Statistical Error in Particle Simulations of Low Mach Number Flows

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Abstract— **We present predictions for the statistical error due to finite sampling in the presence of thermal fluctuations in molecular simulation algorithms. Expressions for the fluid velocity, density and temperature are derived using equilibrium statistical mechanics. The results show that the number of samples needed to adequately resolve the flow-field scales as the inverse square of the Mach number. The theoretical results are verified for a dilute gas using direct Monte Carlo simulations. The agreement between theory and simulation verifies that the use of equilibrium theory is justified.**

I. Introduction

Recently much attention has been focused on the simulation of hydrodynamic problems at small scales using molecular simulation methods such as Molecular Dynamics (MD) [1] or the direct simulation Monte Carlo (DSMC) [2], [3]. Molecular Dynamics is generally used to simulate liquids while DSMC is a very efficient algorithm for simulating dilute gases. In molecular simulation methods the connection to macroscopic observable fields, such as velocity and temperature, is achieved through averaging appropriate microscopic properties over small regions of space. The simulation results are therefore inherently statistical and statistical errors due to finite sampling need to be fully quantified.

Using equilibrium statistical mechanics, we derive expressions for the magnitude of statistical errors due to thermal fluctuations in such simulations for the typical observables of interest, namely, velocity, density and temperature. Since non-equilibrium modifications to thermal fluctuations results are very small, even under extreme conditions [4], we expect our results to be valid for a wide variety of non-equilibrium situations, and certainly in most cases of practical interest where deviations from equilibrium are small. This is verified for the dilute gas case through direct Monte Carlo simulations; dense liquids will be investigated in the future.

II. Statistical error due to thermal fluctuations

We first consider the fluid velocity. In a particle simulation, the flow field is obtained by measuring the instantaneous center of mass velocity, $\vec{u}$, for particles in a statistical cell volume. For steady flows, the statistical mean value of the local fluid velocity, $\langle\vec{u}\rangle$, is estimated over M independent samples. The average fluid velocity, $\vec{u}_0$, is defined such that $\langle\vec{u}\rangle \to \vec{u}_0$ as $M \to \infty$. (The three components of velocity corresponding to the three mutually orthogonal space directions x, y, z, will be denoted u, v, w, respectively.)

Let N_0 be the average number of particles in the statistical cell and $\delta u \equiv u - u_0$ the instantaneous fluctuation in one of the three components of the fluid velocity. Note that all three components are equivalent. From equilibrium statistical mechanics [5],

$$\langle \delta u^2 \rangle = \frac{kT_0}{mN_0} = \frac{c^2}{\gamma \mathrm{Ac}^2 N_0} \tag{1}$$

where T_0 is the average temperature, m is the particle mass, k is Boltzmann's constant, c is the sound speed, and $\gamma = c_P/c_V$ is the ratio of the specific heats. Recall that by the equipartition theorem [5]

$$\frac{3N_0 kT_0}{2} = \sum_j^{N_0} \frac{1}{2} m(\delta u_j^2 + \delta v_j^2 + \delta w_j^2) \tag{2}$$

For a non-equilibrium system, this expression defines T_0 as the average translational temperature. The acoustic number $\mathrm{Ac} = c/c^i$ is the ratio of the fluid's sound speed to the sound speed of a "reference" ideal gas at the same temperature

$$c^i = \sqrt{\gamma kT/m} \tag{3}$$

Note that this reference ideal gas has a ratio of specific heats (γ^i) equal to the *original fluid* specific heat ratio, that is $\gamma^i = \gamma$ as shown in equation (3).

We may define a "signal-to-noise" ratio as the average fluid velocity over its standard deviation; from the above,

$$\frac{u_0}{\sqrt{\langle \delta u^2 \rangle}} = \mathrm{Ac}\,\mathrm{Ma}\sqrt{\gamma N_0} \tag{4}$$

where $\mathrm{Ma} = u_0/c$ is the local Mach number based on the velocity component of interest. This result shows that for fixed Mach number, in a dilute gas simulation ($\mathrm{Ac} = 1$), the statistical error due to thermal fluctuations cannot be ameliorated by reducing the temperature. However, when the Mach number is small enough for compressibility effects to be negligible, favorable relative statistical errors may be obtained by performing simulations at an increased Mach number (to a level where compressibility effects are still negligible).

