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Hydrostatic Boundary Conditions for Lattice Boltzmann Methods

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Abstract

Lattice Boltzmann Methods (LBMs) have been under development for the last two decades and have become another capable numerical method for simulating fluid flow. Recent advances in lattice Boltzmann applications involve simulation of density-dependent fluid flow in closed (Dixit and Babu, 2006) or periodic (Guo and Zhao, 2005) domains. However, standard pressure boundary conditions (BCs) are incompatible with concentration-dependent density flow simulations that use a body force for gravity. An implementation of hydrostatic BCs for use under these conditions is proposed here. The basis of this new implementation is an additional term in the pressure BC. It is derived to account for the incorporation of gravity as a body force and the effect of varying concentration in the fluid. The new hydrostatic BC expands the potential of density-dependent LBM to simulate domains with boundaries other than the closed or periodic boundaries that have appeared in previous literature. With this new implementation, LBM will be able to simulate more complex concentration-dependent density flows, such as salt water intrusion in the classic Henry and Henry-Hilleke thermohaline problems. These new BCs are demonstrated using various examples, beginning with a closed box system, and ending with a system containing two solid walls and two pressure boundaries.

Introduction

LBM is a capable modeling method that can be used to carry out fluid simulations. It is based on the particle distribution function inherent in the Boltzmann equation. Calculations at the microscopic level use discrete velocity directions and time that are upscaled to recover a fluid's macroscopic properties and velocity, which are solutions to the Navier-Stokes equations. LBM has the ability to simulate both multicomponent and multiphase systems (Sukop and Thorne, 2006).

Considerable current LBM research addresses buoyancy and convection simulations. Although many attempts have already been successful, all have been in simplistic domains such as closed (Dixit and Babu, 2006) or periodic domains (Guo and Zhao, 2005) that do not employ non-trivial BCs. Common buoyancy benchmark problems like the thermohaline Henry-Hilleke problem require hydrostatic pressure boundaries. To date hydrostatic pressure boundaries have not been implemented for LBMs that use a body force for gravity (see methods). During an effort to model the thermohaline Henry-Hilleke problem, such hydrostatic pressure BCs were developed. These BCs make simulations of non-trivial domains possible.

Method

To implement a hydrostatic BC in LBM it is essential to understand how a stationary fluid equilibrates under a gravitational body force using a periodic boundary. A periodic boundary implies that the domain is infinitely repeated. When a body force is applied, the actual fluid velocity is calculated by averaging the velocity from before the collision step with the velocity from after the collision step (Shan, 2006). Thus, when gravity is applied in a domain that must equilibrate to a stationary fluid, the vertical velocity before the collision step must be equal and opposite to the vertical velocity after the collision step. This must be manually enforced in the BCs since they are computed immediately before the collision step.

Method Continued

In order to enforce the hydrostatic pressure gradient on the boundary, we assume the fluid is incompressible, since our LBM inherently assumes fluid compressibility, this is achieved by keeping gravity, a body force, small. The smaller gravity, the less compressibility. Thus the familiar expression for pressure difference results:

$$\Delta P = \rho g h$$

The lattice Boltzmann equation of state (EOS) is:

$$P = \frac{\rho}{3}$$

Thus:

$$\frac{\partial \rho}{\partial h} = 3\rho g$$

The above equation holds for all simulations that are limited to one fluid. However, for buoyancy simulations, the density of the second component, whether it be a solute or heat, must be considered. This is done by simply adding another term to density in the equation above:

$$\frac{\partial \rho}{\partial C}(C - C_0)\rho$$

where C is the concentration and C_0 is the reference concentration. Thus the complete pressure gradient becomes:

$$\frac{dP}{dh} = \rho\left(1 + \frac{\partial \rho}{\partial C}(C - C_0)\right)g$$

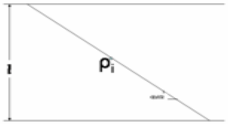
This can be written in terms of density by a simple substitution of the EOS:

$$\frac{\partial \rho}{\partial h} = 3\rho\left(1 + \frac{\partial \rho}{\partial C}(C - C_0)\right)g$$

While the equation above is an important result, it does have limitations. The most prominent is that the density of a system can not fall below zero. Thus

$$\rho_i - \frac{d\rho}{dz}\left(\frac{l - i}{2}\right) > 0$$

must be true, where l represents the height of the domain, and ρ_i represents the density in the middle of the domain.



