbol{u}=0$ ($\gamma=5/3$), and with a small, circular region of initially higher pressure: $P_{\text{in}}=1.0$, $P_{\text{out}}=0.01$. No asymmetry from grid imprinting is evident.

Quiet DSMC fluid calculations have all the advantages of traditional DSMC simulations, and fewer disadvantages. Advantages include unconditional stability; mass, momentum, and energy conservation to machine precision; flexibility,

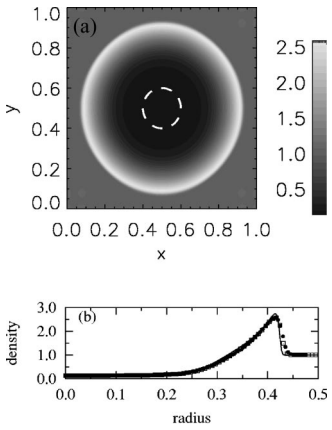

FIG. 3. Panel (a): two-dimensional quiet DSMC simulation of a blast wave from an azimuthally symmetric initial pressure profile (dashed curve). Panel (b): density vs radius for horizontal (circles) and 45° diagonal (squares) cuts across the evolved density profile. The profiles are essentially identical and in good comparison with density from a one-dimensional, first-order Godunov, Roe approximate Riemann solver (solid line). The Cartesian computational mesh used 200×200 grid cells and 4×4 particles per cell, and the simulation ran for 285 time steps.

since complicated boundary conditions and geometries are treated as simple conditions on particle trajectories; and no artificial viscosity required to get convergent results. As has been recognized by many authors [15], dynamic control of the number of simulation particles can dramatically improve dynamical range; in quiet DSMC, the aggressive remapping of fluid quantities onto the particles every time step allows for arbitrary dynamic range, and the results are smooth, exhibiting essentially no statistical noise even with only a few $(\sim2-5)$ particles per cell. All operations in a quiet DSMC fluid calculation are local, so the method would run efficiently and with little message passing on massively parallel computing architectures. Moreover, since the number of particles created per simulation cell is known at the onset of the simulation, ''load balancing,'' or ensuring that each processor in a parallel computer operates near maximum efficiency, can be easily accomplished.

The central themes of quiet DSMC, namely (a) replacing a continuum system with equivalent stochastic differential equations (SDEs) of particle motion, (b) solving these SDEs quietly using a deterministic sampling of the random numbers, and (c) remaking particles every time step from quantities gathered on the grid, have applicability beyond Eulerian hydrodynamics. Step (a) may be performed for any system with dynamics that can be described by a Fokker-Planck kinetic equation [7]. The resulting SDEs are expressed in terms of unit normal random variables $N(0,1)$, for which steps (b) and (c) may be applied. Recently, the authors have used the quiet DSMC technique with success in the simulation of diffusion, radiation transport, magnetohydrodynamics, and kinetic plasma and rarefied gas media [11,12]. Owing to the ubiquity of Fokker-Planck equations in mathematical physics and to the broad use of Monte Carlo techniques to simulate these systems, we feel that quiet DSMC technique may point to a line of thinking that would improve simulation capabilities in many other venues.

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