Monte Carlo Simulation in Molecular Gas Dynamics

By

Katsuhisa KOURA*
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Summary: Two existing techniques of the Monte Carlo simulation in the molecular gas dynamics, namely, the test-particle method and the direct-simulation method, are somewhat critically reviewed.

1. Introduction

The "Monte Carlo method" [1] is generally accepted as the procedure of any use of random sampling in treatment of either deterministic or probabilistic problems [2]. The "Monte Carlo simulation" is the Monte Carlo method involving the "simulation" or "analogue idea" introduced by von Neumann and Ulam [2], where nature is directly modeled in its probabilistic aspects.

In the Monte Carlo simulation in the molecular gas dynamics, the behaviors of molecules (atoms, molecules, electrons, and ions) are probabilistically simulated using the assumptions on which the Boltzmann equation [3] is based, i.e., binary molecular collisions, molecular chaos, and vanishingly short time and small physical space for molecular collisions; the simulated molecules are probabilistically followed using random numbers on a computer through the molecular motions (under the influence of external forces), the molecular collisions, and the boundary interactions; the statistical properties of molecules such as the velocity distribution function, the number density, and the temperature are obtained from the simulated molecules. The existing simulation techniques are distinctly divided into the test-particle method and the direct-simulation method. Both the methods are somewhat critically reviewed in the subsequent sections. General reviews of the Monte Carlo method and simulation and their applications in the molecular flow problems have been made by Sherman (1969) [4] and Bird (1978) [5].

2. Test-Particle Method

Some (one) simulated molecules or test particles without direct mutual interactions are followed through the molecular motions, the boundary interactions, and the molecular collisions with the field molecules whose statistical properties are known. The cumulative history of the test particles yields their statistical properties. This test-particle method was originated by Yarnold (1945) [6] for the electron swarm and by Wannier (1953) [7] for the ion swarm, where the test particles are electrons (ions) and the field molecules are neutral atoms or molecules and the

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* National Aerospace Laboratory

test particles are followed through the electron (ion) motions under the influence of the electric field and the electron (ion)-molecule elastic collisions. Itoh and Musha (1960) [8] developed the test-particle method in the simulation of the electrical discharge in a gas. In the electron-swarm simulation, Thomas and Thomas (1969) [9] and many Japanese researchers Sakai, Tagashira, and Sakamoto (1972) [10]; Makabe, Goto, and Mori (1973) [11]; Hayashi (1976) [12] significantly contributed. In the ion swarm, the simulation method was developed by Skullerud (1968) [13] and Lin and Bardsley (1975) [14]. It is noted that, in the electron (ion) swarm, the electrons (ions) are so diluted in the neutral molecules that the neutral molecules are not disturbed [and the electron-electron (ion-ion) collisions are ignored]; consequently the test particles and the field molecules are in principle separated; this is a linear problem.

In the case of neutral molecules, there also exist linear problems to which the test-particle method is well applicable. Davis (1960)[15] first applied the test-particle method to the free-molecule flow, where the molecular collisions are ignored and the test particles are followed through the molecular motions and the boundary interactions. Perlmutter (1965) [16] applied the test-particle method to the collisionless ion flow in the magnetic field. In the nearly free-molecule flow, the field molecules are taken as the free-stream molecules and the test particles are followed through the molecular motions, the boundary interactions, and the molecular collisions with the free-stream molecules. This is the "first collision" Monte Carlo technique used by Kogan and Degtyarev (1965) [17] and Robertson (1969) [18]. In gas mixtures containing a trace species and predominant species with known statistical properties, the test particles of the trace species are followed through the molecular collisions with the field molecules of the predominant species. This is the "tracer Monte Carlo method" first used by Sinclair and deLeeuw (1969) [19] and recently applied to the isotope-separation problem by Fox and Eaton (1977) [20] and Anderson and Burman (1977) [21], where the statistical properties of the predominant species are obtained by the direct-simulation method.

In the case of the nonlinear molecular flow problems where the test particles and the field molecules can not in principle be separated, Haviland and Lavin (1962) [22] originated the iterative procedure: The test-particles are followed through the molecular motions, the boundary interactions, and the molecular collisions with the field molecules whose velocity distribution function is given by the previous iteration; the cumulative history of the test particles constructs a new field-molecule distribution function for the next iteration; this process is repeated until the test-particle distribution function reproduces the field-molecule distribution function to an acceptable accuracy. A full description of this method is found in a monograph of Haviland (1965) [23]. Perlmutter (1967) [24] reduced the iterative process to that of the macroscopic quantities by assuming the form of the velocity distribution function. This method was employed by Tuer and Springer (1973) [25]. Yoshizawa extended the test-particle method to the analysis of unsteady problems such as a recombination reaction (1967) [26] and a rarefied flow (1969) [27]. Gorelov and Kogan (1968) [28] showed that the test-particle method is effectively

applicable to the small-disturbance (linear) molecular flow problems.

It should be pointed out that the test-particle method of Haviland and Lavin suffers from a significant amount of computer storage due to a cell network in velocity space and the convergence question due to the iterative process. These defects have been overcome by the direct-simulation method.

3. Direct-Simulation Method

The time-dependent velocity distribution function at time $t+\Delta t$ is obtained from that at time t by following simultaneously a large number of simulated molecules over the time step Δt through the molecular motions, the molecular collisions, and the boundary interactions. This direct-simulation method was originated by Bird (1963) [29] with the assumption of uncoupling of the molecular motions and collisions (1965) [30], where the molecular motions and collisions are separately followed provided Δt is much less than the mean collision time τ_c; the molecular collision number n_c during Δt is regulated through the time counter (TC), in which the TC is advanced by a time increment calculated from a collision pair until the TC concurrents with Δt [30]; this procedure is designated as the TC-procedure. It should be pointed out that the TC-procedure tends to yield an unrealistically low n_c [31]. During the development of the simulation technique, Bird (1967) [32] made a significant modification by introducing a cell network in physical space. (A cell network in velocity space is not required.) A full description of the direct-simulation method with the TC-procedure is found in a book by Bird (1976) [31].

