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Citation for published version:
Khajepor, S, Cui, J, Dewar, M & Chen, B 2018, 'A study of wall boundary conditions in pseudopotential lattice Boltzmann models', Computers and Fluids. https://doi.org/10.1016/j.compfluid.2018.05.011

Digital Object Identifier (DOI):
10.1016/j.compfluid.2018.05.011

Link:
Link to publication record in Heriot-Watt Research Portal

Document Version:
Version created as part of publication process; publisher's layout; not normally made publicly available

Published In:
Computers and Fluids

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A study of wall boundary conditions in pseudopotential lattice Boltzmann models

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A R T I C L E   I N F O
Article history:
Received 14 April 2017
Revised 4 April 2018
Accepted 10 May 2018
Available online xxx

Keywords:
Lattice Boltzmann
Boundary condition
Pseudopotential model
Multipseudopotential
Poiseuille flow
Contact angle

A B S T R A C T
The effect of fluid–solid interactions on the hydrodynamics of non-ideal fluids and wettability of surfaces is investigated. We integrate the interaction forces, simulated by pseudopotentials, into two on-site boundary conditions: standard bounce-back (SBB) and Zou and He (ZH) [12] to determine the distribution functions of the boundary nodes. Three different interaction forces are tested: pseudopotential-based interaction (ψ), modified pseudopotential-based interaction (mψ), and a ZH-based interaction, which is proposed by this study based on the ZH method. Therefore, the schemes are ψ-SBB, mψ-SBB, mψ-ZH, and ZH-ZH. The first criterion is the achievement of macroscopic Poiseuille flow. The second criterion is the achievement of a wide range of contact angles. The main method of simulation is multipseudopotential interaction [30]. It is found that the scheme of ψ-SBB creates a relatively large fluctuation of density across the channel. Whilst, the schemes of mψ-SBB, mψ-ZH, and ZH-ZH generate much less density variation across the channel. Among them, ZH-ZH treatment is superior based on density fluctuation and the error associated with the resolution, relaxation time, and compressibility. We found that all four boundary conditions can form a wide range of contact angles. The ψ-SBB scheme creates largest density fluctuation inside a drop on wettable surfaces. The schemes of mψ-SBB and mψ-ZH create almost the same density fluctuation which is larger than ZH-ZH. Moreover, mψ interaction generates spurious velocities as high as six times a free drop with SBB and eight times with ZH while spurious velocities in ψ-SBB and ZH-ZH are very close to the free drop. Therefore, ZH-ZH performs best, also, in wettability tests.

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1. Introduction

Lattice Boltzmann Method (LBM) is a recent and viable solver in a broad range of fluid flow simulations from simple single-phase, to highly complex multiphase flows [1–3]. Since LBM originated from kinetic theory, it has several advantages over other solvers. First of all, it has linear convection or streaming process in phase space. Moreover, without solving a Poisson equation for pressure, which is necessary for incompressible Navier–Stokes solvers, it recovers Navier–Stokes equations. Furthermore, opting for a limited number of velocity directions, instead of covering the whole phase space, it can straightforwardly convert microscopic distribution function to macroscopic quantities [4].

Setting up proper treatments at the boundaries of the simulation domain is necessary to achieve the desired correct results while satisfying the given flow conditions, such as velocity, pressure, or periodic planes. The treatments should keep the accuracy of the solution at a minimum computational cost. In Navier–Stokes based solvers the boundary conditions are directly imposed on macroscopic quantities. However, in LBM, similar to particle-based methods such as molecular dynamics and dissipative particle dynamics, the microscopic characteristics give rise to the desired macroscopic flow conditions. After a streaming process, the distribution functions of a boundary node should be defined. This requires redefining all of them or only the unknowns as the node has some defined particle populations which come from the inside of the domain.

It has been well-studied, and proven, that conventional LBM has the second order of accuracy, in phase space inside of the flow domain [5,6]. Therefore, a proper boundary treatment should provide the same, otherwise degrading the entire simulation accuracy. For example, bounce-back scheme, implemented in lattice gas automation method for straightforward treatment of no-slip boundaries, is found to have the first order of accuracy in the LBM [7,8]. The scheme could be of the second order if the wall line is considered to be halfway between the fluid and solid nodes [9]. He et al.

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[10] found analytical solutions for the lattice Boltzmann fluid in the case of the two-dimensional Poiseuille flow and Couette flow which facilitate the study of the bounce-back scheme. The extrapolation treatments are able to provide the second order of accuracy. The finite difference-based scheme of Chen et al. [4] requests information from two neighboring node layers. The non-equilibrium extrapolation scheme of Zhao-Li et al. [11] needs information from the nearest fluid nodes to determine a new set of distribution functions for the nodes whose pressure or velocity is defined. To keep the great assets of local collision operations which suits parallel processing, an LBM boundary condition better finds the unknown distribution functions of a node merely by use of the information available at the node itself.

On the other hand, the on-site boundary condition proposed by Zou and He [12] imposes pressure or velocity condition on the focused node regardless of neighbors. It finds the unknowns with the aid of conservation of mass and momentum, and bounce-back rule for the non-ideal part of distributions. Moreover, the method keeps the second order of accuracy for simulations. Inamura et al. [13] suggested the missed distributions are found from the equilibrium distribution function that is calculated by a fictitious density and velocity. Skordos [14] filled all the distribution functions on the boundary node using the stress tensor which is related to strain rate tensor. The strain rate tensor can be evaluated by second order finite difference approximation of velocity over neighboring nodes. Latt et al. [15] proposed replacing all the distribution functions of the boundary node by the use of a stress tensor evaluated by the bounce-back of the non-equilibrium part of distribution functions. Latt et al. [15] compared boundary treatments proposed by references [12–14] and found that despite the fact that they all had the second order of accuracy, the ones which determine the other unknown distributions after streaming step through closure relations have better accuracy at low Reynolds number flows. Additionally, the boundary conditions, which fill all the distributions at the boundary node, demonstrate better numerical stability. Therefore, they are suitable for high Reynolds number flows.