A sample domain showing the derivation of the equation below

With some simplistic rearrangement, we obtain a form that can easily be implemented into LBM:

$$\frac{d\rho}{dx} < \frac{2}{l - 1}\rho_i$$

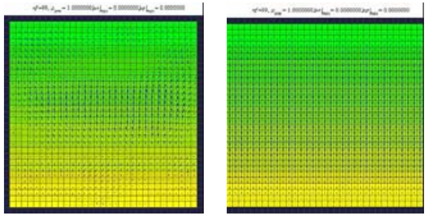
The implementation of the new hydrostatic BC must be applied to the distribution function. For a D2Q9 grid the implementation appears on an East boundary as:

$$f_6 = f_8 - \frac{1}{2}(f_4 - f_2) - \frac{1}{6}\rho_o v + \left(\frac{1}{2}\right)\left(-\frac{1}{2}\right)g\left(\rho_0 + \frac{\partial \rho}{\partial C}(C - C_0)\right)$$

This is an extension of Zou and He's BCs (Zou and He, 1997). North, South and West boundaries can be derived in a similar manner.

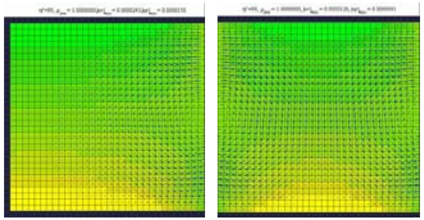
Results

In a closed cavity and a periodic cavity the fluids are naturally hydrostatic without the application of non-trivial BCs. There are residual velocity values with a magnitude of 10^{-16}lu/ts that can be dismissed as numerical noise.



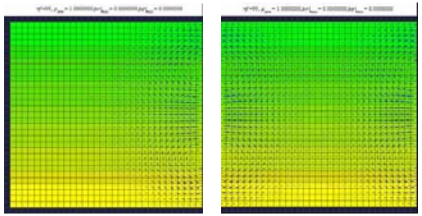
A closed cavity (left) and a periodic cavity (right) showing residual velocity fields with magnitudes of 10^{-16}lu/ts

The problem with buoyancy and convection arises when the walls or periodic boundary conditions are replaced by hydrostatic pressure boundaries. When this occurs, the velocities increase to magnitudes of 10^{-5}lu/ts, and can no longer be dismissed as numerical noise. Thus, it becomes clear that another condition must be implemented.



A cavity with three walls and one hydrostatic pressure boundary (left) and a cavity with two walls and two hydrostatic pressure boundaries (right) showing velocity fields with magnitudes of 10^{-5}lu/ts, indicating the need for the new hydrostatic BC

With implementation of the new hydrostatic BC in LBM the velocities drop to 10^{-11}lu/ts, which is much improved from the previous results of 10^{-5}lu/ts.



A cavity with three walls and a hydrostatic pressure boundary (left) and a cavity with two walls and two hydrostatic pressure boundaries (right) showing residual velocity fields with magnitudes of 10^{-11}lu/ts, proving the importance of the new hydrostatic BC

Results Continued

A number of simulations were carried out. Each contained two components, the main fluid and a solute, and employed varying BCs. Domains with a closed box, and a periodic box gave the same low velocity results seen in previous literature. Most importantly, a domain with three solid walls and one pressure boundary, and a domain with solid walls on the North and South, and pressure boundaries on the West and East, also yielded low velocities, proving the importance of this new hydrostatic BC.

Conclusions

The hydrostatic BC produced hydrostatic results in a number of different simulations. Incorporating this new BC into LBM codes will allow for more accurate and complicated buoyancy and convection simulations. This will make it possible for LBM to be utilized in more applications.

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