

Grad's approximation for missing data in lattice Boltzmann simulations

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Abstract. – Engineering applications of computational fluid dynamics typically require specification of the boundary conditions at the inlet and at the outlet. This issue remains unresolved for kinetic-theory based approaches such as the lattice Boltzmann method. Empirically it is known that the accuracy and stability of simulations is greatly influenced by the boundary conditions even at moderate Reynolds numbers. In this paper, we derive a novel outflow boundary condition for the lattice Boltzmann simulations from non-equilibrium thermodynamics and Grad's moment closure. The proposed boundary condition is validated with a three-dimensional simulation of flow over a backward facing step. Results demonstrate that the new outlet condition significantly extends simulation capacity of the lattice Boltzmann method.

In recent years, the lattice Boltzmann method (LBM) [1–4] has drawn considerable attention as an efficient simulation method for complex flows. The essence of LBM, as inherited from its predecessor, the lattice gas automata [5], is a simple stream-and-collide dynamics on a lattice. The links of the lattice are discrete velocities while the dynamic variables are populations of the links. Although the field of applications of LBM has increased considerably, there remain outstanding issues (stability, boundary conditions, grid-refinement etc) which so far hindered a wider acceptance of LBM for computational fluid dynamics applications. One of these issues, namely numerical stability of simulations of flows at large Reynolds numbers, has been solved in the framework of the entropic formulation of LBM [4, 6, 7]. This solution was essentially based on the choice of time step that does not violate the entropy growth condition (a physically relevant condition prescribed by the second law of thermodynamics). Furthermore, the boundary conditions at solid walls were derived from the continuous kinetic theory [8]. However, other major difficulties that are not related to the sub-grid instability at high Reynolds numbers, still persist. Such difficulties are here referred to as “missing data”, and are typical in situations where off-lattice structures are present (open boundary conditions, curved solid wall boundaries, grid refinement etc.). It is common to these problems that populations of the links at certain nodes become unavailable. It is best to illustrate this with an example.

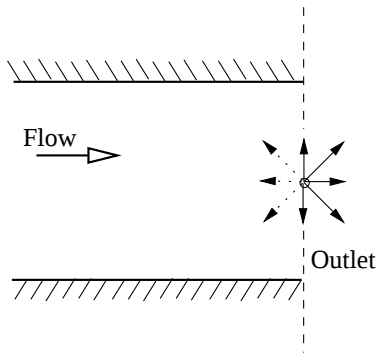


Fig. 1 – Situation at the outlet node. Data is missing for the populations of the velocities pointing into the fluid (dash).

A typical problem of this kind is the specification of the outlet boundary condition in duct-like flows with large aspect ratio. Such flows are most common in engineering and medical applications such as wind tunnels, blood vesicles etc. In Fig. 1, we show a situation at the outlet node. Since there are no lattice nodes beyond the outlet, populations of the three discrete velocities pointing into the fluid are not known and need to be fixed by additional considerations. At present, there is no established way to cope with this problem. Because specification of pressure at the outlet has no significance in long pipes, one relies on interpolation schemes (see, e.g. [9]) lacking physical intuitions. Interpolation often becomes a major source of inaccuracy in the simulations.

In this paper we derive and implement a new outlet boundary condition for the lattice Boltzmann simulations. Our construction is based on the idea of a low-dimensional submanifold in the space of populations which contains most of the dynamics (slow invariant manifold [10]). The main assumption is that this manifold is well approximated by (an analog of) Grad's distribution functions used in the kinetic theory of gases. The Grad distribution is used for extrapolating the missing populations with the resulting outlet condition being local in space, and is thus easy to implement. We report a three-dimensional lattice Boltzmann flow simulation over a step (so-called backwards facing step problem) with this new outlet boundary condition. This setup is a stringent test for the lattice Boltzmann method because of the problems at the outlet. Present results are found to be in good agreement with spectral method and experimental data over a range of Reynolds numbers. This extends the domain of lattice Boltzmann simulations by approximately an order of magnitude.

