Introduction to Perl module lb2d.pm 0.1 for basic Lattice Boltzmann simulations

Danilo Sergi
University of Applied Sciences (SUPSI), The iCIMSI Research Institute, Galleria 2, CH-6928 Manno, Switzerland
(Dated: February 4, 2014)

The Lattice Boltzmann method has been gaining acceptance for hydrodynamic problems involving complex boundaries, non-equilibrium dynamics and interfacial phenomena in multiphase or multicomponent systems. lb2d.pm is a Perl module offering a clear framework for simple Lattice Boltzmann simulations in 2D. The syntax and some basic applications are presented. Mainly, the new version 0.1 enables solute transport and accounts for reactive boundaries leading to surface growth.
I. INTRODUCTION

The present document aims at making viable the use of the module lb2d.pm [1], version 0.1. This is a module for the scripting language Perl that allows to investigate readily simple systems by the Lattice Boltzmann method.

In the next section, we provide a brief account of the theory, along with the basic operations relevant for computations.

In Sec. [III] are listed all the commands, accompanied with a description. The commands are presented in the order they are more likely to be used in a general program. They can be organized into groups as follows:

- Initialization: lattice, processors, read_data, fluids, solute, inlet, outlet, inlet_momentum, outlet_momentum, inlet_solute, outlet_solute, boundary_style, obstacle, surface_reaction, position0, momentum0, concentration0
- Force fields: aveforce, aveacceleration, interface, adhesiveforce, intersolute
- Output: thermo, log, output, write_restart
- Action: iteration

This section should be read at least once completely from the beginning to the end. The examples are given in Perl syntax. In the doubt that it could be expected from us, we say that we tried to reproduce some aspects of the syntax of the molecular dynamics code LAMMPS [2]. The version 0.1 can treat solute transport and surface reaction. The new commands are solute, inlet_solute/outlet_solute, surface_reaction, concentration0 and intersolute. The existing commands read_data, fluids and output have been modified.

In the section Applications, we present some examples worked out in the framework of the module lb2d.pm. In the section Scripts, we discuss the programs used to generate and analyze the data for the proposed case studies.

For more details on the Lattice Boltzmann method, the interested reader is especially addressed to the books [3][4]

- M.C. Sukop and D.T. Thorne Jr., Lattice Boltzmann Modelig: An Introduction for Geoscientists and Engineers, Springer Verlang, Berlin Heidelberg 2010.

- S. Succi, The Lattice Boltzmann Equation for Fluid Dynamics and Beyond, Oxford University Press, Oxford 2009.

This work was committed by iCIMSI-SUPSI for research projects in the fields of mechanical engineering and materials science. The module is freely available at [https://sites.google.com/site/lbmodule/](https://sites.google.com/site/lbmodule/) Questions, comments or suggestions can be sent to lb.module@gmail.com
II. MODEL AND ALGORITHM

The Lattice Boltzmann method is based on the Lattice Boltzmann equation

$$f_i(r + e_i \Delta t, t + \Delta t) = f_i(r, t) \underbrace{- \frac{1}{\tau} \left[ f_i(r, t) - f_{eq}^i(r, t) \right]}_{\text{streaming}} \overbrace{- \frac{1}{\tau} \left[ f_i(r, t) - f_{eq}^i(r, t) \right]}^{\text{collision}}.$$  \hfill (1)

\(\tau\) is the relaxation time; \(r = (x, y)\) are the coordinates of the node of a square lattice. The vector \(e_i\) defines the direction of the \(i\)-th velocity mode. The distribution function of a velocity mode in space and time is given by \(f_i(r, t)\). In the above equation, the first term on the right-hand side accounts for streaming, that is, free propagation, while the second one describes collisions in the BGK approximation [5].

The number of velocity modes and the form of equilibrium distribution functions depend on the specific model. In the d2q9 model, the systems are 2D and there are nine velocity modes. In the module, the equilibrium distribution functions are computed by means of the formula

$$f_{eq}^i(r) = w_i \rho(r) \left[ 1 + \frac{e_i \cdot u}{c_s^2} + \frac{1}{2} \frac{(e_i \cdot u)^2}{c_s^4} - \frac{1}{2} \frac{u^2}{c_s^2} \right] \quad i = 0, \ldots, 8.$$  \hfill (2)

The \(w_i\)'s are weighting factors given by \(w_0 = 4/9, w_i = 1/9\) for \(i = 1, 2, 3, 4\) and \(w_i = 1/36\) for \(i = 5, 6, 7, 8\). \(c_s = 1/\sqrt{3}\) [lu/ts] is the speed of sound. The density and velocity at a given node read respectively

$$\rho(r) = \sum_{i=0}^{8} f_i(r) \quad \text{and} \quad u(r) = \frac{1}{\rho(r)} \sum_{i=0}^{8} f_i(r) e_i.$$  

To keep the notation simple, we omitted the time dependence.

Figure 1 outlines the basic steps of the method employed for computations. After initialization of the system, to every lattice site are attributed its equilibrium distribution functions obtained from Eq. (2). Then, for every lattice site, free propagation is executed. If a velocity mode reaches an obstacle, it is again propagated according to the selected boundary style. (These two steps are performed inside the same loops and shall be referred to as streaming step in the sequel.) Finally, the equilibrium distribution functions are computed with Eq. (2) and the collision term is evaluated. This scheme is repeated from the streaming procedure for the number of timesteps.

![Figure 1](image-url)

Figure 1: Steps of the algorithm for the Lattice Boltzmann dynamics as implemented in the module.
III. COMMANDS

**lattice command**

Syntax:
lattice(style,Nx,Ny,tau)

- style=d2q9
- \(N_x, N_y\)=width of the simulation domain in the directions of \(x\) and \(y\) axes
- \(\tau\)=relaxation time

Example:
&lattice("d2q9",100,100,1);

Description:
This command defines the style of the underlying lattice and the size of the rectangular simulation domain. The last argument fixes the relaxation time \(\tau\).

For the style d2q9, the velocity modes are identified as shown in Fig. 2.
The lattice sites are numbered from 0 to \(N_x (N_y)\).

By default, the boundaries of the simulation domain are periodic.

This command must appear in every script. If this command is used before the read_data command, the definitions of the last three arguments are overridden if the sections relaxation_time and domain are present in the input data file. This command must precede the command processors, otherwise the simulation is interrupted with an error message.

Related commands:
processors read_data

**processors command**

Syntax:
processors(px,py)

- \(px,py\)=\# of processors along each axis

Example:
&processors(3,1);

Description:
With this command the simulations are run in parallel. Specifically, the initialization, streaming and collision steps of the basic algorithm (see Fig. 1) are executed using \(p_x \times p_y\) processors. The principle of space decomposition of the simulation domain is

![Figure 2: Velocity modes for the lattice d2q9.](image-url)
applied. For example, let \( q_x \) and \( r_x \) be integer numbers such that \( N_x = q_x p_x + r_x \). So, the \( x \) side of every subdomain counts \( q_x \) nodes with the exception of the last ones with \( x \geq q_x(p_x - 1) \): in this case the side length is of \( q_x + r_x + 1 \) nodes. The same rule is applied for the other directions.

If this command is used with the serial version of the module, it is disregarded. The parallel version of the module needs a multicore processor and the ForkManager module \(^5\). This command must be used in every script being executed with a parallel version of the module. This command must precede any other command initializing density and momentum: i.e., inlet_momentum/outlet_momentum and momentum0. This command must follow the lattice command.

Warnings: At line 2 of the parallel version of the module, the path of the ForkManager module must be specified. On Windows operating systems we incurred in registry problems.

Related command:
lattice

**read data command**

Syntax:

```
read data(file,arguments)
```

- file=name of data file to read in
- arguments=fluids,solute,equilibrium

Examples:

```
&read data(“../Input/data”);
&read data(“restart.separation”,”fluids”);
&read data(“restart.diffusion”,”solute”,”fluids”);
&read data(“data.separation”,”equilibrium”,”fluids”);
&read data(“data.diffusion”,”solute”,”equilibrium”,”fluids”);
```

Description:

With this command it is defined the starting configuration of the system, partly or completely. The additional arguments fluids, solute and equilibrium can be given in any order. With the additional argument equilibrium, all distribution functions are replaced with their equilibrium values for both fluid flow and solute transport (see Fig. 1). With an additional argument of type fluids, the files defining the state of a two-component system are read in (see write_restart command). For fluid flow, the information of the input data file must be organized into nine sections: relaxation_time, domain, processors, inlet, outlet, boundary, field, density, momentum.

The relaxation_time section is defined as follows:

```
relaxation_time
```

\( \tau_{\alpha} \)

In the case of multicomponent systems, it is possible to specify an additional parameter \( \alpha_{\sigma} \) controlling the density ratio between the substances \( \sigma = 1, 2 \) (see fluids command).

The domain section is defined as follows:

```
domain
```

\( N_x N_y \)

The processors section is defined as follows:

```
processors
```

\( p_x \) and \( p_y \) define the grid of processors.

The inlet and/or outlet sections are defined as follows:

```
inlet
```

```
wall x_0 x_1 label style arguments
```

```
outlet
```

```
wall x_0 x_1 label style arguments
```

Details can be found in the explanation of the commands inlet/outlet and inlet_momentum/outlet_momentum.

