A HYBRID PORE NETWORK - LBM METHOD FOR INTEGRATING FLOW OF IMMISCIBLE PHASES IN DEM.

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Abstract Complex hydro-mechanical couplings with multiple fluid phases is a great challenge for the discrete element methods (DEM). We propose to use for this problem the same pore space decomposition that was used previously for one-phase flow, based on reguar triangulation of the sphere packing. The decomposition lead to a discretization of the pore space as a set of connected throats and the Lattice Boltzman method (LBM) is employed to obtain hydrostatic properties of each throat, which leads to a hybrid Pore Network-LBM framework. An application to the primary drainage of a random packing of spheres is presented and compared to the results of the same problem fully resolved by the Lattice Boltzman method (LBM). The invasion pattern shows a strong fingering effect, correctly reproduced by the hybrid method. The capillary forces estimated with the hybrid method are in semi-quantitative agreement with the reference values.

1 INTRODUCTION

Simulating complex hydro-mechanical couplings in large grain-fluid systems is a great challenge for the discrete element methods (DEM). For materials saturated by only one pore fluid, recent advances in pore-scale methods (in which the porosity is discretized as a network of connected pores [1]) enable the resolution of large coupled problems in three dimensions. These methods can reflect the dominant viscous terms at the particle scale without actually solving a Navier-Stokes problem. The computational cost is thus reduced by orders of magnitudes without sacrifying quantitative correctness, as illustrated by recent examples [3, 4, 2]. Materials with pore space occupied by two or more immiscible pore fluids, leading to surface tension (such as air-water or water-oil systems), pose a greater challenge. Numerical models of partially saturated granular materials based on the DEM have been used extensively, yet the majority of them are strongly limited to the

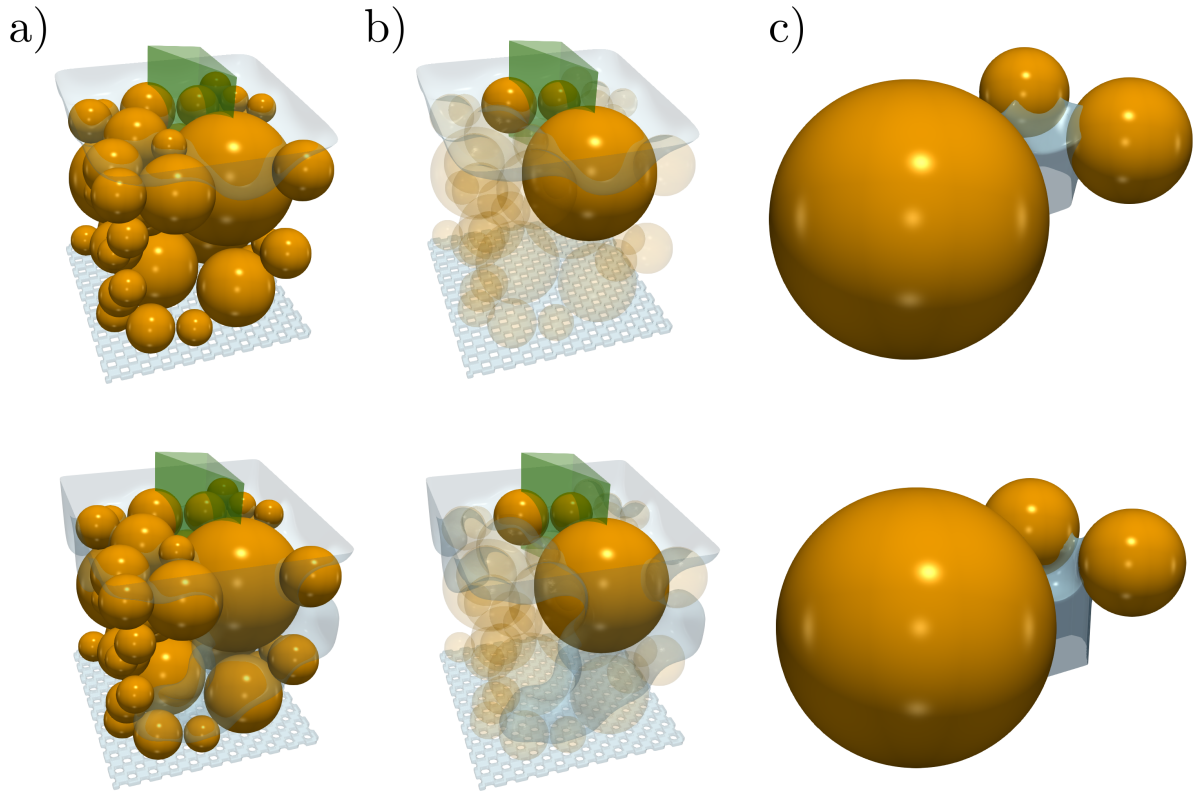

Figure 1: Decomposition of a sphere packing (a) into small subsets of three spheres (b)-(c). Top row shows the initial saturated state of the granular assembly. Bottom row displays the fluid distribution after the first non-wetting intrusion. (b) eviences the position of the subset inside the granular domain while (c) shows a LBM simulation for the selected pore throat.

