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Jin, W.; Kleijn, C. R.; Van Ommen, J. R.

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Direct Simulation Monte Carlo Calculation of Rarefied Gas Drag using an Immersed Boundary Method

W. Jin, C. R. Kleijn and J. R. van Ommen

Delft University of Technology, Department of Chemical Engineering, 2628 BL Delft, The Netherlands

Abstract. For simulating rarefied gas flows around a moving body, an immersed boundary method is presented here in conjunction with the Direct Simulation Monte Carlo (DSMC) method in order to allow the movement of a three dimensional immersed body on top of a fixed background grid. The simulated DSMC particles are reflected exactly at the landing points on the surface of the moving immersed body, while the effective cell volumes are taken into account for calculating the collisions between molecules. The effective cell volumes are computed by utilizing the Lagrangian intersecting points between the immersed boundary and the fixed background grid with a simple polyhedra regeneration algorithm. This method has been implemented in OpenFOAM and validated by computing the drag forces exerted on steady and moving spheres and comparing the results to that from conventional body-fitted mesh DSMC simulations and to analytical approximations.

Keywords: DSMC, immersed boundary method, overlap volume, drag
PACS: 47.45.-n

INTRODUCTION

The Direct Simulation Monte Carlo (DSMC) method [1] has been widely applied to fields where gas rarefaction is important, such as aerospace applications and Micro-Electro-Mechanical Systems (MEMS), where low pressure and small dimensions respectively lead to high Knudsen numbers [2, 3, 4]. When there is an immersed body in the flow domain, conventional DSMC typically requires a body-fitted grid wherein the molecular collisions are computed. However, for a moving immersed body, such as a moving part in MEMS or a Brownian particle, this necessitates a grid regeneration at each time step, which is computationally inefficient.

This problem is common in other grid based simulation techniques as well, such as the continuum finite volume and finite element based computational fluid dynamics (CFD), and the Lattice Boltzmann method (LBM). In these cases, the immersed boundary method (IBM), proposed by [5], has been widely applied to circumvent this problem. However, the immersed boundary method with a fully three dimensional immersed body has not yet been demonstrated in conjunction with the DSMC method. It should be noted that DSMC is a fully particle-based method and thus the flow properties are not calculated at grid points; the boundary conditions are always fulfilled by ensuring a predefined wall interaction law at the immersed boundary. On the other hand, the effective cell volume needs to be computed when a cell is intersected by the immersed boundary in order to render a correct molecular collision probability. This can be done by utilizing the intersecting points to represent the immersed boundary, similar to the Lagrangian points in IBM.

In this paper we present an immersed boundary method in conjunction with DSMC, which allows for the immersed body to move freely on top of the fixed background grid. Rader et al. [6] and Versluis et al. [7] have shown approaches similar to IBM in DSMC. However, in both of their approaches the moving boundaries are limited to flat planes aligned to the grid and the overlap volume with the cell is either greatly simplified or neglected. Here we demonstrate an immersed boundary method with a fully three dimensional immersed moving body and validate the results against that from body-fitted grid simulations and the analytical approximations.

NUMERICAL APPROACH

In DSMC [1] gas dynamics, there are two main steps which are decoupled from each other: 1) the molecular streaming step and 2) the molecular collision step. In the streaming step, the molecules can be accurately bounced back at the immersed boundary by computing the landing points for a given shape and position of the immersed body [8]. On the

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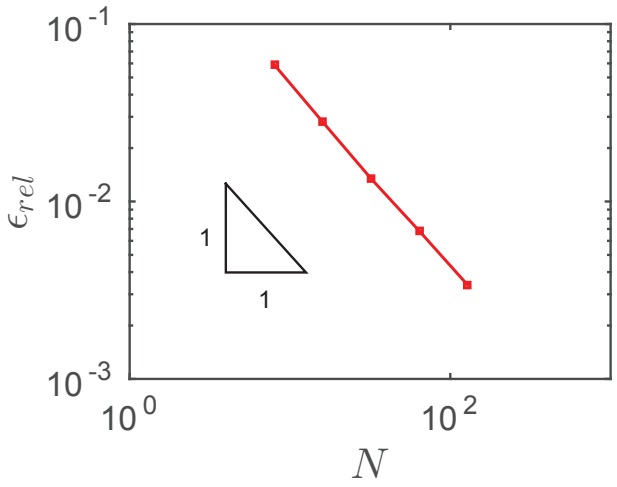

FIGURE 1. Relative errors of the computed overlap volume against different grid resolutions for the immersed sphere.

other hand, the molecular collision step requires computation of the effective cell volume V_c for the correct collision probability P, as shown in equation (1) [1].

$$P = F_N \sigma_T c_r \Delta t / V_c \tag{1}$$

F_N is the number of real molecules that is represented by one simulated molecule, σ_T is the total collision cross-section, c_r is the relative velocity between the two molecules, Δt is the time step.

When a grid cell is intersected by an immersed boundary, the overlap between the cell and the immersed body should be subtracted from the original cell volume to render the effective empty cell volume V_c. The computation of this overlap volume is achieved by constructing polyhedra connecting the intersecting points and the cell vertices that are located inside the immersed body. Due to the fact that the intersecting points may not be on the same plane, there can be multiple possible constructions of polyhedra. In this case, each of the possible polyhedra is decomposed into a number of pyramids by connecting its faces to the center of volume, then the volume of each polyhedron is computed by summing up the volumes of all its pyramids. Finally, an average over the maximum and minimum possible volume of the polyhedra is chosen as a good approximation for the overlap volume.

