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An adaptive procedure for the numerical parameters of a particle simulation

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ABSTRACT

In this article, a computational procedure that automatically determines the optimum time step, cell weight and species weights for steady-state multi-species DSMC (direct simulation Monte Carlo) simulations is presented. The time step is required to satisfy the basic requirements of the DSMC method while the weight and relative weights fields are chosen so as to obtain a user-specified average number of particles in all cells of the domain. The procedure allows the conduct of efficient DSMC simulations with minimal user input and is integrable into existing DSMC codes. The adaptive method is used to simulate a test case consisting of two counterflowing jets at a Knudsen number of 0.015. Large accuracy gains for sampled number densities and velocities over a standard simulation approach for the same number of particles are observed.

1. Introduction

The DSMC (direct simulation Monte Carlo) method is today the most widely used simulation method for high speed rarefied flows [1]. Its accuracy and convergence is mainly determined by the number of particles employed in the simulation, the mesh size and the time step employed. Because of the formulation of DSMC [2], the number of particles in a cell is directly proportional to its number density while the time step of the simulation can be no more than the mean collision time so that the movement and collisions of particles can be decoupled. Similarly, collisions are only performed for particles located in the same cell, so that its characteristic length has to be less than the mean free path for this local assumption to be valid. This in turn signifies that the constraints which the numerical parameters of DSMC have to satisfy are inherently tied to the physics, particularly the number density field, of the test case being simulated. This, however, makes the efficient simulation of flows containing large variations in number density or large disparities between species number densities difficult. Large density variations are commonly encountered in many rarefied flows, particularly jets, while the accurate simulation of trace species, i.e. chemical species with a low concentration relative to others, is important for many applications. This is in particular the case for weakly ionized flows where the electric field is determined by the distribution of charged particles whose concentrations are low compared to neutral particles [3,4]. Trace species also play an important role in chemically reacting [5] and radiating [6] flows. These drawbacks inherent to the DSMC method have led to a number of modifications to the basic DSMC algorithm that are in ubiquitous use today. The first is the use of spatially

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varying weights, particularly for axisymmetric simulations, such as in (amongst many others) [7,8] where the cell volume scales with the distance to the centerline, that allows enough particles to be present close to the centerline while reducing their number further away from it. The second improvement is the use of a spatially varying time step, and an adaptive procedure to calculate the optimum time step field as in, e.g., [9–11]. For multi-species flow, the use of relative weights, also called species weights, is widespread, such as in [6,12,13]. They allow to increase the number of particles representing species with low number densities relative to others thereby allowing the use of fewer particles overall in the simulation. Spatially varying time steps, cell weights and relative weights are, however, almost never used simultaneously and whereas an adaptive procedure for the time step has been proposed before [9,10], one for the cell weights and species relative weights has not. Relative weights are furthermore most often assumed to be spatially uniform thereby forfeiting some of the efficiency gains obtainable by having them vary through the computational domain. The aim of this article is to detail a formulation of an all-encompassing adaptive procedure for the time step, cell weights and relative weights where all are allowed to vary throughout space. Such a procedure greatly facilitates the conduct of efficient DSMC simulations by lessening the need for human inputs, such as e.g., running multiple simulations to determine optimum weight fields. The first part of the article describes the additional considerations that must be taken into account when using spatially varying weights or time steps in terms of particle movement and collisions including the potential deleterious effects of particle cloning. The adaptive procedure for the time step, cell weight and species relative weights is then detailed and its integration into existing DSMC codes discussed. A test case consisting of two counter-flowing axisymmetric jets at a Knudsen number of 0.015 is introduced which is used to illustrate the increased accuracy obtainable with the adaptive method compared to when only a spatially varying time step and weight are used.

2. DSMC framework

2.1. DSMC with spatially varying time step and weights

2.1.1. Definitions

In the canonical version of DSMC, the same cell weight $W_{p,0}$ and time step value Δt_0 are used for all N_c cells of the computational domain while all species are assigned the same relative weight of 1. In the following, spatially variable cellwise constant time step $\Delta t(\vec{x})$, cell weights $W_p(\vec{x})$ and species relative weights $W_{\mathrm{rel},j}(\vec{x})$ are considered. A non-dimensional time step $\widetilde{\Delta} t(\vec{x})$ and cell weight $\widetilde{W}_p(\vec{x})$ are in turn, respectively, defined as

$$\Delta t(\vec{x}) = \Delta t_0 \widetilde{\Delta} t(\vec{x}), \tag{1}$$

$$W_p(\vec{x}) = W_{p,0} \widetilde{W}_p(\vec{x}) \widetilde{\Delta} t(\vec{x}). \tag{2}$$

The non-dimensionalized weight $\widetilde{W}_p(\vec{x})$ is defined as such because it will later be more useful to consider the value of the normalized value of the weight divided by the non-dimensionalized time step, i.e. $\frac{W_p(\vec{x})}{W_{p,0}\widetilde{\Delta t}(\vec{x})}$ instead of $\widehat{W}_p(\vec{x}) \triangleq \frac{W_p(\vec{x})}{W_{p,0}}$. Cellwise constant weights and time step are used, while a total of N_{spec} distinct species are present in the simulation, so that each cell i ($1 \leq i \leq N_c$) is characterized by $\widetilde{\Delta} t_i$, $\widetilde{W}_{p,i}$ and $\{W_{\mathrm{rel},j,i}\}_{j=1}^{N_{\mathrm{spec}}}$. As an example, using the previously defined terminology, the number density $n_{j,i}$ of species j inside cell i of volume V_i, when it contains $N_{j,i}$ particles of species j, is given by:

$$n_{j,i} = \frac{W_{p,0} W_{\mathrm{rel},j,i} \widetilde{W}_{p,i} \widetilde{\Delta} t_i N_{j,i}}{V_i}. \tag{3}$$

2.1.2. Particle movement

When a computational particle of species j moves from one cell i, characterized $\widetilde{W}_{p,i}, W_{\mathrm{rel},j,i}$, $\widetilde{\Delta} t_i$ to cell $i+1$ with different weights $\widetilde{W}_{p,i+1}, W_{\mathrm{rel},j,i+1}$ and a different timestep $\widetilde{\Delta} t_{i+1}$, care must be taken to preserve the flux of particles between the two cells. The number density flux (i.e. the number of physical particles per unit area and time) from cell i to cell $i+1$ through their common face of area $S_{i+1/2}$ from the standpoint of cell i is denoted by $\Phi^k_{i\to i+1|i}(n_j)$ and given as follows:

$$\Phi^k_{i\to i+1|i}(n_j) = \frac{W_{\mathrm{rel},j,i} W_{p,i}}{\Delta t_i S_{i+1/2}} N^k_{j,i\to i+1|i} = \frac{W_{p,0}}{\Delta t_0 S_{i+1/2}} W_{\mathrm{rel},j,i} \widetilde{W}_{p,i} N^k_{j,i\to i+1|i}, \tag{4}$$

where $N^k_{j,i\to i+1|i}$ designates the number of computational particles moving from cell i to cell $i+1$. Similarly, the number density flux of incoming particles from cell i into cell $i+1$ from the standpoint of cell $i+1$ is

$$\Phi_{i\to i+1|i+1}(n_j) = \frac{W_{\mathrm{rel},j,i+1} W_{p,i+1}}{\Delta t_{i+1} S_{i+1/2}} N^k_{j,i\to i+1|i+1} = \frac{W_{p,0}}{\Delta t_0 S_{i+1/2}} W_{\mathrm{rel},j,i+1} \widetilde{W}_{p,i+1} N^k_{j,i\to i+1|i+1}. \tag{5}$$