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Cell size dependence of transport coefficients in stochastic particle algorithms

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Using the Green–Kubo theory, the dependence of the viscosity and thermal conductivity on cell size is obtained explicitly for stochastic particle methods such as direct simulation Monte Carlo (DSMC) and its generalization, the consistent Boltzmann algorithm (CBA). These analytical results confirm empirical observations that significant errors occur when the cell dimensions are larger than a mean free path. © *1998 American Institute of Physics.* [S1070-6631(98)01506-2]

Direct simulation Monte Carlo (DSMC) is a stochastic algorithm that solves the Boltzmann equation by replacing the distribution function with a representative set of particles.[1,2] The two step process consists of the advection term in the Boltzmann equation corresponding to the particles being translated and the collision term modeled by a Markov process with interacting particles selected according to rates given by kinetic theory. As a computational tool, DSMC has been extremely successful in the study of rarefied gas flows,[3] and more recently, for nanoscale problems.[4,5]

Typically, particles are sorted into spatial cells and only those within the same cell are selected at random to be collision partners. The cells are made small enough to restrict collisions to nearby particles but should contain a sufficient number of particles so that the method remains statistically accurate. Empirically, it has been found that cells should be no larger than a mean free path and contain at least twenty particles. On occasion the cell size restriction has been violated,[6] leading to spurious results.[7] In this paper, the Green–Kubo formalism[8,9] is used to quantitatively evaluate the dependence of the viscosity and thermal conductivity on cell size in the DSMC algorithm. As a result, computational expense may be reduced because a larger cell size can be employed since the resulting change in the transport coefficients is known.

Following Wainwright,[9] the shear viscosity, η, is calculated from its Green–Kubo expression as the autocorrelation in time of the stress tensor,

$$\eta = \frac{1}{VkT}\int_0^\infty ds\left[\frac{1}{t_s}\int_0^{t_s} dt J^{xy}(t)J^{xy}(t+s)\right], \tag{1}$$

where V, T, and k are the volume, temperature, and Boltzmann's constant, respectively; t_s is a sufficiently long smoothing time. The particle dynamics in DSMC are stochastic and lead to a Markovian process. The autocorrelation function in Eq. (1) can be evaluated explicitly because, in the Boltzmann limit, correlations due to multiple collisions can be ignored. The xy-component of the stress tensor for a system of N hard spheres of mass m is

$$J^{xy}(t) = m\left[\sum_{i=1}^{N} u_i v_i + \sum_{c=1}^{\infty}(y_i - y_j)\Delta^c u_i \delta(t-t_c)\right], \tag{2}$$

where y_i is the y-coordinate of particle i at time t; u_i, v_i are the x,y-components of its velocity. The change in the x-component of velocity for particle i is $\Delta^c u_i$ where the index c corresponds to a collision between particle i and j which occurs at time t_c. For DSMC collisions, this term is analogous to a ''potential'' contribution to the stress tensor but with the distance determined by the cell size instead of the range of the inter-particle force.

The first term of Eq. (2) gives the contribution to the momentum flux due to the translational motion of the particles (i.e., kinetic term). The second term gives the contribution due to the impulsive change of velocities that occurs at collision. Inserting Eq. (2) into Eq. (1) yields

$$\eta = \eta^K + \eta^C + \eta^P, \tag{3}$$

where the right hand side consists of the kinetic, cross, and potential (i.e., collision) contributions to the viscosity. For hard spheres of diameter σ, the kinetic term gives the Chapman–Enskog viscosity for a dilute gas,

$$\eta^K = \frac{5\pi}{16} m\Gamma\lambda^2, \tag{4}$$

where $\Gamma = 2\sigma^2 n^2\sqrt{\pi kT/m}$ is the Boltzmann collision rate and $\lambda = (\sqrt{2}\pi\sigma^2 n)^{-1}$ is the mean free path. The cross term $\eta^C = 0$ because in DSMC the distance between colliding particles is uncorrelated with their velocities. The potential contribution to the viscosity is, however, cell size dependent,

$$^{P}=\frac{m^2\Gamma}{2kT}\langle(y_i-y_j)^2\rangle\langle(\ \ ^{c}u_i)^2\rangle, \tag{5}$$

where $\langle\ \rangle$ denotes an average over collisions. For a homogeneous rectangular collision cell, $\langle(y_i-y_j)^2\rangle=L_y^2/6$ where L_y is the width of the cell in the y-direction. If the cell geometry is more complicated the coefficient in this expression is modified. Furthermore, unless the cell is spherical, the viscosity (and thermal conductivity) is anisotropic.