RESULTS AND DISCUSSION

Overlap Volume Computation for an Immersed Sphere

The above algorithm is applied to compute the overlap volume for a spherical immersed body, in order to study the convergence behavior of the computational errors. In this case, a sphere with diameter d is placed in a cubic structured grid with cell size Δx. The grid resolution is defined by $N = d/\Delta x$.

Since the molecular collision probability is directly affected by the volume of the intersected cells, the relative error is defined as,

$$\varepsilon_{rel} = \frac{V_{IB} - \sum V_{overlap}}{\sum V_{overlap,\ boundary}} \tag{2}$$

where V_{IB} is the actual volume of the immersed body, $V_{overlap}$ is the computed overlap volume of each cell including the ones that are completely enclosed by the sphere and $V_{overlap,\ boundary}$ is the overlap volume of a boundary cell that is partially overlapped by the immersed sphere.

Figure 1 shows that ε_{rel} from the overlap volume computation decrease linearly with increasing N.

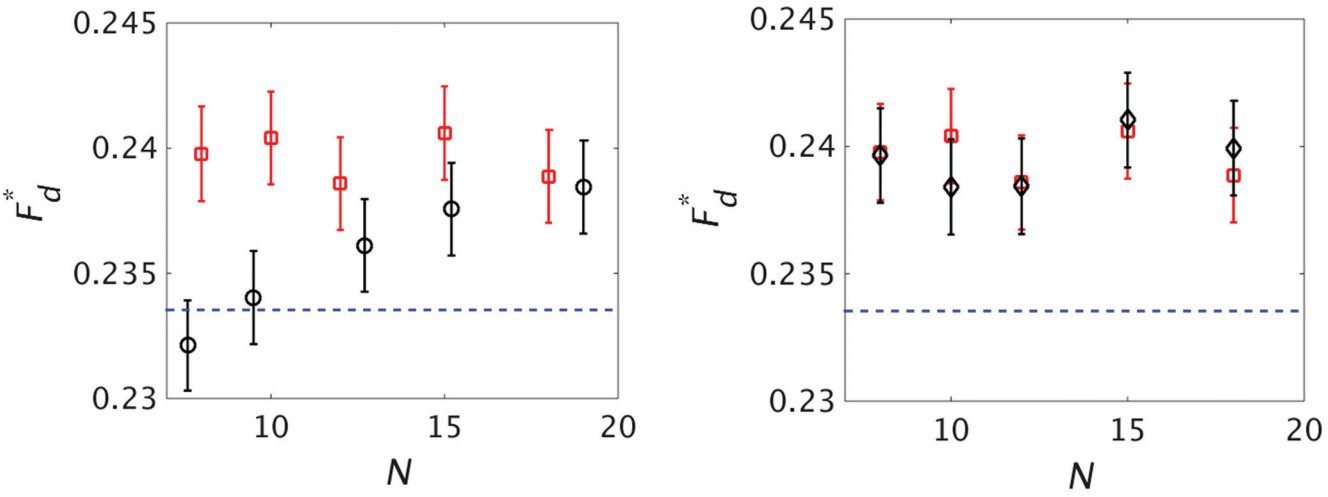

FIGURE 2. Drag forces, normalized by the Stokes drag, versus the grid refinement. Left: sphere with the immersed boundary (red square), with body-fitted mesh (black circle) and analytical approximation. Right: moving sphere (red square), steady sphere (black diamond) and analytical approximation (blue dashed line).

Validation with Drag Forces on the Steady and Moving Spheres

The immersed boundary method described above has been implemented into an open source DSMC solver "dsmcFoam" in OpenFOAM [9] and validated by computing the drag force exerted on an immersed sphere in a rarefied creeping flow. To this end, an immersed sphere is placed at the center of a cubic domain of size $L = 10d$. The boundary conditions are free stream inlet and outlet boundaries at two opposite planes and periodic boundary conditions for the rest of boundaries. Argon with the molecular properties from Bird [1], applying the variable hard sphere (VHS) model, is chosen for the simulated gas. The common DSMC criteria are fulfilled for all the simulations to ensure the well resolved simulations.

A fully diffusive boundary condition is employed at the sphere surface and the drag force is calculated from the summed momentum differences of the molecules reflecting at the sphere surface during a collision step. The drag force F_d is then normalized by the Stokes drag to render the dimensionless drag force ratio $F_d^\star$. The extra computation time required by the immersed sphere is less than 20%. Since this method avoids the grid regeneration at each time step and thus the molecule to cell re-linking, re-computation of the cell based flow properties, etc., this method will be much more efficient than the conventional body-fitted grid method in the case of moving objects. Figure 2 (left) shows $F_d^\star$ at different grid refinement at $Kn = 2.29$ and $Re = 0.02$, compared with the results from body-fitted grid DSMC and with the analytical approximation from Phillips [10]. It shows good agreement among the results while the DSMC with the immersed boundary shows less grid dependency. Figure 2 (right) shows the results for a moving immersed sphere in a stationary gas at $Kn = 2.29$ and $Re = 0.02$, compared to the results from a steady immersed sphere in a moving gas flow. It shows good agreement between two cases and thus validates our novel approach.

CONCLUSION

An immersed boundary method in conjunction with DSMC is presented for simulating rarefied gas flow around an immersed three dimensional moving body. The Lagrangian intersecting points between the immersed boundary and the background grid are utilized to compute the overlap volume. The relative error of this method converges linearly in the grid size. This method has been implemented into OpenFOAM and validated by computing the drag force on an immersed sphere, which showed good agreement with body-fitted grid DSMC and analytical approximations.

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