The structure of the paper is as follows: First the derivation of the lattice Boltzmann equation is revisited. Then we present the Grad approximation pertinent to the discrete-time kinetics before giving details of the outlet boundary condition. Finally, we present the backward-facing step simulation and compare the results with other computational and experimental data.

We consider the simplest setting of the lattice Boltzmann equation. Let $\mathbf{c}_i$ be the links of a regular lattice, $i = 1, \dots, n_d$, and the populations $f_i(\mathbf{x}, t)$ at the location $\mathbf{x}$ and time t obey the kinetic equation,

$$\partial_t f_i + c_{i\alpha} \partial_\alpha f_i = Q_i, \quad (1)$$

where $\partial_t = \partial/\partial t$ and $\partial_\alpha = \partial/\partial x_\alpha$ are dimensionless time and space derivatives, summation convention is assumed, and the relaxation term is in the Bhatnagar-Gross-Krook (BGK) form [11],

$$Q_i = -\frac{1}{\tau}(f_i - f_i^{\text{eq}}(\rho, \mathbf{j})). \quad (2)$$

Here $\tau > 0$ is the dimensionless relaxation time, and the equilibrium $f_i^{\text{eq}}(\rho, \mathbf{j})$ is a function of the locally conserved fields (density ρ and momentum $\mathbf{j}$), tailored in such a way as to reconstruct the Navier-Stokes equation in the hydrodynamic limit of the model (1) when $\tau \rightarrow 0$. Below we use a specific three-dimensional velocity set with $n_d = 15$ (so-called D3Q15 model [2]), with

$$f_i^{\text{eq}}(\rho, \mathbf{j}) = W_i \left[\rho + \frac{j_\alpha c_{i\alpha}}{c_s^2} + \frac{1}{2c_s^4} j_\alpha j_\beta (c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta}) \right]. \quad (3)$$

Here $W_i > 0$ are weights specified for the given velocity set, and $c_s = 1/\sqrt{3}$ is the speed of sound. Kinematic viscosity in the Navier-Stokes recovered in the limit $\tau \ll 1$ is $\nu = \tau \rho c_s^2$. Note that equilibrium (3) is the approximate (accurate to the order j^2) solution to the conditional minimization problem of the entropy function H ,

$$H = \sum_{i=1}^{n_d} f_i \ln \left(\frac{f_i}{W_i} \right) \rightarrow \min, \quad \sum_{i=1}^{n_d} \{1, \mathbf{c}_i\} f_i^{\text{eq}} = \{\rho, \mathbf{j}\}. \quad (4)$$

The lattice Boltzmann method [1–4] is the second-order accurate implicit scheme for the kinetic equation (1). Let us recall the derivation here. After integrating (1) over the time δt , and applying trapezoidal rule in order to evaluate the collision term (second-order accuracy in δt), we get

$$f_i(\mathbf{x} + \mathbf{c}_i \delta t, t + \delta t) - f_i(\mathbf{x}, t) = \frac{\delta t}{2} (Q_i(f(\mathbf{x}, t) + Q_i(f(\mathbf{x} + \mathbf{c}_i \delta t, t + \delta t))) + \text{Err}(\delta t)), \quad (5)$$

where the error term comes from the evaluation of the collision integral, and is of the order,

$$\text{Err}(\delta t) \sim \frac{1}{\tau} \delta t^3. \quad (6)$$

Using in (5) the map,

$$f_i \rightarrow g_i = f_i - \frac{\delta t}{2} Q_i(f), \quad (7)$$

we derive the discrete-time scheme for (1):

$$g_i(\mathbf{x} + \mathbf{c}_i \delta t, t + \delta t) = g_i(\mathbf{x}, t) + \frac{2\delta t}{2\tau + \delta t} \left[g_i^{\text{eq}}(\mathbf{x}, t) - g_i(\mathbf{x}, t) \right]. \quad (8)$$

Furthermore, fixing the grid points in such a way that if $\mathbf{x}$ is a grid point then also $\mathbf{x} \pm \mathbf{c}_i \delta t$ are the grid points, equation (8) becomes the lattice Bhatnagar-Gross-Krook scheme (LBGK). Note that the implicit second-order scheme for the populations f_i (8) can be interpreted as the explicit first-order scheme for the variables g_i (7) obtained from a kinetic equation of the form (1) with a renormalized relaxation time $\tau' = \tau + (\delta t)/2$ ⁽¹⁾.

