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Generation of the Chapman–Enskog Distribution

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A pair of simple, efficient, and robust algorithms for generating random velocities sampled from the Chapman–Enskog distribution is presented.

Particle simulations of a gas require initializing the velocities of molecules. At thermodynamic equilibrium, the velocity distribution for a dilute gas at temperature T is the Maxwell–Boltzmann distribution,

$$f_0(\boldsymbol{\mathcal{C}}) = \frac{1}{\pi^{3/2}} \exp(-\mathcal{C}^2), \tag{1}$$

where $\boldsymbol{\mathcal{C}} = \mathbf{C}/(2kT/m)^{1/2}$ is the normalized thermal velocity and m is the particles' mass. Away from equilibrium the Chapman–Enskog perturbation expansion of the Boltzmann equation gives, to first order in Sonine polynomial expansion, the distribution [1]

$$f(\boldsymbol{\mathcal{C}}) = f_0(\boldsymbol{\mathcal{C}})\Gamma(\boldsymbol{\mathcal{C}}), \tag{2}$$

where

$$\begin{aligned}\Gamma(\boldsymbol{\mathcal{C}}) = 1 &+ (q_x\mathcal{C}_x + q_y\mathcal{C}_y + q_z\mathcal{C}_z)\left(\tfrac{2}{5}\mathcal{C}^2 - 1\right)\\ &- 2(\tau_{x,y}\mathcal{C}_x\mathcal{C}_y + \tau_{x,z}\mathcal{C}_x\mathcal{C}_z + \tau_{y,z}\mathcal{C}_y\mathcal{C}_z)\\ &- \tau_{x,x}\left(\mathcal{C}_x^2 - \mathcal{C}_z^2\right) - \tau_{y,y}\left(\mathcal{C}_y^2 - \mathcal{C}_z^2\right)\end{aligned} \tag{3}$$

and

$$q_i = -\frac{\kappa}{P}\left(\frac{2m}{kT}\right)^{1/2}\frac{\partial T}{\partial x_i} \tag{4}$$

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$$\tau_{i,j} = \frac{\mu}{P}\left(\frac{\partial \boldsymbol{v}_i}{\partial x_j} + \frac{\partial \boldsymbol{v}_j}{\partial x_i} - \frac{2}{3}\frac{\partial \boldsymbol{v}_k}{\partial x_k}\delta_{i,j}\right) \tag{5}$$

are the dimensionless heat flux and stress tensor. The viscosity and thermal conductivity are μ and κ, respectively; P is the pressure and $\boldsymbol{v}_k$ is the fluid velocity. The mean and second moment of the Chapman–Enskog distribution are $\overline{\mathcal{C}}_i = 0$ and $\overline{\mathcal{C}^2} = \frac{3}{2}$. The kinetic theory expressions for the stress tensor and the heat flux are $\tau_{i,j} = \frac{2}{3}\overline{\mathcal{C}^2}\delta_{i,j} - 2\overline{\mathcal{C}_i\mathcal{C}_j}$ and $q_i = 2\overline{\mathcal{C}_i\mathcal{C}^2}$. The Maxwell–Boltzmann distribution suffices in equilibrium situations, but for nonequilibrium flows, for example, when the particle simulation is coupled to a Navier–Stokes finite difference solver, the Chapman–Enskog distribution must be used [2, 3].

The first method for sampling from $f(\boldsymbol{\mathcal{C}})$ uses the acceptance–rejection technique [4]. This requires defining an envelope function $g(\boldsymbol{\mathcal{C}})$ such that $g(\boldsymbol{\mathcal{C}}) \geq f(\boldsymbol{\mathcal{C}})$ for all $\boldsymbol{\mathcal{C}}$. The efficiency of acceptance–rejection (ratio of acceptances to total tries) is $1/A$, where

$$A \equiv \int g(\boldsymbol{\mathcal{C}})\, d\boldsymbol{\mathcal{C}}. \tag{6}$$

The first step is to select a random point from the region beneath $g(\boldsymbol{\mathcal{C}})$ (i.e., the region whose area is given by (6)). All points in this region must be equally likely to be chosen. A simple way to select this point is to use $g(\boldsymbol{\mathcal{C}}) = Af_0(\boldsymbol{\mathcal{C}})$, where f_0 is the Maxwell–Boltzmann distribution (1). A velocity $\boldsymbol{\mathcal{C}}_{\text{try}}$ is drawn from $f_0(\boldsymbol{\mathcal{C}})$ and the point inside the envelope is taken as $(\boldsymbol{\mathcal{C}}_{\text{try}}, \Re g(\boldsymbol{\mathcal{C}}_{\text{try}}))$, where $\Re$ is a uniform deviate in [0, 1). The value of $\boldsymbol{\mathcal{C}}_{\text{try}}$ is accepted if this point lies beneath $f(\boldsymbol{\mathcal{C}})$; this acceptance criterion may be written as $A\Re \leq \Gamma(\boldsymbol{\mathcal{C}}_{\text{try}})$. If this condition is not met, a new point is drawn and the procedure is repeated. The generator is outlined in Table 1.

