Fluid-Structure Interaction with the Entropic Lattice Boltzmann Method

B. Dorschner‡, S.S. Chikatamarla‡ and I.V. Karlin‡

Aerothermochemistry and Combustion Systems Lab,
Department of Mechanical and Process Engineering, ETH Zurich, CH-8092 Zurich, Switzerland
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We propose a novel fluid-structure interaction (FSI) scheme using the entropic multi-relaxation time lattice Boltzmann (KBC) model for the fluid domain in combination with a nonlinear finite element solver for the structural part. We show validity of the proposed scheme for various challenging set-ups by comparison to literature data. Beyond validation, we extend the KBC model to multiphase flows and couple it with FEM solver. Robustness and viability of the entropic multi-relaxation time model for complex FSI applications is shown by simulations of droplet impact on elastic superhydrophobic surfaces.

I. INTRODUCTION

Fluid-structure interaction (FSI) is of significant interest in science and engineering applications, where examples include aeroelasticity such as flutter and buffeting [1][4], or bio-fluidmechanics in order to enhance our understanding of cell aggregation, blood-heart interaction as well as the propulsion mechanisms in flying and swimming [6–10]. Insight in these phenomena through experimental and numerical studies has shown tremendous success for example, the development of cancer diagnostic devices the size of a chip [11][12], optimizing wind turbines [4] or artificial heart valves [13] but also may be used to draw inspirations for the design of novel propulsion system in robotic devices. Yet, such problems remain a challenge to existing methods due to strong nonlinearity and their multidisciplinary nature [14]. Due to inherent limitations of experiments in terms of accuracy, accessibility and cost much research effort has been devoted to the development of numerical methods for the simulation of FSI applications.

In general, there are two main avenues to FSI simulations, namely monolithic and partitioned approaches. The monolithic approach describes the fluid and the structural part with the same discretization scheme in one system of equations, which is solved simultaneously with a single solver. This technique implies consistent fluid-structure interface conditions. On the other hand, in most practical applications the partitioned approach is employed, which uses separate solvers for the fluid and structural part, respectively. The advantage of this approach is its modularity, which allows the use of independently optimized solution strategies in the solid and fluid domain, respectively. Thus partitioned approaches are most common and therefore focus of this paper. On the other hand, consistent solid-fluid interface conditions are not satisfied implicitly and thus pose the main challenge of partitioned fluid-structure approaches. For the simulation of the fluid flow involving complex moving geometries, a broad categorization into body-conforming and non-conforming methods can be identified. Most conventional FSI schemes are based on body-fitted grids, where the interface conditions are treated as boundary conditions and the computational mesh conforms to the moving and deforming solid-fluid interface. Examples of commonly used body-fitted approaches include arbitrary-Lagrangian-Eulerian formulations [15][16] and space-time finite element methods [17][18]. While the interface conditions are easily imposed, the generation of the moving meshes for complex geometries undergoing large deformations is computationally expensive and requires sophisticated procedures to avoid severe mesh distortion to preserve accuracy [18][21]. Viable alternatives are found in non-conforming methods, which we will focus on in this paper.

In particular, we employ the lattice Boltzmann method (LBM), which has matured into an attractive alternative to conventional methods based on a direct discretization of the macroscopic Navier-Stokes equations. The LBM derives from kinetic theory and evolves discretized particle distribution functions (populations) \( f_i(x,t) \), which are associated with a set of discrete velocities \( c_i = 1, \ldots, Q \) and designed to recover the macroscopic Navier-Stokes equations in the hydrodynamical limit. By organizing \( c_i \) into a regular lattice, the LBM reduces to a propagation step, advecting the populations along \( c_i \), and a collision operator, which over-relaxes the populations. In this paper, we chose the entropic multi-relaxation time collision operator [22] for its accuracy and robustness as shown in various challenging set-ups involving a combination of turbulence and complex moving geometries [23]. For modeling complex, moving geometries we employ Grad’s approximation as proposed in [24], which has shown to be reliable for both one- and two-way coupled simulations of moving and deforming objects [25]. The structural domain on the other hand is described by a geometrical nonlinear total Lagrangian formulation in the framework of the finite element method (FEM).

In this paper, we aim to assess the predictive capabilities of the recently developed entropy-based lattice Boltzmann models in combination with Grad’s approximation for fluid-structure interaction problems involving large
deformations. Besides thorough validation by comparison to standard benchmarks, the robustness of the scheme allows us to explore its capabilities in multi-physics applications, where we present a novel multiphase formulation of the entropic multi-relaxation time model and its coupling to the structural solver.

The paper is structured as follows: We begin by briefly introducing the numerical methodology to solve the governing equations for both the fluid and the solid domain, followed by a discussion of their coupling through appropriate boundary conditions. In Section III we report the numerical results obtained by the proposed scheme. We start by a thorough validation of the model in section IIIA and subsequently present the extensions of the FSI scheme for multiphase flows in section IIIB.

II. NUMERICAL APPROACHES

In the following we briefly describe the numerical methodology for the fluid, the elastic solid as well as the coupling methodology. The subscript $f$ and $s$ are used to indicate the fluid and structural quantities, respectively. The time-dependent fluid and solid domain with their common interface are denoted by $\Omega^t_f$, $\Omega^t_s$ and $\Gamma^t_f$ = $\partial \Omega^t_f \cap \partial \Omega^t_s$, respectively. The corresponding reference or initial domains and the interface are referred to as $\Omega_s$, $\Omega^t_s$ and $\Gamma_f$ = $\partial \Omega^t_f \cap \partial \Omega_s$, respectively. Further, Neumann and Dirichlet boundary conditions are identified as $\Gamma_N$ and $\Gamma_D$, respectively.

