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Implementation of a lattice Boltzmann method for immiscible multiphase flow simulations using the level set method

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Abstract. We implemented the lattice Boltzmann method for immiscible multiphase flow simulations and combined it with the level set method according to the paper of G. Thömmes et al. [1]. The level set method is used to calculate the movement of the interface between the two phases. The input for the level set method is computed by the lattice Boltzmann method. We verified our implementation with different test cases.

Key words. Lattice Boltzmann method, Level set method, Free surface, Multiphase

AMS subject classifications.

1. Introduction.

In engineering the immiscible two-phase flow problem often needs to be considered. For example, bubble dynamics are decisive for the design of chemical reactors. Also fingering in oil recovery is a common two-phase problem.

The two-phase flow problem can be described with the Navier-Stokes equations for two incompressible fluids (Eq. 1.1, 1.2). To apply them, we distribute our domain into three parts: Ω_1 and Ω_2 describe the two fluids and $\Gamma = \delta\Omega_1 \cap \delta\Omega_2$ is the interface (Fig. 1). The material properties in each fluid are constant and the interface is assumed to be sharp. Thus the material properties are discontinuous and the fluids will not mix.

The evolution of the flow fields within each fluid can be expressed with the incompressible Navier-Stokes equations,

$$\nabla \cdot \vec{u}_i = 0 \text{ in } \Omega_i, \tag{1.1}$$

$$\frac{\partial \vec{u}_i}{\partial t} + (\vec{u}_i \cdot \nabla)\,\vec{u}_i = -\frac{1}{\varrho_i}\nabla p_i + \nu_i \nabla^2 \vec{u}_i \text{ in } \Omega_i. \tag{1.2}$$

Here, u_i is the velocity, p_i the pressure, ν_i the kinematic viscosity and ϱ_i the mass density.

As boundary conditions and initial conditions we can take for example,

$$\vec{u}_i(x,t) = 0, \text{ on } \delta\Omega_i \backslash \Gamma, \tag{1.3}$$

$$\vec{u}_i(x,0) = \vec{u}_{ini,i}(x), \text{ in } \Omega_i. \tag{1.4}$$

For the interface Γ we have the influence of the surface tension and a no-slip condition, i.e. continuity of the velocities between the fluid phases. Therefore, we get the jump conditions,

$$[\vec{u}] = 0, \tag{1.5}$$

$$[T] \cdot \vec{n} = 2\sigma\kappa\vec{n}. \tag{1.6}$$

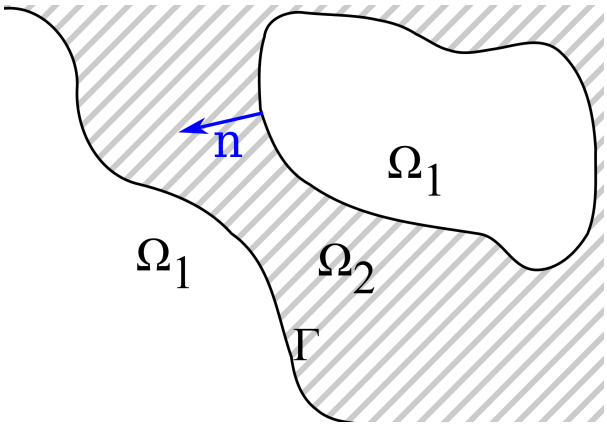

Figure 1. *Two fluid domains Ω_i separated by an interface.*

Here, T is the shear stress tensor, σ the surface tension, and κ the curvature of the interface with respect to its outer normal $\vec{n}$. Brackets denote the jump of a quantity at the interface,

$$[q](\vec{x}) = \lim_{\epsilon \to 0}(q(\vec{x} - \epsilon\vec{n}) - (q(\vec{x} + \epsilon\vec{n})) \text{ with } \vec{x} \in \Gamma. \tag{1.7}$$

In Fig. 1 this is the jump from Ω_1 to Ω_2. For the other direction the sign changes.