The boundary section is defined as follows:

```
boundary
```
style1 argument style2

noslip, slip, mixed and periodic are the available styles. An additional argument is necessary for the mixed style with only one reflection coefficient.

The field section is defined as follows:

text

The density section is defined as follows:

text

The momentum section is defined as follows:

text

The section domain must precede the section processors. If present, the section field must follow the section relaxation_time; the section processors must precede the sections density and momentum; and the section boundary must precede the section density. In all other cases, the sections and their items can be given in any order.

If the read_data command appears before the lattice command and the input file contains the sections relaxation_time and/or domain, this information is overridden. If the input file contains the section processors, the command processors does not redefine the grid of processors. It is possible to redefine the grid of processors of a previous simulation by modifying manually the restart file. If the input file contains force and/or acceleration in the section field, the commands aveforce and aveacceleration in the script add further contributions to the applied forces. If the input file contains interforce and/or adhesiveforce in the section field, the commands interforce and adhesiveforce in the script redefine the parameters $G$, $\psi_0$ and $\rho_0$.

With an additional argument of type solute, the file defining the solute state is read in (see write_restart command). For solute transport, the information of the input data file must be organized into seven sections: relaxation_time, inlet, outlet, reaction, field, concentration and solute_modes.

The relaxation_time section is defined as follows:

text

The inlet and/or outlet sections are defined as follows:

inlet

wall $x_0$ $x_1$ label style arguments

outlet

wall $x_0$ $x_1$ label style arguments

The details are explained in the description of the commands inlet/outlet and inlet_solute/outlet_solute.

The reaction section is defined as follows:

reaction

surface $k_r C_s$ style $b_{\text{max}}$

The various parameters are introduced in the description of the command surface_reaction. This section must precede the section concentration.

The field section is defined as follows:

field

intersolute $G$ $\psi_0$ $C_0$

The parameters are introduced in the description of the command intersolute.

The concentration section is defined as follows:
concentration
\( x \ y \ C \ b \)
x and \( y \) are the coordinates of the lattice site and \( C \) its solute concentration. In the case of surface reaction, \( b \) is the cumulated mass on nodes belonging to the solid surface; for the fluid phase \( b \) vanishes. This quantity is omitted in the absence of surface reaction. For clarity, we suggest to set equal to zero the concentration of the solid nodes not lying on the surface. This section must follow the section reaction.

The solute_modes section is defined as follows:

\[ x \ y \ g_1 \ g_2 \ g_3 \ g_4 \]
x and \( y \) are the coordinates of the lattice site. On a d2q4 lattice, \( g_1, \ldots, g_4 \) are the solute distribution functions. For clarity, we suggest to set all the distribution functions equal to zero for the solid nodes not lying on the surface.

Also for solute transport, the section field must follow the section relaxation_time. In a script, if the solute command is used after the read_data command, the relaxation time is modified. If the input file contains intersolute in the section field, the command intersolute in the script redefines the parameters \( G \), \( \psi_0 \) and \( C_0 \). The same holds for the section reaction and the corresponding command surface_reaction.

In general, the name of a section must be separated by at least one new line character from the data. Different numeric values must be separated by at least one white space character or tabular character. For example, the following line is wrong:

relaxation_time 1

The following lines are instead read correctly:

density
1 0 84.111

The restart file of a previous simulation can be used as input file of a subsequent simulation.

Related commands:
inlet/outlet inlet_momentum/outlet_momentum surface_reaction aveforce aveacceleration interforce adhesiveforce intersolute write_restart

**fluids command**

Syntax:

\[ \text{fluids}(\tau_1, \tau_2, \alpha_1, \alpha_2) \]

- \( \tau_1 = \) relaxation time fluid 1
- \( \tau_2 = \) relaxation time fluid 2
- \( \alpha_1 = \) parameter controlling density ratio
- \( \alpha_2 = \) parameter controlling density ratio

Examples:

&fluids(1,2);
&fluids(0.626,2.5,4/9,0.8);
&fluids(1,1,0,0.998);

Description:

With this command it is possible to simulate systems containing two substances. Details on the formalism can be found in Refs. [3, 7, 8]. If the parameters \( \alpha_\sigma \) are omitted, they are set to \( \alpha_\sigma = 4/9 \) for both fluid components \( \sigma = 1, 2 \). In this case, the equilibrium distribution functions are given by Eq. [2] but using a different velocity. In general, the equilibrium distribution functions take the form [9, 10]

\[
\tilde{f}_i^{\sigma,eq}(\rho_\sigma, \mathbf{u}_\sigma^eq) = w_i \rho_\sigma(r, t) \left[ A_i^\sigma + 3 e_i \cdot \mathbf{u}_\sigma^eq + \frac{9}{2} (e_i \cdot \mathbf{u}_\sigma^eq)^2 - \frac{3}{2} \mathbf{u}_\sigma^eq \cdot \mathbf{u}_\sigma^eq \right] \quad i = 0, \ldots, 8 .
\]

The factors \( w_i \) are the usual weights for the d2q9 lattice (see Eq. [2]). \( \sigma \) designates the fluid component. \( \rho_\sigma \) is the local density; \( \mathbf{u}_\sigma^eq \) is the equilibrium velocity determined as explained in Refs. [3, 7, 8]. The coefficients \( A_i^\sigma \) are given by \( A_0^\sigma = (9/4) \alpha_\sigma \) for \( i = 0 \); \( A_i^\sigma = (9/5)(1 - \alpha_\sigma) \) for \( i = 1 - 8 \). The sound speed of the \( \sigma \)-th component becomes \( (c_s^\sigma)^2 = (3/5)(1 - \alpha_\sigma) \).
**solute command**

Syntax:
solute(taus)

- taus=relaxation time for solute transport

Example:
&solute(1);

Description:
This command enables solute transport for one single species. The relaxation time for solute $\tau_s$ determines the diffusion coefficient

$$D = \frac{1}{2} \left( \tau_s - \frac{1}{2} \right).$$

Solute transport is accounted for using the distribution functions $g_i$ defined on a d2q4 lattice [11]. The dynamics develops through two steps, namely streaming and collision (see Fig. 1). As for fluid flow, the evolution is governed by the BGK equation [5]

$$g_i(r + e_i \Delta t, t + \Delta t) = g_i(r, t) - \frac{1}{\tau_s} \left[ g_i(r, t) - g_i^{eq}(C, u) \right], \quad i = 1, \ldots, 4.$$

In the collision term, the equilibrium functions are of the form [11]

$$g_i^{eq}(C, u) = \frac{1}{4} C [1 + 2 e_i \cdot u], \quad i = 1, \ldots, 4.$$ (3)

The concentration $C$ is given by

$$C(r, t) = \sum_{i=1}^{4} g_i(r, t).$$

$u$ is the velocity of the solvent. In the multicomponent case, it is given by [12]

$$u(r, t) = \left( \sum_{\sigma} \left[ \rho_{\sigma}(r, t) u_{\sigma}(r, t) + \frac{1}{2} F_{\sigma}(r, t) \right] \right) / \sum_{\sigma} \rho_{\sigma}(r, t).$$ (4)

$\rho_{\sigma}$ designates the local density of the fluid components; $F_{\sigma}$ is the force experienced by the fluid component denoted by $\sigma$. The fluid velocity of the $\sigma$-th component is

$$u_{\sigma}(r, t) = \frac{1}{\rho_{\sigma}(r, t)} \sum_{i} f_i^{\sigma}(r, t) e_i.$$

More details on the theory for solute transport can be found in Refs. [11][13][16].

At the surface of the solid phase, the bounce-back rule is applied, unless the surface reaction is enabled.

Related commands:
inlet_solute/outlet_solute surface_reaction boundary_style concentration0

**inlet/outlet commands**

Syntax:
inlet(wall,x0,x1,label1,label2)
outlet(wall,x0,x1,label1,label2)

- wall=xhi,xlo,yhi,ylo is the wall of the simulation domain where the opening lies
- $x_0 < x_1$ =coordinates of the extremities of the opening ($y_0 < y_1$ for xhi and xlo)
- label1=number or string referencing the opening
Figure 3: Hierarchy among the commands of initialization. A command points to another one when it overrides its previous definitions.

- label2=number or string referencing the opening for the second fluid

Examples:
&inlet("xhi",5,10,11);
&outlet("ylo",3,50,"out1");
&inlet("xlo",1,49,"in1","in2");
&inlet("ylo",1,49,11,12);

Description:
With these commands the location of the inlet and/or outlet openings is defined. They override the previous settings via the read_data command as illustrated in Fig. 3.

In the multicomponent case, it is necessary to give two labels, one for every fluid component.