A. Entropic multi-relaxation time lattice Boltzmann method

We solve the weakly compressible Navier-Stokes equations using the entropic multi-relaxation time lattice Boltzmann (KBC) model. For brevity, we only summarize the main steps and refer to the works of [22, 23, 26] for a thorough discussion of the model. The evolution of the population $f_i(x, t)$ is given by the discrete kinetic equation

$$ f_i(x + c_i, t + 1) = f_i^t(x, t) = (1 - \beta) f_i(x, t) + \beta f_i^\text{mirr}(x, t), \quad (1) $$

where the advection step is indicated by the left-hand side and the post-collision state $f_i^t$ is represented on the right-hand side. The populations are expressed in its natural moment basis as the sum of the kinematic part $k_i$, the shear part $s_i$ and the remaining higher-order moments $h_i$ as

$$ f_i = k_i + s_i + h_i, \quad (2) $$

The mirror state may thus be defined as

$$ f_i^\text{mirr} = k_i + (2s_i^{eq} - s_i) + ((1 - \gamma) h_i + \gamma h_i^{eq}), \quad (3) $$

where $s_i^{eq}$ and $h_i^{eq}$ are $s_i$ and $h_i$ evaluated at equilibrium conditions. The equilibrium $f_i^{eq}$ is defined as the minimum of the entropy function

$$ H(f) = \sum_{i=1}^Q f_i \ln \left( \frac{f_i}{W_i} \right), \quad (4) $$

subject to the local conservation laws for mass and momentum

$$ \sum_{i=1}^Q \{1, c_i\} f_i = \{\rho, \rho u_f\}, \quad (5) $$

where the weights $W_i$ are lattice-specific constants.

Finally, the relaxation rate $\gamma$ of the higher-order moments is found by minimizing the discrete entropy function (see Eq. [4]) in the post-collision state $f_i^t$. Thus, at every time step and every grid point the estimate for $\gamma$ is computed by the following analytical expression

$$ \gamma = 1 - \left( 2 - \frac{1}{\beta} \right) \frac{\langle \Delta s | \Delta h \rangle}{\langle \Delta h | \Delta h \rangle}, \quad (6) $$

where $\Delta s_i = s_i - s_i^{eq}$, $\Delta h_i = h_i - h_i^{eq}$ and $\langle X | Y \rangle = \sum_i \langle X_i | Y_i \rangle$.

The entropic multi-relaxation time lattice Boltzmann method recovers the Navier-Stoke equations in the hydrodynamic limit and relates the parameter $\beta$ to the kinematic viscosity as

$$ \nu = c_s^2 \left( \frac{1}{2\beta} - \frac{1}{2} \right), \quad (7) $$

where $c_s = 1/\sqrt{3}$ is the lattice speed of sound.

B. Structural modeling

In the Lagrangian frame, the structural part is governed by the momentum equation as

$$ \rho_s \frac{\partial v_s}{\partial t} - \nabla \cdot P_s = \rho_s b_s, \quad \text{in } \Omega_s $$

$$ v_s = \bar{v}_s, \quad \text{on } \Gamma_D $$

$$ P_s n_s = \bar{t}_s, \quad \text{on } \Gamma_N $$

where $v_s$, $\rho_s$ and $b_s$ are the solid velocity, density and body force per unit mass. The outer normal vector of $\Gamma_f$ or $\Gamma_{s,n}$ is denoted by $n_s$. The prescribed velocities and tractions on the Dirichlet and Neumann boundary are indicated by $\bar{v}_s$ and $\bar{t}_s$, respectively. The first Piola-Kirchhoff stress is denoted by $P_s$ and related to the second Piola-Kirchhoff stress $S_s$ by

$$ P_s = FS_s, \quad (9) $$

where $F$ denotes the deformation gradient

$$ F = I + \nabla u_s, \quad (10) $$
and \( u_s \) is the displacement field of the solid. The second Piola-Kirchhoff stress on the other hand can be mapped to the Cauchy stress tensor \( \sigma_s \) by

\[
S_s = J F^{-1} \sigma_s F^{-T},
\]

(11)

where \( J = \det(F) \). In this paper, we consider the hyperelastic Saint Venant-Kirchhoff constitutive equation, which extents linear elastic models to the geometrically non-linear regime and defines the second Piola-Kirchhoff stress as

\[
S_s = \lambda tr(E)I + 2\mu_s E,
\]

(12)

where

\[
E = \frac{1}{2} (F^T F - I) = \frac{1}{2} (\nabla u_s + \nabla u_s^T + \nabla u_s^T \nabla u_s)
\]

(13)

is the Green-Lagrange strain tensor. The first and second Lamé coefficients are indicated by \( \lambda_s \) and \( \mu_s \), respectively and are related to Young’s modulus \( E_s \) and Poisson’s ratio \( \nu_s \) as

\[
\nu_s = \frac{\lambda_s}{2(\lambda_s + \mu_s)}, \quad E_s = \frac{\mu_s(3\lambda_s + 2\mu_s)}{\lambda_s + \mu_s}.
\]

(14)

In the present work, we employ a two-field formulation and solve for the displacement field separately using the kinematic compatibility condition

\[
\frac{\partial u_s}{\partial t} = -v_s = 0 \quad \text{in} \quad \Omega_s,
\]

\[
u_s - \frac{\partial u_s}{\partial t} = 0 \quad \text{on} \quad \Gamma_D,
\]

(15)

where \( \Gamma_D \) denotes the prescribed displacement on the Dirichlet boundary.

