Journal of Computational Physics 314 (2016) 465–488

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A Cartesian cut cell method for rarefied flow simulations around moving obstacles

G. Dechristé [a,b,*], L. Mieussens [a,b,c,d]

[a] Univ. Bordeaux, IMB, UMR 5251, F-33400 Talence, France
[b] CNRS, IMB, UMR 5251, F-33400 Talence, France
[c] Bordeaux INP, IMB, UMR 5251, F-33400 Talence, France
[d] INRIA, F-33400 Talence, France

ARTICLE INFO

Article history:
Received 12 March 2015
Received in revised form 6 March 2016
Accepted 11 March 2016
Available online 16 March 2016

Keywords:
Kinetic equations
Deterministic method
Immersed boundaries
Cut cell method
Rarefied gas dynamics

ABSTRACT

For accurate simulations of rarefied gas flows around moving obstacles, we propose a cut cell method on Cartesian grids: it allows exact conservation and accurate treatment of boundary conditions. Our approach is designed to treat Cartesian cells and various kinds of cut cells by the same algorithm, with no need to identify the specific shape of each cut cell. This makes the implementation quite simple, and allows a direct extension to 3D problems. Such simulations are also made possible by using an adaptive mesh refinement technique and a hybrid parallel implementation. This is illustrated by several test cases, including a 3D unsteady simulation of the Crookes radiometer.

1. Introduction

In gas dynamic problems, the rarefied regime appears when the mean free path of the molecules of the gas is of the same order of magnitude as a characteristic macroscopic length. The flow has to be modeled by the Boltzmann equation of the kinetic theory of gases. Most of numerical simulations for rarefied flows are made with the stochastic DSMC method [8], especially for aerodynamical flows in re-entry problems. In the past few years, several deterministic solvers have been proposed, that are based on discretizations of the Boltzmann equation or simplified models, like BGK, ES-BGK, or Shakhov models [30]. They are efficient for accurate simulations, multi-scale problems, or transitional flows, for instance.

A recent issue is the account of solid boundary motion in rarefied flow simulations. This is necessary to simulate flows around moving parts of micro-electromechanical systems (MEMS) [19,25], as well as flows inside vacuum pumps. A fascinating illustration of rarefied flows with moving boundaries is the Crookes radiometer, subject of many debates from the late 19th to early 20th century [26]. Recent deterministic simulations help to understand the origin of the radiometric forces [41,46,47,10,48]. The numerical simulation of the Crookes radiometer is difficult because the motion of the vanes is induced by gas/solid interaction (like thermal creep), which means that an accurate prediction of the flow in the vicinity of the boundary is needed in order to predict the correct velocity of the vanes.

There are several numerical methods for moving boundary problems designed for computational fluid dynamics: some of them have recently been extended to deterministic discretizations of kinetic models, and can be divided in two main categories.

* Corresponding author.
E-mail addresses: Guillaume.Dechriste@math.u-bordeaux1.fr (G. Dechristé), Luc.Mieussens@math.u-bordeaux1.fr (L. Mieussens).

http://dx.doi.org/10.1016/j.jcp.2016.03.024
0021-9991/

First, with body fitted methods, the mesh is adapted at each time step so that the boundary of the computational domain always fit with the physical boundary: moving mesh [49] and ALE methods [20,21] fall into this category. Despite their extensive use in computational fluid dynamics, very few similar works have been reported in kinetic theory, except by Chen et al. [11]. Methods of the second category are based on Cartesian grid computations and are usually referred to as immersed boundary methods [31]. The mesh does not change during computations, and hence does not fit with the physical boundary. Special treatment is applied on mesh cells that are located close to the boundary in order to take its motion into account. Various extensions of these methods to kinetic theory have been proposed by several authors in [3,34,16,6]. Two recent variants are the inverse Lax–Wendroff immersed boundary method proposed by Filbet and Yang [18] and the Cartesian grid-based unified gas kinetic scheme of Chen and Xu [9]: the boundary motion is not taken into account in these two works, but these methods could in principle be extended to this kind of problem. We also mention the Lagrangian method: while it falls into the first category in CFD, it does not in kinetic theory. Indeed, whatever the motion of the mesh, the distribution function has to be interpolated at the foot of the characteristic for each microscopic velocity. The accuracy of these methods has been shown in [40,53] for one dimensional problems. Finally, we mention that moving boundary flows can also be treated with DSMC solvers: see, for instance, [33,38,44,45,58].

