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Prediction of Moments in the Particles on Demand Method for LBM

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Abstract. PonD is a method to extend LBM calculations to arbitrary ranges of Mach number and temperature. The current work was motivated by the issue of mass, momentum and energy conservation in the PonD method for LBM. The collision guarantees their conservation, thus, the study involves all aspects of the streaming step: both coordinate and velocity space discretizations, gauge transfer method, resolution of the scheme implicitness. After obtaining the expressions for the change of moments in the system in a time update of the scheme, it was found that the scheme can be formulated as explicit in some cases. Thus, we found the sufficient conditions to make Pond/RegPonD computations explicit and mass, momentum, and energy conserving. The scheme was implemented in the explicit form, and validated for several test cases.

AMS subject classifications: 76N15, 52B10, 65D18, 68U05, 68U07, 65Z05, 65D99

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1 Introduction

Mathematical models of fluid physics are based on the Navier-Stokes-Fourier equations (NSFE) at macroscale and on the Boltzmann equation at mesoscale. The Boltzmann equation defines the evolution of the particle distribution function, and the system of Navier-Stokes-Fourier equations describes the behaviour of its velocity moments. Both models are expressions of the conservation principles. Thus, the property of conservation for the numerical methods in CFD (computational fluid dynamics) is as important as accuracy and stability [1].

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The equations for the moments are often modeled with finite difference, finite volume, or finite element methods [2]. The Boltzmann equation can be modeled with several kinetic schemes, such as discrete velocity models [3,4] and gas-kinetic schemes [5,6]. Among these, the Lattice Boltzmann method [7,8] (LBM) is a very popular method for simulation of fluid dynamics with a kinetic description. The difficulty of the kinetic description is the fact that particle distribution function (PDF) is a 7-dimensional function of 3 coordinates, 3 velocity components and time. Lattice-Boltzmann handles the integration in the velocity space with a small set of Q discrete velocities, thus, gas kinetics is described through the evolution of Q PDF values, which are functions of time and space.

On the one hand, LBM is a node-based method of particle populations propagation on a lattice, which exhibits fluid behaviour. Just like the Chapman-Enskog analysis [9] gives NSFE from the statistics of particle motion, the similar method can be used to obtain NSFE from the motion of virtual particles in LBM. The moment conservation properties are naturally provided by the method construction. On the other hand, it is a method of discretization of the Boltzmann equation [10]. That is its power, since it expresses physics from the kinetic perspective. And that is its weakness, since the discretization of the PDF in the velocity space relies on its closeness to the equilibrium distribution with fixed fluid velocity and temperature.

This issue leads to the understanding that the LBM area of application is limited to low Mach number flows, and problems with very small temperature variations. The examples of such applications are melting and solidification of metals [11, 12], meteorology [13], biological fluid simulation [14], flows in porous media [15], particulate flows [16], automotive industry [17], computer graphics [18].

At the same time, the LBM is very attractive from the computational point of view. The computing cost is significantly less in comparison with the advanced methods of discretization of NSFE, and the method is easy to implement in a parallel program. The locality of the LBM stencil and the simplicity of the calculation in many widely-used variations of the method makes it an attractive platform for the development of the advanced algorithms [19–21], and HPC codes [22].

The latter property in particular raises the question if the method can be used in all parameter ranges of hydrodynamics problems.

Successful simulation of compressible flows are known from the earliest days of LBM existence [23]. Nowadays, there are two major ways to extend LBM capabilities to the compressible regime. One is to use more points in the velocity space to enable accurate integration of higher PDF moments [24–29]. To support high order moment tensor integration in 3D, the number of required points can be several times larger than that in the original LBM, which leads to the memory and performance limitations of the method. At the same time, the velocity and temperature ranges remain limited [30].

The second popular method family is known as DDF (Double Distribution Function) methods [31,32]. The second distribution function is used for higher order moments, for which the accurate computation would require large velocity sets. This way, smaller velocity sets are used for both distributions, but the data storage is doubled. Alternatively,