The structural equations are solved using the finite element method (FEM), which is implemented in the opensource library deal.iI [27]. We follow standard FEM procedures, see, e.g., the textbooks [28, 29] or in the context of monolithic FSI with deal.iI [30, 32]. Using the conventional notation for Lebesgue and Sobolev spaces, we define the following functional spaces for trial and weight functions:

\[
L^2 := \{ w_s \in L^2(\Omega_s) \}
\]

(16)

\[
H^1 := \{ w \in H^1(\Omega_s) : w = 0 \text{ on } \Gamma_s,D \subset \Omega_s \}
\]

(17)

\[
V_0 := \{ w \in H^1(\Omega_s) : w = w_s,D \text{ on } \Gamma_s,D \subset \Omega_s \}
\]

(18)

where \( L^2, H^1 \) denote the Lebesgue space of square integrable functions and the first Sobolev space, respectively. Furthermore, the short-hand notations \( \langle \cdot, \cdot \rangle \) and \( \langle \cdot \rangle \) indicate the scalar product on the \( L^2 \)-space and its boundary, respectively. Thus, following standard procedures, we obtain the following variational formulations for \( \{v_s, u_s\} \in \{L \times V_0\} \)

\[
(\rho_s \partial_t v_s, \psi_{s,v})_{\Omega_s} + (P_s, \nabla \psi_{s,v})_{\Omega_s} = (\rho_s b, \psi_{s,v})_{\Omega_s} + (t, \psi_{s,v})_{\Gamma_s,N_s,N,N} = 0 \quad \forall \psi_{s,v} \in V_0,
\]

(19)

\[
(\partial_t u_s, \psi_{s,u})_{\Omega_s} - (v_s, \psi_{s,u})_{\Omega_s} = 0 \quad \forall \psi_{s,u} \in L,
\]

(20)

where \( \psi_{s,u}, \psi_{s,v}, u_s \) and \( v_s \) are the trial and test functions of the solid displacement and velocity, respectively. Note that the traction \( t \) may also be specified in terms of the Cauchy stress tensor \( \sigma_s \) as

\[
t = J_s \sigma_s F^{-1} n_s
\]

(21)

For simplicity, we use the one step-\( \theta \) scheme for the integration in time, which, for a generic quantity \( g \) with \( \partial_t g(t) = f(t, g(t)) \), reads

\[
\partial_t g \approx \frac{g^{n+1} - g^n}{\Delta t} = \theta f^{n+1} + (1 - \theta)f^n.
\]

(22)

This allows us to choose implicit/explicit Euler or centered/shifted Crank-Nicolson time integration depending on the choice of \( \theta \) but can also easily be extended to the fractional-step-\( \theta \) scheme. Note that the following can be extended in a straightforward manner to other standard time integration schemes such as the Newmark algorithm or alike.

Using the temporal discretization of Eq. (22), the variational formulation of Eq. (19) may be discretized in time as

\[
\rho_s \Delta t^{-1} (v_s^{n+1}, \psi_{s,v})_{\Omega_s} + \theta \left( P_s^{n+1}, \nabla \psi_{s,v} \right)_{\Omega_s} = 0,
\]

(23)

\[
\rho_s \Delta t^{-1} (v_s^n, \psi_{s,v})_{\Omega_s} - \theta \left[ \left( t^n, \psi_{s,v} \right)_{\Gamma_s,N_s,N,N} - \left( \rho_s b^{n+1}, \psi_{s,v} \right)_{\Omega_s} \right] + (1 - \theta) \left[ \left( t^n, \psi_{s,v} \right)_{\Gamma_s,N_s,N,N} - \left( \rho_s b^n, \psi_{s,v} \right)_{\Omega_s} \right] - (P_s^n, \psi_{s,v})_{\Omega_s} \]

\forall \psi_{s,v} \in V_0,

\Delta t^{-1} (u_s^{n+1}, \psi_{s,u})_{\Omega_s} - (1 - \theta) (v_s^n, \psi_{s,u})_{\Omega_s} = 0 \quad \forall \psi_{s,u} \in L,

(24)

With slight rearrangement it should be obvious that Eq. (23) and Eq. (24) can conveniently be expressed in matrix form as

\[
A(U^{n+1}, \Psi) = F(\Psi),
\]

(25)

where \( U^{n+1} = \{v_s^{n+1}, u_s^{n+1}\} \) and \( \Psi = \{\psi_{s,v}, \psi_{s,u}\} \).

Based on the time-discrete equations shown above, we employ a finite element Galerkin discretization in space. We discretize the undeformed or reference domain \( \Omega_s \) in a shape-regular mesh \( \mathcal{M}_h \), which is composed of hexahedral elements \( E \). The finite element spaces are given by

\[
L_h := \{ w_h \in C(\Omega_h), w_h|_E \in Q_p(E) \quad \forall E \in \mathcal{M}_h \subseteq L^2, \}
\]

(26)

\[
V_{0,h} := \{ w_h \in C(\Omega_h), w_h|_E \in Q_p(E) \quad \forall E \in \mathcal{M}_h \}
\]

(27)

\[
V_{D,h} := \{ w_h \in C(\Omega_h), w_h|_E \in Q_p(E) \quad \forall E \in \mathcal{M}_h \}
\]

(28)

\[
\mathcal{W}_h := \{ w_h|_{\Gamma_{s,D,h}} \subseteq L^1, \}
\]

(29)

where \( Q_p(E) \) is the space of tensor product polynomials of degree \( p \). In the following, we restrict ourselves
to the $Q_2$ element for simplicity, but it can straightforwardly be extended to higher order. Further, a bilinear transformation is used to map the physical elements to the unit element.

