



Stochastic algorithm for simulating gas transport coefficients



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ABSTRACT

The aim of this paper is to create a molecular algorithm for modeling the transport processes in gases that will be more efficient than molecular dynamics method. To this end, the dynamics of molecules are modeled stochastically. In a rarefied gas, it is sufficient to consider the evolution of molecules only in the velocity space, whereas for a dense gas it is necessary to model the dynamics of molecules also in the physical space. Adequate integral characteristics of the studied system are obtained by averaging over a sufficiently large number of independent phase trajectories. The efficiency of the proposed algorithm was demonstrated by modeling the coefficients of self-diffusion and the viscosity of several gases. It was shown that the accuracy comparable to the experimental one can be obtained on a relatively small number of molecules. The modeling accuracy increases with the growth of used number of molecules and phase trajectories.

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1. Introduction

The description of transport processes in gases requires knowledge of the corresponding coefficients: diffusivity, viscosity, and thermal conductivity. Of course, there are fairly reliable experimental methods for measuring them. However, that the need for their theoretical calculations or simulations is also understandable. In dilute gases, this problem is solved using kinetic theory of gases (see e.g., [1]). However, calculation of these coefficients is generally not a trivial task because, first, to achieve sufficient accuracy, it is necessary to solve not simple integral equations. Usually it is applied different variational methods using the expansion in a complete set of the Sonine polynomials. To achieve sufficient accuracy it is necessary to take into account different number members of this set to calculate the various transport coefficients [2,3]. This is a rather cumbersome and complicated procedure. On the other hand, so-called Ω -integrals have to be calculated. There are the sufficiently detailed tables of the values of these integrals for the Lennard–Jones potential only. Methods for modeling the transport coefficients of rarefied gases are not available at all, and the molecular dynamics (MD) method is not applicable in this case. This is due to the fact that the corresponding simulation box should have a characteristic linear dimension much larger than the mean free path of molecules and it is therefore necessary to use a huge number of molecules. For dense gases, the MD method has long been used successfully. However, in this case, too, tens of thousands of molecules have to be used to achieve acceptable accuracy (comparable with the experimental accuracy) [4]. In addition, systematic studies of the ideology and results of the MD method have shown that it does not provide true phase trajectories of molecular systems (see [5–7]). Adequate results of MD simulations (e.g., transport coefficients) can be obtained only by averaging

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the corresponding dynamical variables over an ensemble of independent phase trajectories. As a result, MD simulation is a very computer-intensive process. Since this method does not give true phase trajectories of molecular systems, it seems reasonable to employ a certain stochastic method to determine these trajectories. Of course, such stochastic phase trajectories must somehow simulate the molecular system considered. It is the purpose of this paper to develop a stochastic algorithm for simulating the transport coefficients of molecular gases. We consider a rarefied gas, whose molecules interact through the hard spheres potential or the Lennard–Jones potential, and a dense gas of hard spheres (Enskog gas).

2. Algorithm simulating the dynamics of rarefied gases with the hard-sphere intermolecular potential

A gas in which only binary collisions of molecules take place and the molecules themselves are material points is called rarefied. The spatiotemporal scales of the order of the time of interaction between the molecules and their size are indistinguishable. This implies that the intermolecular interaction does not contribute to the transport coefficients and the equation of state. Such contributions appear only in the next approximation for density [8]. For this reason, the transport coefficients of a dilute gas are only functions of the velocities (momenta) of molecules. Therefore, to model the dilute gas dynamics, it is sufficient to consider its evolution in the space of velocities. The second important fact is that transport coefficients are calculated using the equilibrium distribution function and it is sufficient to study the dynamics of the system in local equilibrium.

Thus, we consider a system of N molecules that interact with each other through the hard-sphere potential (d is the diameter of the gas molecule)

$$\Phi(r) = \begin{cases} \infty, & r \leq d \\ 0, & r > d \end{cases} . \quad (1)$$

The velocities of the molecules v_i are distributed according to the Maxwell distribution at a given temperature T

$$f_M(v_i) = n \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left(-\frac{mv_i^2}{2kT} \right) \quad (2)$$

where m is the molecule mass, n is the gas density and k is the Boltzmann's constant. As an equilibrium state is modeled, the initial state of the system must be prepared so that the total momentum of its molecules is equal to zero and the energy corresponds to the given temperature.

As already noted, we need to model the dynamics of the system only in the phase space of all of its velocities. Simulation of the rarefied gas dynamics starts with generating a list of velocities of the molecules at the initial time t . Molecules are introduced in the list in a random order. Changing the order of the particles in the list, we will obtain different phase trajectories (this, of course, is not the only method for obtaining them). Thus, at time t , the molecules have velocities $(\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N)$. It is necessary to obtain the values of the molecular velocities at successive times in the simulation interval (t, t_s) . We select the time interval $\tau_1 = d/v_{max}$, where v_{max} is the maximum magnitude of the velocity of the molecules in the system at the given time. The generation of the list for the time $t + \tau_1$ starts with a consideration of molecule 1. To determine whether molecule 1 collides with another molecule in time τ_1 , a random number uniformly distributed in the interval $(0; 1)$ is generated. If, in time τ_1 , it is less than the average probability of collision $P_{\tau_1} = nd^2\sqrt{\pi kT/m}$ (see [1]), then molecule j with which molecule 1 collides is randomly selected from the remaining $(N - 1)$ molecules. Here n is the number density of the gas. As a result, the velocities of the colliding molecules vary according to the laws of elastic collision

$$\mathbf{v}'_1 = \mathbf{v}_1 + (\mathbf{v}_{1j} \cdot \mathbf{e})\mathbf{e}, \mathbf{v}'_j = \mathbf{v}_j + (\mathbf{v}_{j1} \cdot \mathbf{e})\mathbf{e} \quad (3)$$

where $\mathbf{v}_{j1} = (\mathbf{v}_j - \mathbf{v}_1)$ is the relative velocity vector and \mathbf{e} is the unit direction vector from the center of molecule j to the center of molecule 1.

If the generated number is larger than the average collision probability, molecule 1 does not collide in time interval τ_1 and its velocity remains equal to \mathbf{v}_1 . If it collides, the velocity of molecules 1 and j in the original list are changed. Similarly, the remaining molecules are processed sequentially. As a result, a new list of molecular velocities $(\mathbf{v}'_1, \mathbf{v}'_2, \dots, \mathbf{v}'_N)$ is generated. Some molecules from this list might not have collided during this time, and their velocities then remain unchanged.

After the generation of the list for the time $(t + \tau_1)$, the next time interval is selected as $\tau_2 = d/v_{max}$, where v_{max} is the maximum magnitude of the velocity of the molecules of the system at the time $(t + \tau_1)$ and the procedure is repeated. This procedure is repeated until the given simulation time t_s equal to $t_s = \tau_1 + \tau_2 + \tau_3 + \dots + \tau_N$ is reached. The calculation result is the full set of the velocities of all the molecules of the simulated system at successive times.

In all cases of applying the algorithm the input parameters are initial coordinates and velocities of the molecules, their masses, the gas density and its temperature, the number of molecules in the system, and parameters of the intermolecular interaction potential.

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