⁽¹⁾We note in passing that a nonlinearly stable entropic version of the scheme (8) can be written for the populations f_i rather than for the functions g_i , where the factor $(2\delta t)/(2\tau + \delta t)$ is replaced with $(\alpha \delta t)/(2\tau + \delta t)$, and α is the solution to the entropy estimate, $H(f) = H(f + \alpha Q)$, with $\alpha \rightarrow 2$ in the hydrodynamic limit (see, e. g. Eq. (9) in Ref. [4].)

One simple but important implication of this derivation of the lattice Boltzmann scheme from the kinetic equation (1) deserves to be mentioned. Since the kinetic equation is singularly perturbed ($\tau \ll 1$), the error term gives vanishing contribution to the hydrodynamic (Navier-Stokes) equations if $\text{Err}(\delta t) \sim 1$, that is, $\delta t \lesssim \tau^{1/3}$. Using the standard relation $\text{Re} = \text{Ma}/\text{Kn}$, where Re , Ma and Kn are Reynolds, Mach and Knudsen numbers, this estimate can be recast into a grid resolution requirement. Indeed, since $\text{Kn} \sim \tau$, and $\delta t \sim \delta x \sim N^{-1}$, where $N = L/\delta x$ is the number of grid points along the characteristic length L in the definition of Reynolds number $\text{Re} = UL/\nu$, we find that the error terms do not spoil the Navier-Stokes equation on the time step of the order of δt if $\text{Re} \lesssim N^3 \text{Ma}$. Finally, the Navier-Stokes equation is resolved on the flow time scale $T \sim N\delta t$ if

$$\text{Re} \lesssim N^2 \text{Ma}. \quad (9)$$

For a fixed number of grid points N , (9) estimates the order of magnitude of the Reynolds number up to which the simulation is resolved (that is, the second-order scheme (8) reconstructs the Navier-Stokes equations exactly). The resolution estimate (9) is pertinent to the kinetic scheme, and is flow-independent. It should not be confused with other (flow-dependent) definitions of resolution in computational fluid dynamics, for example, with those based on a characteristic length of fully developed turbulent flows (Kolmogorov's length scale). The estimate (9) simply tells whether the scheme (8) reconstructs the Navier-Stokes equations, or the reconstructed hydrodynamic equations have a feature of a sub-grid model (the sub-grid correction to the Navier-Stokes equation was derived from similar considerations in [12]).

Coming back to the continuous kinetic equation (1), we introduce (an analog of) Grad's moment approximation for the populations. We remind that the classical Grad's distribution functions [13] were obtained as a truncated expansion in Hermite velocity polynomials of the distribution function around the local Maxwellian. Grad's distributions are parameterized by the values of *relevant* moments which include, besides the locally conserved fields, also those which are supposed to vary slower than the rest. These are the stress tensor and the energy flux in the original setting of Grad. Later studies revealed important relations of Grad's distributions to quasi-equilibrium (or maximum entropy) approximations, and suggested extensions for various other macroscopic variables (not obligatory moments) [10,14]. In the context of the lattice Boltzmann method, the Grad approximation was discussed in [3,8]. In the athermal case under consideration, we choose the relevant variables as the locally conserved fields, ρ and $\mathbf{j}$, and the pressure tensor $P_{\alpha\beta}$,

$$P_{\alpha\beta} = \sum_{i=1}^{n_d} f_i c_{i\alpha} c_{i\beta}. \quad (10)$$

Grad's approximation for the populations can be derived by standard techniques (see, e. g. [10,14]), and we write here the final result:

$$f_i^*(\rho, \mathbf{j}, P_{\alpha\beta}) = W_i \left[\rho + \frac{j_\alpha c_{i\alpha}}{c_s^2} + \frac{1}{2c_s^4} (P_{\alpha\beta} - \delta_{\alpha\beta} \rho c_s^2) (c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta}) \right]. \quad (11)$$

Grad's (non-equilibrium) populations (11) span a sub-manifold in the phase space of the kinetic equation (1), parameterized by the values of the density, momentum and pressure tensor.