Finally, the fully time- and space-discrete nonlinear system in matrix notation reads as

$$A(U_h^{n+1}, \Psi_h) = F(\Psi_h),$$  \hspace{1cm} (31)

for $U_h^{n+1} = \{w_{s,h}^{n+1} u_{s,h}^{n+1}\} \in \{\mathcal{L}_h \times \mathcal{V}_{D,h}\}$ and $\Psi_h = \{\psi_{s,v,h}, \psi_{s,a,h}\} \in \{\mathcal{N}_{h,0} \times \mathcal{L}_h\}$.

The non-linear equations arising from the integration procedures and the Saint-Venant Kirchoff constitutive relation are solved using a Newton-Raphson method in combination with a simple line search algorithm. This yields the incremental updating rule for the $k$-th iteration as

$$A'(U_h^{n,k})(\delta U_{n,k}, \Psi_h) = -A(U_h^{n,k}, \Psi_h) + F(\Psi),$$  \hspace{1cm} (32)

$$U_h^{n,k+1} = U_h^{n,k} + \lambda \delta U_h^{n,k},$$  \hspace{1cm} (33)

where $\lambda \in (0, 1]$ is the line search relaxation parameter. For all cases in this paper $\lambda = 0.7$ has proven to be a good choice. The Gâteaux derivatives $A'(U)(\delta U_{n,k}, \Psi_h)$ are analytically computed. In particular, the non-linearity arises due to the Saint-Venant Kirchoff relation, which only depends on the displacement. Thus, for direction $\delta U$ the corresponding derivatives with respect to $U$ may be identified as

$$\partial_U E = \frac{1}{2} (\nabla \delta U F + F^T \nabla \delta U),$$  \hspace{1cm} (34)

which yields

$$\partial_U S = \frac{1}{2} \mu_s (\nabla U F + F^T \nabla U) I + \mu_s (\nabla U F + F^T \nabla U),$$  \hspace{1cm} (35)

and upon substitution

$$A'(U)(\delta U, \Psi_h) = (\nabla \delta U S + F (\mu_s (\nabla U F + F^T \nabla U) + \mu_s (\nabla U F + F^T \nabla U) I, \nabla \Psi_h).$$  \hspace{1cm} (36)

C. Fluid-structure coupling

A consistent coupling of the fluid and structural domain enforces the following interface conditions

$$v_f = v_s \quad \text{on } \Gamma_f,$$  \hspace{1cm} (37)

$$P_f n_s + J \sigma_f F^{-T} n_s = 0 \quad \text{on } \Gamma_f,$$  \hspace{1cm} (38)

where the $\sigma_f = -p_f I + \rho_f v_f (\nabla v_f + \nabla v_f^T)$ is the fluid stress tensor.

Within the context of partitioned approaches, one can distinguish between weakly(loose)- and strongly-coupled FSI schemes. While weakly-coupled methods do not enforce the fluid-solid interface constraints, strongly-coupled methods typically utilize subiterative schemes to converge to the solution of the monolithic system. Weakly-coupled methods are computationally less expensive but have shown to generate artificial energy at the interface due to the staggered nature of the evolution of the fluid and structural part \[33\]. This so-called added-mass effect can cause fatal instabilities for small solid-fluid density ratios and thus may limit their range of applicability \[34–38\].

However, the added-mass effect is proportional to the time step size for compressible flows, and convergences to a non-zero value only in the fully incompressible regime. Thus, for the weakly compressible LBM at the incompressible limit and the corresponding small time step size this effect has only a limited influence \[39\].

Hence, for simplicity, we chose a weakly-coupled partitioned approach using the conventional serial staggered (CSS) approach. The fluid is solved by the LBM and the solid by an appropriate finite element discretization, which accounts for geometric nonlinearity. The coupling between both domains is achieved through appropriate boundary conditions. On one hand, the Grad boundary condition accounts for the coupling from the solid to the fluid. On the other hand, the fluid is coupled to the solid by the traction force as computed through a pressure tensor extrapolation scheme similar to \[39\].

Thus, in the CSS algorithm, we first perform a fluid step (including boundary conditions) and compute the force (traction) on the solid. Subsequently, the structural solver computes its deformation, where the traction is imposed as a boundary condition. Finally, we transfer velocity and displacement of the solid to the fluid solver, update the solid geometry in the fluid solver and incorporate the boundary velocity in the fluid boundary conditions.

In the following, we briefly summarize the implementation of the corresponding boundary conditions needed to perform full coupling.

1. Fluid boundary conditions

In the FSI simulations, the fluid boundary condition imposes the no-slip condition and accounts for the momentum exerted from the solid to the fluid. In the realm of LBM many variants exist in literature ranging from simple bounce-back schemes to implicitly corrected immersed boundary methods. However, only a few have shown to be stable, accurate and universally applicable. A viable alternative was proposed in \[24\] using an analog of Grad’s approximation for the missing populations. This boundary condition was shown to be second-order accurate and consistent with the entropy-based LBM. Accuracy and robustness has been demonstrated for various challenging set-ups involving complex, moving and deforming geometries in one- and two-way coupled sim-
ulations in both laminar and turbulent flows [23, 25, 40].