For hard spheres, the collision probability is proportional to the relative speed between particles, so $\langle(\ ^{c}u_i)^2\rangle=\frac{8}{9}kT/m$, leading to

$$^{P}=\frac{2}{27}m\Gamma L_y^2. \tag{6}$$

A similar line of calculation gives the Chapman–Enskog thermal conductivity, $\kappa^K=(75\pi/64)\,k\Gamma\lambda^2$, and a potential contribution of

$$\kappa^P=\frac{1}{6}k\Gamma L_y^2. \tag{7}$$

There is no cell size dependence for the self-diffusion coefficient since only the kinetic term contributes to the diffusion. The pressure is not affected by the cell size because the virial, $\langle(y_i-y_j)\ \ ^{c}u_i\rangle$, is zero, by symmetry, in DSMC.[10,11]

The shear viscosity and thermal conductivity, including the cell size corrections, are thus

$$=\frac{5}{16\sigma^2}\sqrt{\frac{mkT}{\pi}}\left(1\quad\frac{32}{135\pi}\frac{L_y^2}{\lambda^2}\right), \tag{8}$$

and

$$\kappa=\frac{75}{64\sigma^2}\sqrt{\frac{k^3T}{m\pi}}\left(1\quad\frac{32}{225\pi}\frac{L_y^2}{\lambda^2}\right), \tag{9}$$

for hard spheres. Other collision models used in DSMC, such as the generalized hard sphere model,[1,12] give different coefficients but the functional dependence of and κ on cell size will be the same. Unless the cell dimensions are smaller than a mean free path, the fractional errors can be significant; for example, when the collision cells are one mean free path wide the errors in the hard sphere viscosity and thermal conductivity are 7.5% and 4.5%, respectively.

The effect of cell size on viscosity is demonstrated in a planar Couette problem, that is, for a dilute gas between parallel, thermal walls moving in opposite directions with constant speed. The transverse momentum flux measured in DSMC simulations is plotted in Fig. 1 as a function of cell size; these values are normalized by $F^K=\ ^{K}\nabla u$, the momentum flux when $L_y\to 0$. For cells smaller than 4λ, the data is in good agreement with Eq. (8) for a constant velocity gradient, but when the cells are very large, the velocity profile is no longer linear (see Fig. 2). In that case, the cell size correction becomes larger than the physical viscosity, given by the kinetic term, and there is little velocity change across a cell. Instead a steep gradient develops at the boundary between cells with the velocity change restricted to within

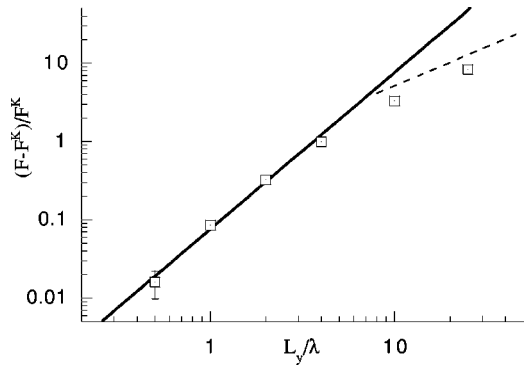

FIG. 1. Normalized transverse momentum flux, $(F-F^K)/F^K$, versus cell size, L_y/λ, in Couette flow. The solid line is the Green–Kubo result, $32L_y^2/135\pi\lambda^2$, and the dashed line is the free-molecule limit, $24L_y/15\pi\lambda$. Data points are from DSMC simulation; when not explicitly drawn the error bar is smaller than the symbol size. The distance between the moving walls is 100λ and their velocities are $\pm 0.5\sqrt{kT/m}$.

about a mean free path from this interface. For a step function profile, the momentum flux is given by the free-molecular limit, namely,

$$F^*=n\sqrt{\frac{mkT}{2\pi}}\ \ U, \tag{10}$$

where U is the velocity difference between adjacent cells,[13] so that

$$\frac{F^*-F^K}{F^K}=\frac{24}{15\pi}\frac{L_y}{\lambda}, \tag{11}$$

which is in close agreement with the simulation data in Fig. 1.

The cell size effect on transport coefficients is also present in stochastic particle algorithms based on DSMC, such as the Consistent Boltzmann Algorithm (CBA)[10] and its extensions.[11] Because the separation between particles selected for collision is uncorrelated with the CBA displacement performed after a collision, ^{P} and κ^P are again given by Eqs. (6) and (7) with the collision rate Γ augmented by the Enskog Y-factor. The CBA transport coefficients for

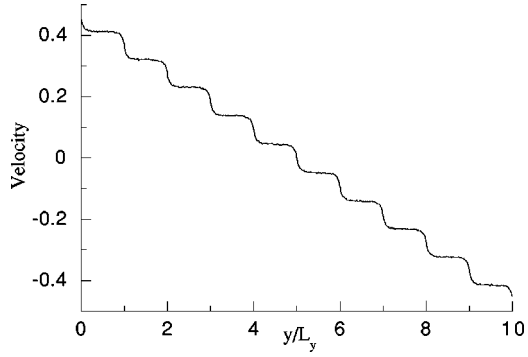

FIG. 2. Fluid velocity, $u/\sqrt{kT/m}$, versus position, y/L_y, from a DSMC simulation of Couette flow with cell size $L_y=10\lambda$. The steps in the velocity profile occur at the boundaries of the rectangular cells; velocity is sampled at grid points $\frac{1}{5}\lambda$ apart. The distance between the moving walls is 100λ and their velocities are $\pm 0.5\sqrt{kT/m}$.

dense hard spheres have the same cell size corrections as DSMC, Eq. (8) and Eq. (9), with λ being the Enskog mean free path.

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