The cell network in physical space was independently devised by Koura [33, 34] in 1967, where it was indicated that the introduction of the cell network leads to the additional time-step condition $\Delta t \ll \tau_m$ in order that the assumption of uncoupling is valid, in which $\tau_m = \lambda/v$ is the characteristic molecular motion time, λ is the characteristic cell dimension, and v is the characteristic molecular velocity; when there exists an external force, Δt should satisfy the additional condition $\Delta t \ll \tau_f$, where $\tau_f = v/a$ is the characteristic force time and a is the characteristic acceleration of force [34]. The fact that a molecular collision occurs almost independently and uniformly during Δt owing to the small change in the velocity distribution function during Δt due to the condition $\Delta t \ll \min(\tau_c, \tau_m, \tau_f)$ leads to the collision-frequency (CF) procedure [33, 34], which is essentially different from the TC-procedure of Bird: The collision frequency ν in each cell is calculated at time t and taken to be constant during Δt; the collision number n_c during Δt in each cell is taken deterministically as $n_c = \nu \Delta t$ or probabilistically as $\sum_{k=1}^{n_c} (\Delta t_c)_k = \Delta t$, where Δt_c is the collision-time interval between successive molecular collisions assigned by the probability $p(\Delta t_c) = \nu \exp(-\nu \Delta t_c)$.

The CF-procedure originated by Koura for gas mixtures (1969) [33–38] has been extended by Koura to gas mixtures with internal degrees of freedom such as vibration (1974) [39, 40] and rotation (1976) [41–44], chemical reactions (1973) [40, 45–49] involving electrons (1975) [42, 43, 50] and ions (1975) [50, 51], and interactions with radiation (1980) [52], using the semi-classical molecular model with

the discrete internal energy described by the semi-classical Boltzmann equation [52, 53]. It is noted that the CF-procedure makes it possible to simulate the behavior of trace molecules in heat-bath molecules (1975) [50] and the model collision terms such as the BGK model [54, 55] owing to the use of the collision frequency ν.

The CF-procedure was employed by Takagi (1971) [56], Murakami and Oshima (1974) [57], Anderson and Burman (1977) [21], Deshpande, Subba Raju, and Ramani (1979) [58], Nanbu (1980) [59] in little different appearance with no improvement [60], and Ogawa (1982) [61]. Yoshikawa (1979) [62] used an unreliable method with a phenomenologically adjustable parameter in the semi-classical treatment of molecular rotation.

The range of application of the TC direct-simulation method has been extended especially by Bird to gas mixtures (1968) [63], gases in the gravitational field (1971) [64], near continuum flows (1974) [65], small-disturbance (linear) flows (1977) [66], and three-dimensional flows (1979) [67]. Sugimura and Vogenitz (1975) [68] applied the TC method to weakly ionized flows using a finite-difference solution of the Poisson equation for the electric field.

The TC method has also been extended to polyatomic gases with internal degrees of freedom using the classical and phenomenological molecular models. Bird (1970 [69] used the classical rough-sphere model. Macpherson (1971) [70] solved the classical equations of motion for each molecular collision in the simulation procedure. Melville (1972) [71] used the classical loaded-sphere model. Bird (1971) [72] put forward the phenomenological energy-sink model, which, however, reveals an unrealistic distortion of the velocity distribution function. This defect has been overcome by the phenomenological model of Larsen and Borgnakke (1974) [73], which was used by Bird (1977) [74] in the simulation of a dissociation and recombination reaction. Similar phenomenological models were proposed by Pullin (1978) [75] and Ogawa (1982) [61].

It should be noted that both the classical and phenomenological models deal with the continuous internal energy and have some macroscopically adjustable parameters such as the relaxation time. On the other hand, in Koura's semi-classical treatment, the internal energy is taken to be discrete and no macroscopically adjustable parameters are included owing to the use of the differential cross section for the transition of the discrete internal quantum state, which is provided by quantum or classical calculations and experiments.

4. Future Prospects

Although the future prospects of the numerical method in the molecular gas dynamics are strongly influenced by the developments in the computer technology, the following remarks are made on the future prospects:

1. The test-particle method may continue a most effective simulation method for the behavior of particles without direct mutual interactions in dilute or dense matters. This method has been successfully applied to (linear) problems such as the electron or ion swarm and the photon [76] or neutron [77] transport, although the

test-particle method in the dilute-gas simulation has some disadvantages as compared with the direct-simulation method.

2. The direct-simulation method may continue a most effective simulation method for the (nonlinear) Boltzmann equation.

3. The Monte Carlo sampling technique developed by Nordsieck, Hicks, and Yen (1967) [78, 79] for the evaluation of the collision integral in the Boltzmann equation appears to become an effective numerical method for the Boltzmann equation, although it requires a cell network in velocity space and an iterative process and, consequently, suffers from essentially the same disadvantages of a large amount of computer storage and the convergence question as the test-particle method of Haviland and Lavin. The effective ordinary numerical quadrature for the collision integral may still be desired in order to solve the Boltzmann equation by the ordinary numerical method free from the statistical error.

4. Dilute or dense gases (liquids) can in principle be simulated by the molecular-dynamics method originated by Alder and Wainwright (1957) [80], where the trajectories of a large number of simulated molecules are followed by solving the simultaneous equations of motion. Since this method may require no special assumptions, it appears to become an effective simulation method in the molecular gas dynamics [81] especially for dense gases and in the plasmas, although the magnitude of computational task is required.

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