The Grad approximation is a parametrization of the population in terms of its moments and in the athermal case it has shown to be sufficient to include the pressure tensor $\Pi$ besides the conserved quantities. An explicit expression is given by

$$f_i^* (\rho, v_f, \Pi) = W_i \rho + \frac{\rho}{c_s^2} \xi_i \cdot v_f + \frac{1}{2c_s^4} (\Pi - \rho c_s^2 I) : (\xi_i \otimes \xi_i - c_s^2 I),$$

where the pressure tensor $\Pi$ is approximated by

$$\Pi = \Pi^\text{eq} + \Pi^\text{neq},$$

with

$$\Pi^\text{eq} = \rho c_s^2 I + \rho v_f \otimes v_f,$$

$$\Pi^\text{neq} = -\frac{\rho c_s^2}{2\beta} (\nabla v_f + \nabla v_f^T).$$

Thus, by appropriately specifying density $\rho$, velocity $v_f$ and the pressure tensor $\Pi$ we account for the momentum exerted from the fluid to the solid as well the mass swept by the object. For this purpose, the concept of target values was introduced, where the details are discussed at length in our previous contributions [24, 25] and we will only highlight important FSI specifics here. While the target density is given by the implied bounce-back density with an additional contribution in order to account for the object motion, the velocity gradients are evaluated using a finite difference scheme. The velocity at the locations of the Eulerian fluid mesh on the other hand involves interpolation of the velocity from the intersection point $x_{w,i}$ with the boundary along the lattice vector $c_i$.

To that end, in the case of FSI, we use the FEM mesh to construct a surface mesh, which is passed to the fluid solver. In particular, we partition the quadrilateral surface elements of the FEM solver into triangular elements for an efficient detection of the intersection location and update the vertex locations using the displacements as computed by the FEM solver. Furthermore, the corresponding velocity values are transferred to the fluid solver and used to interpolate the velocity values at the intersection locations $x_{w,i}$. This completes the fluid boundary condition.

2. **Solid boundary conditions**

For the coupling of the fluid to the solid, we impose a traction boundary condition as

$$t = J_s \sigma_f F_s^{-T} n_s.$$  

Thus, we need to evaluate $\sigma_f$ at the quadrature points of the FEM mesh. Fortunately, in LBM the fluid stress tensor can conveniently computed as

$$\sigma_f = -p I - (1 - \beta) \Pi^{(1)},$$

where $p = \rho c_s^2$ in the athermal case and $\Pi^{(1)} = \sum \xi_i f_i^{(1)} \xi_i \otimes \xi_i$, which is evaluated using $f_i^{(1)} \approx f_i - f_i^\text{eq}$. As $\sigma_f$ needs to be evaluated at all quadrature point on the solid surface mesh, we use an extrapolation scheme, similar to [39].

### III. NUMERICAL RESULTS

#### A. Validation

1. **Turek Benchmark**

For the validation of FSI schemes a comprehensive test suite was proposed in [41], which consists of a rigid circular cylinder with a flexible flag attached to its downstream side. The structure is placed asymmetrically in a laminar channel flow and therefore induces an oscillatory motion of the elastic beam as the flow evolves. The setup is schematically shown in Figure 1. While the boundary conditions in pitchwise directions are no-slip boundaries, the inflow at the left boundary has a prescribed parabolic

| Contribution | $u_x$ | $u_y$ | $f$ |
|--------------|------|------|-----|
| [41]        | $-0.01431 \pm 0.01431$ | $-0.06361 \pm 0.06516$ | 1.0995 |
| Present     | $-0.01460 \pm 0.01460$ | $-0.06463 \pm 0.06492$ | 1.10 |

TABLE I. Results for CSM3.
we do not consider the surrounding fluid of the setup ing a time-dependent large deformation test case. Thus, we first validate the structural solver separately us-

assumed to follow the hyperelastic Saint Venant-Kirchoff respectively. The constitutive law for the solid part is

strain boundary conditions for the fluid and the solid,
thickness we consider the FSI3 benchmark of [41] for which the

marks of the fully coupled FSI scheme. To that end, validated the structural, we proceed with bench-

cial damping in the simulations of [41] both results agree

Figure 3 and it is obvious that apart from minor artifi-

cial damping in the simulations of [41] both results agree well. This validates our implementation of the structural model.

For brevity, we avoid presenting the pure CFD val-

in Figure [1] but only account for a gravitational force 

profile according to

\[ u(0, y) = 1.5\bar{U}y(H - y)/(H/2)^2, \]  

(45)

where the mean inflow velocity is \( \bar{U} \) and the channel height \( H \). As initial condition for the unsteady simulation we use a smooth ramping function for the inflow. The cylinder with diameter \( D \) is placed asymmetrically at \((2D, 2.1D)\), while the beam has length \( L = 3.5D \) and thickness \( h = 0.2D \). Note that while in [11] all computations were carried out in two dimension, we perform a quasi two-dimensional simulation by using only a few points in spanwise direction and apply periodic and plane strain boundary conditions for the fluid and the solid, respectively. The constitutive law for the solid part is assumed to follow the hyperelastic Saint Venant-Kirchoff model.

Before attempting to solve the fully coupled FSI system, we first validate the structural solver separately using a time-dependent large deformation test case. Thus, we do not consider the surrounding fluid of the setup.