Related commands:
inlet_momentum/outlet_momentum position0 momentum0

inlet_momentum/outlet_momentum commands
Syntax:
inlet_momentum(label,style,arguments)
outlet_momentum(label,style,arguments)

- label specifies the opening previously defined with the commands inlet/outlet
- style=poiseuille, uniform, dirichlet and gradient are available for both inlet and outlet
- arguments depend on the style of the opening:
  - If the opening is of style poiseuille, it is necessary to specify the maximal velocity $v_{\text{max}}$ and the initial density $\rho$ at the opening nodes.
  - For the uniform style, it is necessary to give the velocity and the initial density $\rho$ of the opening nodes.
  - dirichlet means constant pressure. In this case, it is necessary to specify the initial density $\rho$ to hold constant at the opening nodes.
  - For the gradient style, it is necessary to enter the initial density of the opening nodes.

Examples:
&inlet_momentum("in1","poiseuille",0.07,24);
&inlet_momentum(100,"uniform",0.05,24);
&inlet_momentum("in3","dirichlet",24.25);
&outlet_momentum("out3","dirichlet",24);
&outlet_momentum("out2","gradient",24);

Description:
These commands determine how to update the momentum at the nodes of the inlet and/or outlet openings. More precisely, for an inlet opening on the wall xlo, after streaming and the treatment of collisions with solid boundaries the velocity modes $f_1$, $f_3$
and \( f_8 \) remain undetermined. For the styles poiseuille and uniform, they are updated according to the following rules [17]:

\[
\rho = \frac{1}{1-v_x} \left[ f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7) \right],
\]

\[
f_1 = f_3 + \frac{2}{3} \rho v_x,
\]

\[
f_5 = f_7 - \frac{1}{2} (f_2 - f_4) + \frac{1}{6} \rho v_x,
\]

\[
f_8 = f_6 + \frac{1}{2} (f_2 - f_4) + \frac{1}{6} \rho v_x.
\]

\( v_x \) is the velocity imposed at the inlet node. For the poiseuille style we have

\[
v_x(y) = \frac{4v_{\text{max}}}{(y_1 - y_0 + 1)^2} \left[ \left( \frac{y_1 - y_0 + 1}{2} \right)^2 - \left( \frac{2y - y_1 - y_0}{2} \right)^2 \right] \quad \text{for} \; y = y_0, \ldots, y_1.
\]

The velocity \( v_x \) is of course constant in the uniform case. The collision step is then performed including also the nodes of the opening [17]. For the other walls, the formulas are given in Appendix A.

For the style dirichlet, the pressure \( P \) is kept constant at the inlet and/or outlet openings \( (P = c_s^2 \rho) \). Let us consider the wall xhi for example. After streaming, the velocity \( v_x \) and the populations \( f_3, f_6, f_7 \) are unknown. They are determined as follows:

\[
\rho = \frac{1}{1-v_x} \left[ f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7) \right] - 1,
\]

\[
f_3 = f_1 - \frac{2}{3} \rho v_x,
\]

\[
f_6 = f_8 + \frac{1}{2} (f_4 - f_2) - \frac{1}{6} \rho v_x,
\]

\[
f_7 = f_5 - \frac{1}{2} (f_4 - f_2) - \frac{1}{6} \rho v_x.
\]

Then, the collision step is performed also for the nodes of this opening [17]. The openings on the other walls are treated as explained in Appendix A.

For the style gradient, after the collision step, the velocity modes are updated with the values of their neighbors. For example, for an outlet opening on the xhi wall, we have \( f_i(N_x, y) = 2f_i(N_x - 1, y) - f_i(N_x - 2, y) \) for \( i = 0, \ldots, 8 \).

With two substances (see fluids command), it is necessary to specify how to update the momentum for every fluid component: the first label in the inlet/outlet command refers to fluid1 and the second one to fluid2.

Warning: The thermo information is not correct with the gradient style (see thermo command).

Related commands:

\textit{inlet/outlet thermo}

\textbf{inlet\_solute/outlet\_solute commands}

Syntax:

\begin{verbatim}
inlet_solute(label,style,arguments)
outlet_solute(label,style,arguments)
\end{verbatim}

- label specifies the opening previously defined with the commands inlet/outlet
- style=flux, dirichlet and adiabatic are available for both inlet and outlet
- arguments depend on the style of the opening:
  - If the opening is of style flux, it is necessary to specify the velocity \( v \) and the solute concentration \( C_0 \).
  - For the dirichlet style, the solute concentration is kept constant. The initial and imposed solute concentration is an input parameter.
  - For the adiabatic style, the initial solute concentration must be specified.
Examples:
&inlet_solute(“in1”,“flux”,0.01,1.1);
&inlet_solute(99,”dirichlet”,1);
&outlet_solute(“out1”,“dirichlet”,1.1);
&outlet_solute(“out2”,“adiabatic”,1);

Description:
These commands determine how to update the solute concentration at the nodes of the inlet and/or outlet openings. As for fluid flow, after the streaming step some distribution functions remain undetermined. For example, for an inlet opening on the wall xlo, the distribution function \(g_1\) is not defined (transport occurs on a d2q4 lattice, see solute command). For the style flux, it is determined according to the rules [3]:

\[
C = v C_0 + D C_1 \quad \text{and} \quad g_i = g_i^{eq}, \quad i = 1, \ldots, 4.
\]

\(C\) is the solute concentration at the inlet node. \(C_0\) is the concentration of the solution injected into the system and \(v\) is the associated velocity. \(C_1\) is the solute concentration of the nearest node inside the simulation domain. The collision step is applied also to the nodes of this opening. The formulas for the other walls are given in Appendix [B].

For the style dirichlet, the concentration \(C\) is kept constant at the inlet and/or outlet openings. For example, for the wall xhi, after streaming, the distribution \(g_3\) is unknown (transport on a d2q4 lattice, see solute command). It is determined according to the following rules [3]:

\[
C = \bar{C} \quad \text{and} \quad g_3 = \bar{C} - C'.
\]

\(C\) is the solute concentration at the opening. \(\bar{C}\) is the desired solute concentration; \(C'\) is the actual value immediately after the streaming step. The collision step is then performed also for the nodes of this opening. The formulas for the other walls can be found in Appendix [B].

For the style adiabatic, we impose a vanishing flux at the nodes of the openings. For example, for an outlet opening on the xhi wall, we simply have \(g_3 = g_1\). The collision step is then applied also for these lattice sites.

With two substances (see inlet/outlet commands), it is possible to use the label of any fluid component.

Related commands:
solute inlet/outlet

**boundary_style command**

Syntax:
boundary_style(style,argument)

- style=noslip, slip, mixed, hybrid
- argument=reflection coefficient for the mixed style (argument ≤ 1)

Examples:
&boundary_style(“slip”);
&boundary_style(“noslip”);
&boundary_style(“mixed”,0.5);
&boundary_style(“hybrid”);

Description:
With this command it is specified how to treat the collisions at the solid boundaries. This command must precede the obstacle command, otherwise the simulation is interrupted with an error message.

In the absence of this command all boundaries are for sure periodic: in the restart file the style of the boundaries is indicated as periodic, even with inlet/outlet openings.

The noslip style is suited for describing rough surfaces. The velocity modes reaching an obstacle are simply bounced back [3][4].

The slip style is useful for simulating smooth surfaces (mirror reflection). The velocity modes \(f_1, f_2, f_3 \) and \(f_4\) are still bounced back when they meet an obstacle. The diagonal modes are treated differently. Let us consider for example the velocity mode \(f_5\)
at node \((i,j)\). If the node \((i+1, j+1)\) is not an obstacle, the velocity mode \(f_5\) propagates freely. Otherwise, for the arrangements illustrated in Fig. 4 we apply the rules

\[
f_8(i+2, j) = f_5(i, j) \quad \text{or} \quad f_6(i, j+2) = f_5(i, j)
\]

In all the remaining cases, the velocity mode is bounced back. Similar rules apply for the other diagonal modes. Care is taken in order to avoid that velocity modes cross inlet/outlet openings.

The mixed style is a combination of the slip and noslip rules. When a velocity mode hits a solid site, a fraction \(R\) is propagated forward (slip rule) and the remaining fraction \(1-R\) backward (noslip rule).

The mode hybrid allows to use more than one style for the boundaries. The type of a solid node is specified via the command obstacle with additional arguments (the extra arguments double jointly with the fluids command). In simulations, the collision is treated according to the style of the target solid node.

