Investigation of Galilean Invariance of multi-phase lattice Boltzmann methods

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Abstract

We examine the Galilean invariance of standard lattice Boltzmann methods for two-phase fluids. We show that the known Galilean invariant term that is cubic in the velocities, and is usually neglected, is the main source of Galilean invariance violations. We show that incorporating a correction term can improve the Galilean invariance of the method by up to an order of magnitude. Surprisingly incorporating this correction term can also noticeably increase the range of stability for multi-phase algorithms. We found that this is true for methods in which the non-ideality is incorporated by a forcing term as well as methods in which non-ideality is directly incorporated in a non-ideal pressure tensor.

Key words: Lattice Boltzmann, Liquid-Gas, Galilean invariance.

1 INTRODUCTION

The issue of Galilean invariance for lattice Boltzmann methods, and in particular for non-ideal fluid simulations based on an input pressure tensor[1], has received considerable attention in the past[2,3,4]. It was noticed that these methods had a severe problems with Galilean invariance and careful expansion methods elucidated a set of correction terms for the pressure tensor to improve Galilean invariance. The attraction of methods based on an input pressure tensor is that this pressure tensor can be easily derived from an input free energy. This immediately delivers predictions for the phase-diagram, the interface profiles and the surface tension.

Others held that the problem lay deeper, and that it was inappropriate to include the non-ideal terms for the method in an input pressure tensor, and that it is appropriate to put the non-ideal terms in a Vlasov-like forcing term[5,6]. Unfortunately, it has been difficult to relate the approach by Shan and Chen[5]
to a free energy. Meanwhile others have taken to use a forcing term that corresponds to the divergence of the pressure tensor[6]. This should, in principle, lead to an equivalent model to the pressure tensor approach. We will show later, that there are subtle differences though. On the up-side, using a forcing approach does not require similar correction terms to the pressure tensor approach, and therefore it has been labeled “Galilean invariant”.

Recently we have been working on including Lees-Edwards-like boundary conditions in lattice Boltzmann [9] to simulate sheared systems. It turns out that these boundary conditions are very sensitive to Galilean invariance violations. None of the above methods seemed to show a sufficient level of Galilean invariance which lead us to this closer investigation of the origins of Galilean invariance in lattice Boltzmann methods.

In a lattice based method the lattice represents a fixed reference frame, and it is not surprising that this should show up to some order. So we measured the error for a variety of situations and tried to quantify the main contribution. We found that the well known \( \nabla^2 (\rho u^3) \) term in the Taylor expansion of the momentum equations, which is usually neglected, is responsible for the majority of the error. We then demonstrate how including an additional correction term can significantly increase the Galilean invariance of lattice Boltzmann methods.

2 The lattice Boltzmann method

We can write the lattice Boltzmann method in a general way that neatly separates the ideal gas contributions from the non-ideal contributions. To do this we write

\[
f_i(r + v \Delta t, t + \Delta t) - f_i(r, t) = \frac{1}{\tau} (f_i^0(x, t) - f_i(x, t) + G_i) + F_i
\]

where \( f_i^0 \) is the contribution function for an ideal gas, the \( F_i \) are the contributions of a forcing term and the \( G_i \) allow us to manipulate the pressure tensor. As usual the moments for the ideal-gas distribution function are

\[
\sum_i f_i^0 = \rho, \quad \sum_i f_i^0 v_{i\alpha} = \rho \bar{u}_\alpha, \quad \sum_i f_i^0 v_{i\alpha} v_{i\beta} = c_s^2 \rho \delta_{\alpha\beta} + \rho \bar{u}_\alpha \bar{u}_\beta,
\]

\[
\sum_i f_i^0 v_{i\alpha} v_{i\beta} v_{i\gamma} = \frac{1}{3} \rho (\bar{u}_\alpha \delta_{\beta\gamma} + \bar{u}_\beta \delta_{\alpha\gamma} + \bar{u}_\gamma \delta_{\alpha\beta}) + \rho \bar{u}_\alpha \bar{u}_\beta \bar{u}_\gamma + Q_{\alpha\beta\gamma}
\]

where \( \rho = \sum_i f_i \) is the mass density, \( \bar{u} = \sum_i f_i v_i / \rho \) is the mean fluid velocity before the action of the forcing term \( F_i \). The velocity of sound is given by \( c_s = \)
1/\sqrt{3}. For all models with \( v_{i\alpha}^2 = 1 \) (like D1Q3, D2Q7, D2Q9, D3Q15, D3Q19 or D3Q27) we have \( v_{i\alpha}^3 = v_{i\alpha} \) which means that e.g. \( \sum_i f_i v_{i\alpha}^3 = \sum_i f_i v_{i\alpha} = \rho u_x \) making a correction term \( Q \) necessary for the third moment. One usually chooses \( Q_{\alpha\beta\gamma} = -\rho u_\alpha u_\beta u_\gamma \). It is this term that will lead to the leading Galilean invariance problems.