TABLE II. FSI3: Mean and amplitude of the flag tip deflection.

| Contribution | \( u_x \) | \( u_y \) | \( f_x \) | \( f_y \) |
|--------------|---------|---------|---------|---------|
| ALE-FEM [41] | -0.00288 ± 0.000271 | 0.000148 ± 0.000351 | 11 | 5.5 |
| LB-FEM [39]  | -0.00269 ± 0.000253 | 0.000148 ± 0.000343 | 10.9 | 5.3 |
| present      | -0.00268 ± 0.000257 | 0.000145 ± 0.000338 | 11 | 5.5 |

For brevity, we avoid presenting the pure CFD validation as done in [11]. The fluid solver however was thoroughly validated as witnessed by many of our preceding contributions (see, e.g., [12]). Thus, having validated the structural solver, we proceed with benchmarks of the fully coupled FSI scheme. To that end, we consider the FSI3 benchmark of [11] for which the density ratio is \( \rho_s/\rho_f = 1 \) and the Reynolds number \( Re = UD/\nu = 200 \). The aeroelastic coefficient was taken as \( Ac = E_s/(\rho_f \bar{U}^2) = 1.4 \cdot 10^3 \), where \( E_s \) indicates Young’s modulus for the structure and the Poisson ratio was set to \( \nu_s = 0.4 \). In the fluid domain, we use two levels of refinement as shown in Figure [2] which effectively resolves the cylinder diameter by \( D_{lb} = 40 \) lattice points. The elastic beam was discretized using \( (140, 10, 1) \) elements and evolved with a time step of \( \Delta t = 8.75 \cdot 10^{-5} \).
two-dimensional setting, we next consider a fully three-
dimensional flow. To that end, we investigate the non-
linear dynamics of a flag in a uniform fluid flow. Despite
being a classical model problem for FSI, the complex mo-
tion of the flag challenges numerical methods and thus
only a few cases have been reported in literature [43–45].
Here, we use the case as provided in [43, 44] for valida-
tion. While in [44] a diffuse-interface immersed boundary
method was employed, [43] used an immersed boundary
method coupled with a nonlinear FEM solver. As shown
in Figure 5, the leading edge of a square flag of length $L$
and thickness $h = 0.01L$ is placed at the origin of the do-
main. In addition, zero displacement and velocity bound-
ary conditions are imposed at the leading edge. The rect-
gle fluid domain spans from $[-2L \times -1L \times -4L]$ to
$[8L \times 1L \times 4L]$ in streamwise, spanwise and transverse
direction, respectively, where periodic boundary conditions
are applied in spanwise direction and free-stream bound-
aries are imposed in transverse direction. Using two lev-
els of refinement, the flag was resolved by $L = 100$ lattice
units in the finest level. The flexible flag is discretized
with a uniform mesh of $[50 \times 50 \times 2]$ elements. The Pois-
son ratio is set to $\nu_s = 0.4$ and the bending rigidity is
$Eh^3/(12(1-\nu_s^2))\rho_f U_\infty^2 L^3 = 10^{-4}$. The density ratio
is taken as $\rho_s/\rho_f = L/h$ and the Reynolds number is
$Re = U_\infty L/\nu = 200$. Initially, the flag coincides with the
$xy$-plane and a small perturbation is used to trigger the
periodical flapping behavior. During the evolution, we
record the displacement of the Point B, which is located
at $B = (L, 0, 0)$ in the undeformed configuration and compare it to the reference data of [43, 44] in Figure 7. Note that in [43] two flag models were considered, namely
a plate model with infinitesimal thickness (Flag 1) and
three dimensional model with thickness $h = 0.01L$ (Flag
2). Both cases demonstrate negligible discrepancies due
to the low Reynolds number in this case. After the initial
transient, the flow quickly converges to a periodic flap-
ning as seen in Figure 7. The comparison of the present
simulations to the references shows good agreement. Be-
sides the displacement, we computed the evolution of the
drag coefficient $C_d = F_d/(1/2\rho_f U_\infty^2 L^2)$ and compare it
values reported in [43] in Figure 7. Significant noise can

2. Flow past a flapping flag

Having validated the proposed scheme in the quasi
two-dimensional setting, we next consider a fully three-

![FIG. 5. FSI3: Evolution of the flag tip deflection in $x$- and $y$-direction.](image1)

![FIG. 6. Schematic of the flow past a flapping flag.](image2)
be observed for the simulations by [43], which, according to the authors, originates from the noisy prediction of the thin plate. In contrast, the results from the present method appear smooth and do not exhibit oscillations. Overall, both results agree qualitatively but do exhibit discrepancies, likely due to the noise. Unfortunately, no data regarding the drag evolution was reported in [44] and thus eludes a comparison. Finally, in Figure 8, the vortical structures in the wake of the flag are visualized by isosurfaces of the Q-Criterion, which are colored by streamwise velocity. The vortices shed from the trailing edge connect with the vortices shed from the side edges to form hairpin-type vortices along with two separate co-rotating vortices. Notably, this wake structure bears significant resemblance to self-propelled anguilliform swimmers [25]. Analogous vortex structures have been observed in the references [43, 44].

3. Beam in crossflow

So far we have successfully validated the proposed scheme for quasi-two dimensional and three-dimensional flows. As a final validation, we include a simulation involving turbulence. To that end, we consider a flexible beam in a cross flow. This set-up has been studied both experimentally and numerically in [43] and [46], respectively and aims to model the deformation of aquatic plants caused by the flow. The beam is vertically mounted in a uniform flow and has the length $L$, the thickness $h$ and the width $b$. As in the references, the Reynolds number is set to $Re = U_\infty L/\nu = 8000$ and the geometrical properties of the beam are given by $L/b = 5$ and $h/b = 0.2$. The solid material has the non-dimensional Young’s modulus $\tilde{E}_s = E_s/\rho U_\infty^2$ and the Poisson’s ratio $\nu_s = 0.4$. The density ratio is set to $\rho_s/\rho_f = 0.678$ and a buoyancy force $f_b = (\rho_f - \rho_s)gh/(\rho_f U_\infty^2) = 0.2465$ is applied. The rectangular domain ranges from $[-5b, -8b, -8.5b]$ to $[16b, 8b, 8.5b]$ in which the centroid of the beam is placed at the origin of the undeformed configuration. Using one level of refinement, the fluid domain discretizes the beam width with $b = 40$ lattice points and the solid mesh employs $[2 \times 20 \times 140]$ elements to represent the beam.