In this paper, we try to mix the advantages of body fitted and Cartesian methods: we present a cut cell method for computing rarefied gas flows around moving obstacles. The method consists in extracting a body fitted mesh from an initial Cartesian mesh. This approach has first been proposed to study inviscid flows [13,5,59]. It has later been extended to viscous flow simulations [54,57] and also adapted to moving wall problems [55,32,56]. A more extensive review of its applications can be found in [24]. However, this is the first extension to moving boundary problems in kinetic theory (complex 3D stationary DSMC simulations have already been investigated in [28,60]). This approach is well suited to deterministic approximations of the Boltzmann equation and is easy to implement because of the Cartesian structure of the mesh. Moreover, this is, up to our knowledge, the only immersed boundary method to be conservative. The versatility and robustness of the technique is illustrated by various 2D flows, and by the simulation of the unsteady rotation of the vanes of a 3D Crookes radiometer. This article is an extended version of our work announced in [16]. Here, the Boltzmann collision operator is replaced by BGK like models, that are approximated by a discrete velocity method. However, this is not a restriction: other collision operators could be used, and any velocity approximation (like the spectral method) could be used.

Generally, the problem of cut cell methods is that it is difficult to take into account the various shapes of cells that are cut by the solid boundary: for instance, in 2D, a cut cell can be a triangle, a quadrangle, or a pentagon, and this is worse in 3D. Here, we propose a simple representation of these cells by using the notion of virtual cells that are polygons (or polyhedrals) with possibly degenerated edges (or faces). This makes the treatment of any cut cell completely generic: in the implementation, the different kinds of cut cells and the non-cut cells are treated by the same algorithm. This makes the extension of the method to 3D problems very easy. However, to make large scale 3D simulations possible, we also use an adaptive mesh refinement (AMR) technique and a special parallel implementation.

The outline of our paper is as follows. In section 2, we give the governing equations of rarefied gas flows and introduce some notations. Our cut cell method is presented in section 3 for 2D problems. It is validated on three different numerical examples in section 4. Then, in section 5, our algorithm is extended to 3D simulations, and a 3D unsteady simulation of the Crookes radiometer is presented. Finally, some conclusions and perspectives are discussed in section 6. Technical details like computations of geometric parameters of the cells are presented in the Appendix.

2. Rarefied gas dynamics

2.1. Boltzmann equation

In rarefied regimes, a monoatomic gas is described by the Boltzmann equation:

$$\frac{\partial F}{\partial t} + \vec{v} \cdot \nabla F = Q(F). \tag{1}$$

The distribution function $F(t, \vec{x}, \vec{v})$ is the mass density of molecules at time t that are located at the space coordinate $\vec{x} \in \mathbb{R}^3$ and that have a velocity $\vec{v} \in \mathbb{R}^3$. For our approach, it is more relevant to look at the integral form of (1) in a time dependent volume $V(t)$. The Reynolds transport theorem leads to:

$$\frac{\partial}{\partial t} \int_V F \, \mathrm{d}V + \int_{\partial V} (\vec{v} - \vec{w}) \cdot \vec{n} F \, \mathrm{d}S = \int_V Q(F) \, \mathrm{d}V, \tag{2}$$

where $\partial V(t)$ is the surface of the volume $V(t)$. Let $\vec{x}$ be a point of this surface: it is moving at a velocity $\vec{w}(t, \vec{x})$ and the vector $\vec{n}(t, \vec{x})$ is the outward normal vector to the surface at this point.

The density ρ, momentum $\rho\vec{u}$, total energy E and stress tensor $\overline{\overline{\Sigma}}$, are computed by the first moments of the distribution function with respect to the velocity: