Assesment of applicability of the Lattice Boltzmann Method for multi-scale simulation of fluid flows

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Abstract

In multiple technical and scientific applications it is common to observe physical phenomena involving large range of temporal and spatial scales. In order to properly model with high precision those situations, it is neccesary to have numerical tools that allow to obtain accurate predictions in the whole range on involved physical scales. Nevertheless, most of the traditional simulation techniques are primarily focused on specific sub-ranges of the involved scales. For instance, the majority of the numerical methods based on continuum medium models are centered on the so-called macro-scales, i.e. ranges of temporal and spatial scales of the same magnitude order of the involved system's extent. On the other hand, the so-called atomistic methods, which are primarily concentrated on spatial and temporal ranges of about the order of microscopic scales, are essentially based on lagrangian-type approaches with an emphasis on the modeling of the interaction of particles constituing the system's substance.

In general, macroscopic models are not suitable for modelling situations where microscopic effects become relevant. A specific example is the case of flows featuring slip-velocity in walls, which are usually observed in micro- and nano-systems. In these cases the Navier-Stokes equations are no longer valid, and produce very low levels of accuracy in the numerical predictions. Contrastively, atomistic models, although accurate in modeling phenomena at small scales, are practically unpractical for modelling phenomena at meso- and macro-scales, due to the excessively high computational costs involved. Therefore, it seems clear then that it is convenient to develop and implement methods combining the best of the different modelling approaches: able to adequately solve the characteristics associated to the micro-scales, and coupling with models focused on meso- and macro-scales. The main target would be to efficiently solve the aspects of large scales that may be involved, without loosing accuracy of the micro- and nano-scales physics. This type of methodologies are generally known as hybrid simulation methodologies.

The hybrid methods essentially focus on simultaneously simulating multiple physical scales, coupling macro-scale and atomistic modelling approaches. In such cases each model is oriented on a specific range of scales, both spatial and temporal, sharing evolution information of the variables studied with the other methods employed.

Meso-scale methods, such as the Lattice-Boltzmann method, constitute as first approaches to hybrid-type modelling techniques. These methods allow to use atomistic-based mathematical models on macroscopic scale problems. Another alternative for hybrid methods is to combine the use of atomistic approaches with the techniques featuring the computational efficiency of mesoscopic models. Another alternative is to increase the accuracy of mesoscopic models to combine with continuum medium models. It is worth to mention that one of the problems of hybrid methods is that the coupling between the different models it is usually not straightforward, mainly because they are based on different theoretical frameworks.

The present work is focused on assesing, exploring and implementing a numerical methodology that allows to study multiscale phenomena by extending the Lattice Boltzmann model (LBM) to improve its accuracy. It is also pursued to combine the LBM with a macroscopic model in order to study high Reynolds fluid flows. One of the possible modifications for the LBM would be to increase the numerical order schemes, so increaseing its accuracy. The expected result is to obtain a modelling methodology to explore multiscale fluid flow problems.