Journal of Computational Physics 301 (2015) 230–246

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Free surface Neumann boundary condition for the advection–diffusion lattice Boltzmann method

Matthias Markl *, Carolin Körner

Chair of Metals Science and Technology, Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstr. 5, 91058 Erlangen, Germany

ARTICLE INFO

Article history:
Received 17 June 2015
Accepted 15 August 2015
Available online 28 August 2015

Keywords:
Neumann boundary condition
Lattice Boltzmann method
Free surface
Advection–diffusion equation

ABSTRACT

The main objective of this paper is the derivation and validation of a free surface Neumann boundary condition for the advection–diffusion lattice Boltzmann method. Most literature boundary conditions are applied on straight walls and sometimes on curved geometries or fixed free surfaces, but dynamic free surfaces, especially with fluid motion in normal direction, are hardly addressed. A Chapman–Enskog Expansion is the basis for the derivation of the advection–diffusion equation using the advection–diffusion lattice Boltzmann method and the BGK collision operator. For this numerical scheme, a free surface Neumann boundary condition with no flux in normal direction to the free surface is derived. Finally, the boundary condition is validated in different static and dynamic test scenarios, including a detailed view on the conservation of the diffusive scalar, the normal and tangential flux components to the free surface and the accuracy. The validation scenarios reveal the superiority of the new approach to the compared literature schemes, especially for arbitrary fluid motion.

1. Introduction

The lattice Boltzmann (LB) method [1] is commonly applied to hydrodynamic fluid flow [2–4] described by the Navier–Stokes equations. Additionally, the LB method is suitable to solve the diffusion and advection–diffusion equation. Possible applications are thermal flows [5,6], multi-component flows [7] or solute transport in porous media [8]. Most of the LB implementations use the Bhatnagar–Gross–Krook (BGK) collision operator [9], which limits its applications to isotropic diffusion phenomena. By replacing the BGK with a multi-relaxation time (MRT) operator, an anisotropic diffusion behavior is possible [10].

A Neumann boundary condition specifies the solution of a first derivative at a boundary. Regarding the advection–diffusion LB method, the boundary condition is defined on the flux, which is the spatial derivative of the diffusive scalar. This paper focuses on a zero flux condition in normal direction to the free surface. Additionally, there are no physical restrictions in tangential direction.

Neumann and other boundary conditions are usually applied on straight walls [8]. Towards curved or free surface boundaries there are only few approaches in literature. The easiest way to impose a boundary condition is the bounce-back scheme [11], resulting in a zero flux in normal direction. Unfortunately, the tangential parts also vanish. Modified bounce-back schemes, altered by the boundary direction [12,13], still affect the tangential flux. A Neumann boundary condition is

* Corresponding author.
E-mail address: matthias.markl@fau.de (M. Markl).

http://dx.doi.org/10.1016/j.jcp.2015.08.033

presented in [14], which interpolates the macroscopic quantities at the boundary, and demonstrates an appropriate reconstruction of the tangential flux. However, if interpolation is not possible, the fall-back boundary condition is the bounce-back rule. A similar interpolation approach basing on the bounce-back approach and using the particle distribution functions is presented in [15]. Fixed curved boundaries are examined and a first order accuracy for the Neumann boundary condition with arbitrary fluxes is achieved.

Most of these schemes are derived for static boundary problems, like simulations of porous media or curved channels. But considering free surface flows, especially movements in normal direction occur. All mentioned schemes are not appropriate to model these kinds of moving boundary problems [14], because the first order moment of the LB method is not conserved resulting in an unphysical concentration of the diffusive scalar at the boundary depending on the velocity.

The free surface LB method described in [5] provides a suitable boundary condition for arbitrary free surface flows. Nevertheless, some drawbacks are identified during the revision of this approach. Therefore, after a short introduction into the free surface advection–diffusion LB method, a new approach is derived, where these drawbacks are eliminated or minimized. Finally, the boundary condition is validated in different static and dynamic test scenarios, including a detailed view on conservation of the diffusive scalar, the normal and tangential flux components to the free surface and the accuracy.

