Hybrid lattice Boltzmann-Direct Simulation Monte Carlo approach for non-equilibrium flows in complex geometries

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HYBRID LATTICE BOLTZMANN-DIRECT SIMULATION MONTE CARLO APPROACH FOR NON-EQUILIBRIUM FLOWS IN COMPLEX GEOMETRIES

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KEY WORDS

kinetic theory, hybrid method, lattice Boltzmann method, Grad's velocity probability distribution function

SHORT SUMMARY

In this contribution, we present the results of a comparative study performed by using three numerical methods based on the kinetic theory of gases and applied to a flow of industrial relevance characterized by large compressibility and rarefaction effects. The employed methods are the Lattice Boltzmann Method (LBM), in a regularized formulation, the Direct Simulation Monte Carlo (DSMC), and the hybrid method, coupling the LBM and the DSMC, recently developed by the authors and here extended to the case of flow simulations in complex geometries involving hundreds of millions of cells and billions of computational particles. The good efficiency and parallelization scalability properties of the individual in-house LBM and DSMC codes are maintained also in the hybrid code implementation allowing to study with high accuracy the physics of flows showing large non-equilibrium effects in realistic geometries.

EXTENDED ABSTRACT

The Navier-Stokes equations represent an accurate model to describe the flow behavior in the hydrodynamic limit and when non-equilibrium effects can be treated perturbatively with respect to the equilibrium state, [1]. Whenever these assumptions are not satisfied anymore, commonly when the molecular-level spatial scale size is comparable to the macroscopic flow scale, a more fundamental approach based on the Boltzmann equation has to be followed. The Direct Simulation Monte Carlo has shown to be the most successful approach to approximate the Boltzmann equation in the rarefied flow regime, [2].

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In addition to this, for a large number of industrial applications, such as micro-electromechanical systems and material processing tools, a wide range of non-equilibrium/rarefaction flow conditions are present. The idea to study gas flows with such characteristics applying only the DSMC, however, faces a large computational cost associated to the near-continuum flow regions and basically due to the particle-based nature of the method and the explicitness of the interparticle collision mechanism. To deal with the current limitations from computational and modelling points of view, therefore, a hybrid method coupling near-continuum and rarefied flow solvers is needed.
In the hybrid method proposed by the authors, the DSMC is in charge of the rarefied/non-equilibrium flow regions while the LBM is used as solver for the near-continuum flow conditions. The adoption of the LBM, which shares common kinetic theory roots with the DSMC [3], in fact, aims at reducing the time and space scale separations typical of other hybrid methods where classical Navier-Stokes or Euler equations solvers are applied, e.g. [4]. LBM, moreover, has shown to be able to capture to some extent typical rarefied gas flow phenomena, such as the Knudsen paradox [5]. In [6], we introduced the schemes, based on the Grad's moment method approach to reconstruct the local single particle distribution function at a given order of truncation by using Gauss quadratures, and needed to extract and transfer information about the flow conditions at the interface between the DSMC and the LBM domain. In [7], we applied these schemes to a two-dimensional flow configuration adopting a domain decomposition technique. In the present contribution, we show the results reported in a recent work, [8], where the hybrid model is validated in terms of accuracy and assessed from a computational cost reduction point of view for a complex three-dimensional flow (see Fig.1 for a representation of the flow domain), involving a very large number of computational particles (in the order of 10^9) and cells (in the order of 10^8).

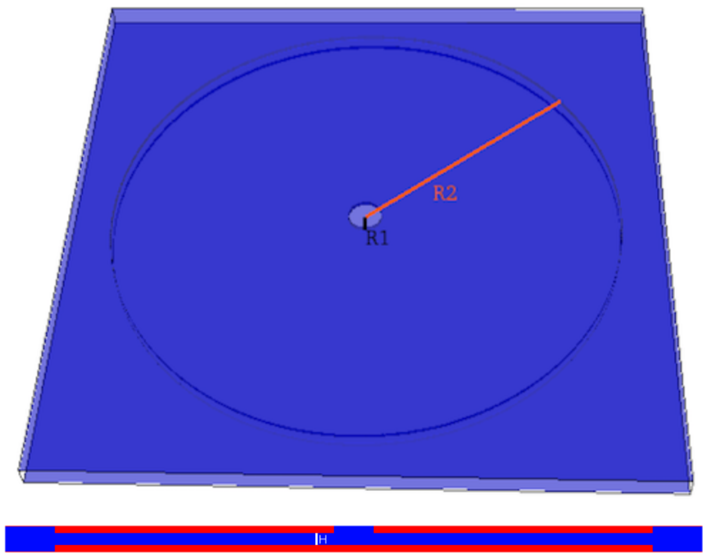

Figure 1: Top and side views of the investigated geometry. The flow inlet is realized through a circular duct of radius R_1. At R_2, an expansion of the flow section is present. The outlet is located at the lateral outer surfaces of the simulation box. The height of the channel between the top and bottom red disks is equal to H. Reproduced from [8].