There are different approaches to solve the immiscible two-phase problem. The most spread among these approaches is the colour gradient method of Gunstensen and Rothman [3, 4, 5]. The downside of this method is that it is only applicable for small density and viscosity differences. Another approach is the concept of *interaction potentials* by Shan and Chen [6, 7]. This method actually models miscible fluids and can only approximately describe the behavior of immiscible fluids. Furthermore there are free surface methods which only take one fluid in account for computation ([8]). They work best for big density and viscosity ratios.

In this publication we use a hybrid lattice Boltzmann level set method. Thereby, the interface motion is calculated by the level set method. The input data for the level set method is given by the lattice Boltzmann method, which is calculated independently for each fluid. This method has the advantage that it allows big ranges of density and viscosity ratios between the fluid phases and has a high accuracy but requires only little memory .

This paper is organized as follows: Section 2 gives an introduction to the lattice Boltzmann method and the level set method and explains the coupling of these. In section 3 we present our results and finally in section 4 we draw a conclusion.

2. Numerical Methods.

The algorithm we describe in this paper uses the lattice Boltzmann method and the level set method. With the lattice Boltzmann method we calculate the velocity field for each fluid independently. The level set method uses this velocity field to

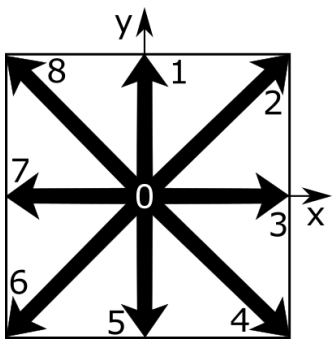

Figure 2. *The vectors of one cell in LBM.*

compute the movement of the interface. We will shortly introduce both methods and show how they can be coupled.

2.1. The Lattice Boltzmann Method. To solve the incompressible Navier-Stokes equations, we use the lattice Boltzmann method (LBM). This method describes the evolution of the particle density $f(\vec{x}, \vec{v}, t)$ in phase space, with $(\vec{x}, \vec{v})$ as the phase space variables and t as time. The LBM algorithm discretizes with a regular grid in space and with restricted number of velocities adapted to this grid [9, 10, 11, 12]. We use the D2Q9 model in 2D, which has 9 velocity vectors on a plane grid with unit spacing including one zero velocity (Fig. 2). The vectors are given by the columns of the matrix,

$$c = \begin{bmatrix} 0 & 0 & 1 & 1 & 1 & 0 & -1 & -1 & -1 \\ 0 & 1 & 1 & 0 & -1 & -1 & -1 & 0 & 1 \end{bmatrix}. \tag{2.1}$$

The corresponding particle distributions are denoted by $f_i(\vec{x}, t) = f(\vec{x}, \vec{c_i}, t)$. We get the density and velocity from the particle distribution functions with,

$$\rho(\vec{x}, t) = \sum_{i=1}^{9} f_i(\vec{x}, t), \qquad \vec{u} = \sum_{i=1}^{9} f_i(\vec{x}, t)\vec{c_i}. \tag{2.2}$$

In the interior, the LBM alternates collision step and propagation step. For the collision step we use the Bhatnagar-Gross-Krook (BGK) approximation [13],

$$f_i^+(\vec{x} + \vec{c_i}, t + 1) = f_i(\vec{x}, t) - \frac{1}{\tau}(f_i - f_i^{eq}) + G_i. \tag{2.3}$$

The propagation step is denoted by,

$$f_i(\vec{x} + \vec{c_i}, t + 1) = f_i^+(\vec{x}, t + 1). \tag{2.4}$$

The parameter τ is the relaxation parameter for the BGK collision operator and controls the kinematic viscosity in lattice units $\nu = \frac{1}{6}(2\tau - 1)$. Note, that we assume the cell spacing Δx

and the time step Δt to be unity here. The lattice speed of sound equals to $c_s = \frac{1}{\sqrt{3}}$. G_i is an additional force, e.g. gravity. In our case we set $G_i = 0$. Furthermore, we use the equilibrium distribution,