It should be noted that bounce-back applicability is not limited by the geometry of the wall. However, the others need to find the vectors tangent and normal to the wall, for which various probable situations should be assessed beforehand. They also require further treatments for corner nodes. Bounce-back has been going through considerable extensions; it is combined with spatial interpolations to handle moving boundaries [16]. Junk and Yang [17] modified bounce-back to increase the accuracy of velocity and pressure fields whilst keeping the procedure completely local. Nash et al. [18] studied this category of boundary condition treatments regarding accuracy and performance in various types of flow. It should be noted for curved boundaries, the standard bounce-back reduces the accuracy of the system. In such cases, Mei et al. [19,20] proposed a treatment based on the work of reference [21] that keeps the second order of accuracy in LBM.

One of the well-known capabilities of the LBM is the straightforward simulation of multiphase and multicomponent systems without the need for marker-function advective and front tracking methods. The two-phase systems are formed as a result of Van der Waals (VW) loop seen in equations of state (EOSs) of non-ideal fluids. The most popular model is the pseudopotential model proposed by Shan and Chen [22] at the early stage of LBM development. It is consistently developing and widely used in simulations and analyses of bubble or drop characteristics, multiphase flow in porous media, and nucleate boiling [23–29]. Multi-pseudopotential interaction (MPI) [30–32] is a new scheme which ameliorates SC model in different aspects; it removes the inconsistency of SC model, can be applied to a liquid-vapor system with large density ratios, gives the flexibility of changing the interface width, and raises the system stability. In spite of the popularity, the boundary treatments for pseudopotential models have not been studied thoroughly. The SC model utilizes a lattice force, based on the pseudopotential of each node, to model interactions of fluids, and also fluids with solids at a wall boundary.

The lattice force at the boundaries can affect fluid flow behavior in channels and change the wettability of solid surfaces. Therefore, it is possible to model wetting and non-wetting multiphase flow in channels and porous media. The aim of this paper is to study and compare several popular pseudopotential boundary conditions and find out how they perform in modeling fluid flows in channels and wettability of surfaces. For the latter, a liquid drop, which is in equilibrium with its vapor, is placed on surfaces with different levels of wettability. For the former, to narrow down the study, we focus only on single-phase pseudopotential fluids in the channels. The first example of this idea is when pseudopotential model is used to decrease the compressibility of a fluid and decrease the compressibility error in the lattice Boltzmann equation [33]. The second example is a half-saturated porous geometry. There exist channels where a single-phase fluid is flowing and its interactions with solid should be correctly modeled. The third example is the simulation of two-phase flows in which some solid walls are merely interacting with one phase such as the flow regime of slug, annular and dispersed in a pipe. During this, one phase flows in the center of the pipe and the other one is interacting with the pipe wall.

In this paper, we implement different solid-liquid force interactions into the standard bounce-back and on-site Zou and He [12] treatments, to build non-slip wall boundary conditions. Then these methods are assessed for a single-phase fluid, the compressed water, which flows in a two-dimensional channel and recovers macroscopic Poiseuille flow. The accuracy of simulations, density variation, and velocity profiles due to these treatments are studied. We also demonstrate that the choices of solid-liquid interaction can significantly change the flow behavior. Then those boundary conditions are investigated for two-phase systems, a drop on wettable surfaces. In this case, the availability of contact angles, fluctuation of density near the wall, and magnitude of spurious velocities are examined.

2. Methodology

The BGK lattice Boltzmann equation (LBE), as a particular discretization of Boltzmann equation [34] for simulation of a flow field, with a general forcing term is defined as

\[
 f_i(x + e_i \Delta t, t + \Delta t) - f_i(x, t) = -\frac{1}{\tau} \left[ f_i(x, t) - f_i^{eq}(x, t) \right] + \Delta t f_i^p,
\]

(1)

where \( f_i \) are particle distribution functions or particle populations at position \( x \) and time \( t \), \( i = 0 \ldots q - 1 \) are the indices of neighboring nodes, \( e_i \) are the discrete velocity vectors to neighboring nodes, \( \tau \) is the nondimensional relaxation time, \( f_i^{eq} \) is the local equilibrium distribution function obtained from the Chapman–Enskog expansion of Maxwellian to the second order at constant temperature [35,36], and \( f_i^p \) is the forcing term. For a flow field near its equilibrium state without internal or external forces, the momentum flux tensor can be obtained by employing the equilibrium distribution function and considering its isotropy on the lattice

\[
 q^{-1} \sum_{i=0}^{q-1} e_i^a e_i^b f_i \approx q^{-1} \sum_{i=0}^{q-1} e_i^a e_i^b f_i^{eq} = \rho \theta \delta_{ab} + \rho u_a u_b,
\]

(2)

where \( \theta \) and \( \beta \) are Cartesian coordinates, \( \theta \) is lattice temperature, and \( u \) is velocity. The density and velocity are respectively found
from zeroth order and first order moments of distribution functions

\[ \rho = \sum_{i=0}^{q-1} f_i, \]  
(3)

\[ u_a = \sum_i f_i e_{ai} / \rho. \]  
(4)

The definition of velocity is modified when internal or external forces are added to the system which will be explained in the following discussions. The lattice temperature depends on the underlying lattice structure. For the case of the D2Q9 lattice, the discrete velocities are \( e_0 = 0 \), and \( e_1 = (c, 0), e_2 = (c, c), e_3 = (0, c), e_4 = (-c, c), e_5 = (-c, -c), e_6 = (-c, c), \) where \( c = \Delta x / \Delta t \) is micro-velocity and \( \Delta x \) is lattice spacing. This choice of lattice sets the lattice temperature as \( \theta = c^2 / 3 \). It can be found from Eq. (2) that such a system is governed by the ideal gas pressure. To model non-ideal fluids and two-phase systems, Shan and Chen [22] introduced a lattice force into the LBE,

\[ F = -G \psi(x, t) \sum_{j=1}^{N} w(|c_j|^2) \psi(x + c_j, t) c_j. \]  
(5)

to describe the interaction potentials (pseudopotentials) between fluid particles, where \( G \) is the amplitude of the force, \( N \) the number of neighboring nodes that interact with the node of interest, \( c_j \) the vectors linking to those neighbors, and \( w \) the weight function that makes the interaction force dependent on the distance. The distance to the nearest neighbor is \( c \). The SC force can be incorporated into the LBE through the forcing term and equilibrium distribution functions.

