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Introducing a variable speed of sound in single-component lattice Boltzmann simulations of isothermal fluid flows

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ABSTRACT

To simulate the hydrodynamics and mixing characteristics of chemical reactors by means of a lattice Boltzmann method (LBM), it is essential to consider components with varying molecular weights (and therefore speeds of sound). This option requires modification of the standard equilibrium distribution function and the use of an extended velocity set. In this paper, we show that, for isothermal incompressible single-component non-reactive flows, tuning the speed of sound with a modified equilibrium distribution and an extended velocity set allows for reproducing the proper flow characteristics with strongly reduced errors (compared to LBM simulations on standard lattices). This is done for two isothermal benchmarks, viz. a damped standing pressure wave and a decaying viscous Taylor–Green Vortex. The convergence as a function of the number of lattice nodes used improves substantially for varying values of the speed of sound.

1. Introduction

This paper reports on our results with respect to introducing, exploiting and assessing variable speeds of sound in isothermal lattice Boltzmann (LBM) flow simulations. Our wish to introduce variable speeds of sound stems from our interest in computationally simulating chemical reactors operated either in batch, semi-batch, or continuous flow modes. A rather unexplored aspect of simulating reactive flows by means of lattice Boltzmann methods (LBMs), however, relates to the differences in molecular mass that are typical of chemical reactions where mass is conserved but the number of moles and molecular mass vary between reactants and products [1,2]. One of the options for dealing with these variations in molecular mass is by means of a tunable speed of sound.

In LBM, the speed of sound c_s plays a major role although it is not a physically meaningful property of an incompressible fluid [3]. It figures predominantly in the Chapman–Enskog multi-scale analysis that relates the (discretized) Boltzmann equation to the macroscopic continuum description [4–6]. In the LBM approach, (partial) pressure, temperature and kinematic viscosity are all proportional to c_s^2, as in an ideal gas. In general, we have the isothermal sound speed $c_s^2 = \frac{RT}{M}$, where R is the universal gas constant, T is temperature, and M is the molecular mass. This follows from the ideal equation of state $p = \frac{\rho RT}{M}$ and $c_s^2 = \frac{\partial p}{\partial \rho}|_T$. In the standard isothermal LBM, the speed of sound is fixed and determined by the lattice. For certain applications, however, such as the chemical reactors of our interest, it is necessary to simulate components with different molecular masses and therefore different sound speeds. Specifically, we require a component σ to have different equations of state $p_\sigma = \frac{\rho_\sigma RT}{M_\sigma} = \rho_\sigma c_{s,\sigma}^2$ and the total pressure $p = \sum_\sigma p_\sigma$. For such systems, we must be able to tune the speeds of sound of the components while retaining a correct description of the hydrodynamics.

With eventual applications to flows in chemical reactors in mind, the purpose of this paper is to demonstrate the feasibility of retaining correct hydrodynamics while using a variable isothermal sound speed. The meso-scale LBM is known to be excellently capable of simultaneously dealing with thermodynamic, hydrodynamic and chemical phenomena and processes in a computationally efficient and elegant way. It is also known, however, that in non-isothermal flows satisfying the constraints posed by the thermohydrodynamic equations requires the extension of the LBM velocity set beyond the minimum number that is used in the standard isothermal LBM [7–10]. Since in the LBM the speed of sound is proportional to temperature, it is clear from these studies that also under isothermal conditions tuning the speed of sound, while

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not necessarily spatially or temporally variant, requires the use of lattices with additional velocities to retain correct hydrodynamics.

In this paper, we first show we must both modify the equilibrium distribution and use an extended velocity to allow a variable speed of sound. For our present purpose, simulations of a single component system are sufficient to demonstrate the ability to vary a component's speed of sound, while, compared to multi-component systems, such single-component simulations allow a more transparent analytical treatment (Chapman–Enskog), easier numerical implementation, and test cases with simpler boundary conditions compared to multi-component systems. Nonetheless, our eventual purpose is to exploit the combination of a tunable speed of sound, a modified equilibrium distribution and an extended velocity set for the purpose of simulating convective transport and mixing in both stirred and continuous-flow chemical reactors with multiple components. This application of the present work will be the topic of a future paper. Compressibility artifacts and acoustics topics are explicitly outside the scope of the present paper as they are irrelevant to the chemical reactors of interest and we consider only flows with low Mach numbers.

In general, to vary the speed of sound in isothermal LBMs, we can choose between two types of lattice implementations which may be denoted as off-lattice and on-lattice propagation schemes, respectively. Alternative methods have also been investigated, e.g. it was shown by Buick and Cosgrove [11] that a variable speed of sound may be introduced through a modified body force. However, within the scope of this work we will limit the discussion solely to lattice implementations.

