

## Supplementary Materials

These Supplementary materials contain the details/description of lattice Boltzmann method for single-phase fluid flow and non-reactive advection-diffusion simulations and the set of parameters used in this work.

### S1 Lattice Boltzmann method for fluid flow

The discretized Boltzmann equation adopted in this paper is:

$$f_i(x + \mathbf{e}_i \Delta x, t + \Delta t) = f_i(x, t) + \Omega_i(f(x, t)), \quad (\text{S1.1})$$

where  $f_i$  represents the distribution function of particles moving along the  $i$ -directions of the chosen lattice with velocity  $\mathbf{e}_i$ .  $\Delta x$  and  $\Delta t$  are respectively the lattice spacing and time interval between two successive iterations, conventionally unitary and expressed in lattice units.  $\Omega_i$ , defined as the collision operator, defines the rate at which the distribution functions exchange momentum when locally collide. The most widely used form of this term is the linearized Single Relaxation Time (Succi, 2001; Sukop and Thorne, 2006):

$$\Omega_i = -\frac{1}{\tau} (f_i(x, t) - f_i^{eq}(x, t)), \quad (\text{S1.2})$$

where  $\tau$  is the relaxation time that controls the rate of distribution functions  $f_i(x, t)$  tend to the local equilibrium, indicated by the equilibrium distribution function  $f_i^{eq}(x, t)$ . This latter is a truncated expansion of Maxwell distribution, which in case of fluid flow solver is defined as:

$$f_i^{eq}(x, t) = \rho \omega_i \left[ 1 + 3 \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2} + \frac{9}{2} \frac{(\mathbf{e}_i \cdot \mathbf{u})^2}{c_s^4} + \frac{3}{2} \frac{u^2}{c_s^4} \right]. \quad (\text{S1.3})$$

$c_s^2$  is the sound of speed of the model and  $\omega_i$  are the lattice weights. Both parameters are constant once the lattice's geometry is chosen. Here, the scheme used for 3D fluid flow simulations is the  $D_3Q_{19}$  (i.e. three space dimensions and nineteen directions for particle distribution function). The value of  $c_s^2$  is equal to 1/3, whereas the lattice weights are:

$$\omega_i = \begin{cases} \frac{1}{3} & i = 0 \\ \frac{1}{18} & i = 1, \dots, 7. \\ \frac{1}{36} & i = 8, \dots, 18 \end{cases} \quad (\text{S1.4})$$

The macroscopic variables, the density  $\rho$  and the velocity  $\mathbf{u} = (u, v, w)$  are defined locally as the first two moments of the distribution functions:

$$\rho = \sum_{i=0}^{18} f_i, \quad \mathbf{u} = \frac{1}{\rho} \sum_{i=0}^{18} \mathbf{e}_i f_i. \quad (\text{S1.5})$$

It is well documented that through a Chapman-Enskog expansion (Succi, 2001), the following Navier-Stokes equations are retrieved in the case of incompressible fluids and low Mach numbers:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (\text{S1.6})$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \mathbf{u} \nabla \cdot (\rho \mathbf{u}) = -\nabla p + \nabla \cdot (\rho \nu \nabla \mathbf{u}). \quad (\text{S1.7})$$

The kinematic viscosity is directly related to the relaxation time  $\tau$  as  $\nu = c_s^2 (\tau - \frac{1}{2}) \Delta t$ . The pressure is linearly related to density through the equation of state  $p = c_s^2 \rho$ .

The transition from LBM units to real dimensions is straightforward through the definition of conversion factors for the primary quantities (e.g. length, time and density for fluid flow) (Wang et al., 2016; Krüger et al., 2017).

## S2 Lattice Boltzmann method for advection-diffusion

The lattice Boltzmann equation for transport processes follows a similar rule as the fluid flow solver. In this case it is necessary to add a new particle distribution functions:

$$g_i(x + \mathbf{e}_i \Delta x, t + \Delta t) = g_i(x, t) - \frac{1}{\tau_s} (g_i(x, t) - g_i^{eq}(x, t)). \quad (S2.1)$$

We adopt even in this case the Single Relaxation Time scheme, with a different relaxation time  $\tau_s$ . Differently from fluid flow solver, we use a D<sub>3</sub>Q<sub>7</sub> lattice scheme, because in case of solute transport the concentration is the only quantity conserved, the molecular diffusion is isotropic and to reduce the memory demand. This choice brings to a simplified equilibrium distribution function, which does not consider quadratic terms of velocity as:

$$g_i^{eq} = t_i C (1 + 3 \frac{\mathbf{e}_i \cdot \mathbf{u}}{c_s^2}) \quad (S2.2)$$

The local concentration is calculated as  $C = \sum_{i=0}^6 g_i$  and  $\mathbf{u} = (u, v, w)$  is the local velocity field calculated with the fluid dynamics solver. Here, the speed of sound of the model is equal to 1/4 and the lattice weights  $t_i$  depending on the lattice scheme are:

$$t_i = \begin{cases} 1/4 & i = 0 \\ 1/8 & i = 1, \dots, 6 \end{cases} \quad (S2.3)$$

Similar to Navier-Stokes equations, the following advection-diffusion equation for non-reactive dissolved phase is retrieved by a Chapman-Enskog expansion (Succi, 2001):

$$\frac{\partial C}{\partial t} + \nabla \cdot (C \mathbf{u}) = \nabla \cdot (D_m \nabla C) \quad (S2.4)$$

In this case, the molecular diffusivity is related to the relaxation time  $\tau_s$  as  $D_m = c_s^2 (\tau_s - \frac{1}{2}) \Delta t$ .

## S3

### List of acronyms and abbreviation

$A_s$ = Surface Area of grains	$\bar{U}$ = Average seepage velocity
$C$ = Solute concentration	$V$ = Volume of domain
$D_m$ = Molecular diffusivity	$WI$ = Washout index
$D_{eff}$ = Effective diffusion coefficient	$Pe$ = Peclet number
$D_{WI}$ = Delay washout index	$Re$ = Reynolds number
$k$ = permeability	$Sc$ = Schmidt number
$L$ = Length of domain	$\xi$ = Correlation length (corresponding to pore size)
$L_e$ = Average length of streamlines	$\tau$ = Tortuosity
$M$ = Solute mass in the domain	$\nu_m$ = Matèrn smoothness parameter
$SSA$ = Specific Surface Area	$\phi$ = porosity
$t$ = time	$\nu$ = kinematic viscosity
$\mathbf{u}$ = Fluid velocity	