Using these flow and structural conditions and parameters, the plate converges to a steady deformation. A snapshot of the deformed state is presented in Figure 9, where the wake behind the deformed beam is visualized by isosurfaces of the Q-Criterion and colored by velocity magnitude. Qualitatively this is in line with the reference. For a more thorough comparison, we computed the drag coefficient $C_d = F_x/(1/2 \rho_f U_\infty^2 bL)$ along with the deflection of the beam’s free end in the deformed state. Along with the reference values, the results of the present simulation are listed in Table III. It is apparent
TABLE III. Flexible plate in a cross flow. Comparison of drag coefficient $C_d$ and plate deflection $D_x/b$ and $D_y/b$ in stream- and pitchwise direction, respectively.

| Contribution                      | $C_d$ | $D_x/b$ | $D_y/b$ |
|----------------------------------|-------|---------|---------|
| Tian et al. (2014), IMB-FEM      | 1.03  | 2.12    | 0.54    |
| Luhar & Nepf (2011), exp.        | 1.15  | 2.14    | 0.59    |
| present                          | 1.13  | 2.14    | 0.55    |

FIG. 9. Flexible plate in a cross flow: Isosurfaces of $Q$-criterion, colored by velocity magnitude.

that the results are in good agreement with the reference data. While some discrepancies may be observed to the numerical study of the present simulation matches that the results are in good agreement with the reference data. While some discrepancies may be observed to the numerical study of the present simulation matches the experimental study well.

**B. Extensions to fluid-structure interaction in multiphase flow**

Two-phase flows are of fundamental interest in science and engineering applications, which exhibits various complex phenomena at multiple temporal and spatial event scales. These include droplet breakup, droplet reconnection as well as droplet impact on a surface, where effects such as splash, skating, rebound, or the trampoline effect have been observed.

In recent years, much attention has been devoted to droplet impact on so-called superhydrophobic surfaces. Super-hydrophobic surfaces exhibit strong repellence of liquid droplets, which can be exploited for anti-icing, self-cleaning, drag reduction and many other applications. The most known example of a natural super-hydrophobic surface is the surface of the lotus leaf, i.e. Nelumbo nucifera. Numerous studies suggested that the combination of surface chemistry and roughness on multiple scales on the surface is responsible for its repellence. Thus, modern synthetic designs of superhydrophobic surfaces, combine the effects of micro-texturing and chemistry to enhance the hydrophobic effect. To that end, many studies have investigated the underlying physics of droplet impact on superhydrophobic surfaces using different designs and conditions with the ultimate goal to reduce the contact time.

Note however that most studies have focused on rigid surfaces and neglected the flexibility of the substrate, which is inherent to most naturally occurring repellent surfaces such as leaves, textiles or butterfly wings. Notable is the recent study of the effect of elasticity on hydrophobicity was investigated experimentally.

In this section, we aim to go beyond classical benchmark cases and explore the capabilities of the KBC-FSI solver in the context of multiphase flows by considering droplet impact on flexible superhydrophobic surfaces, similar to. From the numerical point of view, simulations of such a kind are challenging. However, the LBM offers an attractive alternative to conventional schemes, due to the ease of implementing inter-molecular forces and complex boundaries without sacrificing efficiency. While various LB models for multiphase flow exist, restrictions on density ratio, kinematic viscosity and interface thickness remained for long. Among others, a viable alternative was proposed in , where combining the notion of a discrete entropy function, the free-energy based formulation and an appropriately regularized equation of state significantly increased the range of applicability of LB models for multiphase flow. This approach has been thoroughly validated by simulations of droplet impact on flat and micro-textured superhydrophobic surfaces for a variety of different bouncing regimes. Here, we build on these results and extend it to the KBC model, the Grad boundary condition and the coupling to the structural solver. The equation of state and the forcing approach is kept same.

On the fluid side, following, the phase separation and wetting properties are implemented through a body force

$$ F = F_f + F_s. $$

The mean field force

$$ F_{f,\alpha} = \partial_\beta \left( \rho \kappa^2 \delta_{\alpha\beta} - P^K_{\alpha\beta} \right), $$

accounts for the phase separation by implementing the Korteweg stress tensor

$$ P^K_{\alpha\beta} = \left( p - \kappa \rho \partial_\gamma \partial_\gamma \rho - \frac{\kappa}{2} (\partial_\gamma \rho)(\partial_\gamma \rho) \right) \delta_{\alpha\beta} + \kappa (\partial_\alpha \rho)(\partial_\beta \rho), $$

where the pressure $p$ is prescribed through a non-ideal equation of state and $\kappa$ controls the surface tension. This yields

$$ F_{f,\alpha} = 2 \varphi \partial_\alpha \varphi - \kappa \rho \partial_\alpha (\partial_\beta \rho), $$
\[ \varphi = \sqrt{\rho c_p^2} - p. \]  

(50)

The equation of state is a polynomial regularization of Peng-Robinson form \([67]\) as introduced in \([64]\) and reads

\[ p = 5.3 \times 10^{-2} \rho - 3.818183621928911 \times 10^{-2} \rho^2 + 4.139745482116905 \times 10^{-3} \rho^3 + 3.748484095210317 \times 10^{-4} \rho^4 - 1.455265965531227 \times 10^{-4} \rho^5 + 1.2746947442749278 \times 10^{-5} \rho^6, \]  

(51)

which yields an effective density ratio of \( \rho_v/\rho_l \approx 100 \) with liquid and vapour densities \( \rho_l \approx 7.55 \) and \( \rho_v \approx 0.073 \), respectively.