To simulate fluids with a non-ideal equation of state we can introduce either a forcing term \( F_i \) with the moments

\[
\sum_i F_i = 0, \quad \sum_i F_i v_{i\alpha} = \rho a_\alpha, \quad \sum_i F_i v_{i\alpha} u_{i\beta} = \rho (a_\alpha u_\beta + a_\beta u_\alpha),
\]

\[
\sum_i F_i v_{i\alpha} v_{i\beta} v_{i\gamma} = \frac{1}{3} (\rho a_\alpha \delta_{\beta\gamma} + \rho a_\beta \delta_{\alpha\gamma} + \rho a_\gamma \delta_{\alpha\beta})
\]

or a pressure term \( G_i \) with the moments

\[
\sum_i G_i = 0, \quad \sum_i G_i v_{i\alpha} = 0, \quad \sum_i G_i v_{i\alpha} u_{i\beta} = A_{\alpha\beta}, \quad \sum_i G_i v_{i\alpha} v_{i\beta} v_{i\gamma} = 0.
\]

Here \( \rho a_\alpha \) is a forcing term and \( A \) is a pressure term. We will see below how these terms can be used to introduce non-ideal terms into the equation of state or simply to correct the above mentioned deficiencies of the velocity set.

The knowledge of these moments is sufficient to perform a Taylor expansion (or equivalently a Chapman Enskog multi-scale expansion) of equation (1). If we define the macroscopic velocity \( u \) as \( u = \bar{u} + a/2 \) we obtain the continuity equation

\[
\partial_t \rho + \partial_\alpha (\rho u_\alpha) = 0
\]

and a momentum conservation equation

\[
\partial_i (\rho u_\alpha) + \partial_\beta (\rho u_\alpha u_\beta) = -\partial_\beta (\rho c_s^2 \delta_{\alpha\beta} + A_{\alpha\beta}) + \rho a_\alpha \\
+ \partial_\beta [\nu (\partial_\beta u_\alpha + \partial_\alpha u_\beta + \partial_\gamma u_{\alpha\beta})] \\
- \nu \partial_\beta [u_\alpha \partial_\gamma A_{\beta\gamma} + u_\beta \partial_\gamma A_{\alpha\gamma} + \partial_\rho A_{\alpha\beta} \partial_\gamma (\rho u_\gamma) + \partial_\gamma Q_{\alpha\beta\gamma}]
\]

where the kinematic viscosity is \( \nu = (\tau - 1/2) c_s^2 \). This equation is the Navier-Stokes equation, except for the terms in the last line. The condition of Galilean invariance requires that a description in a reference frame \( S \) another reference frame \( S' \) translating with a constant velocity \( u_0 \) be related by a spatial coordinate transformation \( x = x' - u_0 t \) and a translation of velocities \( u = u' - u_0 \).

It is easy to see that only the terms in the last line of eqn. (3) are not Galilean invariant.
Let us first consider (3) for an ideal gas. In this case $a = 0$ and $A = 0$ so the only non-Galilean invariant term to second order is $Q$. We can eliminate this error term by introducing a well crafted forcing term of the form

$$\rho a_\alpha = \nu \partial_\beta \partial_\gamma Q_{\alpha\beta\gamma}$$

(4)

We should mention here that we can avoid this problem and choose $Q = 0$ if we use a velocity set that is large enough[7]. But for now we want to stay with the standard velocity sets.

To simulate a non-ideal system we want to obtain a pressure term in the first line of (3) that is the divergence of a pressure tensor derived from Thermodynamics. In particular we need

$$\partial_\beta P_{\alpha\beta} = \partial_\beta (c_s^2 \rho \delta_{\alpha\beta} + A_{\alpha\beta}) + \rho a_\alpha$$

(5)

to first order. For the forcing approach we choose $A = 0$ and this equation defines $a$. We will refer to this approach as “Forcing” in our comparisons. To improve Galilean invariance for this approach we can add the same additional forcing term (4) to restore Galilean invariance to second order. This approach we will refer to as “ForcingQ”.