Related command:

obstacle

**obstacle command**

Syntax:

\[
\text{obstacle(rectangle,} x_0, x_1, y_0, y_1, \text{style1,argument,style2,argument)} \\
\text{obstacle(circle,} x_c, y_c, r, \text{style1,argument,style2,argument)}
\]

- shape=rectangle,circle
- \(x_0 < x_1\)=lower and higher \(x\) coordinates for the rectangle. The same holds for \(y_0\) and \(y_1\)
- \(x_c,y_c\)=coordinates of the center of the circle
- \(r\)=radius of the circle
- style1,style2=noslip,slip,mixed
- argument=reflection coefficient for the mixed style (argument \(\leq 1\))

Examples:

\&obstacle("rectangle",4,10,5,5); \\
\&obstacle("circle",5,5,10); \\
\&obstacle("rectangle",0,0,50,"slip"); \\
\&obstacle("circle",20,10,5,"noslip");
&obstacle("rectangle",0,60,0,0,"noslip","noslip");
&obstacle("rectangle",2,7,12,17,"mixed",0.3);
&obstacle("rectangle",10,20,10,30,"mixed",0.7,"mixed",0.5);

Description:
This command defines the lattice sites that will be considered as occupied by a solid phase. This command overrides any previous definition of these lattice sites via the read_data, inlet/outlet and/or position0 commands (see Fig. 3). This command must follow the boundary_style command, otherwise the simulation is interrupted with an error message.
If the boundary style is hybrid, the command takes extra arguments specifying one of the available methods for the treatment of collisions. In the multicomponent case, the additional arguments double.
With the mixed style, at most 99 different reflection coefficients can be defined for the first substance in the multicomponent case.
Related commands:
read_data boundary_style position0

**surface_reaction command**

Syntax:
surface_reaction(kr,Cs,style,b0,bmax)

- kr=reaction-rate constant
- Cs=saturated concentration
- style=growth
- b0,bmax=initial and threshold value for cumulated mass at solid-liquid interface

Example:
&surface_reaction(0.25,1,"growth",0.5,1);

Description:
This command introduces a surface reaction for solute transport. At the reactive boundary, the solute concentration $C$ satisfies the macroscopic equation \[11, 13–16\]

$$D \frac{\partial C}{\partial n} = k_r (C - C_s),$$

where $D$ is the diffusion coefficient, $C_s$ is the saturated concentration and $k_r$ is the reaction-rate constant. After the streaming step for solute transport, at the solid surface the incoming modes into the fluid phase are undetermined. The unknown quantities are updated according to the following rules \[11\]:

$$C = \frac{2g_{\chi(i)} + k_r C_s}{k_r + 1/2} \quad \text{and} \quad g_i = -g_{\chi(i)} + \frac{1}{2} C.$$ 

The distribution functions $g_i$ describe solute transport (see solute command). $i' = \chi(i)$ is the index for the opposite direction associated with that of $i$. More details on the implementation can be found in Appendix C. The subsequent collision step is performed also for the nodes at the solid-liquid interface. After the collision step, at the solid boundaries mass precipitates. The mass deposited on a solid node is updated as follows \[15,16\]:

$$b(t + \Delta t) = b(t) + \Delta b \quad \text{with} \quad \Delta b = k_r (C - C_s),$$

if $\Delta b > 0$. The initial mass on solid nodes is $b_0$. The amount $\Delta b$ is subtracted from the incoming modes in the fluid phase \[16\]. Solute transport in the solid phase is neglected. For surface growth, when for a solid node $b(t + \Delta t)$ exceeds $b_{\text{max}}$, one of its direct neighbors in the fluid phase becomes a solid node; it is chosen randomly and every occurrence is equiprobable.

Related command:
solute
**position0 command**

Syntax:

position0(rectangle,x₀,x₁,y₀,y₁)
position0(circle,xₜ,yₜ,r)

- shape=rectangle,circle
- x₀ < x₁=lower and higher x coordinates for the rectangle. The same holds for y₀ and y₁
- xₜ,yₜ=coordinates of the center of the circle
- r=radius of the circle

Examples:
&position0(“rectangle”,8,9,11,20);
&position0(“circle”,5,7,11);

Description:
This command defines regions of rectangular and/or circular shape for which the user specifies the starting populations via the momentum0 command.

The previous definitions of the lattice sites via the read_data command are modified. Inlet/outlet nodes and/or obstacle nodes are not reinitialized (see Fig.3).

This command must precede the command momentum0, otherwise the simulation is interrupted with an error message.

Related command:
momentum0

**momentum0 command**

Syntax:
momentum0(mode,value,fluid)

- mode=e₀,e₁,e₂,... velocity mode
- value=population value
- fluid=1,2 indicates the substance

Examples:
&momentum0(“e₀”,4);
&momentum0(“e₇”,1);
&momentum0(“e₁”,4,1);

Description:
This command allows to set the populations of the lattice sites selected via the position0 command. If two commands are used with the same mode, the populations are summed. Every momentum0 command refers to the last region defined with the position0 command: regions with different densities can be so defined. Negative population values are subtracted.

This command must be used after the command position0, otherwise the simulation is interrupted with an error message. The other priority relations are illustrated in Fig.3.

In the multicomponent case, it is necessary to specify the fluid component with an extra argument: 1 for fluid1, 2 for fluid2.

Related commands:
inlet/outlet position0

**concentration0 command**

Syntax:
concentration0(value)
• value=concentration value

Example:
&concentration0(1.3);

Description:
This command allows to define the solute concentration for the lattice sites selected via the position0 command. Every concentration0 command refers to the last region defined with the position0 command: regions with different concentrations can be so defined. Negative concentration values are subtracted.
This command must be used after the command position0, otherwise the simulation is interrupted with an error message.
Related command:
solute

aveforce command
Syntax:
aveforce(mode,value,fluid)

• mode=e0,e1,e2,… velocity mode
• value=intensity of the force
• fluid=1,2 indicates the substance

Examples:
&aveforce("e1",3.11*10**−3);
&aveforce("e1",4.33*10**−3,1);

Description:
With this command an average force is applied to all lattice sites occupied by the fluid phase. If two commands are used with the same mode, the components of the force vector are summed. This command must be used after the lattice or fluids commands.
In the multicomponent case, it is necessary to specify the fluid component with an extra argument: 1 for fluid1, 2 for fluid2.
Related command:
aveacceleration

aveacceleration command
Syntax:
aveacceleration(mode,value,fluid)

• mode=e0,e1,e2,… velocity mode
• value=intensity of the acceleration
• fluid=1,2 indicates the substance

Examples:
&aveacceleration("e1",2.22*10**−4);
&aveacceleration("e3",1.55*10**−4,2);

Description:
With this command an average acceleration is added to all lattice sites occupied by the fluid phase. If two commands are used with the same mode, the components of the vector acceleration are summed. This command must be used after the lattice or fluids commands.
In the multicomponent case, it is necessary to specify the fluid component with an extra argument: 1 for fluid1, 2 for fluid2.
Related command:
**interforce command**

Syntax:

\[
\text{interforce}(G, \psi_0, \rho_0)
\]

- \(G\) = interaction strength
- \(\psi_0\) = factor
- \(\rho_0\) = average density

Examples:

\&interforce(-120,4,200);
\&interforce(0.9);

Description:

This command introduces van der Waals forces between nearest-neighbor lattice sites occupied by the fluid phase. The force is computed with the formula

\[
F(x,y) = -G\psi(x,y) \sum_{i=1}^{8} w_i \psi(r + e_i \Delta t) e_i .
\]

We use the notation \(r = (x,y)\) for a two dimensional lattice; time dependence omitted for clarity. The constants \(w_i\) are defined by the lattice style. The function \(\psi(x,y)\) is defined as

\[
\psi(x,y) = \psi_0 e^{-\rho_0 \rho(x,y)} .
\]

In the multicomponent case, the above formula becomes

\[
F_{\sigma}(x,y) = -G\rho_{\sigma}(x,y) \sum_{i=1}^{8} w_i \rho_{\sigma}(r + e_i \Delta t) e_i \quad \sigma = 1,2 .
\]

Given \(\sigma\), the other fluid component is denoted as \(\bar{\sigma}\). Of course, the arguments \(\psi_0\) and \(\rho_0\) must be omitted in this case.

Warning: The thermo information is not correct when this command is used (see thermo command).

**Related command:**

 thermo

**adhesiveforce command**

Syntax:

\[
\text{adhesiveforce}(G, \psi_0, \rho_0, \text{fluid})
\]

- \(G\) = interaction strength
- \(\psi_0\) = factor
- \(\rho_0\) = average density
- \(\text{fluid}=1,2\) indicates the substance

Examples:

\&adhesiveforce(-200,4,200);
\&adhesiveforce(0.2,1);

Description:
This command introduces adhesive forces between lattice sites occupied by the fluid phase in the proximity of solid boundaries. The force is computed with the formula

\[ F(x, y) = -G\psi(x, y) \sum_{i=1}^{8} w_i s(r + e_i \Delta t) e_i . \]

We use the notation \( r = (x, y) \) for a two dimensional lattice; time dependence omitted for clarity. The constants \( w_i \) are defined by the lattice style. The function \( \psi(x, y) \) is given by

\[ \psi(x, y) = \psi_0 e^{-\rho_0 / \rho(x, y)} . \]

The function \( s(x, y) \) is defined as

\[ s(x, y) = \begin{cases} 
1 & \text{if site (}x, y\text{) solid} \\
0 & \text{if site (}x, y\text{) fluid} 
\end{cases} . \]

In the multicomponent case, it is necessary to specify the fluid component with an extra argument: 1 for fluid1, 2 for fluid2. The force is evaluated with the formula

\[ F_{\sigma}(x, y) = -G_{\sigma} \rho_{\sigma}(x, y) \sum_{i=1}^{8} w_i s(r + e_i \Delta t) e_i \quad \sigma = 1, 2 . \]

Of course, the arguments \( \psi_0 \) and \( \rho_0 \) must be omitted in this case.