The authors introduced the concept of the multipseudopotential interaction (MPI), over the single-pseudopotential interaction (SPI), to describe the hydrodynamics of practical fluids, under the condition that each potential satisfies a thermodynamic requirement [31]

\[ F_{\text{total}} = F^{(1)} + F^{(2)} + ... + F^{(n)} = \sum_{j=1}^{N} -G_j \psi_j(x, t) \sum_{i=1}^{N} w(|c_i|^2) \psi_j(x + c_i, t) c_i. \]  
(6)

where \( n \) is the number of forces (or pseudopotentials), \( G_j \) the amplitude, and \( \psi_j \) the consistent pseudopotential of the \( j \)-th part of the force

\[ \psi_j(\rho) = \left( \frac{\rho}{\lambda_j \epsilon_j + \zeta_j \rho} \right)^{1/\epsilon_j}. \]  
(7)

where \( \lambda_j \) and \( \zeta_j \) are arbitrary constants, \( \epsilon_j = -2(a_1 + 12\Delta t s_j G_j) / a_2 \) in which \( a_1 = 0, \) and \( a_2 = 3 \) for nearest-neighbor interactions [30], \( s_j \) is an arbitrary constant, \( w(|c_i|^2) = 0 \) for \( |c|^2 > 2 \) and from fourth-order isotropy of the force on the lattice \( w(1) = 1 / 3 \) and \( w(2) = 1 / 12 \). The physics of MPI is to present the inter-particle potential with the contributions from a set of sub-forces at various potentials, which are functions of particle densities. The forcing term is

\[ \begin{aligned} F_i = 3w_i \Delta t \left( 1 - \frac{1}{2 \tau} \right) & \left[ e_{ix} - \frac{\rho}{c^2} \right] + \frac{3w_i \Delta t}{c^4} \sum_{j=1}^{N} \left[ s_j \epsilon_j \psi_j^{(i)} \left( 3F^{(i)}_j \epsilon_j \rho \epsilon_j - c^2 F^{(i)}_j \epsilon_j \right) \right] \end{aligned} \]  
(8)

and the actual fluid velocity, \( v \), applied in the equilibrium distribution function, is defined as,

\[ v_a = u_a + F_a \Delta t / 2 \rho \]  
(9)

where Einstein summation convention is adopted. Meanwhile, the MPI EOS is found to be

\[ p = \rho T \left( 1 - \frac{a^2}{b^2} \right) + \frac{a^2}{b^2} \rho + \frac{aa}{b^2} \frac{\rho}{(1 + b \rho)} \]  
(10)

which is suitable to implement cubic EOSs by adopting proper parameters and number of pseudopotentials, the details can be found in Khajepor and Chen [30]. In this study, we chose Soave–Redlich–Kwong (SRK) EOS for the MPI system to present the thermodynamic behavior of water. SRK is the well-known two-parameter cubic equation of state [37] and is defined by rearrangement as,

\[ p = \rho T \left( 1 - \frac{a}{b} \right) + \frac{a}{b} \rho + \frac{a}{b} \frac{\rho}{(1 + b \rho)} \]  
(11)

where \( a \) and \( b \) is determined by the acentric factor and the reduced temperature respectively. The compressibility of fluid is proportional to the factor, \( Y = b^2 / a \). The relevant parameters of pseudopotentials of the MPI scheme for SRK EOS are listed in Table 1.

### 3. Boundary conditions

We begin with a brief discussion on the Standard bounce-back (SBB) scheme which will be tested. We then demonstrate how the fluid–solid interaction forces can be implemented into Zou and He scheme [12] for the pseudopotential model. Finally, the various schemes of fluid–solid interactions are discussed.

#### 3.1. Standard bounce-back

The standard bounce-back (SBB) is the simplest but popular LBM scheme to treat non-slip boundary conditions. It reverses and sends back the distribution functions penetrated to the stationary solid surface. For a fluid node in contact with the wall, the unknown distribution functions, \( f_i \), coming from the solid surface can be found from

\[ f_i(x, t + 1) = f_j(x, t^+). \]  
(12)

where \( i \) is the opposite direction to \( i \) and \( t^+ \) is a post-collision time but before streaming. If the nearest solid nodes are the solid surface especially in complex boundaries, the method is of first-order accuracy [7,8]. However, if the surface line drawn at halfway between the solid and fluid nodes, the second order of accuracy is achieved [9]. It should be noted in the case of a moving boundary, SBB can be applied straightforwardly by taking into account solid to fluid momentum transfer [1].

#### 3.2. Zou and He treatment with interaction force

Zou and He (ZH) [12] proposed a boundary condition scheme, which can be used to set density or velocity at a particular node.
The idea is to find unknown distribution functions with the aid of macroscopic values and known distribution functions. Here, in a D2Q9 lattice, we revisit ZH treatment to incorporate the pseudopotential interaction force. For a solid or boundary node, A, at the bottom of a domain shown in Fig. 1, the distribution functions \( f_2, f_3, \) and \( f_5 \) have to be defined after every collision-and-stream step.

For 2D pseudopotential LBM, we consider interaction forces acting on node A, namely \( F_r \) and \( F_f \). We can set three neighboring nodes at the bottom as three ghost nodes. Ghost nodes are the nodes which are not a part of the physical domain but form a virtual layer around the boundary of the domain. The densities of wall surface nodes are copied on to the nearest ghost nodes to calculate interaction force through Eq. (6). The bounce-back rule is valid for the non-equilibrium part of the distribution function perpendicular to the wall [12],

\[
f_2 = f_4 + \frac{2}{3} \rho v_y. \tag{13}
\]

From Eqs. (3), (4) and (9), it can be found that

\[
\rho = \frac{2(f_0 + f_1 + f_3) + 4(f_4 + f_5 + f_b) - F_y}{2(1 - v_y)}. \tag{14}
\]

\[
f_5 = f_7 + \frac{1}{6} \rho v_y + \frac{1}{2} \rho v_x + \frac{1}{2} (-f_1 + f_3) - \frac{1}{4} (F_x + F_y). \tag{15}
\]

\[
f_6 = f_5 + \frac{1}{6} \rho v_y - \frac{1}{2} \rho v_x + \frac{1}{2} (f_1 - f_3) - \frac{1}{4} (-F_x + F_y). \tag{16}
\]

For a stationary solid node, velocity in the above equations are set to \( v_x = v_y = 0 \). It should be noted that since pseudopotential LBM pressure is directly related to density via EOS, the pressure boundary condition can be applied straightforwardly. However, the velocity component tangent to boundary surface, in this example \( v_x \), should be defined along with the density, or a relation between velocity components should be given, for example, the angle of the velocity vector is known. In such a case, Eq. (14) can be solved for velocity and Eqs. (13),(15), and (16) are treated the same as velocity boundary condition to find \( f_2, f_3, \) and \( f_5 \).