$$f_i^{eq}(\rho, \vec{u}) = f_i^*(\rho + 3\vec{c_i} \cdot \vec{u} + \frac{9}{2}(\vec{c_i} \cdot \vec{u})^2 - \frac{3}{2}\vec{u} \cdot \vec{u}) \tag{2.5}$$

with the corresponding D2Q9 weight factors,

$$f_i^* = \begin{cases} \frac{4}{9}, & i = 0 \\ \frac{1}{9}, & i = 1, 3, 5, 7 \\ \frac{1}{36}, & i = 2, 4, 6, 8 \end{cases}.$$

We use two types of boundary conditions. To simulate static walls, we use simple bounce-back boundary conditions,

$$\tilde{f}_i = f_{i^*}^+(\vec{x_b}, t), \text{ with } \vec{x_b} \in \delta\Omega, \tag{2.6}$$

where i^* is the index of the opposite direction $c_{i^*} = -c_i$. To simulate a flow, we use moving no-slip boundary conditions,

$$\tilde{f}_i = f_{i^*}^+(\vec{x_b}, t) + 6 f_i^* \vec{c_i} \vec{v}, \text{ with } \vec{x_b} \in \delta\Omega, \tag{2.7}$$

where $\vec{v}$ is the speed of the moving wall. To enable inflow and outflow of fluids we have periodic boundary conditions,

$$\tilde{f}_i(\vec{x_a}, t) = f_i^+(\vec{x_b}, t), \tag{2.8}$$

where x_a and x_b are points of opposite boundaries.

One time step in the LBM algorithm is achieved by the following sub-steps:

1. Collision step: $f_i^+ = f_i - \frac{1}{\tau}(f_i - f_i^{eq}) + G_i$
2. Propagation step: $f_i(\vec{x} + \vec{c_i}, t + 1) = f_i^+(x, t)$, for interior nodes
3. Boundary conditions: $f_i(\vec{x} + \vec{c_i}, t + 1) = f_i(\vec{x} + \vec{c_i}, t)$, if $\vec{x} \notin \Omega$

2.2. The Level Set Method. We deal with the movement of the interface between the two fluids by using the level set method. The method captures the surface that represents the interface with a continuous signed distance function, where the interface is implicitly given as the zero level set.

Let Γ_t be our interface at time t. Within the level set method, Γ_t is the zero iso-surface of the level set function φ. Thus, for $\vec{x} \in \Gamma_t$ we have $\varphi(\vec{x}, t) = 0$, in direction of the surface normal we get $\varphi > 0$, and in the other direction we get $\varphi < 0$. For this level set function we get the level set equation introduced by Osher and Sethian in [14] for the evolution of free surfaces,

$$\frac{\partial \varphi}{\partial t} + \vec{v} \cdot \nabla \varphi = 0, \tag{2.9}$$

with the velocity $\vec{v} = \vec{u}(\vec{x}(t))$ for $\vec{x}(t) \in \Gamma_t$, which we obtain from the LBM.

To solve this equation we use the Toolbox of Ian Mitchell [15] for Matlab. This toolbox takes as input the velocity field we get from the lattice Boltzmann method and computes the movement of the interface. The toolbox also provides functions to calculate the normal and the curvature of the surface. We will need this information for the coupling of the methods.

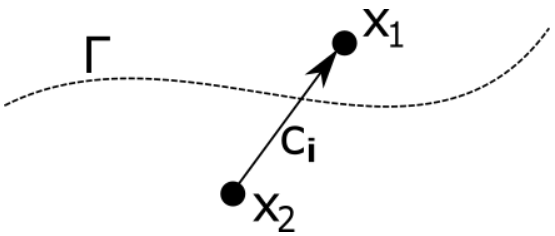

Figure 3. *Link between two points in different fluids.*

2.3. Coupling of LBM and level set method. The lattice Boltzmann method requires a boundary treatment at the interface which implements the jump conditions (1.6). For sake of simplicity, we do not write arrows for every vector, i.e., $\vec{u} \to u$. One should consider that every position, direction, and velocity is two-dimensional.