Finally, in order to use the Grad approximation within the second-order scheme (8), populations (11) should be interpreted with the transform (7):

$$g_i^* = f_i^* - \frac{\delta t}{2} Q_i(f^*). \quad (12)$$

The main assumption in using Grad's approximations is that the sub-manifold (12) approximates well the slow manifold of the dynamic system (8). While in most of the cases of applications of Grad's approximation this indeed remains an assumption, for some lattice Boltzmann models, this was recently verified affirmatively in a simulation of the lid-driven cavity flow [15].

With this assumption, we impose the outlet condition (see Fig. 1) by the following rule: On the time step $n + 1$, the populations of the links at the outlet pointing into the fluid are assigned the values (12), whereas the values of the moments ρ , $\mathbf{j}$, and $P_{\alpha\beta}$ are taken from the previous time step n at the same nodes. Initially, all links are at equilibrium.

The three-dimensional backwards-facing step flow was used to validate the outlet boundary condition. The standard $D3Q15$ lattice Boltzmann model with the polynomial equilibrium (3) was used. Geometry of the setup was chosen in such a way as to mimic the experiment of Armaly et al [16]: The channel length (X) was $20S$, where S is the step height, the channel width (Y) was $2S$. The step height was $S = 10$ (lattice units), the step length was $2S$. The ratio of the span width (Z) to the step height was equal $36 : 1$ (that is, the span width was $36S$ lattice units). The total number of grid points was about 1.5×10^6 . Kinetic boundary conditions [8] were applied on the wall nodes. The inflow was a fully developed velocity profile in a duct flow (simulated separately in the duct with the dimension $15S \times S \times 36S$). The inflow velocity maximum ranged between 10^{-2} to 4×10^{-2} while the kinematic viscosity was fixed at $\nu = 10^{-3}$. The outlet condition (12), (11) was applied both in the backwards-facing step channel and in the auxiliary duct simulations. All simulations were done on a single-processor facility (PC), a single run time ranged between one to several hours depending on the Reynolds number, $Re = (2US)/\nu$, where U is cross-section averaged inlet velocity. According to (9), the kinetically resolved maximal Reynolds number is $Re_{\max} \sim 10$.

Before reporting the results, we need to admit that, for example, the same three-dimensional lattice Boltzmann model with the outlet boundary conditions based on a simple second-order interpolation formula for the missing populations (see, e. g. [9]) failed at Reynolds number $Re < 50$. The reason for such a poor performance, as we mentioned it already, is the errors which start at the outlet and propagate upstream.

The range of Reynolds number covered in our simulation with the new outlet was $100 < Re < 392$ (that is, essentially in the unresolved regime in the sense of (9), which is typical of most of the lattice Boltzmann simulations). In Fig. 2, snapshots of the velocity on the mid-plane at $Re = 270$ are shown in the full computation domain, including the outlet. It is visible in Fig. 2 that the velocity profile stays smooth during the whole simulation. In Fig. 3, the primary flow reattachment length (the distance at which the velocity field on the bottom wall becomes directed towards the outlet) is compared with the results of the simulations of the incompressible Navier-Stokes equation by various numerical techniques [17, 18], with the recent two-dimensional lattice Boltzmann simulation on a non-uniform grid [9], as well as with the experimental data of Armaly et al [16], and was found to be in excellent agreement. We stress that the accuracy and stability achieved with the new outlet boundary condition allowed to use a small step size of only ten grid points, much less than it would be required with different boundary conditions.