In addition to the intersection of a solid wall and periodic boundary, corner nodes are almost inevitable situations. For a D2Q9 lattice, a corner node leaves five unknown and three known distribution functions. For example, node B placed at the bottom left of the domain in Fig. 2 has \( f_1, f_2, f_5, f_6, \) and \( f_8 \) as unknowns and \( f_3, f_4, \) and \( f_7 \) as known values. To calculate the interaction force on this node, the densities of solid surface nodes are considered for nearby ghost nodes. We set \( v_x = v_y = 0 \) and assume the density of the node is known due to the side pressure (density) boundary or extrapolation over nearby nodes. From the bounce-back rule of non-equilibrium part of both perpendicular distribution functions, we find \( f_2 = f_4, f_1 = f_5 \). Therefore, the rest can be found from Eqs. (3), (4) and (9),

\[
f_5 = f_7 - \frac{1}{4} F_x - \frac{1}{4} F_y. \tag{17}
\]

In pseudopotential LBM, the interaction between liquid and wall is considered to control the wettability of a solid surface in contact with a two-phase fluid. This idea, in fact, mimics the interactions observed at the molecular level and scales up to macro-scale. In the cases where pseudopotential fluid is in the form of the single phase, such as a compressed liquid in contact with stationary solid boundaries, the wettability is less focused but obtaining correct density and velocity profiles along and across the channel are of importance.

The most well-known pseudopotential fluid–solid interactions can be formulated as

\[
F_{fs} = -G_{fs} \frac{\phi_f(x)}{\phi_s(x)} \sum_i \delta_{\rho_i} (x + c_i) \mathbf{w}_i s(x + c_i) c_i. \tag{20}
\]

where \( G_{fs} \) is the amplitude, \( \phi_f \) and \( \phi_s \) are fluid and solid potentials respectively, \( \delta \) is a switch function gives 0 for fluid–fluid interactions and 1 for fluid–solid interactions. If a non-wetting fluid is simulated \( G_{fs} \) should be positive otherwise negative. Marty and Chen [38] defined a fluid–solid interaction force setting \( \phi_f(x) = \rho(x) \) and \( \phi_s = 1 \) for a single component system. Raiksnmäki al. [39] and Sukop al. [40] proposed to replace the fluid density factor with pseudopotential as \( \phi_f(x) = \psi(x) \) and \( \phi_s = 1 \). Kang et al. [41] consider a constant density for solid nodes \( \phi_f(x) = \rho(x) \) and \( \phi_s = \rho_s \) where \( \rho_s \) is an imaginary density set for a solid node. The pseudopotential version of this model is introduced by Benzi et al. [42] where \( \phi_f(x) = \psi(x) \) and \( \phi_s = \psi(\rho_s) \). Li et al. [43] assumed the solid node has a density equal to the fluid node which is interacting with, \( \phi_f(x) = \psi(x) \) and \( \phi_s = 1 \). In this way, the fluid–solid force has the same order of magnitude as fluid–fluid interactions if \( G \) and \( G_{fs} \) are in the same order. They called their interaction model modified pseudopotential-based interaction (m\( \psi \)-based).

Marty and Chen [38] and Kang et al. [41] models are the same because \( \rho_s \) is a constant and can be merged with \( G_{fs} \); they are called density-based interactions. The same applies to versions of Raiksnmäki al. [39] and Benzi et al. [42], pseudopotential-based interactions (\( \psi \)-based), where \( \psi(\rho_s) \) can be considered as the amplitude of the force. Li et al. [43] assessed all these forces regarding static contact angles and found that pseudopotential-based interaction is more suitable for modeling small contact angles and

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**Please cite this article as:** S. Khajepor et al., A study of wall boundary conditions in pseudopotential lattice Boltzmann models, Computers and Fluids (2018), https://doi.org/10.1016/j.compfluid.2018.05.011
\( \psi \)-based interaction performs better than the others for achieving greater contact angles.

When using the ZH boundary condition to construct solid nodes, i.e., imposing the no-slip boundary condition, a density, \( \rho \), for the solid node is calculated by Eq. (14). As such, we define the fluid–solid interaction, ZH-based interaction,

\[
F_{fs} = -G_f \psi (x) \sum_i w_i \psi (x + c_i, \rho \text{ZH}) s(x + c_i) c_i. 
\] (21)

This force similar to modified \( \psi \)-based force keeps the order of magnitude as fluid–fluid interactions which is the most important point of defining such an interaction force [40].

To apply the fluid–solid interactions in the MPI framework, they are considered in the same shape as fluid–fluid interactions. Therefore, Eq. (20) becomes

\[
P_{fs}^{total} = \sum_{j=1}^{n} -G_{f}^{(i)} \phi_{f}^{(j)} (x) \sum_{i=1}^{n} \phi_{f}^{(j)} (x + c_i) w_i s(x + c_i) c_i. 
\] (22)

In this study, the focused interactions are the schemes of \( \psi \)-based interaction, modified \( \psi \)-based interaction, and ZH-based interaction in combinations with either the bounce-back or the ZH boundary treatments.

4. Results and discussion

The boundary treatments discussed in Section 3 are assessed based on their viability in modeling non-ideal fluid flows in 2D channels (Section 4.1) and drop contact angles for two-phase systems (Section 4.2). The results from simulations are discussed in comparison with the analytical incompressible solution. The focused parameters for the flows are compressibility, resolution, density fluctuation, and viscosity. The important parameters for the drop on surfaces are the availability of contact angles, density fluctuation, and the magnitude of spurious velocities.

4.1. Non-Ideal Poiseuille Flow

All simulations are run on a two-dimensional square lattice including nine velocities (D2Q9). The detail of domain sizes for each case will be given individually. The general setting, unless otherwise stated, is listed as follows. The nondimensional relaxation time and lattice spacing parameter are set to unity \( \tau = 1, c = 1 \). ZH pressure boundaries are used for driving force of walled Poiseuille flow. The MPI forces are calculated by use of Eqs. (6) and (7) whose parameters, for the SRK EOS, can be found in Table 1. The internal forces are embedded in the LBE using Eq. (8), which reproduces Navier–Stokes equations to the second order. The thermodynamic values of SRK EOS at the saturation state \( T_b = 0.7 \) are listed in Table 2. The amplitudes of fluid–solid interaction are kept at fluid–fluid interactions \( c_{f}^{(i)} = G_i \) where \( G_i \) is the amplitude of fluid–fluid interaction.