For the coupling, we use a bounce back type boundary condition that prescribes the velocity as Dirichlet value as described in [1, p. 1146]. For example, in Fig. 3 for a point $x_2 \in \Omega_2$ that is next to the phase interface we set,

$$f_i(x_2, t+1) = f_{i*}^{+}(x_2, t) + 6 f_i^* c_i \cdot \tilde{u} + R_i. \tag{2.10}$$

Here, $\tilde{u}$ describes the linear interpolation of the velocity along the direction c_i, evaluated at the location $\tilde{x} = x_1 + q c_i = x_2 + (q-1)c_i$ on the interface,

$$\tilde{u} = q u(x_2, t) + (1-q) u(x_1, t).$$

The additional term R_i ensures the jump conditions of the normal stress and corrects the error terms that is introduced by the first order accurate bounce back treatment,

$$R_i = 6 f_i^* \Lambda_i : A \text{ with } A = -q(1-q)[S] - (q - \frac{1}{2}) S^{(2)}, \tag{2.11}$$

with

$$\Lambda_i = c_i \otimes c_i - \frac{1}{2}(c_i \cdot c_i)\mathbf{I}. \tag{2.12}$$

That is an orthogonal projection of the column vectors of the (symmetric) deviatoric shear rate jump tensor on the link direction weighted with the interface distance and a compensation term for the interpolation error. This error arises, when the interface is not on the exact middle between two LBM grid cells. The tensor product is $a \otimes b = ab^T$ and the double contraction $A : B = \text{trace}(AB^T)$. We can rewrite formula (2.11) in the form,

$$R_i = 6 f_i^* (-q)(1-q)\Lambda_i : [S] - (q - \frac{1}{2})\Lambda_i : S_2, \tag{2.13}$$

and use the following first-order estimate to obtain the shear rate from the non-equilibrium parts of the distributions (see [17])

$$S_k = -\frac{3}{2\tau} \sum_{i=1}^{9} c_i \otimes c_i (f_i - f_i^{eq})(t, x_k). \tag{2.14}$$

Furthermore, we have,

$$\Lambda_i : [S] = ([S] : n \otimes n)((n \cdot c_i)^2 - \frac{1}{2}(c_i \cdot c_i)) + 2([S] : n \otimes t)(n \cdot c_i)(t \cdot c_i), \tag{2.15}$$

which is obtained by a coordinate transformation onto a basis (n, t) of normal and tangential vector to the interface. From the fluid mechanical jump condition (1.6) and the relation $[\mu S] = \bar{\mu}[S] + [\mu]\bar{S}$ it can be seen,

$$[S] : n \otimes n = \frac{1}{2\bar{\mu}}([p] + 2\sigma\kappa) - \frac{[\mu]}{\bar{\mu}}\bar{S} : n \otimes n, \tag{2.16}$$

$$[S] : n \otimes t = -\frac{[\mu]}{\bar{\mu}}\bar{S} : n \otimes t. \tag{2.17}$$

Here $\mu_k = \varrho_k \nu_k$ are the dynamic viscosities, with $\bar{\mu} = (\mu_1 + \mu_2)/2$ and $\bar{S} = (S_1 + S_2)/2$ as averaged quantities, κ the interface curvature, and the viscosity jump $[\mu] = \mu_2 - \mu_1$. The pressure jump is approximated by,

$$[p] \approx \frac{1}{3}(\rho(x_2, t)\varrho_2 - \rho(x_1, t)\varrho_1). \tag{2.18}$$

and with that, all variables for the boundary conditions are well defined. A refill method is still missing. Due to the fact that the interface moves, some cells change their fluid type. We use an equilibrium/non-equilibrium refill as it is described in [16] consisting out of the four following steps:

1 Interpolate density and velocity from interior neighbors.
2 Compute the corresponding equilibrium.
3 Copy the non-equilibrium part from a direct interior neighbor.
4 Reinitialise by adding equilibrium and non-equilibrium parts.