**Intersolute command**

Syntax:
\[
\text{intersolute}(G, \psi_0, C_0)
\]

- \( G \)=interaction strength
- \( \psi_0 \)=factor
- \( C_0 \)=average concentration

Example:
\[
\&\text{intersolute}(-5*10^{-3}, 1, 5*10^{-3});
\]

Description:

With this command it is possible to introduce interfaces for solute transport. In analogy with multiphase fluid flow, the mechanism consists in adding to the velocity \( u \) in Eq. 3 a term of the form \( \tau_s F(r, t) / C(r, t) \). The function \( F \) is obtained by

\[ F(x, y) = -G\psi(x, y) \sum_{i=1}^{4} \psi(r + e_i \Delta t) e_i . \]

We use the notation \( r = (x, y) \) for a two dimensional lattice; time dependence omitted for clarity. The function \( \psi(x, y) \) is defined as

\[ \psi(x, y) = \psi_0 e^{-C_0 / C(x, y)} . \]

Related commands:
- solute interforce

**Thermo command**

Syntax:
\[
\text{thermo}(N_f)
\]
• $N_t$=print general information on screen every this many timesteps

Example:
&thermo(50);

Description:
When this command is used, general information is printed on screen during the simulation. Mass is the weight of the overall fluid phase of the system. It is obtained by summing the density of the lattice sites occupied by the fluid phase. Momentum returns the $x$ and $y$ components of the overall momentum vector. Mass_eq is the equilibrium mass of the overall fluid phase; it is calculated from the equilibrium densities. At $t = 0$, this information refers to the state of the system before the routine of streaming (see Fig. 1). At the beginning and at the end of a run the local time is printed. At start, it is also indicated if the program runs in serial or parallel mode. For example, $1 \times 1$ is used for serial; $2 \times 1$ means that the $x$ side of the simulation domain is partitioned between 2 processors.

The basic computations for the thermo information are performed in the collision step, thus without additional loops. When the command interforce is used, the contribution of this force to the velocity is not computed correctly because all the densities are updated only at the end of the loops. Similarly, with the gradient style for inlet/outlet openings, the thermo information is not correct because all the momenta are updated after the collision step. If necessary, we suggest to derive these quantities from the output files.

Related commands:
inlet/outlet interforce log output

log command
Syntax:
log(file)

• file=name of log file

Example:
&log("Log/log.poiseuille");

Description:
By default, the information printed on screen is also written in the file log.lb. The command log allows to specify the name of the log file.

Related command:
thermo

output command
Syntax:
output(file,$N_t$)

• file=name of output file

• $N_t$=print output every this many timesteps

Example:
&output("../Dump/output",50);

Description:
With this command it is specified the frequency with which information on the system state is printed in an output file. To the given file name is appended the suffix ".dat" for dat files. The fields of every line of the output file are defined as follows:

$x$ $y$ $\rho$ $v_x$ $v_y$

$x$ and $y$ are the coordinates of the lattice site, $\rho$ the corresponding density, $v_x$ and $v_y$ the components of the velocity vector, including also the contributions from the applied forces. The first block of $(N_x + 1) \times (N_y + 1)$ lines defines the state of the first frame; the second block of $(N_x + 1) \times (N_y + 1)$ lines defines the state of the second frame; etc. This information refers to the state of the system after the collision step (see Fig. 1).
In the multicomponent case, an output file is written for every substance. The strings “.fluid1.dat” and “.fluid2.dat” are appended to the specified file name. In these files there are four velocity components:
\[ x, y, \rho, v_x, v_y, v_x, v_y \]
The first two velocity components refer to the single substance. The last two values are the \( x \) and \( y \) components of the velocity of the overall fluid, Eq. 4.

If solute transport is enabled, an output file is written for the solute component. The string “.solute.dat” is appended to the specified file name. The fields of every line of the output file are defined as follows:
\[ x, y, C, b \]
\( x \) and \( y \) are the coordinates of the lattice site and \( C \) its solute concentration. For solid sites, \( b \) is the mass deposited on the reactive boundary; \( b \) vanishes in the fluid phase. This last quantity is omitted in the absence of surface reaction. The data are organized into blocks as for the fluid phase. The information refers to the state of the system after the collision step and the cumulation of mass on the solid surface.

It is possible to write only one output file.

**write_restart command**

**Syntax:**
write_restart(file, \( N_t \))

- file= name of restart file
- \( N_t \)= print restart file every this many timesteps

**Example:**
&write_restart(“../Restart/restart.example”, 100);  

**Description:**
This command defines the frequency with which a restart file is written. The restart file is written at the end of the simulation if the number of timesteps is a multiple of \( N_t \). To the given file name is appended the string “.timesteps”, where timestep is the timestep number at which the restart file is written. The restart file has the format of an input data file including all sections. The density value \(-11\) is attributed to the sites belonging to the solid phase in the section density, while all the velocity modes are set equal to 0 in the section momentum.

In the multicomponent case, a restart file is written for every substance. The file name of the first component ends with the string “.fluid1” and that of the second one ends with the string “.fluid2”.

If solute transport is enabled, a restart file is written for the solute component. The file name of the restart file ends with the string “.solute”.

This command must be used before the iteration command.

**Related commands:**
read_data iteration

**iteration command**

**Syntax:**
iteration(\( N_t \))

- \( N_t \)= \# of timesteps

**Example:**
&iteration(20000);  

**Description:**
This command fixes the number of iterations to be done. The iteration command must follow any other command of the module. Without this command the simulation is not performed.

**Related command:**
write_restart
IV. APPLICATIONS

A. Poiseuille flow

A channel is obtained from the simulation domain with \( N_x = 60 \) and \( N_y = 30 \) [lu] (d2q9 style). At \( x = 0 \) and \( N_x \) [lu] the boundaries are periodic and at \( y = 0 \) and \( N_y \) [lu] the boundaries are solid, of type noslip. The channel is filled with fluid: the initial populations of the rest and slow modes are set to 4 and those of the fast modes to 1 [mu/lu]. A constant acceleration in the \( e_1 \) direction is applied, of general form

\[
g = \frac{4}{3} \frac{u_{\text{max}}}{(N_y - 1)^2} (2\tau - 1) .
\]

We choose \( u_{\text{max}} = 0.07 \) [lu/ts] and \( \tau = 1 \) [ts], leading to \( g = 1.11 \cdot 10^{-4} \) [lu/ts^2]. In this way, the velocity component \( v_x \) develops a parabolic profile in the course of time. In the stationary regime, the theoretical velocity profile is given by

\[
v_x(y) = \frac{3g}{2\tau - 1} \left[ \left( \frac{N_y - 1}{2} \right)^2 - \left( y - \frac{N_y}{2} \right)^2 \right] , \quad \text{with} \quad y = \frac{1}{2}, \ldots, N_y - \frac{1}{2} .
\]

This behavior is usually referred to as Poiseuille flow. Figure 5 shows the velocity profile as obtained after 10'000 timesteps.

![Figure 5: Velocity profile for Poiseuille flow. Points are obtained from simulation. The solid line is the theoretical prediction, Eq. 5.](image)

B. Phase separation

Let us consider a lattice of style d2q9 with \( N_x = N_y = 100 \) [lu]. The initial density of every site is given by \( d(x,y) = d_0 + \delta d \) with \( d_0 = 200 \) [mu/lu^2] and \( \delta d \) a random number in the interval \([0, 1]\) (uniform distribution). Cohesive forces are introduced via the interfource command with arguments \( G = -120 \) [mu·lu/ts^2], \( \psi_0 = 4 \) and \( \rho_0 = 200 \) [mu/lu^2]. The system is let evolve for 20'000 timesteps with relaxation time \( \tau = 1 \) [ts]. Figure 6 shows four different frames of the system dynamics. It clearly appears that the liquid phase, higher density, separates from the vapor phase, lower density. For the cohesive forces, small droplets merge together to form a single droplet immersed in its own vapor phase.

C. Contact angles I

We consider a fluid confined in a rectangular box of size \((N_x + 1) \times (N_y + 1)\), with \( N_x = 200 \) and \( N_y = 50 \) [lu] (d2q9 style). The boundaries of the simulation domain are solid, of type noslip, and the initial density of the other lattice sites is initialized as in the previous application. van der Waals forces are defined by the set of parameters \( G = -120 \) [mu·lu/ts^2], \( \psi_0 = 4 \) and \( \rho_0 = 200 \).
Figure 6: Top: The state of the system at the beginning and after 2′000 timesteps: many small droplets rapidly form. Bottom: State of the system after 4′000 and after 20′000 timesteps. A single droplet forms for the cohesive forces. Color map based on density.

[mu/lu^2]. Adhesive forces between the solid and liquid phases are introduced with the parameters \(\psi_0 = 4\) and \(\rho_0 = 200\) [mu/lu^2]. The interaction strength \(G\) is varied in order to obtain different contact angles [20]. Figure 7 shows the state of the systems after 10′000 timesteps; relaxation time \(\tau = 1\) [ts]. The hydrophilic regime is reproduced with \(G = -250\) [mu·lu/ts^2]; \(G = -187.16\) [mu·lu/ts^2] leads to the neutral behavior; the hydrophobic regime is reproduced with \(G = -70\) [mu·lu/ts^2] [3].