The simulations are run for at least \( 10^5 \) steps and velocity of nodes all over the system is monitored to verify that the equilibrium state is reached by

\[
\frac{v_{\text{max}}(t) - v_{\text{max}}(t-1)}{v_{\text{max}}(t-1)} \leq 10^{-10}.
\] (23)

where \( v_{\text{max}} \) is the velocity magnitude of the node which has the maximum value in the computational domain. The equilibrium time depends on viscosity, domain size, and type of boundary conditions.

We assess the results in comparison with the analytical solution of Poiseuille flow in a no-slip channel. It is assumed that the flow is fully developed and uniform in x direction and pressure drop is linear along the channel \( dp/dx = \Delta p/L_x \). The results from simulations are discussed in comparison with the analytical incompressible solution. The focused parameters for the flows are compressibility, resolution, density fluctuation, and viscosity. The important parameters for the drop on surfaces are the availability of contact angles, density fluctuation, and the magnitude of spurious velocities. The first set of simulations is run for Poiseuille flow where no solid boundary condition is applied [44] as an ideal test case that the fluid itself creates a Poiseuille profile. To do so, we charge MPI fluid in a fully periodic rectangular domain and exert two equal but opposite body forces. The first one only acts on the top half and the other one moves the bottom half. The sketch of the simulation domain is shown in Fig. 3. The body force is added to Eq. (9), thus, \( F_{total} = F_b + F_{MPI} \). Fig. 4 shows the velocity profile for half of the periodic domain. Different results are coming from various channel resolutions \( N_y = 4, 8, 16 \). The errors against resolutions for different relaxation times \( \tau = 0.6, 0.8, 1.1 \) are shown in Fig. 5. The errors show that the pseudopotential LB has the second order of accuracy same as conventional LB. In fact, after inspection of density throughout the domain, we found that no density change is observed in the whole domain in all simulations. It means the pseudopotential forces are neutralizing each other since pseudopotentials are calculated by node density and, therefore, the model acts similar to conventional LB.

4.1.2. Pseudopotential-based interaction

To simulate Poiseuille flow in between two stationary plates, we first employ \( \psi \)-based interaction and set SBB, Eq. (12), at top and bottom of the channel, abbreviated as \( \psi \)-SBB. The MPI fluid at density \( \rho_{\text{init}} = 1.03 \) is initially charged in the channel which is equivalent to 3% compressed water at \( T_b = 0.7 \). The domain size is \( 120 \times 16 \). The flow is driven by pressure (or density) difference at

Table 2: Pressure, density, and temperature of SRK EOS for water at \( T_b = 0.7 \) for \( \alpha = 0.01 \) and \( s = 0.2 \) and \( \omega = 3.44 \). The numbers are in lattice unit, \( \beta_s \) is reduced compressibility.

| \( T \times 10^3 \) | \( T_r \times 10^4 \) | \( \rho_{\text{sat}} \times 10^5 \) | \( \rho \times 10^5 \) | \( \rho_s \times 10^5 \) | \( \rho_t \times 10^5 \) | \( \alpha \) | \( \beta_s(\rho) \times 10^5 \) |
|---------------|---------------|--------------|--------------|--------------|--------------|--------|----------------|
| 7.093690      | 1.013384      | 1.986763     | 4.389998     | 3.786023     | 2.948138     | 1.299605 | 1.353599      | 1.554878 |

Fig. 3. Sketch of the periodic Poiseuille domain.
are found from Eq. (20) which is calculated for each potential of MPI scheme.

Fig. 7(a) depicts profiles of density across the channel at $x = L_x/2$ with $\rho_\text{left} = 1.1\rho_\text{initial}$ for $a = 0.1, 0.01, 0.001$, and $b = 0.2$ i.e. $Y = b^2/a = 0.4, 4, 40$. In the case $Y = 40$, which repulsion part of SRK EOS is dominant and the fluid acts more compressible, the density of fluid from wall decreases smoothly in a parabolic distribution to a minimum density slightly lower than the average density. By increasing the attraction parameter or decreasing $Y$, where the fluid is more approaching to incompressible fluid, the density forms plateau in the center closer to average density but density fluctuations near the wall increases. The velocity profile of these cases are shown in Fig. 7(d). The best agreement with analytical results (incompressible fluid flow) comes from $Y = 0.4$, but with the increase of $Y$ the fluid moves faster than incompressible one.

The relatively same results are observed when $\rho_\text{left} = 0.9\rho_\text{right}$ which are demonstrated in Fig. 7(c). The density of liquid increases from wall density to the average density at the center and decrease of $Y$ moves the profile of density from smooth parabolic shape to flat profile at the center with fluctuations close to the wall. The associated velocity profiles are shown in Fig. 7(f). The best consistency between simulation and the incompressible theory Eq. (24) is for $0.4 < Y < 4$. The worse deviation is seen at the highly compressible fluid, $Y = 40$.

According to Fig. 7(b), the less density gradient is seen across the channel if wall density is set to average density $\rho_\text{left} = \rho_\text{ave}$. However, we show in Section 4.1.3 that this only happens here because the sample is taken at the halfway along the channel. The velocity profiles, seen in Fig. 7(e), stay relatively the same as previous cases.

4.1.3. ZH-based and modified pseudopotential-based interaction

To simulate walls in Poiseuille flow, here, we investigate three cases of fluid–solid treatment: ZH-based fluid–solid interaction coupled with ZH zero velocity (ZH-ZH), modified $\psi$-based interaction with bounce-back (m$\psi$-SBB), and modified $\psi$-based interaction with ZH zero velocity (m$\psi$-ZH). The MPI fluid and inlet (or left), and outlet (or right) boundaries are set the same as Section 4.1.2. The tests focus on density fluctuations across the channel and errors due to resolution, relaxation time, and parameter $Y$. The error is defined as a deviation from macroscopic Poiseuille flow, Eq. (24).