In conclusion, we have derived a new outlet condition for lattice Boltzmann simulations of hydrodynamic problems. The derivation is based on the physically intuitive picture that

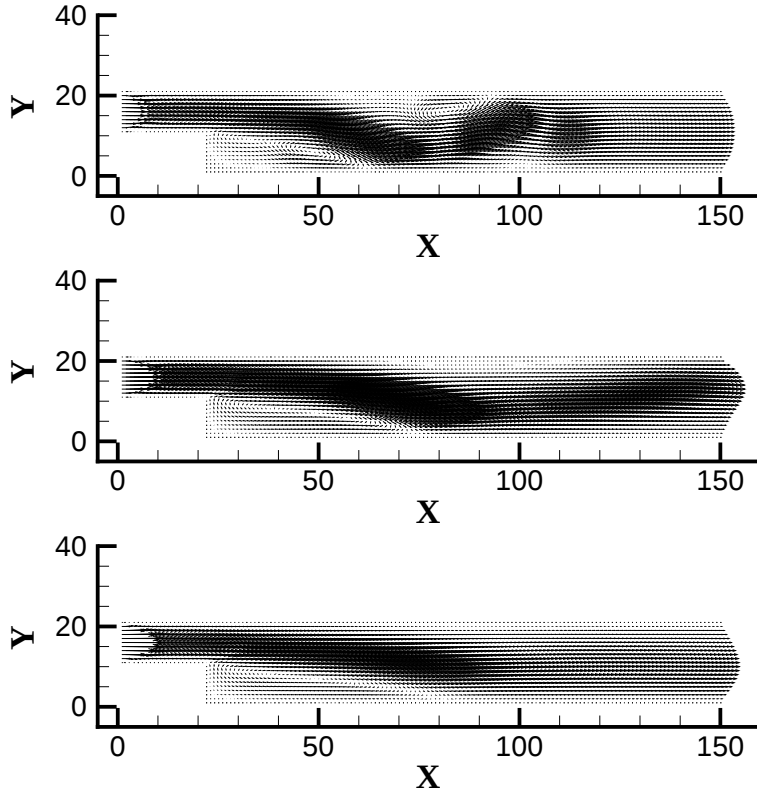


Fig. 2 – Snapshots of the velocity field on the mid-plane at $Re = 270$ at 9×10^3 , 18×10^3 , and 40×10^3 time steps in lattice units (from top to bottom).

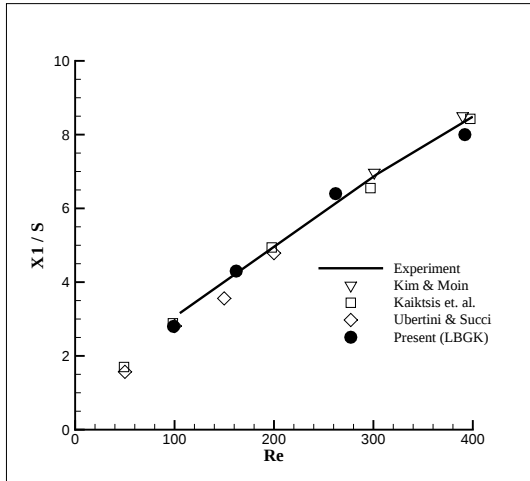


Fig. 3 – Primary reattachment length X_1 normalized by the step height S . Comparison of the present simulation with the experiment of Armaly et al [16], and simulations of Kaiktsis et al [17], Kim and Moin [18], and Ubertini and Succi [9].

Grad's approximation contains most of the dynamics of the kinetic model. The outlet condition was verified in the three-dimensional simulation of the benchmark problem, and clearly outperformed other suggestions in terms of stability and accuracy. Similar considerations should be applicable in a variety of other problems where one faces off-grid structures such as grid refinement and curved boundary. IVK was supported by the BFE-Project Nr. 100862.

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