The one-standard-deviation error bar for the sample estimate $\langle u \rangle$ is $\sigma_u = \sqrt{\langle \delta u^2 \rangle}/\sqrt{M}$ and the fractional error in

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the estimate of the fluid velocity is

$$E_u = \frac{\sigma_u}{u_0} = \frac{1}{\sqrt{MN_0}} \frac{1}{\mathrm{Ac}\,\mathrm{Ma}\sqrt{\gamma}}, \tag{5}$$

yielding

$$M = \frac{1}{\gamma \mathrm{Ac}^2 N_0 \mathrm{Ma}^2 E_u^2}. \tag{6}$$

For example, with $N_0 = 100$ particles in a statistical cell, if a one percent fractional error is desired in a Ma $= 1$ flow, about $M = 100$ independent statistical samples are required (assuming Ac ≈ 1). However, for a Ma $= 10^{-2}$ flow, about 10^6 independent samples are needed. Since most particle methods require $10 - 100$ time steps between independent samples, this makes the resolution of the flow velocity computationally expensive for low Mach number flows.

Note that equation (2) suggests that the variance in the fluctuation of the magnitude of the total velocity in a statistical cell is given by

$$\langle (\delta u^2 + \delta v^2 + \delta w^2) \rangle = \frac{3kT_0}{mN_0} \tag{7}$$

that is, the expected error in estimating the magnitude of the total velocity is $\sqrt{3}$ larger than in estimating a velocity component.

Next we turn our attention to the density. From equilibrium statistical mechanics, the variance in the fluctuation in the number of particles in a cell is

$$\langle \delta N^2 \rangle = -N^2 \frac{kT}{V^2} \left(\frac{\partial V}{\partial P} \right)_T = \kappa_T N_0^2 \frac{kT_0}{V} \tag{8}$$

where $\kappa_T \equiv -V^{-1}(\partial V/\partial P)_T$ is the isothermal compressibility. Note that for a dilute gas $\kappa_T = 1/P$ so $\langle \delta N^2 \rangle = N$ and, in fact, the probability distribution of N is Poissonian. The fractional error in the estimate of the density is

$$E_\rho = \frac{\sigma_\rho}{\rho_0} = \frac{\sigma_N}{N_0} = \frac{\sqrt{\langle \delta N^2 \rangle}}{N_0 \sqrt{M}} = \frac{\sqrt{\kappa_T k T_0}}{\sqrt{MV}} \tag{9}$$

where V is the volume of the cell. The above expression can also be written as

$$E_\rho = \frac{\sigma_\rho}{\rho_0} = \frac{\sqrt{\kappa_T / \kappa_T^i}}{\sqrt{MN_0}} \tag{10}$$

where $\kappa_T^i = V/N_0 kT_0$ is the isothermal compressibility of the reference dilute gas ($\gamma^i = \gamma$) at the same density and temperature. Since $c \propto 1/\sqrt{\kappa_T}$,

$$E_\rho = \frac{1}{\sqrt{MN_0}} \frac{1}{\mathrm{Ac}} \tag{11}$$

Note that for fixed M and N_0, the error decreases as the compressibility decreases (i.e., as the sound speed increases) since the density fluctuations are smaller.