Fig. 8 shows the contours of density field over the computational domain for $\psi$-SBB, m$\psi$-SBB, m$\psi$-ZH, and ZH-ZH treatments. The density variation across the channel for $\psi$-SBB is much larger than the others. It is seen that only around halfway through the channel an almost vertical contour level, 1000($\rho/\rho_\text{ave} - 1$) = 0, is formed. Since the wall density is set at $\rho_\text{left} = \rho_\text{ave}$, that is the location where the density of fluid coincides with the density of the wall. Therefore, any density difference between fluid and solid causes the density fluctuation. Due to high fluid fluctuation, this treatment is not comparable with the others, and hereafter we concentrate on the other treatments.

Fig. 9 demonstrates the density variation across the channel for the three cases ZH-ZH, m$\psi$-SBB, and m$\psi$-ZH. Since at macro-scale desired flow field has a constant density across the channel, we define a simple parameter, fluctuation = $(\rho_{\text{max}} - \rho_{\text{min}})/\rho_{\text{max}}$. In Section 4.1.2, we have seen that at $Y = 0.4$ the system shows highest density fluctuations close to the boundary wall, therefore, this value is chosen for these simulations. The density fluctuation is very small in all of these cases. The schemes of m$\psi$-SBB and m$\psi$-ZH show the same accuracy but ZH-ZH treatment gives one order of magnitude less in fluctuation. Moreover, when using ZH-ZH, the wall density calculated by ZH method will be well in accordance with interior nodes. The jump of density near the wall, filled circles, can be observed in m$\psi$-ZH treatment.

Please cite this article as: S. Khajepor et al., A study of wall boundary conditions in pseudopotential lattice Boltzmann models, Computers and Fluids (2018), https://doi.org/10.1016/j.compfluid.2018.05.011
The error is depicted versus vertical resolution of the domain in Fig. 10. As expected, the error decreases with the increase of domain resolution. ZH-ZH treatment is superior at different resolutions. After that, \( \psi \-SBB \) placed which shows lesser error than \( \psi \-ZH \). It should be noted the horizontal resolution is accordingly increased to make sure that the dynamics of the simulations stay the same.

The effect of relaxation time is shown in Fig. 11. In the range of \( 0.6 \leq \tau \leq 1.1 \), the \( \psi \-ZH \) method shows more error than the others but the error almost reaches a plateau after \( \tau = 0.8 \). Similar behavior is seen for ZH-ZH treatment which has the lowest error. However, \( \psi \-SBB \) error increases proportionally with \( \tau \).

If we increase \( Y \) in SRK EOS, in fact, the compressibility of the liquid is increased which intensify compressibility error of lattice.
Fig. 9. Profile of density across the channel for three boundary treatments ZH-ZH, mψ-SBB, and mψ-ZH. The filled circle and triangles represent wall nodes defined by ZH boundary treatment.

Fig. 10. Error due to vertical resolution of the channel for three boundary treatments ZH-ZH, mψ-SBB, and mψ-ZH.

Fig. 11. Error due to change of relaxation time for three boundary treatments ZH-ZH, mψ-SBB, and mψ-ZH.

Fig. 12. Error due to parameter Y for three boundary treatments ZH-ZH, mψ-SBB, and mψ-ZH.

Boltzmann. Such behavior can be seen in Fig. 12 which demonstrates the error dependency to parameter Y. ZH-ZH treatment is better than the others and mψ-SBB is placed after mψ-ZH.

4.2 Wettability assessment

For two-phase systems, the selected boundary conditions are assessed regarding achievable contact angles, density behavior near the wall, and spurious velocities. The domain size is considered as 300 × 100 in lattice unit (lu). Top and bottom of the domain are wall boundary conditions. Left and right boundaries are periodic. The nondimensional relaxation time and lattice spacing parameter are set to unity τ = 1, c = 1. A drop with the radius of R = 30 lu is placed on the wall while it is wetting the surface slightly, so the drop center is (x_c, y_c) = (Lx/2, R − 5). As the initialized system is not in the perfect equilibrium state, there is a slight pressure wave forming at the beginning of the simulation which may cause the drop to separate from the surface. To avoid such a problem, a small gravity force, G = −10^{-6} lu, is exerted in the system which is removed after a few thousand steps. For the case of mψ-SBB, mψ-ZH, and ZH-ZH the wettability of the surface is controlled via G_{fs}^{(j)} = A_C × G_j, where A_C is a multiplier and G_j is the amplitude of fluid–fluid interaction. For the case of ψ-SBB, G_{fs}^{(j)} = G_j and the wettability is controlled via density of the solid wall as a function of vapor density, ρ_v = A_p × ρ_0, where A_p is an arbitrary multiplier. The fluid thermodynamic properties are mentioned in Table 3.

The results from the simulations of a static drop on surfaces made with different boundary conditions can be found in Figs. 13–16. It is identified that the drop forms a wide range of contact angles from ~15° to ~180°. When the contact angle approaches 180°, it becomes difficult to keep the drop near the wall because of hydrophobicity. The density of the drop and the vapor around it are deviated from the free drop state due to the change in solid–liquid and solid–vapor surface tension forces, γ_sl and γ_sv respectively.

The effect of fluid–solid interaction strength, which is presented by A_C for the schemes of mψ-SBB, mψ-ZH, and ZH-ZH and A_p for the scheme of ψ-SBB, on contact angles are summarized and plotted on Figs. 17 and 18. It shows that both A_C and A_p play the same role because the stronger the fluid–solid interactions, the smaller the contact angles. The sound correlations between contact angles and the fluid–solid interaction strengths can be formulated as the polynomial, \( \theta = \sum_{i=0}^{3} k_i A^i \), where A is A_C or A_p, and the values of k_i are listed in Table 4.

