Physica A 411 (2014) 104–112

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

# Analysis of transport properties determined by Langevin dynamics using Green–Kubo formulae

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## HIGHLIGHTS

- We employ Green–Kubo formulae to investigate the transport properties of Langevin model.
- Langevin velocity model predicts the Prandtl number to be 3/2 for monatomic gas.
- Langevin acceleration model could adjust the Prandtl number with an additional time scale.

## ARTICLE INFO

*Article history:*
Received 23 October 2013
Received in revised form 26 February 2014
Available online 18 June 2014

*Keywords:*
DSMC
Langevin dynamics
Green–Kubo formulae
Transport coefficients

## ABSTRACT

Recently, the Langevin dynamics method has been applied to simulate gas flows. It is very crucial to evaluate whether the Langevin dynamics could correctly predict transport properties of gas or not. In this paper, the transport properties of Langevin velocity model and acceleration model are analyzed by using Green–Kubo formulae. For the Langevin velocity model, the time correlation functions have the exact exponent forms, and the Prandtl number for monatomic gas is predicted to be 3/2. For the Langevin acceleration model with an additional time scale, the molecular movements change from Markovian process to Non-Markovian process, and the Prandtl number could be adjusted to some extent. In the limit of equilibrium, there is a minimum about 1.298 for the Prandtl number of monatomic gas when the two time scales are equal in Langevin acceleration model. Besides theoretical analyses, molecular simulations according to the Langevin velocity model and acceleration model are performed, and the simulation results validate our analytical solutions.



## 1. Introduction

A stochastic algorithm based on Langevin equation, has been proposed to simulate rarefied gas flows recently [1–3]. Here we call it Langevin simulation Monte Carlo (LSMC) method. Comparing with the direct simulation Monte Carlo (DSMC) method [4,5], which has been very popular in the simulation of rarefied gas flows, the LSMC method is more efficient for simulating small Knudsen number flows. It is known that in DSMC method, the molecular movements and inter-molecular collisions are assumed uncoupled during small time intervals. Molecular motions are modeled deterministically, while inter-molecular collisions are treated statistically. For accurate DSMC applications, the sizes of cell within which molecular collision partners are selected should be less than mean free path of molecules, and the time steps should be less than mean collision time. Therefore, DSMC would become computationally very expensive for the simulation of small Knudsen number flows. On the other hand, the Langevin equation uses drift term and diffusion term to describe molecule movements, and no direct molecular collisions have to be modeled. This allows the LSMC method to proceed with much larger time step than that used in DSMC method. Using Langevin simulation, very good agreement of molecular stresses and mean velocity in comparison with DSMC, linearized Boltzmann and experiment has been achieved [1,3].

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http://dx.doi.org/10.1016/j.physa.2014.06.012
0378-4371/

According to the principle of stochastic process, the Langevin equation is closely related to the Fokker–Planck equation [6], and the LSMC method could be regarded as a stochastic solution of the Fokker–Planck equation. The relation between LSMC method and Fokker–Planck equation is similar to the relation between DSMC method and Boltzmann equation. Based on gas kinetic theory, the Fokker–Planck equation could be considered as an approximation of Boltzmann equation [7]. Many researchers have discussed the Fokker–Planck description as a model equation for gas dynamics. For example, Lebowitz et al. [8] and Pawula [9] tried to approximate the Boltzmann equation by a Fokker–Planck equation with a simple drift model, which results in a wrong Prandtl number for monatomic gas molecules. Since the Prandtl number is very important for the heat transport phenomena, many efforts have been made for the Fokker–Planck model to provide correct Prandtl number. Heinz [10] introduced an acceleration model with an additional time scale, which could be used to adjust the Prandtl number. With the acceleration model, the molecule movements change from Markovian process to Non-Markovian process. Yano et al. [11] proposed a Fokker–Planck equation with a source term to correct Prandtl number. Recently, Gorji et al. [2] introduced a cubic non-linear drift term in Fokker–Planck equation, and this model leads to the correct Prandtl number for monatomic gas. In the equilibrium limit, the non-linear drift model automatically regresses to be linear.