Finally we consider the measurement of temperature. First we should remark that the measurement of instantaneous temperature is subtle, even in a dilute gas. But given that temperature is measured correctly, equilibrium statistical mechanics gives the variance in the temperature fluctuations to be

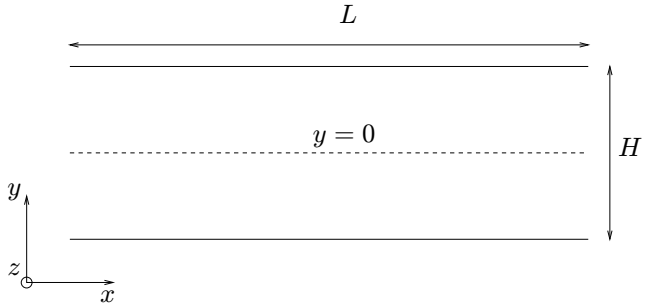

Fig. 1. Channel geometry

$$\langle \delta T^2 \rangle = \frac{kT_0^2}{c_V N_0} \tag{12}$$

where c_V is the heat capacity per particle at constant volume. The fractional error in the estimate of the temperature is

$$E_T = \frac{\sigma_T}{T_0} = \frac{\sqrt{\langle \delta T^2 \rangle}}{T_0 \sqrt{M}} = \frac{1}{\sqrt{MN_0}} \sqrt{\frac{k}{c_V}} \tag{13}$$

Because the fluctuations are smaller, the error in the temperature is smaller when the heat capacity is large; note that for a monatomic dilute gas $c_V = \frac{3}{2}k$.

The fractional error in the density and temperature depend only on the density and temperature of the fluid and are independent of the flow speed. Although typically undesirable in isothermal low speed flows, density and temperature gradients develop due to compressibility and viscous heating effects. The magnitude of these effects is proportional to the square of the Mach number, making them particularly challenging to resolve. Consider for example the case of viscous heat dissipation: if we express the local temperature as $T_0 = T_G + \Delta T$, where T_G is the global mean temperature, then the fractional error in the temperature deviation can be approximated by

$$E_{\Delta T} = \frac{\sigma_T}{|\Delta T|} \approx E_T \left| \frac{T_G}{\Delta T} \right| \propto \frac{E_T}{\mathrm{Ma}^2} \tag{14}$$

assuming $|\Delta T/T_G| \propto (\nabla u_0)^2 \propto \mathrm{Ma}^2$. Although this expression is only approximate, it serves to highlight the typical scaling of signal-to-noise ratios found in low speed flows.

A final note: In DSMC simulations one considers each particle as "representing" a large number of molecules in the physical system. In all the expressions given here, N_0 is the number of particles used by the simulation, so the fluctuations can be reduced by using larger numbers of particles (i.e., using a lower molecule-to-particle ratio).

III. Numerical Simulations

We performed simulations of an ideal gas under flow conditions to verify the validity of the expressions derived above. The DSMC method used in the simulations is briefly described below.

A. The direct simulation Monte Carlo

The DSMC method [2] is a particle-based stochastic numerical scheme for solving the nonlinear Boltzmann equation [7]. The motion of a representative set of particles is simulated in time in a series of timesteps, each of which involves a ballistic advection of each molecule and stochastic collisions between pairs of molecules. This "coarse-grained" molecular description contains the essential physics to fully capture both the hydrodynamic and kinetic regimes [2]. DSMC offers significant modeling advantages compared to continuum techniques in situations where molecular information is required to achieve closure of the governing hydrodynamic equations, or when the continuum hydrodynamic equations are not valid.

For the sake of brevity we will not present a more detailed description of the DSMC algorithm. Excellent introductory [3] and detailed [2] descriptions can be found in the literature, as well as comparisons of DSMC simulation results with solutions of the linearized Boltzmann equation [6] for flows in microchannels. Comparisons of DSMC results with experiments for diverse non-equilibrium phenomena spanning the whole Knudsen range can be found in [8], [2].

B. Simulations

Standard DSMC techniques [2], [3] were used to simulate flow of gaseous argon (molecular mass $m = 6.63 \times 10^{-26}$ kg, hard sphere diameter $\sigma = 3.66 \times 10^{-10}$ m) in a two-dimensional channel of length L and height H (see fig. 1). The simulation was periodic in the x direction (along the channel axis). The simulation was also periodic in the $z-$direction in which the flowfield is also homogeneous. Flow in the $x-$direction was generated by applying a constant acceleration field in that direction.

