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Parallel Fokker–Planck-DSMC algorithm for rarefied gas flow simulation in complex domains at all Knudsen numbers

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ABSTRACT

A major challenge for the conventional Direct Simulation Monte Carlo (DSMC) technique lies in the fact that its computational cost becomes prohibitive in the near continuum regime, where the Knudsen number (Kn)—characterizing the degree of rarefaction—becomes small. In contrast, the Fokker–Planck (FP) based particle Monte Carlo scheme allows for computationally efficient simulations of rarefied gas flows in the low and intermediate Kn regime. The Fokker–Planck collision operator—instead of performing binary collisions employed by the DSMC method—integrates continuous stochastic processes for the phase space evolution in time. This allows for time step and grid cell sizes larger than the respective collisional scales required by DSMC. Dynamically switching between the FP and the DSMC collision operators in each computational cell is the basis of the combined FP-DSMC method, which has been proven successful in simulating flows covering the whole Kn range. Until recently, this algorithm had only been applied to two-dimensional test cases. In this contribution, we present the first general purpose implementation of the combined FP-DSMC method. Utilizing both shared- and distributed-memory parallelization, this implementation provides the capability for simulations involving many particles and complex geometries by exploiting state of the art computer cluster technologies.

1. Introduction

Many real-world flows exhibit large variations of the molecular mean-free path length. For example, nozzle flow into vacuum as it occurs in space vehicle thrusters or hypersonic flows encountered during atmospheric reentry. The conventional Navier–Stokes–Fourier (NS) description, on which continuum flow solvers are based, brakes down where the Knudsen number (Kn)—characterizing the degree of rarefaction—becomes large. In these situations, the flow description needs to be directly based on the Boltzmann equation. While there exist different numerical techniques for solving the Boltzmann equation [1], the most prominent one certainly is the Direct Simulation Monte Carlo (DSMC) method introduced by Bird [2]. While DSMC enjoys widespread success [3], its computational cost becomes prohibitive in the near continuum regime. Hence, the previously mentioned flow situations—which are characterized by a large Kn range—are notoriously difficult to simulate. One approach is, for example, to couple NS and DSMC solvers, as presented by Schwartzentruber et al. [4] for hypersonic flows.

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The Fokker–Planck (FP) based particle Monte Carlo scheme introduced by Jenny et al. [5] and further developed at ETH's Institute of Fluid Dynamics [6,7], allows for computationally efficient simulations of rarefied gas flows in the low Kn regime. In contrast to DSMC—where binary collisions are computed explicitly—the FP based method works by integrating continuous stochastic processes for the evolution of the system in phase space. This allows for time step and grid cell sizes larger than required to resolve the collisional scales, as is necessary in DSMC. Recently, the Fokker–Planck-DSMC (FP-DSMC) algorithm, combining the FP and DSMC schemes, was introduced and successfully applied to flows covering the whole Kn range [8]. The FP-DSMC algorithm combines the efficiency of the FP method for small to moderate Kn with the accuracy of DSMC for large Kn. Since both DSMC and the FP algorithm are particle methods, the FP-DSMC algorithm uses the same computational particles and merely employs different collision operators in different regions. Switching between DSMC and FP collision operators is performed dynamically such that accuracy and optimal efficiency are guaranteed.

Accuracy and computational efficiency of the (diatomic) FP method and of the FP-DSMC algorithm have been successfully demonstrated for one- and two-dimensional flows [7–9]. In the present paper, a general purpose solution algorithm and its parallel implementation are described. The new method is capable of simulating 3D flows of diatomic molecules in and around complex geometry, which is demonstrated by its application to various relevant test cases. The flexibility of the new algorithm—which does not require explicit specification of an interface between continuum and rarefied regions—makes it ideally suited for the study of complex flows. The present implementation is both flexible in terms of treatment of various flow types, from internal flows in micro devices to hypersonic reentry type flows, as well as efficient, i.e. it scales well with a large number of computational particles.