Different wetting states can be modeled by means of the force \( F_s \), which reads

\[ F_{s,\alpha}(x, \tau, t) = \kappa_w \rho(x, \tau, t) \sum_i w_i s(x + c_{i,\alpha} \delta t) c_i,\alpha, \]  

(52)

where \( \kappa_w \) allows us to choose the equilibrium contact angle in accordance with the Young-Laplace equation. The term \( s(x + c_{i,\alpha} \delta t) \) is an indicator function that is equal to one for the solid domain nodes and is equal to zero otherwise; \( w_i \) are appropriately chosen weights \([64]\). To model superhydrophobic surfaces, the equilibrium contact angle was set to \( \theta = 165^\circ \), which corresponds to \( \kappa_w = -0.145 \).

The total body force \( F \) is imposed through the exact difference method \([68]\) with the velocity increment

\[ \delta u_i = \frac{F_i}{\rho \delta t}. \]  

(53)

Hence, the LB equation can be written as

\[ f_i(x + \delta v_i, t + \delta t) = f_i(x, t) + \beta f_i^{\text{mirr}}(x, t) + F_i(x, t), \]  

(54)

with

\[ F_i = f_i^{\text{eq}}(\rho, \delta u + u) - f_i^{\text{eq}}(\rho, u). \]  

(55)

Unlike the entropic LBM of \([64]\), we here use the KBC realization of LBM, where we incorporate the force term into the KBC model through the shifted entropic scalar product

\[ \langle X | Y \rangle' = \sum_i \frac{X_i Y_i}{f_i^{\text{eq}}(\rho, u + \delta u)}, \]  

(56)

which is used to compute the stabilizer \( \gamma \) from Eq. \([6]\).

Also in the multiphase model, we use Grad’s boundary condition. For the fluid-structure coupling, we employ the same methodology as outlined above but include the pressure \( p \) as prescribed by the equation of state in Eq. \([51]\). Note however that the diffuse nature of the liquid-vapour interface necessitates a pressure regularization. This arises from the fact that the numerical integration of the pressure over the solid surface is prone to numerical errors, due to sharp pressure gradients and large negative values in the interface region, which are sampled only relatively coarsely on the FEM mesh. This leads to an artificial negative pressure, which is compensated in our simulations by a regularization procedure, where we use a simple linear interpolation between the liquid and vapor density to evaluate the pressure.

Motivated by the experimental study of \([63]\), we investigate the effect of elasticity on the droplet impact on a superhydrophobic, elastic beam for a wide range of Weber numbers.

In all simulations, the droplet is resolved by \( D = 80 \) lattice points, the surface tension is set to \( \sigma = 0.295 \) (\( \kappa = 0.295 \)) and the computational domain of the fluid is given by \([320 \times 250 \times 320]\). The beam has dimensions \([300 \times 200 \times 5]\) and Lamé coefficients are set to \( \lambda = 1500 \) and \( \mu_s = 1000 \). While one end of the beam is clamped, the other end is only simply supported and the droplet impacts the center of the beam.

We simulated Weber numbers in the range of \( \text{We} \in [7, 72] \) for both rigid and flexible beams and recorded the maximum spreading diameter \( D_{\text{max}}/D_0 \) as shown in Figure 10.

![Figure 10](image.png)

FIG. 10. Maximum droplet spreading diameter on a rigid and elastic superhydrophobic surface, respectively.

For the entire range of Weber numbers, it is apparent that the maximum spreading diameter decreases when elasticity of the beam is taken into consideration. Analogously, the experimental study conducted in \([63]\) also observed a reduction of the apparent spreading diameter. While a quantitative comparison is out of reach for the current preliminary simulations due to the large dimensions of the beam used in the experiment, the proposed scheme does capture the effect of elasticity qualitatively. A natural explanation for the cause of the reduction of the spreading diameter is that the momentum of the droplet is transferred to the beam, which decreases...
the effective Weber number perceived by the droplet and thus reduces the maximum spreading of the droplet. It is only long after the droplet has reached its maximum spread that the momentum is transferred back (no damping is applied) to the liquid. A similar explanation was proposed in [63]. A sequence of snapshots of the droplet impact on both the rigid and the elastic beam is shown in Figure 11. It is clear that initially both the rigid and the elastic beam behave similar, but the elastic case exhibits faster rebound and take off. Note that the density ratio between solid and fluid is roughly $\rho_s/\rho_f \approx 100$, which explains the delayed response of the fluid. Further, the observed asymmetry in the elastic case is due to the asymmetric boundary conditions of the beam.

These results are promising and underline the robustness and viability of multi-physics simulations based on the KBC-FSI solver. A detailed investigation of FSI for multiphase flows will be published in a subsequent paper.

IV. CONCLUDING REMARKS

In this paper we have presented a partitioned fluid-structure interaction approach. On one hand, the fluid flow is computed by the entropic multi-relaxation time lattice Boltzmann model in combination with Grad boundary conditions and multi-domain grid refinement. On the other hand, the elastic solid was modeled by the hyperelastic Saint Venant-Kirchoff model, which accounts for large, geometrically non-linear deformations and was solved by a corresponding FEM formulation.

The proposed scheme was validated for various challenging set-ups for quasi-two dimensional and fully three dimensional simulations of laminar and turbulent flows. Finally, extensions to multi-physics simulations were explored. An extension of the KBC model to multiphase flows and its coupling to the solid solver was presented. Promising results, in qualitative agreement with recent experiments, were shown for the simulation of droplet impact on elastic superhydrophobic surface, which demonstrate the viability of proposed scheme.

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