For non-flowing systems, McCracken and Abraham [12] exploited both off-lattice and on-lattice schemes for simulating diffusive mass transfer in binary mixtures with varying molecular masses. Off-lattice schemes represent a multiple lattice approach where components, depending on their relative weights, travel only fractions of the lattice spacing in a lattice time step [12–14]. An off-lattice scheme was used by Arcidiacono et al. [13] to describe the behavior of several chemical species when simulating the oxidation of methane in a channel with catalytic walls. While physically sound, off-lattice schemes require computationally expensive interpolation steps and also complicate the boundary conditions required in many engineering applications.

Compared to off-lattice schemes, on-lattice schemes are more attractive since they require little modification in standard numerical codes and preserve the local nature of LBMs. The idea behind on-lattice propagation schemes is to manipulate the equilibrium moments in such a way as to properly recover the required hydrodynamic equations in the macroscopic limit.

Applied to standard velocity lattices, however, on-lattice schemes, as described in the literature [3,5,12,15–19] suffer from an inherent flaw as they do introduce unphysical error terms into the Navier–Stokes equation (see Section 2.2 and Appendix A). These error terms are the result of the limited number of velocities available in standard LBM lattices and render the scheme less accurate when applied to systems involving fluid flow. It can be shown that in 1D the error terms associated with varying the sound speed on standard LBM lattices take the form of a viscous stress and can be mitigated by rescaling the viscosity [3]. This, however, is not possible in higher dimensions, where a hydrodynamically correct modification of the sound speed requires a lattice with additional velocities.

Many of the above-cited researchers sticking to the standard velocity lattice were interested in acoustics and compressibility effects. For example, Alexander et al. [15] implemented fluid compressibility effects by modifying the equilibrium distribution without extending the velocity lattice. In spite of the resulting incorrect formulation of the hydrodynamics they used this approach while relaxing the low-Mach number restriction of the conventional LBM; this allowed them to simulate shock-wave formation through the viscous Burgers equation by using the LBM framework. As said, acoustics and compressible flows are beyond the scope of this paper.

To resolve the issue of the unphysical error terms in the Navier–Stokes equation, more velocity directions must be added to the LBM lattice. We refer to these lattices, with an extended velocity set, as "extended velocity lattices". To the best of our knowledge, only a few researchers used an extended velocity lattice with the view to tune the isothermal speed of sound in LBM [7,20]. Qian [7] proposed extended velocity sets along with modified equilibrium distributions for simulating 1D, 2D and 3D thermohydrodynamic cases – which can be simplified for isothermal conditions. In their paper on multiphase systems, Chai and Zhao [20] proposed a multiple-relaxation-time scheme to allow for the use of different speeds of sound for different components of different molecular mass. This effectively introduced a modified equilibrium distribution on a D2Q13 lattice, however this was done without further derivation or analysis. However, a general and systematic theoretical treatment and evaluation of the accuracy and applicability of a variable-speed-of-sound approach for isothermal single-phase flows has not yet been reported.

In the present paper, we will therefore first set the scene by showing once more that modifying the equilibrium distribution on a standard D1Q3 or D2Q9 lattice does not allow tuning of the speed of sound and that resolving this problem requires extending the velocity lattice, i.e. to D1Q5 or D2Q13. We will then introduce equilibrium distribution functions on these extended lattices in the BGK collision framework. While several early papers on (multi-component) LBM, such as [17], already mention the importance of a 'proper choice' of the equilibrium distribution in order to change the sound speed, most studies were conducted on standard velocity lattices and do not recover correct hydrodynamics.

We will investigate the accuracy of this novel approach for two canonical isothermal single-phase single-component flows and will find just marginal errors in the velocity and density fields. The novelty of our work is that we provide a systematic theoretical treatment, including a derivation that proves the necessity of using extended velocity lattices to extend the isothermal LBM sound speed and an evaluation of the accuracy and range of applicability of this approach. Furthermore, compared to Qian's as well as Chai and Zhao's papers, we use a different equilibrium distribution, and our validation focuses on flow field predictions while their validation focused on viscosities, (self-)diffusion coefficients and phase separation.

The remainder of this paper comprises of the following sections: Section 2 reviews the need for extended velocity lattices when changing the sound speed in isothermal LBMs. It also presents the newly proposed on-lattice propagation scheme using a modified equilibrium distribution. Then, the improved accuracy of our scheme is assessed with the help of two canonical cases of fluid flow; in Section 3, we compare numerical simulations with the analytical solution for the case of a viscously damped standing pressure wave, while in Section 4 we do the same for the Taylor–Green Vortex.

2. An alternative on-lattice propagation scheme

2.1. Conventional theory

The kinetic LBM equation which governs the evolution of a mass distribution function f_i is given by:

$$\frac{f_i(x_\alpha + e_{i,\alpha}\triangle t, t+\triangle t) - f_i(x_\alpha, t)}{\triangle t} = \Omega_i(x_\alpha, t) \tag{1}$$