Please cite this article as: S. Khajepor et al., A study of wall boundary conditions in pseudopotential lattice Boltzmann models, Computers and Fluids (2018), https://doi.org/10.1016/j.compfluid.2018.05.011
Table 3
Pressure, density, and temperature of SRK EOS for water at $T_b = 0.7$, $a = 0.04$, $b = 0.2$ and $\omega = 0.344$. The numbers are in lattice unit. $\rho_b$ is reduced compressibility.

| $T \times 10^2$ | $T_b \times 10^2$ | $\rho_b \times 10^4$ | $\rho_b^m \times 10^4$ | $\rho_b^m \times 10^2$ | $\rho_b$ | $\alpha$ | $\rho_b(\rho_b^m) \times 10^2$ |
|----------------|------------------|----------------------|-----------------------|------------------------|--------|-------|--------------------------|
| 2.837476       | 4.053537         | 7.947053             | 1.755999              | 3.786023               | 2.948138 | 1.299605 | 1.353599                 | 1.554878 |

Table 4
The parameters of the correlations of the contact angle with interaction strengths.

| Boundary condition scheme | $k_0$ | $k_1$ | $k_2$ | $k_3$ | $A$ | Adjusted R-Squared |
|---------------------------|-------|-------|-------|-------|-----|-------------------|
| ZH-ZH                     | 2620.29 | -7408.23 | 7574.99 | -2698.99 | $A_\theta$ | 1.0 |
| $\psi$-SBB                | 488.45  | -622.12 | 198.91  | 0.0    | $A_\theta$ | 0.99 |
| $\psi$-ZH                 | 553.29  | -774.01 | 277.58  | 0.0    | $A_\theta$ | 0.99 |
| $\psi$-SBB                | 166.020 | -2.067  | 0.006   | 0.0    | $A_\theta$ | 0.998 |

Fig. 13. A static drop on surfaces with different levels of wettability. By changing the density of the wall, $\rho_b$, $\psi$-SBB boundary condition creates different contact angles. (a) $A_\theta = 100$, $\theta = 21^\circ$ (b) $A_\theta = 70$, $\theta = 52.30^\circ$ (c) $A_\theta = 50$, $\theta = 76.75^\circ$ (d) $A_\theta = 30$, $\theta = 110.92^\circ$ (e) $A_\theta = 10$, $\theta = 144.52^\circ$ (f) $A_\theta = 4$, $\theta = 161.38^\circ$.

Fig. 14. A static drop on surfaces with different levels of wettability. By changing the multiplier of fluid–solid interactions, $A_\theta$. $\psi$-SBB boundary condition creates different contact angles. (a) $A_\theta = 1.3$, $\theta = 15.2^\circ$ (b) $A_\theta = 1.1$, $\theta = 45.46^\circ$ (c) $A_\theta = 0.9$, $\theta = 90.02^\circ$ (d) $A_\theta = 0.8$, $\theta = 115.97^\circ$ (e) $A_\theta = 0.7$, $\theta = 148.35^\circ$ (f) $A_\theta = 0.66$, $\theta = 167.66^\circ$.

Fig. 15. A static drop on surfaces with different levels of wettability. By changing the multiplier of fluid–solid interactions, $A_\theta$. ZH-ZH boundary condition creates different contact angles. (a) $A_\theta = 1.25$, $\theta = 20.55^\circ$ (b) $A_\theta = 1.0$, $\theta = 57.56^\circ$ (c) $A_\theta = 0.9$, $\theta = 83.33^\circ$ (d) $A_\theta = 0.8$, $\theta = 110.98^\circ$ (e) $A_\theta = 0.7$, $\theta = 145.42^\circ$ (f) $A_\theta = 0.66$, $\theta = 165.94^\circ$.

Fig. 16. A static drop on surfaces with different levels of wettability. By changing the multiplier of fluid–solid interactions, $A_\theta$. ZH-ZH boundary condition creates different contact angles. (a) $A_\theta = 1.14$, $\theta = 18.7^\circ$ (b) $A_\theta = 1.08$, $\theta = 55.51^\circ$ (c) $A_\theta = 1.02$, $\theta = 80.09^\circ$ (d) $A_\theta = 0.92$, $\theta = 114.93^\circ$ (e) $A_\theta = 0.84$, $\theta = 142.46^\circ$ (f) $A_\theta = 0.79$, $\theta = 164.7^\circ$.

Except for the scheme of ZH-ZH, a parabolic correlation works well for the curve-fitting. The contact angle created by ZH-ZH scheme is larger than those by schemes of $\psi$-SBB and $\psi$-ZH when $A_\theta > 1.1$ and it is smaller for $A_\theta < 1.1$. The contact angle is more sensitive to the interaction strength as the slope of contact angle-$A_\theta$ for ZH-ZH scheme is much steeper than those of the other schemes.

Fig. 19 depicts the density change about the drop–wall contact line. Higher than $y/\Delta y = 7$, all schemes showing the density of their drops. However, getting closer to the wall at $y/\Delta y = 6$, hydrophobic $\psi$-SBB deviates quickly from the drop density. The more hydrophilic, the less deviation is seen from $\psi$-SBB. The width of the solid–liquid interface is in the range of 1–5 lattices. The boundary schemes of $\psi$-SBB and $\psi$-ZH affect density profiles almost identically. Their first deviation is seen at $y/\Delta y = 4$ in their hydrophobic version. They get closer to drop density by decreasing hydrophobicity. However, the very hydrophilic surface of them can create densities greater than inside of the drop. In these cases, the width of the solid–liquid interface is 1–3 lattices. This scenario is generally true for the ZH-ZH method but with considerable less deviation. The hydrophobic version of ZH-ZH separates at $y/\Delta y = 3$. The width of the solid–liquid interface, in a wide range of contact angle, is only 1–2 lattices. It should be noted that a smaller density deviation is generally more desirable as it describes a scale much bigger than molecular levels.

Fig. 20 demonstrates the magnitude of maximum spurious velocity, $|u_{\text{max}}|$, in the domain as a function of contact angle for different methods. $|u_{\text{max}}|$ is normalized with the magnitude of the velocity.
Fig. 17. Contact angle as a function of $A_0$ for $\psi$-SBB, $\psi$-ZH, and ZH-ZH boundary conditions. The lines are polynomial functions fitted onto the results.

Fig. 18. Contact angle as a function of $A_0$ for boundary conditions $\psi$-SBB boundary condition. The line is a parabola function fitted on the results.

Fig. 19. Profiles of density change near the wall along a vertical line passing the center of the drops for $\psi$-SBB, $\psi$-SBB, $\psi$-ZH, and ZH-ZH boundary conditions. Density, $\rho$, for each case is normalized by the density of its drop, $\rho_{\text{drop}}$, because $\rho_{\text{drop}}$ is different in different cases.

Fig. 20. Maximum spurious velocity as a function of contact angle for $\psi$-SBB, $\mu$-SBB, $\mu$-ZH, and ZH-ZH boundary conditions. The magnitude of maximum spurious velocity, $|u_{\text{max}}|$, normalized by the magnitude of the maximum spurious velocity of a free drop $|u_{\text{max}}^{\text{Free drop}}|$.