D. Contact angles II

Let us consider a rectangular domain with \(N_x = 200\) [lu] and \(N_y = 50\) [lu] with rigid boundaries of type noslip (d2q9 model). The simulation domain is filled with two substances so that to be left with a single droplet of the first fluid in the middle. Inside a rectangle of base 51 [lu] centered in the simulation domain, the density for the first fluid is \(f_0 = 2\) [mu/lu^2] and that of the second one \(f_0 = 0.1\) [mu/lu^2]; elsewhere we choose \(f_0 = 0.1\) [mu/lu^2] and \(f_0 = 2\) [mu/lu^2] for the first and second component, respectively. Interparticle forces are introduced with parameter \(G = 0.9\) [lu/mu/ts^2] [8]. The interaction strength with the solid boundaries is \(G_1 = 0.2\) [lu/ts^2] for the first fluid and \(G_2 = -0.2\) [lu/ts^2] for the second fluid [8]. Figure 8 shows the densities of the two substances after 20′000 timesteps (relaxation time \(\tau = 1\) [ts]). The fluid with lower density is interpreted as dissolved in the other one. It appears that a single droplet forms in the middle with the first component exhibiting hydrophilic behavior while the second one hydrophobic.
Figure 7: Liquid phase confined in a rectangular box displays hydrophilic, neutral and hydrophobic behavior, from Top to Bottom. The contact angle is indeed $< 90^\circ$, $\approx 90^\circ$ and $> 90^\circ$, respectively. Color map based on density. Black points represent solid boundaries.

E. Parallelization

Let us consider a two-component fluid confined in the simulation domain with $N_x = 350$ [lu] and $N_y = 200$ [lu] (d2q9 model). The wall ylo is solid, of type noslip, and centered above it we place a square of side length 129 [lu] with densities $f_0 = 2$ [mu/lu$^2$] for the first substance and $f_0 = 0.1$ [mu/lu$^2$] for the second one. Elsewhere the densities are $f_0 = 0.1$ [mu/lu$^2$] and $f_0 = 2$ [mu/lu$^2$] for the first and second fluid, respectively. These initial conditions guarantee the formation of a single droplet of the first component. Interparticle forces are defined by $G = 0.9$ [lu/mu/ts$^2$]; the interaction strengths for adhesive forces are $G_1 = 0.3$ [lu/ts$^2$] and $G_2 = -0.3$ [lu/ts$^2$] for the first and second fluid component, respectively. The wall xhi and xlo are periodic and the relaxation time is $\tau = 1$ [ts]. The system is let evolve for 500 timesteps in the parallel mode with different number of processors; the timings are shown in Fig. 9. We used a Desktop PC with operating system Windows 7 equipped of an Intel processor of the family i7. Figure 10 shows the state of the system after 40'000 timesteps.

F. Surface growth

The simulation domain is $N_x = 200$ [lu] long and $N_y = 200$ [lu] wide with periodic boundary conditions (d2q9 model). A solid obstacle of square shape with side length 11 [lu] is placed in the center. The collisions with the solid boundaries are treated according to the bounce-back rule corresponding to the noslip style. The rest of the simulation domain is filled uniformly with a single component fluid and solute. The initial density of the fluid is defined by $f_0 = 24$ [mu/lu$^2$]. The initial concentration of the solute is $C_0 = 1.5$ [mu/lu$^2$]. The parameters controlling the surface reaction are chosen as follows. The saturated concentration is set to $C_s = 0.5$ [mu/lu$^2$] and the initial mass on the solid surface is $b_0 = 0.5$ [mu/lu$^2$]. The surface grows whenever the cumulated mass on the solid surface exceeds the threshold value of $b_{\text{max}} = 1$ [mu/lu$^2$]. For the reaction-rate constant $k_r$, different values are considered. The dynamics amounts to 20'000 timesteps with relaxation times $\tau = 1$ [ts] for fluid flow and $\tau_s = 1$ [ts] for solute transport. The properties of the growing surface depend on the relative saturation $\psi = C_0/C_s$ and the Damkohler number $Da = k_rL/D$. $L$ is a characteristic length of the system and $D$ the diffusion coefficient. Figure 11 shows the resulting final states.
Figure 8: Final state for the solution of two immiscible substances. Color map based on density; solid phase indicated by black points. Top: Representation for the first fluid; Bottom: Representation for the second fluid. There remain two distinct fluid components forming complementary contact angles with the surface.

Figure 9: Timing for different processor grids. The parallelization for four or more processors is inefficient.

for different Damkohler numbers.
Figure 10: Fluid immersed in another one in contact with a solid boundary. A spherical droplet forms exhibiting hydrophobic behavior since for the contact angle holds $\theta > 90^\circ$. Color map based on density; black points represent solid nodes.

Figure 11: Surface growth in the purely diffusive regime from a small seed. Final configuration for systems with different Damköhler number $Da$. As the Damköhler number increases the structures become more dendritic or, equivalently, less compact.
V. SCRIPTS

A. Poiseuille flow

The data of Sec. IV A were generated with the following Perl program.

```perl
#!/usr/bin/perl
use lib "D:\LB_data\Module";
use strict;
use lb2d qw( lattice processors read_data fluids solute inlet outlet inlet_momentum
outlet_momentum inlet_solute outlet_solute boundary_style obstacle
surface_reaction position0 momentum0 concentration0
aveforce aveacceleration interforce adhesiveforce intersolute
 thermo log output write_restart

iteration);

my $Nx=60;
my $Ny=30;
my $Nt=10000;

&lattice("d2q9",$Nx,$Ny,1);

&boundary_style("noslip");
&obstacle("rectangle",0,$Nx,0,0);
&obstacle("rectangle",0,$Nx,$Ny,$Ny);

&position0("rectangle",0,$Nx,1,$Ny-1);

&mmomentum0("e0",4);
&mmomentum0("e1",4);
&mmomentum0("e2",4);
&mmomentum0("e3",4);
&mmomentum0("e4",4);
&mmomentum0("e5",1);
&mmomentum0("e6",1);
&mmomentum0("e7",1);
&mmomentum0("e8",1);

&aveacceleration("e1",1.11*10**-4);

&thermo(100);
&log("log\poiseuille");
&output("v_profile",int($Nt/20));

&write_restart("restart.v_profile",$Nt);

&iteration($Nt);
```
The command `use lib "D:\LB\data\Module"` specifies the location of the module. If the command under commentary is typed in the command line, it is possible to have a list of the directories that Perl scans by default. If the module is in one of these directories, this line is not necessary. With the command `use lb2d qw(...)`, the listed functions of the module `lb2d.pm` are loaded. This command is of initialization and must appear in any program.

All the commands of the module are used in a straightforward way. Note that operations and variables can be used as arguments of the functions. As an example, in the command output, with `int($Nt/20)` it is specified to write in the file `v_profile` 20 evenly spaced frames.

The raw data can be analyzed with the following Matlab program.

```matlab
clear;
clf;
%==============================================
frame=21;
Nx=60;
Ny=30;
tau=1;
g=1.11*10^-4;

nu=(tau-0.5)/3;

nodes=(Nx+1)*(Ny+1);

%==============================================
load D:\LB\data\Poiseuille\v_profile.dat;

x=[v_profile(:,1)];
y=[v_profile(:,2)];
d=[v_profile(:,3)];
ux=[v_profile(:,4)];
uy=[v_profile(:,5)];

%==============================================
X=0:1:Nx;
Y=0:1:Ny;

[A,B]=meshgrid(X,Y);
[sx,sy]=meshgrid(0:Nx,0:Ny);

for i=1:frame
    from=1+(i-1)*nodes;
    to=nodes+(i-1)*nodes;
    k=0;
    q=0;
    for j=from:to
        if d(j)==-11
            q=q+1;
            ox(q,i)=x(j);
            oy(q,i)=y(j);
        end
        k=k+1;
        u(k,i)=x(j);
    end
```

```
In the first block are entered the general settings of the Lattice Boltzmann simulation. In the second block, the data are loaded. In the third block, the data are read and organized into matrices for the usual quantities. The last entry of these matrices always refers to the frame number. Finally, the data are displayed frame after frame with the instructions of the last block. The color map is based on the $x$ component of velocity (contourf command) and the vector field is also given by the velocity vector (quiver command). By enabling the streamline command, streamlines derived from the velocity field are drawn. With the command saveas, a figure in the format jpg is created for every frame. The second figure displays the velocity profile (see Fig. 5).

**B. Phase separation**

The following Perl commands generate the data presented in Sec. IV B.

```perl
my $Nx=100;
my $Ny=100;
my $Nt=20000;
&lattice("d2q9",$Nx,$Ny,1);
```
The initialization is omitted since already discussed for the first example. In this case, the initial state of the system is imported from the input data file `phase_data`, read with the command `read_data`. At the beginning, the distribution functions are replaced with their equilibrium values because of the additional argument `equilibrium`.

The raw data are analyzed with a Matlab program similar to that given for Poiseuille flow.

### C. Contact angles I

The Perl commands specific to the case of hydrophilic behavior are given below (see Sec. IV C).