The two walls at $y = -H/2$ and $y = H/2$ were fully accommodating and smooth with fixed temperature $T_0 = 273$ K. The equilibrium density was $\rho_0 = 1.78\text{kg/m}^3$ and approximately 40 particles per cell were used. The channel height ($H = 5 \times 10^{-7}$m) was significantly larger than the mean free path $\lambda = m/(\sqrt{2}\pi\rho_0\sigma^2) \sim 6 \times 10^{-8}$m at the density of the simulation.

The number of cells was chosen so that the cell linear dimension is less than 1/3 of a mean free path. Alexander et al. [9] have shown that the transport coefficients deviate from the dilute gas Enskog values as the square of the cell size Δx with the proportionality constant such that for cell sizes of the order of one mean free path an error of the order of 10% occurs. For $\Delta x \leq 1/3\lambda$ the difference between the viscosity of the gas and the viscosity of a dilute hard-sphere gas is less than 1.5%.

The timestep of the simulation Δt was taken to be significantly smaller than the mean free time λ/c_o, where $c_o = \sqrt{2RT}$ is the most probable velocity. It has been shown [10], [11] that the error in the transport coefficients is proportional to the square of the timestep, with a proportionality constant such that for timesteps of the order of one mean free time the error is of the order of 5%. In our simulations, $\Delta t < \lambda/(7c_o)$, thus making the error negligible.

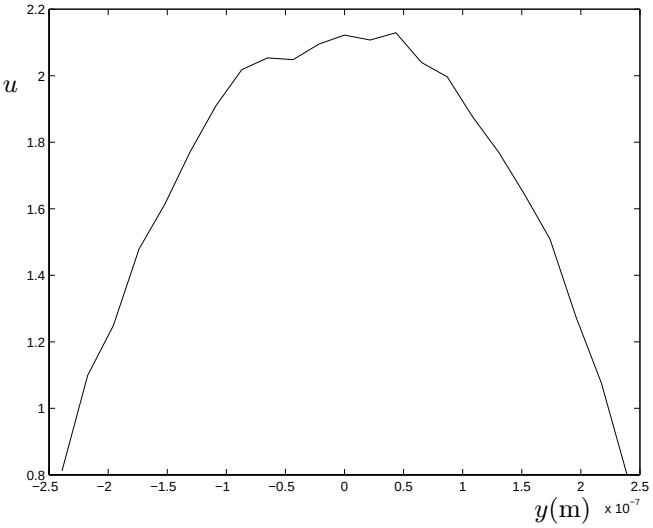

Fig. 2. Velocity profile (in m/s) as a function of the transverse channel coordinate, y.

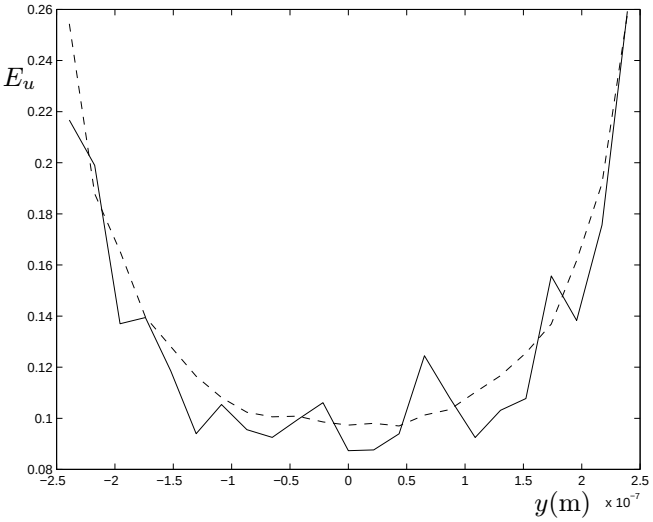

Fig. 3. Fractional error in velocity for Poiseuille flow in a channel as a function of the transverse channel coordinate, y. The dashed line denotes equation (5) and the solid line denotes DSMC simulation results.