To guarantee that the envelope function is everywhere greater than the Chapman–Enskog distribution requires that the constant A be selected such that $A \geq \Gamma(\boldsymbol{\mathcal{C}})$. In principle, this is impossible because $|\Gamma(\boldsymbol{\mathcal{C}})| \to \infty$ as $\boldsymbol{\mathcal{C}} \to \infty$. In practice, given τ and q, one can select an A such that the envelope contains almost all of the Chapman–Enskog distribution beneath it. For this purpose, a "breakdown" parameter, $B \equiv \max(|\tau_{i,j}|, |q_i|)$, is defined [5]. When this parameter exceeds 0.1, the validity of the Chapman–Enskog distribution is suspect anyway, since the perturbation from equilibrium is no longer small. For example, when $q_i = 0.1$, the temperature gradient is such that T varies by about 25% over a distance of only 10 mean-free paths.

An analysis of the function Γ, which contains terms of the form $\mathcal{C}_i(\frac{2}{5}\mathcal{C}^2 - 1)$, $2\mathcal{C}_i\mathcal{C}_j$, and $\mathcal{C}_i^2 - \mathcal{C}_j^2$, shows that for about one in 10^6 draws of $\boldsymbol{\mathcal{C}}_{\text{try}}$ the magnitude of the first term

TABLE 1
Outline of the Acceptance–Rejection Random Velocity Generator for the Chapman–Enskog Distribution

1. Given $\tau_{i,j}$ and q_i, find $B \equiv \max(|\tau_{i,j}|, |q_i|)$.
2. Set amplitude parameter $A = 1 + 30B$.
3. Draw $\boldsymbol{\mathcal{C}}_{\text{try}}$ from Maxwell–Boltzmann distribution $f_0(\boldsymbol{\mathcal{C}})$.
4. Accept $\boldsymbol{\mathcal{C}}_{\text{try}}$ if $A\Re \leq \Gamma(\boldsymbol{\mathcal{C}}_{\text{try}})$ where $\Re$ is a uniform deviate in [0, 1); else go to step 3.
5. Generated particle velocity is $\boldsymbol{c} = (2kT/m)^{1/2}\boldsymbol{\mathcal{C}}_{\text{try}} + \boldsymbol{v}$.

will exceed 15; similarly for one in 10^6 draws one of the latter two terms will exceed 12. However, the values of the separate terms are correlated thus, if one term is large, the other terms, even taking into account the different signs, are more likely to contribute significantly in making Γ large. For typical applications, setting $A = 1 + 30B$ will result in $\Gamma > A$ for roughly one in 10^6 draws of $\mathcal{C}_{\text{try}}$. The efficiency of the routine ($=1/A$) is 25% when $B = 0.1$ and the efficiency approaches 100% near equilibrium. In the rare case when $\Gamma(\mathcal{C}_{\text{try}}) > A$, the value of $\mathcal{C}_{\text{try}}$ is simply accepted, causing a negligible error in the generated distribution.

The second method of generating velocities from the Chapman–Enskog distribution is developed from the Metropolis Monte Carlo scheme of equilibrium statistical mechanics [6]. The idea is to design a Markov chain with a transition probability between states, $P(\mathcal{C}_{\text{old}} \to \mathcal{C}_{\text{new}})$, such that

$$f(\mathcal{C}_{\text{old}})P(\mathcal{C}_{\text{old}} \to \mathcal{C}_{\text{new}}) = f(\mathcal{C}_{\text{new}})P(\mathcal{C}_{\text{new}} \to \mathcal{C}_{\text{old}}). \tag{7}$$

A simple way to satisfy this condition is to take

$$P(\mathcal{C}_{\text{old}} \to \mathcal{C}_{\text{new}}) = f_0(\mathcal{C}_{\text{new}}) \begin{cases} 1 & \text{if } \Gamma(\mathcal{C}_{\text{new}}) \geq \Gamma(\mathcal{C}_{\text{old}}), \\ \Gamma(\mathcal{C}_{\text{new}})/\Gamma(\mathcal{C}_{\text{old}}) & \text{if } \Gamma(\mathcal{C}_{\text{new}}) < \Gamma(\mathcal{C}_{\text{old}}). \end{cases} \tag{8}$$

with the probability that the system remains at $\mathcal{C}_{\text{old}}$ fixed by the normalization of P. The procedure for generating the set of values can be understood as a sequence of Monte Carlo "moves." Given an initial $\mathcal{C}_{\text{old}}$, a new velocity $\mathcal{C}_{\text{new}}$ is drawn from the Maxwell–Boltzmann distribution. The "move" to this new velocity is automatically accepted if the new value of Γ is greater than the old value; this is considered a "downhill move." If $\Gamma(\mathcal{C}_{\text{new}}) < \Gamma(\mathcal{C}_{\text{old}})$ then the "uphill move" is accepted with probability $\Gamma(\mathcal{C}_{\text{new}})/\Gamma(\mathcal{C}_{\text{old}})$; otherwise the move is rejected and the value of $\mathcal{C}_{\text{old}}$ is unchanged. The two conditions for accepting a move may be combined by accepting a move if $\Gamma(\mathcal{C}_{\text{new}}) \geq \Re\Gamma(\mathcal{C}_{\text{old}})$. The algorithm for this generator is outlined in Table 2.