```perl
my $Nx=200;
my $Ny=50;
my $Nt=10000;
&lattice("d2q9",$Nx,$Ny,1);
&read_data("box_data","equilibrium");

&boundary_style("noslip");
&obstacle("rectangle",0,0,0,$Ny);
&obstacle("rectangle",$Nx,$Nx,0,$Ny);
&obstacle("rectangle",0,$Nx,0,$Ny);
&obstacle("rectangle",0,0,$Ny,$Ny);

&interforce(-120,4,200);
&adhesiveforce(-250,4,200);

&log("log\phase");
&interforce(-120,4,200);
&log("log\phase");
&thermo(100);
&output("phase",int($Nt/20));

&write_restart("phase",$Nt);
&iteration($Nt);
```

Note that the obstacle commands override the definitions of density and momentum with the command `read_data`.

The raw data can be analyzed after small changes to the Matlab program for Poiseuille flow (see Sec. V A).

### D. Contact angles II

The data of the application of Sec. IV D are generated with the following Perl program.
#!/usr/bin/perl

use lib "D:\LB_data\Module";  #perl -e 'print join "\n", @INC'
use strict;
use lb2d_par qw(
    lattice processors read_data fluids solute inlet outlet inlet_momentum
    outlet_momentum inlet_solute outlet_solute boundary_style obstacle
    surface_reaction position0 momentum0 concentration0
    aveforce aveacceleration interforce adhesiveforce intersolute
    thermo log output write_restart
    iteration);

my $Nx=200;
my $Ny=50;
my $Nt=20000;
my $fluid1=1;
my $fluid2=2;
my $tau1=1;
my $tau2=1;
&lattice("d2q9",$Nx,$Ny,1);

&processors(2,1);
&fluids($tau1,$tau2);

&boundary_style("noslip");
&obstacle("rectangle",0,$Nx,0,0);
&obstacle("rectangle",0,$Nx,$Ny,$Ny);
&obstacle("rectangle",0,0,0,$Ny);
&obstacle("rectangle",$Nx,$Nx,0,$Ny);
&position0("rectangle",1,$Nx/2-26,1,$Ny-1);
&momentum0("e0",0.1,$fluid1);
&momentum0("e0",2,$fluid2);

&position0("rectangle",$Nx/2-25,$Nt/2+25,1,$Ny-1);
&momentum0("e0",2,$fluid1);
&momentum0("e0",0.1,$fluid2);

&position0("rectangle",$Nt/2+26,$Nt/2+26,1,$Ny-1);
&momentum0("e0",0.1,$fluid1);
&momentum0("e0",2,$fluid2);

&interforce(0.9);
&adhesiveforce(0.2,$fluid1);
&adhesiveforce(-0.2,$fluid2);

&log("log\theta_fluids");
The command use lb2d_par qw(...) loads the parallel version of the module. The list of functions is the same as for the serial version. The simulation is run on two CPUs (processors command). It should be noted that the commands momentum0 and adhesiveforce have one extra argument specifying the fluid component since two substances are present (fluids command). On a cluster with a queue system, it is necessary to submit the job with a shell script similar to the following.

```bash
#!/bin/sh
#$ -N fluids
#$ -S /bin/sh
#$ -cwd
#$ -j y
#$ -q long.q
#$ -pe smp 2
#$ -l h_rt=24:00:00

echo "Starting job fluids at " 'date'
mpirun -np $NSLOTS perl < theta_fluids.pl
echo "Ending job fluids at " 'date'
```

The second line attributes the name fluids to the job; the third line specifies the shell interpreter; the current directory becomes the working directory with line 4; with the next line, STDERR is redirected to STDOUT; the sixth line selects the queue long.q; at line 7 the user requests two CPUs on the same node and the variable $NSLOTS is set to this value; at line 8 it is specified the walltime. With the command mpirun, the Perl program is executed in parallel on $NSLOTS cores. The echo commands print in the STDOUT file the local time at the beginning and at the end of the simulation.

The data can be visualized and analyzed with a Matlab program similar to that of Sec. V A.

E. Parallelization

The data of Fig. 10 in Sec. IV E were generated with the following Perl program.

```perl
#!/usr/bin/perl
#-----------------------------------------------
use lib "D:\\LB_data\\Module";  #perl -e 'print join "\n", @INC'
use strict;
use lb2d_par qw( lattice processors read_data fluids solute inlet outlet inlet_momentum outlet_momentum inlet_solute outlet_solute boundary_style obstacle surface_reaction position0 momentum0 concentration0
aveforce aveacceleration interforce adhesiveforce intersolute
 thermo log output write_restart
iteration);
#-----------------------------------------------
```
This simulation can be continued for other 20'000 timesteps with the following commands.

my $Nx=350;
my $Ny=200;
my $Nt=20000;

my $L=64;
my $fluid1=1;
my $fluid2=2;
my $tau1=1;
my $tau2=1;

&lattice("d2q9",$Nx,$Ny,1);
&processors(3,1);
&fluids($tau1,$tau2);
&boundary_style("noslip");
&obstacle("rectangle",0,$Nx,0,0);
&position0("rectangle",0,$Nx,2*$L+1,$Ny);
&momentum0("e0",0.1,$fluid1);
&momentum0("e0",2,$fluid2);
&position0("rectangle",0,$Nx/2-$L-1,0,2*$L);
&momentum0("e0",0.1,$fluid1);
&momentum0("e0",2,$fluid2);
&position0("rectangle",$Nx/2+$L+1,$Nx,0,2*$L);
&momentum0("e0",0.1,$fluid1);
&momentum0("e0",2,$fluid2);
&position0("rectangle",$Nx/2-$L,$Nx/2+$L,0,2*$L);
&momentum0("e0",2,$fluid1);
&momentum0("e0",0.1,$fluid2);
&interforce(0.9);
&adhesiveforce(0.3,$fluid1);
&adhesiveforce(-0.3,$fluid2);
&log("log\_droplet\_fluids");
&thermo(100);
&output("droplet\_fluids",$Nt);
&write_restart("restart\_droplet\_fluids",$Nt);
&iteration($Nt);
The data were visualized with a Matlab program similar to that discussed in Sec. VA.

F. Surface growth

The simulations presented in Sec. IV F were carried out using the following Perl commands.

