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Citation for published version (APA):
Di Staso, G., Clercx, H. J. H., Succi, S., & Toschi, F. (2015). Hybrid DSMC-LBM scheme for rarefied and continuum gas flows. In *Proceedings of the 2nd European Conference on Non-equilibrium Gas Flows - NEGF15, December 9-11, 2015, Eindhoven, The Netherlands* (pp. 1-2)

Document status and date:
Published: 01/01/2015

Please check the document version of this publication:

• A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
• The final author version and the galley proof are versions of the publication after peer review.
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Download date: 14. Jan. 2025

Proceedings of the 2^{nd} European Conference on Non-equilibrium Gas Flows - NEGF15
December 9-11, 2015, Eindhoven, the Netherlands
NEGF15-13

HYBRID DSMC-LBM SCHEME FOR RAREFIED AND CONTINUUM GAS FLOWS

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KEY WORDS

Grad's moment method, single-particle distribution function, coupling scheme, Gauss-Hermite quadrature, Boltzmann equation, non-equilibrium effects

ABSTRACT

The kinetic description of gases, based on the Boltzmann equation, is particularly appealing as it allows to cover flow conditions ranging from the extremely rarefied regime to the hydrodynamic limit [1]. The two limits, rarefied and continuum, have been studied numerically by approximating the Boltzmann equation via the Direct Simulation Monte Carlo (DSMC) method [2] and, since more than two decades, via the Lattice Boltzmann method (LBM), [3]. While the former approach is particularly suited to rarefied flow conditions, its computational costs make it unpractical to study hydrodynamic flows. The LBM has largely proved itself to be a computationally efficient method in the hydrodynamic limits even though its use under rarefied flow conditions comes at a cost of additional modeling or computational resources [4], [5]. Here we present results on the development of a hybrid scheme capable of coupling the LBM and the DSMC methods. The key point of the LBM-DSMC coupling, in fact, is that both methods operate at the same length- and time-scales. The coupling scheme we developed is based on a theoretical framework grounded on Grad's moment method approach [6] and it is able to construct the local single particle distribution function at a given order of truncation by using the Hermite expansion approach and Gauss quadrature. In particular, for the LBM to DSMC step, the mapping scheme prescribes that the coefficients of the expansion should be computed from the LBM non-equilibrium discrete distribution functions and the obtained distribution function is sampled via acceptance/rejection method to generate DSMC particles velocities. For the reciprocal step, DSMC to LBM, the mapping scheme prescribes that the coefficients of the expansion should be computed from the DSMC hydrodynamic moments and the obtained distribution function is evaluated at the set of discrete speeds used in LBM so that the discrete populations can be reconstructed. The standard D3Q19 LBM model, however, is not able to quantitatively reproduce non-equilibrium effects beyond the Navier-Stokes level. To extend the range of applicability of the LBM also for flows at finite Knudsen number, so avoiding the use of DSMC whenever it becomes prohibitively expensive, we chose to adopt a larger than the standard set of discrete speeds (39 instead of 19 speeds), and to apply the kinetic boundary conditions, which impose diffuse reflection at the solid walls similarly to what is done in DSMC. Moreover, we applied the regularization procedure, which, by ensuring that both the equilibrium and non-equilibrium discrete distributions lie in the subspace spanned

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by the same Hermite polynomials basis used to build the truncated local distribution function in the coupling step, allows to filter out all higher-order contributions not sufficiently supported by the set of discrete speeds, [7], [8]. The capabilities of the kinetic hybrid approach for simulating gas flows in the early transition regime are illustrated in the case of plane Poiseuille flows, and connections between the order of truncation in Hermite polynomials expansion, the degree of accuracy of Gauss quadrature and the accuracy at Chapman-Enskog expansion level are also shown. In this view, it is evident the role of a larger set of discrete speeds for LBM in order to better capture non-equilibrium effects. Fig.1 shows the velocity profiles and deviations between the solutions obtained from DSMC and two different LBM sets of discrete speeds for a plane force-driven Poiseuille flow at $Kn = 0.10$ (based on channel height) and with Mach number at centerline equal to $Ma = 0.10$. While the conventional 19 speeds set, recovering hydrodynamic moments only up to Navier-Stokes level, reproduces DSMC velocity profile only in the bulk of the flow, the 39 speeds set, satisfying higher order isotropy conditions, allows to accurately resolve the flow also within the Knudsen layer, where non-equilibrium effects are stronger. These results suggest rules to determine the breakdown of LBM as accurate solver and to identify not only the domain boundary where the passage from a smaller to a larger set of discrete speeds for the LBM solver is needed but also, eventually, to indicate the need to switch from the LBM to the DSMC solver. Finally, based on the established theoretical framework and mapping schemes, an operating algorithm that is capable to couple the LBM and the DSMC methods and that is able to solve flows with variable rarefaction, is currently under development.

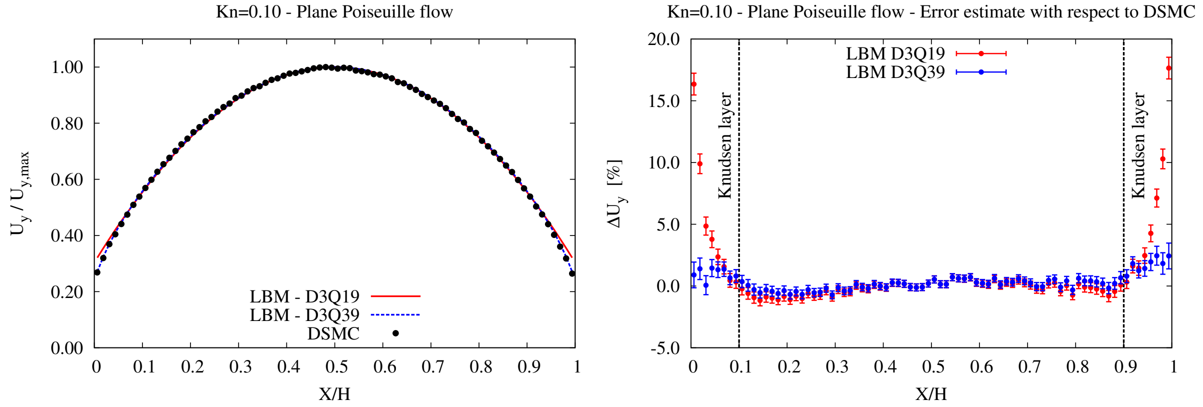

Figure 1: (Left panel) Comparison between the DSMC and LBM velocity profiles for plane Poiseuille flow at $Kn = 0.10$ and $Ma = 0.10$ in correspondence of the channel centerline; (right panel) Deviations between LBM and DSMC velocity profiles for two different sets of discrete speeds: 19 and 39.

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