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Employing Per-Component Time Step in DSMC Simulations of Disparate Mass and Cross-Section Gas Mixtures

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Abstract. A new approach to simulation of stationary flows by Direct Simulation Monte Carlo method is proposed. The idea is to specify an individual time step for each component of a gas mixture. The approach consists of modifications mainly to collision phase simulation and recommendations on choosing time step ratios. It allows lowering the demands on the computational resources for cases of disparate collision diameters of molecules and/or disparate molecular masses. These are cases important e.g., in vacuum deposition technologies. Few tests of the new approach are made. Finally, the usage of new approach is demonstrated on a problem of silver nanocluster diffusion in argon carrier gas under conditions of silver deposition experiments.

AMS subject classifications: 65C05, 76M28

Key words: Direct Simulation Monte Carlo, time step, disparate masses, gas mixture, nanoclusters.

1 Introduction

The Direct Simulation Monte Carlo (DSMC) method [1] is a standard for the simulation of nonequilibrium rarefied gas flows described by the Boltzmann equation. This method is based on tracking individual molecules (simulators), considering them moving independently with occasional discrete events of pair collisions applied according to a statistical model. After the steady state is reached, the average of simulator parameters over many time steps delivers macroparameters of the flow. The method has three discretization parameters:

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First, displacement and collision phase are uncoupled to speed up a computation, this defines the time step parameter Δt.

Second, a considerably limited, reduced number of simulators is used to simulate a large number of physical molecules. The symmetry of the Boltzmann equation allows reducing the number density n of molecules by increasing the collision cross-section σ_T, keeping the local mean free path λ unchanged:

$$n \to \frac{n}{F}, \qquad \sigma_T \to F\sigma_T, \qquad \lambda = \frac{1}{\sqrt{2}n\sigma_T},$$

here F is the number of physical molecules represented by a simulator.

Third, for a reduced number of simulators, collisions can no longer be a point event, as it should in the Boltzmann equation, so, the simulation area is divided into cells of linear size h and collision partners are chosen randomly within the same cell, causing spatial collision separation.

As is said, DSMC is the most practical method for the numerical simulation of nonequilibrium rarefied gas flows. However, the statistical nature of DSMC forces to calculate a lot of time steps to collect enough samples to get good statistical averages, as the noise amplitude is inversely proportional to the square root of the simulated period of time. When the flow is close to equilibrium, gradients of macroparameters are too small to resolve. This forces to use modified DSMC [2–5] or even alternative [6, 7] methods to solve the Boltzmann equation.

Discretization causes distortion of flow parameters and effective transport coefficients, the error is of second order in cell size and time step, i.e., $\sim (h/\lambda)^2$ [8] and $\sim (v_C\Delta t)^2$ [9] (v_C is the local mean collision frequency) and first order in F, i.e., $\sim h/(\lambda\overline{N})$ [10] ($\overline{N}$ is the mean number of simulators in a cell and $\lambda\overline{N}$ is invariant on local density). Simulating a d-dimensional flow of characteristic linear size L and characteristic mean free path λ, keeping the same distortion, requires $\sim(L/\lambda)^d$ cells and a proportional number of simulators, these determine demands on computer memory and on number of operations per time step. With the increase of flow density, the time step has to shrink, while relaxation of the flow slows down, therefore, the number of time steps to reach steady state is $\sim(L/\lambda)^2$. Sometimes reaching a steady state is more costly than collecting a good average of flow properties. When reaching a steady state is not obvious, convergence detection algorithms have to be used [11].

The majorant collision frequency (MCF) scheme [12] assumes that each possible pair (i,j) of simulators in a cell has its own collision frequency:

$$v_{ij} = \frac{F\sigma_T c_r}{V_C}, \tag{1.1}$$

here c_r is the relative velocity and V_C is the cell volume. The algorithm to accomplish this is as following. First, a value of the majorant collision frequency $v_{\max}$ is chosen in each