The rest of the paper is organized as follows: In Section 2, the Fokker–Planck algorithm for diatomic gas flows is reviewed and the dynamic coupling with DSMC is described. Section 3 describes key implementation issues, specifically data structure, parallelization and the treatment of complex geometries. In Section 4, we present results obtained with the new implementation for hypersonic flow past a corner profile, a sphere, as well as flow expansion through a 3D micro-nozzle geometry into vacuum. The results of the FP-DSMC algorithm are compared to those obtained by pure DSMC in terms of field quantities as well as computational cost.

2. Review of the Fokker–Planck-DSMC algorithm

A detailed derivation of the Fokker–Planck model and the Fokker–Planck-DSMC algorithm for diatomic gas flow were given in the articles by Gorji and Jenny [8,9]. In the following, the main results relevant for the new method and its implementation are summarized.

2.1. The Fokker–Planck model for diatomic gas flow

2.1.1. Particle system, phase space and sample space

As previously mentioned, the FP method—like DSMC—is a stochastic particle based method in which an ensemble of N computational particles, each with index i, weight w^i, random velocity vector $\mathbf{M}^i(t) \in \mathbb{R}^3$, random vector $\boldsymbol{\omega}(t) \in \mathbb{R}^2$ of rotational degrees of freedom, random vector $\boldsymbol{\xi}(t) \in \mathbb{R}^2$ of vibrational degrees of freedom, and random position vector $\mathbf{X}^i(t) \in \mathbb{R}^3$, is used to approximate the joint probability density function (PDF) $f_{\boldsymbol{\Phi}}(\boldsymbol{\Psi}; \mathbf{x}, t)$ of the state $\boldsymbol{\Phi} = (\mathbf{M}, \boldsymbol{\omega}, \boldsymbol{\xi})^T \in \mathbb{R}^7$ in the associated sample space $\boldsymbol{\Psi} = (\mathbf{V}, \boldsymbol{\Omega}, \boldsymbol{\Xi})^T \in \mathbb{R}^7$ at physical location $\mathbf{x}$ and time t. The state vector $\boldsymbol{\Phi}$ is normalized such that the energy of a single particle with index i may be calculated (with Einstein's summation convention implied) as

$$e^i_{\text{tot}} = e^i_{\text{tr}} + e^i_{\text{rot}} + e^i_{\text{vib}} = \frac{1}{2}\boldsymbol{\Phi}^i_{jj}. \tag{1}$$

The specific energy $e^i_{\text{s,tot}}$ of particle i is consequently given by

$$e^i_{\text{s,tot}} = e^i_{\text{s,tr}} + e^i_{\text{s,rot}} + e^i_{\text{s,vib}} = \frac{1}{2}\left(\boldsymbol{\Phi}^i - \overline{\boldsymbol{\Phi}}\right)_{jj}. \tag{2}$$

In the limit of $N \to \infty$, the particle approximation converges to the PDF

$$f_{\boldsymbol{\Phi}}(\boldsymbol{\Psi}; \mathbf{x}, t) = \lim_{N\to\infty} \frac{\sum_{i=1}^N w^i \delta(\boldsymbol{\Phi}^i(t) - \boldsymbol{\Psi})\delta(\mathbf{X}^i(t) - \mathbf{x})}{\sum_{i=1}^N w^i \delta(\mathbf{X}^i(t) - \mathbf{x})}, \tag{3}$$

where $\delta(\cdot)$ is the Dirac functional. The mass density function (MDF) is defined as

$$\mathscr{F}(\mathbf{x}, \boldsymbol{\Psi}; t) = \rho(\mathbf{x}, t) f_{\boldsymbol{\Phi}}(\boldsymbol{\Psi}; \mathbf{x}, t), \tag{4}$$

where $\rho(\mathbf{x}, t)$ is the fluid density.