Fig. 21. Contact radius as a function of time for a drop which is put on surfaces with different equilibrium contact angles using ZH-ZH boundary conditions. $R$ is the drop radius. Time is normalized with the aid of inertial time $t_\rho = \sqrt{\rho R^2 t}$. The curves are fitted based on the power law equation $r/R = C(t/t_\rho)^\gamma$.

maximum spurious velocity of the same drop in a periodic domain without wall boundary conditions, $|u_{\text{Free drop}}|$. For the cases $\psi$-SBB and ZH-ZH and $\theta > 50^\circ$, the maximum spurious velocity is almost equal to that of a free drop. For smaller angles $\theta \leq 50^\circ$, spurious velocities of ZH-ZH grow linearly in contrast to $\psi$-SBB which decreases linearly. Both $\mu$-SBB and $\mu$-ZH show a considerable increase of spurious velocities at lower angles about 6 times and 8 times, respectively, of what is seen in the free drop. Their magnitude decreases with the decrease of hydrophilicity, but they are still much bigger than those from the $\psi$-SBB and ZH-ZH.

We test the applicability of ZH-ZH in dynamic wetting processes. A drop is placed on a hydrophobic surface to form a contact angle about $\theta \approx 180^\circ$. When the system reaches equilibrium, it is considered as the initial state for three different surfaces: $\theta = 114.9^\circ$, $\theta = 64.2^\circ$, $\theta = 18.7^\circ$. In each case, we monitor dynamic spreading of the drop and record contact radius, $r$, which is the radius of the wetted area. Based on Tanner’s law [45–47] at the final stage, a drop spreads on a very wettable surface $\theta = 0^\circ$ with the relationship $r \sim t^{1/2}$ in 3D cases and $r \sim t^{1/3}$ in 2D cases. However, during the initial stage of spreading, the capillary force is at its maximum to reshape the drop. Therefore, the drop spreads faster.
at the early stage. Experiments and simulation results of references [48,49] showed that, for a fully wetting surface, relationship \( r \sim t^{1/2} \) is dominant during the initial stage and, for partially wetting surfaces, the exponent, 1/2, decreases with the increase of the static contact angle. The results from our simulations on this dynamic wetting are given in Fig. 21. The data are analyzed with the aid of \( r/R = C(t/t_p)^n \) where \( t_p = \sqrt{\rho R/g} \) is the inertial time scale. \( R \) is the initial drop radius, and \( \gamma \) is surface tension, and \( C \) and \( n \) are free parameters, which can be determined from curve-fitting. In all three cases, we see the linear behavior at the beginning; it has the exponent of \( n = 0.5 \) for the very wettable surface, \( \theta = 18.7^\circ \). The exponent decreases to \( n = 0.46 \) for \( \theta = 64.2^\circ \) and further down to \( n = 0.38 \theta = 114.9^\circ \) which is generally in good agreement with experiment observations.

5. Conclusion

We have chosen the two most popular boundary treatments, SBB and ZH. They are combined with fluid–solid interaction forces originating from SC model. These boundary treatments are compared and assessed in two scenarios: Poiseuille flow for compressed liquids and contact angles achieved by putting a drop on wettable surfaces. The MPI scheme with SRK EOS is utilized to model water. Three force interactions between fluid and solid are considered, the \( \psi \)-based, the modified \( \psi \)-based, which are found in the literature, and the ZH-based which is proposed and defined by this study. For a hydrodynamic study, the criterion is closeness to single-phase macroscopic Poiseuille flow and, for a hydrostatic study, the availability of drop contact angles is considered.

The periodic Poiseuille flow is studied as an ideal Poiseuille flow which is purely made of LB equation without boundary conditions. It is shown that the pseudopotential LB method is second-order accurate as density is constant all over the channel and the method coincides with conventional LB without pseudopotential interactions.

\( \psi \)-based interaction along with SBB gives high-density gradient and fluctuations near the wall. The choice of wall density plays the key role. The closer it is to the neighboring fluid nodes, the less fluctuation is observed which makes it difficult to use in complex geometries. The velocity profile is very close to analytical Poiseuille flow unless the parameter \( Y \) is greatly increased which makes the fluid more compressible and consequently strengthens the compressibility error of LB method.

The density fluctuations of ZH-ZH, \( m\psi \)-SBB, and \( m\psi \)-ZH, in the channel, are far less than and not comparable to those from \( \psi \)-SBB. Therefore, those three treatments are studied together. The performance of them assessed based on density variation across the channel, and error because of domain resolution, relaxation time, and Y parameter. ZH-ZH in all cases is superior. It has one order of magnitude less density across the channel in comparison with others. It shows less error in different resolutions, a low relaxation time dependency and less compressibility error. In all cases, \( m\psi \)-ZH takes the third place after \( m\psi \)-SBB.

For a drop on wettable surfaces, all boundary treatments successfully form a wide range of contact angles. The profiles of the contact angle versus the interaction strength can be formulated with cubic and parabolic polynomial. \( \psi \)-SBB shows largest density deviation near the wall. ZH-ZH keeps the density close to drop density. The schemes of \( m\psi \)-SBB and \( m\psi \)-ZH show the same density behavior and are placed between \( \psi \)-SBB and ZH-ZH. Spurious velocities of \( m\psi \)-SBB and \( m\psi \)-ZH are considerably higher (about 6 and 8 times at lower contact angles) than a free drop while \( \psi \)-SBB and ZH-ZH effects on spurious velocities are negligible. ZH-ZH is tested for a dynamic drop-spreading process. It successfully follows the power law which is seen in the literature.

To summarize, ZH-ZH shows best results in the Poiseuille flows and wettability tests. The schemes of \( m\psi \)-SBB and \( m\psi \)-ZH act well in single-phase flow, however, if there is two-phase interaction near the wall, they tend to intensify spurious velocities. The scheme of \( \psi \)-SBB demonstrates a large density fluctuation/deviation near the wall when there are density gradients in a simulation domain.

Acknowledgments

This research has received funding from the European Union’s Horizon 2020 Research and Innovation Programme under grant agreement no. 654462 STEMM-CCS, supported by the FP7 Cooperation Work Programme under grant no. 265847-FP7-OCEAN, the Natural Environment Research Council under grant no. NE/H013970, and the Research Council of Norway through the CLIMIT Program BayMoDe project no 254711.

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