2. Free surface advection–diffusion lattice Boltzmann method

The single phase-continuum conservation equations to simulate incompressible fluid transport are the incompressible Navier–Stokes equations. Suppose an additional diffusive scalar ϱ, e.g., representing the thermal energy density or the concentration of an additive. Due to diffusion and the dynamics of the fluid the diffusive scalar is distributed described by the advection–diffusion equation

$$\partial_t \varrho + \nabla \cdot \left(\varrho \underline{u}\right) = \nabla \cdot \left(a(\varrho) \nabla \varrho\right), \tag{1}$$

where t is the time and $\underline{u}$ the divergence free macroscopic velocity and a the diffusion coefficient, which can either depend on ϱ or is a constant value.

LB models base on particle distribution functions (pdf) $f\left(\underline{x}, \mathbf{v}, t\right)$, describing the probability of finding a particle with microscopic velocity $\mathbf{v}$ at position $\underline{x}$ at time t. The basic idea for the derivation of the LB method [2,4,16,17] is to solve the linear transport equation for pdfs in the physical momentum space. The D3Q19 stencil [18], a finite set of 19 discrete velocities $\underline{c}_i$ with lattice weights ω_i, discretizes the microscopic phase space. The domain is covered by a regular lattice consisting of cubic cells with side length δ_x. In each cell the diffusive scalar is modeled by the discretized pdfs f_i and the macroscopic quantity is computed by

$$\varrho = \sum_i f_i. \tag{2}$$

For all cells the pdf values collide and stream to the neighbor cells using the lattice displacement vector $\underline{e}_i = \underline{c}_i \delta_t$ and the time resolution δ_t. The so-called BGK collision operator [9] uses a single relaxation time τ to relax towards the local equilibrium, which reads in the discretized form

$$f_i\left(\underline{x} + \underline{e}_i, t + \delta_t\right) = f_i\left(\underline{x}, t\right) + \frac{\delta_t}{\tau}\left(f_i^{\mathrm{eq}}\left(\underline{x}, t\right) - f_i\left(\underline{x}, t\right)\right), \tag{3}$$

where f_i^{eq} is the Maxwell equilibrium distribution [16]

$$f_i^{\mathrm{eq}}\left(\underline{x}, t\right) = \omega_i \varrho \left(1 + \frac{\underline{c}_i \cdot \underline{u}}{c_s^2}\right), \tag{4}$$

where $c_s = \delta_x / (\sqrt{3}\delta_t)$ is the lattice speed of sound. The relaxation time τ is related to the diffusion coefficient a by

$$a = c_s^2 (\tau - 0.5\delta_t). \tag{5}$$

The Mach number describes the ratio of the characteristic fluid velocity to the lattice speed of sound. In the incompressible flow limit, i.e., for small Mach numbers $Ma < 0.1$, the advection–diffusion equation (1) is derived by a Chapman–Enskog expansion in Appendix A.

The validation scenarios require a Dirichlet boundary condition for straight walls, which ensures a constant value ϱ_w by a non-equilibrium bounce-back approach [12]

$$f_i\left(\underline{x}, t\right) = f_i^{\mathrm{eq}}\left(\varrho_w\right) + f_{\bar{i}}^{\mathrm{eq}}\left(\varrho_w\right) - f_{\bar{i}}\left(\underline{x}, t\right), \tag{6}$$

where $\bar{i}$ denotes the inverse direction of i.

A free surface advection–diffusion LB method is necessary for the simulation of moving interfaces between immiscible gas and liquid fluids. It has to be guaranteed that the gas phase is separated by a closed interface layer from the fluid phase [19]. Thus each lattice cell has a certain state: gas, interface or liquid. To ensure mass conservation a volume of