Suppose we choose an inward pointing direction c_i in a boundary point $x \in \Omega_1$, e.g., the direction of biggest angle with the surface normal. Then the density is interpolated by,

$$\tilde{\rho}(x) = 3\rho(x + c_i, t) - 3\rho(x + 2c_i, t) + \rho(x + 3c_i, t). \tag{2.19}$$

Figure 4 shows the cells we use for the interpolation. In [1] the velocity is interpolated by using the velocity of the interface. The Ian-Mitchell toolbox does not provide a function to access this value. Therefore, we use the formula given in [18] that is basically the same we use for density,

$$\tilde{u}(x) = 3u(x + c_i, t) - 3u(x + 2c_i, t) + u(x + 3c_i, t). \tag{2.20}$$

We can now calculate the new equilibrium part of the particle densities in x, $f_i^{eq}(\tilde{\rho}, \tilde{u})$ and add them to the non-equilibrium part which we copy from a nearest neighbor,

$$f_i(\vec{x}, t + 1) = f_i^{eq}(\tilde{\rho}, \tilde{u}) + f_i^{neq}(x + c_i, t + 1).$$

This completes the refill algorithm.

Finally, we can couple the two methods in the following way:

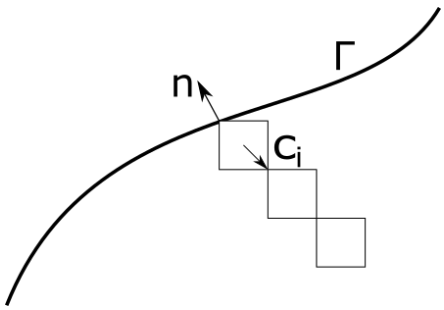

Figure 4. *Cells that are used for the refill method.*

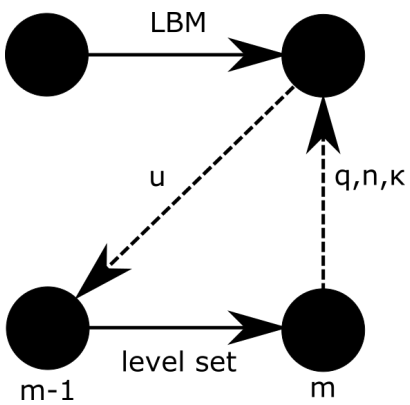

Figure 5. *Data exchange between LBM and level set method.*

1. Create the initial interface Γ_0.
2. Run the level set code once to create the surface description for LBM.
3. Run the LBM using the data from the level set for a prescribed number of steps
4. Pass the current velocity field to the level set code and run it for the same number of steps (see Fig. 5).
5. Repeat step 3 and 4 until the end of the simulation.

3. Results and Examples. To verify the correctness of our implementation we firstly built a Couette flow and compared our results with the one we get from the analytic solution. Secondly, we used the Young-Laplace experiment for a bubble to validate the implementation of surface tension.

3.1. Couette channel flow. The Couette channel flow consists of a fixed lower wall at $y = 0$ and an upper wall at $y = 1$ that is moving with a constant velocity. At these walls we use no-slip boundary conditions. To generate a channel flow, we use periodic boundary conditions for the boundaries at the inflow $x = 0$ and the outflow $x = 1$. The two fluids are distributed in a way that the interface is parallel to our walls.

For the Couette channel flow exists an analytic solution that can be derived from the Navier-Stokes equations

$$v(x) = \begin{cases} v_0(\frac{\mu_1}{\mu_1+\mu_2}x + \frac{\mu_2}{\mu_1+\mu_2}), & x \geq 0 \\ v_0(\frac{\mu_2}{\mu_1+\mu_2}x + \frac{\mu_2}{\mu_1+\mu_2}), & x < 0, \end{cases}$$

where μ_1 denotes the dynamic viscosity in the lower fluid and μ_2 the viscosity in upper fluid.