If we chose to introduce the non-ideal term in $A$ we can recover the algorithm of Swift et al.[1]. This corresponds to choosing $A_{\alpha\beta} = P_{\alpha\beta} - \rho c_s^2$ and $a = 0$. We refer to this approach in the following as “Pressure”.

This approach is deficient in as much as the correction terms in the third line in (3) are unphysical and will lead to severely non-Galilean invariant behavior. This problem was addressed by Holdych et al.[2] and independently by Inamuro et al.[3]. Because the divergence of the pressure tensor is small to first order, the main contribution to the error terms comes from the density alone. Therefore choosing

$$A_{\alpha\beta} = P_{\alpha\beta} - \rho c_s^2 \rho \delta_{\alpha\beta} - \nu (\partial_\alpha \rho u_\beta + \partial_\beta \rho u_\alpha + \partial_\gamma \rho u_\gamma)$$

(6)

will only leave error terms of the order $\partial^2 P$ which can be assumed to be small in systems close to equilibrium. This approach will be referred to as “Holdych”. The restriction of being close to equilibrium was late revisited by Kalarakis et al.[4] who suggested an improvement to these corrections.

However, the Holdych approach as well as all other later approaches are still deficient in that they do not correct the Q term. Clearly there is a multitude of possible combinations of choices for $A$ and $a$ that will lead to a Galilean invariant form of eqn. (3). One other choice we examined is
\[ A_{\alpha\beta} = P_{\alpha\beta} - \rho c_s^2, \]
\[ a_\alpha = -\partial_\beta \{ \nu \partial_\gamma [u_\alpha (P_{\beta\gamma} - \rho c_s^2 \delta_{\beta\gamma}) + u_\beta (A_{\alpha\gamma} - \rho c_s^2 \delta_{\alpha\gamma}) + (\partial_\rho A_{\alpha\beta} - c_s^2 \delta_{\alpha\beta}) \partial_\gamma (\rho u_\gamma)] \}. \]

which has in common with the Kalarakis\cite{4} approach that it is not limited to systems close to equilibrium. The above choice leads to a Galilean invariant momentum equation given by

\[ \partial_t (\rho u_\alpha) + \partial_\beta (\rho u_\alpha u_\beta) = -\partial_\beta (\rho c_s^2 \delta_{\alpha\beta} + A_{\alpha\beta}) + \rho a_\alpha \\
+ \partial_\beta [\nu (P_{\beta\gamma} \partial_\gamma u_\alpha + P_{\alpha\gamma} \partial_\gamma u_\beta + P_{\alpha\beta} \partial_\gamma u_\gamma)] \tag{7} \]

This scheme has a tensorial interface viscosity. We refer to the resulting method as “PressureQ”.  

3 The non-ideal gas

For simplicity we will consider a non-ideal gas with a $\phi^4$-free energy\cite{8}. For such a system we can calculate the phase diagram and the surface tension analytically, simplifying the analysis.

For a critical density $\rho_c$, critical temperature $T_c$ and critical pressure $p_c$ we obtain for the pressure tensor

\[ P_{\alpha\beta} = [p_c(\phi + 1)^2 (3\phi^2 - 2\phi + 1 + 2\theta) - \kappa \rho \nabla^2 \rho - \frac{\kappa}{2} (\nabla \rho)^2] \delta_{\alpha\beta} + \kappa \partial_\alpha \rho \partial_\beta \rho \tag{8} \]

where $\phi = (\rho - \rho_c)/\rho_c$ is the reduced density and $\theta = \beta (T - T_c)/T_c$ is the reduced temperature, where $\beta$ is an arbitrary constant. The equilibrium values for the density are given by

\[ \rho^0 = \rho_c \pm \sqrt{-\theta}. \tag{9} \]

The definition of the pressure tensor is all that is needed to define the lattice Boltzmann methods for non-ideal fluids as we explained in section 2.

We performed simulations of an equilibrium system containing one domain of gas and one of liquid at different imposed velocities. As mentioned above, while the different approaches are very similar as far as the expansion to second order is concerned, there are noticeable differences in the behavior of the methods. Firstly let us compare the numerical results for the phase-diagram shown in Figure 1. On the one hand we notice that the ability of the pressure based methods to reproduce the analytical phase-diagram is noticeably better than the corresponding forcing method. On the other hand we we see that the range
Fig. 1. Phase diagram for $p_c=0.1$, $\kappa = 0.1$, $n_c = 1$, $p_c = 0.1$ and $\nu = 1/6$ for the “ForcingQ” and “Holdych” approaches. Note that the Holdych approach is better at reproducing the analytical phase diagram where as the ForcingQ approach has a larger range of stability.