As the number of attempted moves, N, becomes large, the distribution of $\mathcal{C}_{\text{old}}$ approaches $f(\mathcal{C})$. In practice, only a small number of attempted moves is required to obtain the Chapman–Enskog distribution to high accuracy when $a(N)$, the probability that the Nth attempted move is accepted, is close to one. Indeed, this probability is typically greater than 0.9 when $B \leq 0.1$. The error in the generated distribution may be estimated from

TABLE 2

Outline of the Random Velocity Generator for the Chapman–Enskog Distribution Based on the Metropolis Monte Carlo Method

1. Draw $\mathcal{C}_{\text{old}}$ from Maxwell–Boltzmann distribution $f_0(\mathcal{C})$; select a new value if $\Gamma(\mathcal{C}_{\text{old}}) < 0$.
2. Draw a new velocity $\mathcal{C}_{\text{new}}$ from Maxwell–Boltzmann distribution.
3. If $\Gamma(\mathcal{C}_{\text{new}}) \geq \Re\Gamma(\mathcal{C}_{\text{old}})$ then accept the "move" and set $\mathcal{C}_{\text{old}} = \mathcal{C}_{\text{new}}$; otherwise keep the current value of $\mathcal{C}_{\text{old}}$ ($\Re$ is a uniform deviate in [0,1)).
4. Repeat steps 2 and 3 until $N = 1 + 30B$ attempted moves have been made (counting both accepted and unaccepted moves); $B \equiv \max(|\tau_{i,j}|, |q_i|)$.
5. Generated particle velocity is $\boldsymbol{c} = (2kT/m)^{1/2}\mathcal{C}_{\text{old}} + \boldsymbol{v}$.

$\Delta \equiv |1 - a(N)/a(\infty)|$. Due to the Markov properties of the algorithm this difference goes as $e^{-\alpha N}$ so it decreases rapidly with N. However, the rate of convergence, α, depends on the difference between f and f_0, that is, on the breakdown parameter B. Taking the number of attempted moves as $N = 1 + 30B$ results in a fractional difference of $\Delta < 10^{-4}$. The computation time for this generator is comparable to that of the acceptance–rejection method for the above error criterion.

Because the Chapman–Enskog distribution comes from a perturbation expansion, the probability distribution can become negative. For example, when $B = 0.1$, $f(\mathcal{C}_{\text{try}})$ is negative about 0.05% of the time and this fraction rises to an alarming 4% for $B = 0.4$. In the acceptance–rejection generator the value of $\mathcal{C}_{\text{try}}$ is always rejected where the distribution is negative. Similarly, according to the rules of the Metropolis generator, a move is automatically rejected if $\Gamma(\mathcal{C}_{\text{new}}) < 0$. The moments of the generated distribution are slightly different from those of $f(\mathcal{C})$ when the gradients are large but again the use of the Chapman–Enskog distribution is questionable anyway under these circumstances.

The cumulative distribution functions for $f(\mathcal{C})$ could, in fact, also be obtained analytically in terms of error functions [3]. A random velocity generator may be constructed using the inversion method [4]; however, the roots of three complicated functions must be found numerically. The computation time is independent of the breakdown parameter, but for $B = 0.1$ the inversion method is about nine times slower than the two generators presented here. Another disadvantage of inversion is that it has difficulties where the distribution is negative. In such cases, since the cumulative distribution is no longer monotonic, the root-finding scheme may encounter difficulties; e.g., Newton's method can diverge. On the other hand, using the inversion method can be advantageous if all but the high speed tail of the distribution will be discarded (e.g., high Mach number downwind boundary), since each component of $\mathcal{C}$ is generated separately.

Finally, in some applications only particles moving in one direction need to be generated. For example, particles created in a reservoir cell to the left of a boundary plane at $x = 0$ are discarded if their x-component of velocity is negative. Taking the absolute value of the x component of velocity after $\mathcal{C}$ has been generated is incorrect since the Chapman–Enskog distribution is not symmetric. Instead, to correctly generate only those particles with a thermal velocity in the $+x$ direction, after drawing $\mathcal{C}_{\text{try}}$ in step 3 of the acceptance–rejection method, take the absolute value of its x component of velocity. Similarly, in the Metropolis generator, after drawing $\mathcal{C}_{\text{old}}$ in step 1 or $\mathcal{C}_{\text{new}}$ in step 2, take the absolute value of its x component of velocity. The fraction of particles moving in the $+x$ direction is $\delta = \frac{1}{2} - q_x/10\pi^{1/2}$ so, if the reservoir cell would normally contain N particles, only δN need to be generated.

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