3.2. Young-Laplace experiment for a bubble. The Couette-Flow is not influenced by surface tension due to the fact that the surface tension is multiplied with the curvature in Equation 2.15 and the curvature is zero in the Couette-Flow. We use the Young-Laplace experiment to validate the implementation of surface tension. The pressure p inside a bubble of radius r is proportional to the surface tension coefficient σ according to the Young-Laplace law

$$p = \frac{2\sigma}{r} = 2\sigma\kappa. \tag{3.1}$$

4. Conclusion.

REFERENCES

[1] G. THÖMMES, J. BECKER, A lattice Boltzmann method for immiscible multiphase flow simulations using the level set method, J. Comput. Phys. 228 (2009), 1139-1156.

[2] D. ADALSTEINSSON, J.A. SETHIAN, A fast level set method for propagating interfaces, J. Comput. Phys. 118 (2) (1995) 269-277.

[3] A.K. GUNSTENSEN, D.H. ROTHMAN, S. ZALESKI, G. ZANETTI, Lattice Boltzmann model of immiscible fluids, Phys. Rev. A 43 (8) (1991) 4320-4327.

[4] A.K. GUNSTENSEN, D.H. ROTHMAN, Macroscopic modeling of immiscible flows in three dimensions by a lattice Boltzmann method, Europhys. Lett. 18 (2) (1998) 157-161.

[5] K. SANKARANARAYANAN, I.G. KEVREKIDIES, S. SUNDARESAN, J. LU, G. TRYGGVASON, A comparative study of lattice Boltzmann and front-tracking finite-difference methods for bubble simulations, Int. J. Multiphase Flow 29 (1) (2003) 109-116.

[6] X. SHAN, H. CHEN, Lattice Boltzmann model for simulation flows with multiple phases and components, Phys. Rev. E 47 (3) (1999) 567-603.

[7] X. SHAN, H. CHEN, Simulation of nonideal gases and liquid-gas phase transition by the Lattice Boltzmann equation, Phys. Rev. E 49 (4) (1994) 2941.

[8] C. KÖRNER, M. THIES, T. HOFMANN, N. THÜREY, U. RÜDE, Lattice Boltzmann Model for Free Surface Flow for Modeling Foaming, J. Stat. Phys. 121 (2005) 179-196.

[9] S. CHEN, G.D. DOOLENM, Lattice Boltzmann method for fluid flows, Ann. Rev. Fluid Mech. 30 (1998) 329-364.

[10] X. HE, L.S. LUO, Lattice Boltzmann model for the incompressible Navier-Stokes equation, J. Stat. Phys. 88 (1997) 927-944.

[11] S. SUCCI, The Lattice Boltzmann Equation for Fluid Dynamics and Beyond, Clarendon Press, Oxford, ISBN 978-0-19-850398-9 (2001).

[12] D.A. WOLF-GLADOW, Lattice-Gas Cellular Automata and Lattice Boltzmann Models, An Introduction, Springer, 2000.

[13] P. BHATNAGAR, E. GROSS, M. KROOK, A model for collision processes in gases: 1. Small amplitude processes in charged and neutral one-component systems, Phys. Rev. 94 (1954) 511.
[14] S. OSHER, J. SETHIAN, Fronts propagating with curvature-dependent speed: algorithms based on Hamlton-Jacobi formulations, J. Comput. Phys. 79 (1988) 12-49.
[15] I. MITCHELL, A Toolbox of Level Set Methods, August 2015, URL: http://www.cs.ubc.ca/~mitchell/ToolboxLS/.
[16] A. CAIAZZO, Asymptotic analysis of lattice Boltzmann method for fluid-structure interaction problems, Ph.D. Thesis, Kaiserslautern (Germany) and Pisa (Italy), 2007.
[17] T. KRÜGER, F. VARNIK, D. RAABE, Shear stress in lattice Boltzmann simulations, Phys. Rev. E 79 (4) (2009) 046704.
[18] P. LALLEMAND, L.-S. LUO, Lattice Boltzmann method for moving boundaries, J. Comput. Phys. 184 (2003) 406-421.