Fig. 2. Deviation from the analytical density difference for the different methods as a function of $u_0$. $\kappa = 0.1$, $n_c = 1.0$, $p_c = 0.42$, $\beta = 0.1$, $\theta = -0.03$ and $\nu = 1/6$. The data end at values of $u_0$ at which the methods became unstable.

Next we examine the effect of an imposed velocity on the equilibrium densities. In Figure 2 we show the deviation of the predicted liquid-gas density difference from the measured one. We notice that the original pressure method has excessive deviations even for small $u_0$. We were surprised to see that in these simulations the gas and liquid domains were actually stationary, even with an imposed velocity $u_0$. The domains made up for the imposed velocity by evaporation and condensation mechanisms and a faster velocity in the gas than in the fluid. We see that the error is generally less for the corrected pressure methods than for the forcing methods.

We were very surprised to see that the $Q$ corrections did not only improve that Galilean invariance of the method, they substantially increased the range of stability. This is true both for the range of stable velocities $u_0$ as well as the accessible density ratios (even at $u_0 = 0$. This was an unexpected benefit
of our study and we still do not understand why the correction term has such beneficial effects on the stability.

We now need to quantify the Galilean invariance error for the advection of an interface profile. For the velocity the analytical solution is a constant, so we can define an error function

$$E_D(u_0) = \sqrt{\sum_x (u(x) - u_0)^2 / L_x.}$$  (10)

This measure is effectively time independent, as is appropriate for this equilibrium consideration.

In Figure 3 we show the Galilean invariance error $E_D(u_0)$ for the different methods we described. As mentioned above the original pressure approach performs very poorly, in fact refusing to advect the domains relative to the lattice. The Holdych approach improves on this significantly leading to an advection of the profile. We were surprised by the non-monotonic behavior of the error, leading to a minimum at $u_0 = 0.2$. We will come back to this later. Adding the $Q$ correction to the Holdych approach leads to a noticeable improvement for velocities as small as $u_0 = 10^{-3}$. The Forcing approach leads to a good behavior at small $u_0$ but increases rapidly with $u_0$. Its behavior is significantly improved for $u_0 > 0.03$ by including the $Q$ correction in the in the method.

When interpreting the above results, it is important to remember that the parameter space for the Galilean invariance problem includes not only $u_0$ but also the parameters determining the equilibrium density profile $\kappa$, $\theta$ and $p_c$ as well as the relaxation time $\tau$. This parameter space is so large as to make it nearly impossible to examine it exhaustively. But we want to discuss at least the dependence on $\kappa$, which is related to the interface width and the surface tension. It is also important to look at this when one wants to
fairly compare the pressure and forcing approaches. It turns out that while the pressure approach reproduces the analytical interface profile fairly, the forcing approach does not, at least not for the nominal value of $\kappa$. The forcing approach leads to a much wider interface so that it would be fairer to compare the forcing approach to a pressure approach with a larger $\kappa$. In Figure 4 we can see that this matters a lot. The Galilean invariance error $E_D$ is largest for small values of $\kappa$ corresponding to thin interfaces. And for small values of $\kappa$ this absolute error decreases much slower with decreasing $u_0$. This is probably the reason that the pressure approach performed much worse than the forcing approach (with the same nominal $\kappa$ value) for small $u_0$.

A close examination of Fig 4 also shows that the non-monotonic behavior of $E_D(u_0)$ is related to the small $\kappa$ behavior. The graph suggests that the error function becomes monotonic for large $\kappa$.

4 Summary

We have shown that the usually neglected error term in the Navier Stokes level momentum equation derived for standard lattice Boltzmann methods leads to noticeable Galilean invariance violations. These violations are noticeable even in the range of usual velocities of $u < 0.1$, but become dominant for larger velocities.

A carefully defined forcing term can remove the non-Galilean invariant terms recovering the Navier Stokes equation. We have shown that this approach is also effective in practice, reducing the Galilean invariance error substantially. The correction term also had the added benefit of increasing the range of stability for the multi-phase applications, leading to a larger range of stable velocities and even, perhaps surprisingly, to a larger range of density ratios that can be simulated by the methods.
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