Sample independence is very important when accurate determination of the sample standard deviation is required [1]. To ensure that the samples taken were independent, one sample every 250 timesteps was taken starting after 1 million timesteps ensuring that the system was in steady state. A total of 10 million timesteps were run. Figure 2 shows the velocity profile as determined using 36000 samples.

C. Results

Figures 3–5 show the measured fractional error, obtained from the standard deviation of cell values in the x and z directions. The velocity profile (Fig. 2) is close to parabolic,

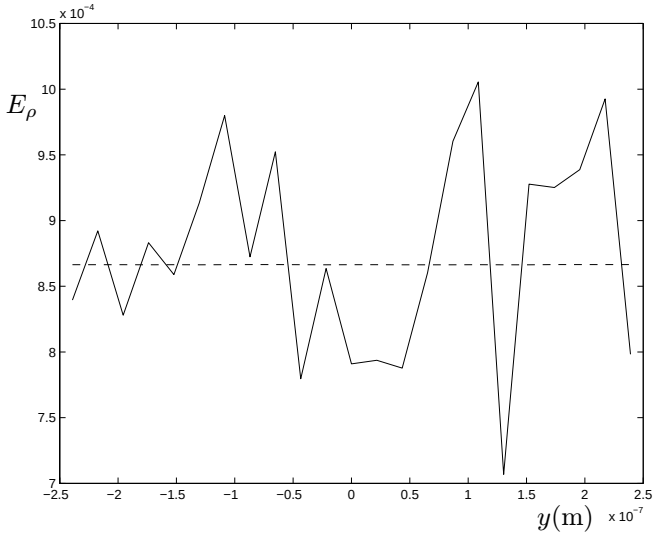

Fig. 4. Fractional error in density for Poiseuille flow in a channel as a function of the transverse channel coordinate, y. The dashed line denotes equation (11) and the solid line indicates DSMC simulation results.

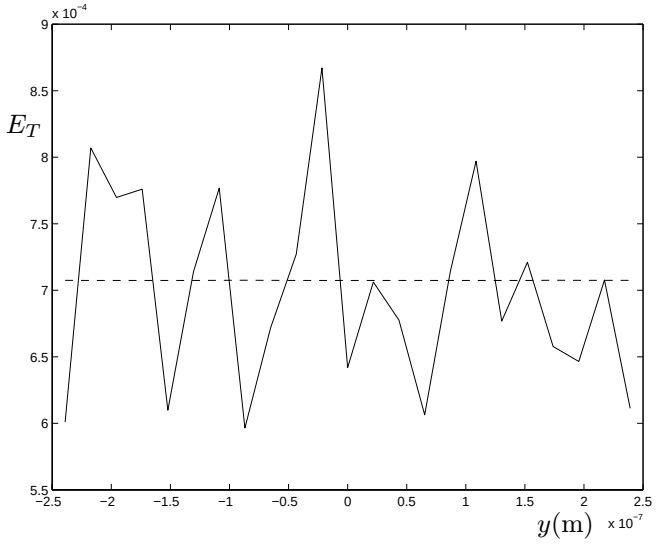

Fig. 5. Fractional error in temperature for Poiseuille flow in a channel as a function of the transverse channel coordinate, y. The dashed line denotes equation (13) and the solid line indicates DSMC simulation results.

so the fractional error in the velocity measurement is minimum at the centerline. The number of particles was nearly constant everywhere in the system so the fractional errors in density and temperature are nearly constant. In all cases, the simulation measurements are in good agreement with the theoretical predictions.

IV. Conclusions

We have presented expressions for the statistical error in estimating the velocity, density and temperature in molecular simulations. These expressions were validated for flow of a dilute gas in a two-dimensional channel using the direct simulation Monte Carlo technique. Despite the non-equilibrium nature of the validation experiment, good agreement is found between theory and simulation, verifying that modifications to non-equilibrium results are very small. We thus expect these results to hold for general non-equilibrium applications of interest. The validity of the above expressions for dense fluid flows is currently under investigation.

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