```perl
my $label=0;
my $Nx=200;
my $Ny=200;
my $Nt=20000;
my $tau=1;
my $taus=1;
my $mass0=0.5;
my $mass1=2*$mass0;
my $kr=5*10**-3;
my $Cs=0.5;
my $C0=1.5;
&lattice("d2q9",$Nx,$Ny,$tau);
&processors(2,1);
&solute($taus);
&surface_reaction($kr,$Cs,"growth",$mass0,$mass1);
&boundary_style("noslip");
&obstacle("rectangle",100-5,100+5,100-5,100+5);
&position0("rectangle",0,$Nx,0,$Ny);
&momentum0("e0",24);
```
&concentration0($C0);

&thermo(1000);
&log("log\.growth".$label);
&output("growth".$label,int($Nt/20));
&write_restart("growth".$label,$Nt);

&iteration($Nt);

The module is loaded as for the previous examples. The commands solute and concentration0 initialize solute transport. The parameters controlling the surface reaction are entered via the command surface\_reaction.

The data were displayed with a Matlab program similar to that discussed in Sec V.A.
Appendix A: Formulas for inlet/outlet openings in d2q9 model

For the inlets on the other walls, when the velocity is prescribed, we use

\[ \rho = \frac{1}{1 - v_x} \left[ f_0 + f_2 + f_4 + 2(f_3 + f_8) \right], \]

\[ f_3 = f_1 + \frac{2}{3} \rho v_x, \]

\[ f_6 = f_8 + \frac{1}{2} (f_4 - f_2) + \frac{1}{6} \rho v_x, \]

\[ f_7 = f_3 - \frac{1}{2} (f_4 - f_2) + \frac{1}{6} \rho v_x \quad \text{for xhi}; \]

\[ \rho = \frac{1}{1 - v_y} \left[ f_0 + f_1 + f_3 + 2(f_2 + f_6) \right], \]

\[ f_4 = f_2 + \frac{2}{3} \rho v_y, \]

\[ f_7 = f_5 + \frac{1}{2} (f_1 - f_3) + \frac{1}{6} \rho v_y, \]

\[ f_8 = f_6 - \frac{1}{2} (f_1 - f_3) + \frac{1}{6} \rho v_y \quad \text{for yhi}; \]

\[ \rho = \frac{1}{1 - v_y} \left[ f_0 + f_1 + f_3 + 2(f_4 + f_7) \right], \]

\[ f_2 = f_4 + \frac{2}{3} \rho v_y, \]

\[ f_5 = f_7 - \frac{1}{2} (f_3 - f_1) + \frac{1}{6} \rho v_y, \]

\[ f_6 = f_8 + \frac{1}{2} (f_3 - f_1) + \frac{1}{6} \rho v_y \quad \text{for ylo}. \]

In the case of outlet, the formulas read

\[ \rho = \frac{1}{1 + v_x} \left[ f_0 + f_2 + f_4 + 2(f_3 + f_8) \right], \]

\[ f_3 = f_1 - \frac{2}{3} \rho v_x, \]

\[ f_6 = f_8 + \frac{1}{2} (f_4 - f_2) - \frac{1}{6} \rho v_x, \]

\[ f_7 = f_3 - \frac{1}{2} (f_4 - f_2) - \frac{1}{6} \rho v_x \quad \text{for xhi}; \]

\[ \rho = \frac{1}{1 + v_x} \left[ f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7) \right], \]

\[ f_1 = f_3 - \frac{2}{3} \rho v_x, \]

\[ f_5 = f_7 - \frac{1}{2} (f_2 - f_4) - \frac{1}{6} \rho v_x, \]

\[ f_8 = f_6 + \frac{1}{2} (f_2 - f_4) - \frac{1}{6} \rho v_x \quad \text{for xlo}; \]
\[ \rho = \frac{1}{1 + v_y} [f_0 + f_1 + f_3 + 2(f_2 + f_5 + f_6)] , \]
\[ f_4 = f_2 - \frac{2}{3} \rho v_y , \]
\[ f_7 = f_3 + \frac{1}{2} (f_1 - f_3) - \frac{1}{6} \rho v_y , \]
\[ f_8 = f_6 - \frac{1}{2} (f_1 - f_3) - \frac{1}{6} \rho v_y \quad \text{for yhi;} \]

\[ \rho = \frac{1}{1 + v_y} [f_0 + f_1 + f_3 + 2(f_4 + f_7 + f_8)] , \]
\[ f_2 = f_4 - \frac{2}{3} \rho v_y , \]
\[ f_5 = f_7 + \frac{1}{2} (f_3 - f_1) - \frac{1}{6} \rho v_y , \]
\[ f_6 = f_8 - \frac{1}{2} (f_3 - f_1) - \frac{1}{6} \rho v_y \quad \text{for ylo.} \]

In the style dirichlet, for the other walls we apply the rules:

\[ v_x = 1 - \frac{f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)}{\rho} , \]
\[ f_1 = f_3 + \frac{2}{3} \rho v_x , \]
\[ f_5 = f_7 - \frac{1}{2} (f_2 - f_4) + \frac{1}{6} \rho v_x , \]
\[ f_8 = f_6 + \frac{1}{2} (f_2 - f_4) + \frac{1}{6} \rho v_x \quad \text{for xlo;} \]

\[ v_y = \frac{f_0 + f_1 + f_3 + 2(f_2 + f_5 + f_6) - 1}{\rho} , \]
\[ f_4 = f_2 - \frac{2}{3} \rho v_y , \]
\[ f_7 = f_3 - \frac{1}{2} (f_1 - f_3) - \frac{1}{6} \rho v_y , \]
\[ f_8 = f_6 + \frac{1}{2} (f_1 - f_3) - \frac{1}{6} \rho v_y \quad \text{for yhi;} \]

\[ v_y = 1 - \frac{f_0 + f_1 + f_3 + 2(f_4 + f_7 + f_8)}{\rho} , \]
\[ f_2 = f_4 + \frac{2}{3} \rho v_y , \]
\[ f_5 = f_7 + \frac{1}{2} (f_3 - f_1) + \frac{1}{6} \rho v_y , \]
\[ f_6 = f_8 + \frac{1}{2} (f_3 - f_1) + \frac{1}{6} \rho v_y \quad \text{for ylo.} \]
Appendix B: inlet/outlet openings for solute transport on a d2q4 lattice

In the case of inlet openings, for the flux style the solute concentrations are updated by applying the following rules [3]:

\[
C = \frac{\nu C_0 + DC_{-1}}{D + v} \quad \text{and} \quad g_i = g_i^{eq}, \quad i = 1, \ldots, 4, \quad \text{for xhi};
\]

\[
C = \frac{\nu C_0 + DC_{-1}}{D + v} \quad \text{and} \quad g_i = g_i^{eq}, \quad i = 1, \ldots, 4, \quad \text{for yhi};
\]

\[
C = \frac{\nu C_0 + DC_1}{D + v} \quad \text{and} \quad g_i = g_i^{eq}, \quad i = 1, \ldots, 4, \quad \text{for ylo}.
\]

For outlet openings the formulas become

\[
C = \frac{\nu C_0 - DC_{-1}}{D + v} \quad \text{and} \quad g_i = g_i^{eq}, \quad i = 1, \ldots, 4, \quad \text{for xhi};
\]

\[
C = \frac{\nu C_0 - DC_1}{D + v} \quad \text{and} \quad g_i = g_i^{eq}, \quad i = 1, \ldots, 4, \quad \text{for xlo};
\]

\[
C = \frac{\nu C_0 - DC_{-1}}{D + v} \quad \text{and} \quad g_i = g_i^{eq}, \quad i = 1, \ldots, 4, \quad \text{for yhi};
\]

\[
C = \frac{\nu C_0 - DC_1}{D + v} \quad \text{and} \quad g_i = g_i^{eq}, \quad i = 1, \ldots, 4, \quad \text{for ylo}.
\]

\(C_0\) is the concentration of the solution injected into the system; \(\nu > 0\) is the associated velocity. Given a node belonging to the opening, \(C_1\) and \(C_{-1}\) represent the solute concentration for the nearest node inside the simulation domain.

For openings of type dirichlet, the solute concentration is updated using the following rules [3]:

\[
C = \bar{C} \quad \text{and} \quad g_1 = \bar{C} - C' \quad \text{for xlo};
\]

\[
C = \bar{C} \quad \text{and} \quad g_4 = \bar{C} - C' \quad \text{for yhi};
\]

\[
C = \bar{C} \quad \text{and} \quad g_2 = \bar{C} - C' \quad \text{for ylo}.
\]

\(\bar{C}\) is the prescribed solute concentration and \(C'\) is the solute concentration obtained after the streaming step.
Appendix C: Implementation of surface reaction on the lattice d2q4

We provide details for the implementation of the surface reaction on the lattice d2q4. The following rules are applied:

1. Two opposite unknown modes can not occur.

2. Two orthogonal unknown modes are possible at corners. The two $g_i$’s are determined separately and the solute concentration is assumed to be the average value $C = (C_1 + C_2) / 2$. As an example, for the lower left corner of Fig. 12 we have

   \[ C_1 = \frac{2g_3 + k_r C_s}{k_r + 1/2} \quad g_1 = -g_3 + \frac{1}{2} C_1, \]

   \[ C_2 = \frac{2g_4 + k_r C_s}{k_r + 1/2} \quad g_2 = -g_4 + \frac{1}{2} C_2, \]

   \[ C = \frac{C_1 + C_2}{2}. \]

3. When the surface grows, the neighbors in the fluid phase of a solid node have the same probability to become a solid node.

4. The deposited mass is subtracted from the solute concentration, as well as from the incoming modes in the fluid phase in equal parts [16].

5. The cumulated mass of the solid node triggering surface growth is set to zero.

[1] D. Sergi, e-print arXiv:1202.0442, 2012.
[2] S.J. Plimpton, R. Pollock, and M. Stevens, in Proc. of Eighth SIAM Conf. on Parallel Processing for Scientific Computing, Minneapolis, MN, March (1997); Available at [http://lammps.sandia.gov/download.html](http://lammps.sandia.gov/download.html).
[3] M.C. Sukop and D.T. Thorne Jr., *Lattice Boltzmann Modeling: An Introduction for Geoscientists and Engineers* (Springer Verlang, Berlin Heidelberg, 2010).
[4] S. Succi, *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond* (Oxford University Press, Oxford 2009).
[5] P. Bhatnagar, E. Gross, and M. Krook, Phys. Rev. 94, 511 (1954).
[6] Available at [http://search.cpan.org/~dlux/Parallel-ForkManager-0.7.9/lib/Parallel/ForkManager.pm](http://search.cpan.org/~dlux/Parallel-ForkManager-0.7.9/lib/Parallel/ForkManager.pm).
[7] N.S. Martys and H. Chen, Phys. Rev. E 53, 743 (1996).
[8] H. Huang, D.T. Thorne Jr., M.G. Schaap, M.C. Sukop, Phys. Rev. E 76, 66701 (2007).
[9] S. Chibbaro, Eur. Phys. J. E 27, 99 (2008).
[10] S. Chibbaro, L. Biferale, F. Diotallevi, S. Succi, Eur. Phys. J. Special Topics 171, 223 (2009).
[11] Q. Kang, P.C. Lichtner, and D. Zhang, Water Resour. Res. 43, 5551 (2007).
[12] X. Shan and G.D. Doolen, J. Stat. Phys. 81, 379 (1995).
[13] Q. Kang, D. Zhang, S. Chen, X. He, Phys. Rev. E 65, 36318 (2002).
[14] Q. Kang, D. Zhang, and S. Chen, J. Geophys. Res. 108, 2504 (2003).
[15] Q. Kang, D. Zhang, P.C. Lichtner, I.N. Tsimpanogiannis, Geophys. Res. Lett. 43, 21107 (2004).
[16] G. Lu, D.J. DePaolo, Q. Kang, D. Zhang, J. Geophys. Res. 114, 11087 (2009).
[17] Q. Zou and X. He, Phys. Fluids 9, 1591 (1997).
[18] X. Shan and H. Chen, Phys. Rev. E 47, 1815 (1993).
[19] X. Shan and H. Chen, Phys. Rev. E 49, 2941 (1994).
[20] P.G. de Gennes, Rev. Mod. Phys. 57, 827 (1985).