In this paper, we employed the Green–Kubo formulae [12] to analyze the transport properties of Langevin equation, including velocity model and acceleration model proposed by Heinz [10]. The Green–Kubo relations give the exact mathematical formulae for transport coefficients in terms of integrals of time correlation functions of some specific microscopic flux. Based on the Langevin model and Ito calculus [13], we could directly obtain the analytical solution of velocity for each molecule, and then the time correlation functions are determined. Using Green–Kubo formula, we obtain the analytical solutions of transport coefficients, and the corresponding results are presented in Sections 2 and 3 for the Langevin velocity model and acceleration model, respectively. In order to validate our analytical results, molecular simulations under equilibrium condition are performed, and the corresponding results are shown in Section 4. The discussions and conclusions are presented in Section 5.

## 2. Analysis of Langevin velocity model

Let us consider simple Langevin model for the velocity $u_x$ of one molecule in $x$ direction,

$$\frac{\mathrm{d}u_x}{\mathrm{d}t} = -\frac{1}{\tau}(u_x - \langle u_x\rangle) + \left(\frac{4e_s}{3\tau}\right)^{1/2}\frac{\mathrm{d}w}{\mathrm{d}t}, \tag{1}$$

where $\langle u_x\rangle$ is the mean, or macroscopic velocity of molecules, $\tau$ is the characteristic relaxation time scale of molecular velocities, $e_s$ refers to the specific kinetic energy of molecules, i.e., $e_s = \frac{3}{2}\langle u_x^2\rangle$, and $w(t)$ is a Wiener process with the following properties

$$\left\langle \frac{\mathrm{d}w}{\mathrm{d}t}(t)\right\rangle = 0, \tag{2}$$

$$\left\langle \frac{\mathrm{d}w}{\mathrm{d}t}(t)\,\frac{\mathrm{d}w}{\mathrm{d}t}(t')\right\rangle = \delta(t-t'). \tag{3}$$

Note that our analysis is performed under equilibrium condition, and hence $\langle u_x\rangle$ equals zero. Meanwhile, the kinetic energy is constant and equal to $\frac{3}{2}RT$, where $R$ is the gas constant, and $T$ is the temperature of system.

Using Ito calculus [13], the exact solution of Eq. (1) could be written as

$$u_x(t) = u_x(0)\,\mathrm{e}^{-\frac{t}{\tau}} + \left(\frac{4e_s}{3\tau}\right)^{\frac{1}{2}}\int_0^t \mathrm{e}^{-\frac{t-s_x}{\tau}}\frac{\mathrm{d}w}{\mathrm{d}s_x}(s_x)\,\mathrm{d}s_x. \tag{4}$$

Similarly, the evolutions of velocities in $y$ and $z$ direction are

$$u_y(t) = u_y(0)\,\mathrm{e}^{-\frac{t}{\tau}} + \left(\frac{4e_s}{3\tau}\right)^{\frac{1}{2}}\int_0^t \mathrm{e}^{-\frac{t-s_y}{\tau}}\frac{\mathrm{d}w}{\mathrm{d}s_y}(s_y)\,\mathrm{d}s_y, \tag{5}$$

$$u_z(t) = u_z(0)\,\mathrm{e}^{-\frac{t}{\tau}} + \left(\frac{4e_s}{3\tau}\right)^{\frac{1}{2}}\int_0^t \mathrm{e}^{-\frac{t-s_z}{\tau}}\frac{\mathrm{d}w}{\mathrm{d}s_z}(s_z)\,\mathrm{d}s_z. \tag{6}$$

Having these expressions of velocity evolutions, the transport coefficients can be obtained by using Green–Kubo relations [12], which give the diffusion, viscosity and thermal conductivity coefficients as follows:

$$D = \int_0^{+\infty}\langle u_x(0)u_x(t)\rangle\,\mathrm{d}t, \tag{7}$$

$$\mu = \frac{1}{k_BVT}\int_0^{+\infty}\langle P_{xy}(0)P_{xy}(t)\rangle\,\mathrm{d}t, \tag{8}$$

$$\kappa = \frac{1}{k_BVT^2}\int_0^{+\infty}\langle J_x(0)J_x(t)\rangle\,\mathrm{d}t, \tag{9}$$