Burnett Order Stress and Spatially-Dependent Boundary Conditions for the Lattice Boltzmann Method

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Abstract. Stress boundary conditions for the lattice Boltzmann equation that are consistent to Burnett order are proposed and imposed using a moment-based method. The accuracy of the method with complicated spatially-dependent boundary conditions for stress and velocity is investigated using the regularized lid-driven cavity flow. The complete set of boundary conditions, which involve gradients evaluated at the boundaries, are implemented locally. A recently-derived collision operator with modified equilibria and velocity-dependent collision rates to reduce the defect in Galilean invariance is also investigated. Numerical results are in excellent agreement with existing benchmark data and exhibit second-order convergence. The lattice Boltzmann stress field is studied and shown to depart significantly from the Newtonian viscous stress when the ratio of Mach to Reynolds numbers is not negligibly small.

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1 Introduction

Since its initial developments [1–3], the lattice Boltzmann method (LBM) has become an established branch of computational fluid dynamics (CFD). Its foundations can appear to be conceptually different from traditional methods of CFD: rather than discretising continuum mass, momentum, and possibly constitutive equations directly, the LBM is derived from a velocity-space truncation of Boltzmann's equation for gases [4]. This kinetic formulation yields a linear, constant coefficient hyperbolic system of equations in which all nonlinearities are confined to algebraic source terms. The linear differential operators are discretised exactly by integrating along their characteristics and the governing equations of motion are recovered by seeking slowly varying solutions to the kinetic

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equation. The locality of the lattice Boltzmann algorithm gives it the opportunity to exploit massively parallel modern computer architectures, including graphics processing units (GPUs), leading to very fast computations [5].

The lattice Boltzmann equation converges with second-order accuracy in grid spacing to the solution of the discrete Boltzmann equation, which at fixed Mach and Reynolds numbers differ from the (weakly) compressible Navier-Stokes equations only by finite Mach number artefacts and $\mathcal{O}(Kn^2)$ contributions to the stress, where Kn is the Knudsen number [6–8]. By von-Karman's relation, $Kn \propto Ma/Re$. The finite Mach number errors in standard lattice Boltzmann models are of order $\mathcal{O}(Ma^3)$. They appear in the stress tensor and break Galilean invariance. They arise because the discrete Maxwellian equilibria are truncated at second-order in velocity and cannot be removed completely on the standard nearest neighbour integer lattices that are commonly in use (e.g D2Q9, D3Q15, D3Q19, or D3Q27 lattices). Hazi and Kavran [9] proposed adjusting the third order moment to restore Galilean invariance in axis-aligned shear flows but defects still existed in the diagonal components of the momentum flux tensor. Building on this, Dellar [10] showed that these defects can be eliminated when the LBM density is constant and reduced to $\mathcal{O}(Ma^5)$ otherwise if a collision operator with velocity-dependent relaxation times is used. A similar approach was proposed by Geier et al. [11] to reduce the defects under diffusive scaling by adjusting the equilibria in the cumulant lattice Boltzmann method.

Although usually neglected, the deviatoric stress that is naturally embedded in the LBM moment PDE system is governed by non-Newtonian constitutive equation that includes "Burnett order" contributions, as shown by Dellar [12]. Thus, computations of the stress with the LBM with large relaxation times can yield physically meaningful results that do not agree with the Navier-Stokes equations. This has implications for lattice Boltzmann methods for rarefied flow, the LBM at low Reynolds numbers, and the calculation of forces on bodies using the LBM (since the non-equilibrium contribution to the moment flux $\Pi_{\alpha\beta}^{(1)} = -\mu(\partial_{\alpha}u_{\beta} + \partial_{\beta}u_{\alpha}) + \mathcal{O}(\tau^2)$) and, as discussed in detail here, the implementation of boundary conditions. Imposing stress boundary conditions that are local, second-order accurate, and consistent with the moments of the truncated Boltzmann PDE is not easily achieved with most lattice Boltzmann implementations. Furthermore, the stress at a boundary may depend on the velocity in a non-trivial way and even constraints on the velocity field can be difficult to implement precisely with lattice Boltzmann when $\mathbf{u}_{wall} = \mathbf{u}_{wall}(\mathbf{x})$ is not constant.

At first, imposing boundary conditions on the lattice Boltzmann algorithm appears straightforward: one must supply values for the distributions f_i (see equation 2.1) on "incoming" characteristics pointing into the domain. The popular D2Q9 lattice (Fig. 2) has three unknown incoming distributions at boundaries aligned with grid points and lattice Boltzmann boundary conditions specify the values of these distribution functions in terms of those that are known. Incoming distributions at boundary nodes can be determined by a simple reversal in the particles' velocity; an approach known as "bounce-back". Some steady state solutions of the linearised (continuous) Boltzmann equation