For this flow set-up, characterized by conditions ranging from the near-continuum regime in proximity of the flow inlet up to the rarefied one, found close to the outlet section, the application of the DSMC method provides a reliable description but it is time consuming and the near-continuum method is fast but inaccurate. The domain decomposition between the LBM and the DSMC areas is performed according to the simultaneous fullfilment of two criteria: a global one, which prescribes that the DSMC is used only when Kn=λ/H ≥0.1, where λ is the mean free path and H is the channel height; and a local one, which imposes the passage from LBM to DSMC when $\mathrm{Kn}_\ell \geq 0.1$, with

$$\mathrm{Kn}_\ell = \lambda \left| \frac{\nabla |\mathbf{u}|}{c_s} \right|. \quad (1)$$

In Eq.(1), $|\mathbf{u}|$ is the flow velocity magnitude and c_s is the speed of sound. Using such criteria, about 20% of the total number of cells, corresponding to about 20 millions of cells, are solved with the DSMC method.
In Fig.2(left), the velocity magnitude profile measured at the mid-height section $y = H/2$ as obtained from the three numerical methods are compared with the solution generated using dsmcFoam, [9], taken as reference. While in the present study DSMC and hybrid LBM-DSMC methods provide a solution comparable to the reference one throughout large part of the flow domain, the LBM solution shows larger difference for radial positions closer to the outlet section. This can be easily explained because of the increasing importance of the non-equilibrium/rarefaction effects, and because of the adoption of a D3Q19 lattice which can only provide a flow description at the Navier-Stokes level of representation, [10].

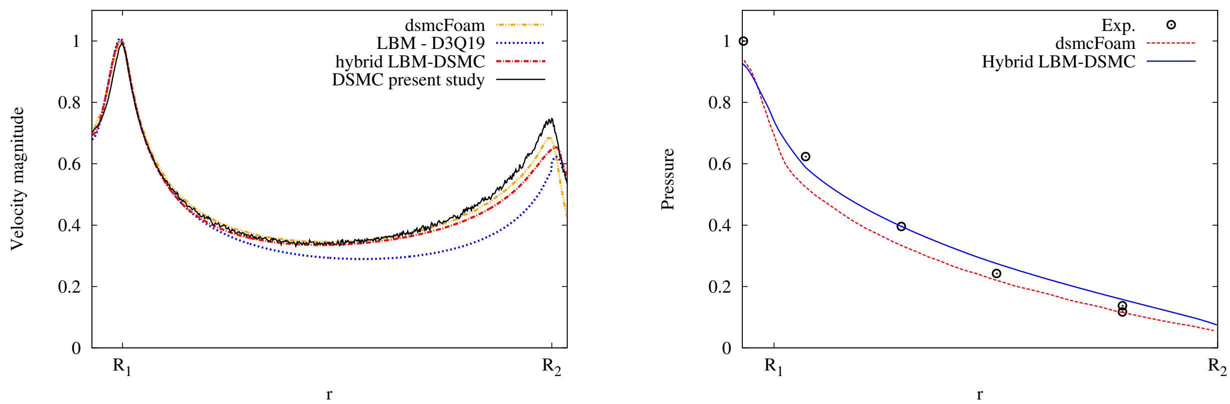

Figure 2: (Left) Velocity magnitude normalized with the maximum value found in the dsmcFoam solution as a function of the radial position, r, measured at $y = H/2$, for the three different numerical methods and dsmcFoam. $r = 0$ corresponds to the centerline of the inlet section. The two peaks at $r = R_1$ and $r = R_2$ occur as a consequence of the large variation of the flow area section. Going further downstream, the found velocity decrease can then be attributed to the increase of the flow area section and to the fact that the flow is subsonic. (Right) The pressure profile at the floor section, $y = 0$, obtained from the hybrid method solution is compared with the dsmcFoam and the experimental data. The pressure data are normalized with respect to the maximum value found from experiments. Reproduced from [8].

In Fig.2(right), the pressure measured at the section $y = 0$ and obtained from the hybrid LBM-DSMC method and dsmcFoam are compared with the experimental data (black hollow circles). A good accordance of the hybrid solution is found.
The computational cost associated with each method is assessed in Tab.1. The LBM and hybrid LBM-DSMC simulations are stopped when the convergence criterion:

$$\sum_i^N \frac{|\mathbf{u}(\mathbf{x}_i, t) - \mathbf{u}(\mathbf{x}_i, t-1)|}{|\mathbf{u}(\mathbf{x}_i, t)|} \cdot \frac{1}{N} < 10^{-6}, \quad (2)$$

is fulfilled. The DSMC simulation, instead, is stopped when the number of cumulated samples is such that a 1% fractional error is reached on the expected smallest flow velocity magnitude, defined as:

$$E_{u_i} = \frac{\sigma_{u_i}}{|u_i|} = \frac{\sqrt{< \delta u_i^2 >}}{\sqrt{S}|u_i|} \approx \frac{1}{\sqrt{SN}}\frac{1}{\mathrm{Ma}}, \tag{3}$$

In Eq.(3), N is the average number of particles, S is the number of required samples and Ma=u_i/c_s is the Mach number.

A large speed-up (more than four-fold) is guaranteed by the adoption of the hybrid formulation, while the final solution is still accurate and comparable to the DSMC solution.

Finally, ways to extend the current range of applicability of the hybrid models in order to accurately capture thermal effects are presented.

Method	Comp. Time [h]	Scaling
LBM - D3Q19	1.9	0.016
DSMC	120	1
Hybrid LBM-DSMC	29	0.242

Table 1: Computational cost of the three employed numerical methods. The same discretization of the flow domain for the three methods (1600×52×1600 grid cells) and the number of CPU cores (1600) is adopted. The DSMC and hybrid LBM-DSMC simulations initially evolve about $2.6{\cdot}10^9$ and $0.5{\cdot}10^9$ particles, respectively. Reproduced from [8].

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