so-called pendular regime in which the wetting phase is present in such a little amount that it only forms pendular bridges associated to pairs of particles. In the other saturation regimes one hardly avoid time consuming surface minimization techniques or even the direct resolution of a 2-phase fluid dynamics problem at the microscale to capture the geometry of phases and interfaces. The pore-scale approach of this problem, discussed hereafter, aims at a drastic decrease of the computational cost, as was done for single phase flow. For a range of micro-scale processes this approach is known to give accpetable results. For instance, the primary drainage of a saturated sample can be reproduced accurately [5]. However, a number of processes remain which still need significant efforts from both phenomenological and algorithmic points of view, such as bubble entrapement, coalescence of wetting phases, or viscous effects leading to mixed scenario of drainage-imbibition at the local scale. The determination of capillary forces in this framework is also an open issue.

In this paper the following question is examined: is the pore-scale decomposition employed previously for single-phase flow applicable to multiple (two) immiscible pore fluids

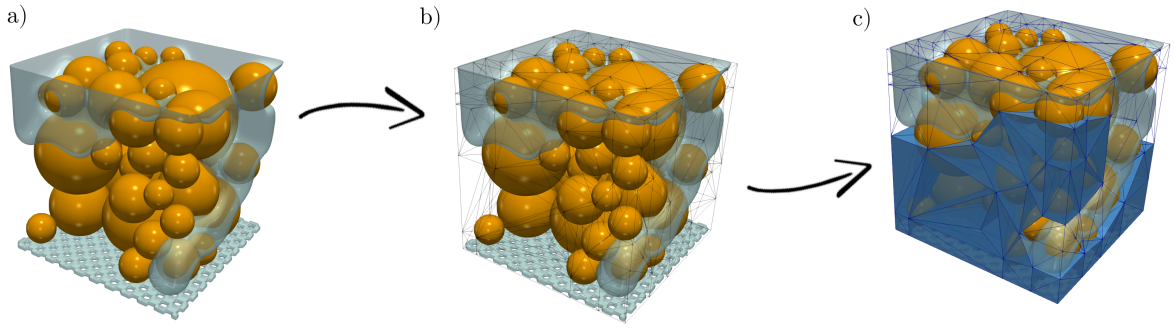

Figure 2: a) Fluid distribution after the first non-wetting phase intrusion using a fully resolved LBM solution. $p_c^* = \dfrac{p_c R}{\gamma} = 4.2$, where R is the average radius and γ the surface tension. b) Tetrahedrized granular domain. c) Comparison of the invasion path between the fully resolved LBM simulation (translucid blue isosurface) and the Hybrid model (wetting phase is illustrated in blue).

with capillarity effects, to predict phases geometry and capillary forces on the solid particles? We show how the movements of the fluid phases and the fluid-solid interactions can be described by introducing relevant geometrical objects in a tetrahedrized granular domain, together with evolution laws. Direct simulations with the Lattice-Boltzman method (LBM) are used to produce reference results at a packing scale. Then domain decomposition is applied to the packing to identify the elementary units of the micro-structure. LBM simulations are also performed for those elementary object under particular boundary conditions to establish local rules of interface displacement, in order to assemble a global hybrid two-phase flow problem to be solved by a pore-network solver. The capillary forces on the particles are determined from the full LBM approach and from the hybrid method for comparison.

2 PACKING AND PORE-SPACE DECOMPOSITION

We consider a random packing of fourty polydisperse spheres generated by growing the spheres in a cubic box. The packing is decomposed by regular triangulation and each triangular face of the triangulation define a *pore-throat*, i.e. a narrow region of the pore space surrounded by three spheres, where a stable meniscus may form, following [5]. In order to simulate the position of the meniscus in each throat as a function of capillary pressure we define a LBM model for each throat independently. The model geometry is defined by a cylinder of triangular cross-section modified locally by the presence of the three spheres as illustrated by the green domain in Fig. 1. The throat-scale simulation starts from a throat domain saturated by the wetting phase, while the boundary conditions impose a progressive invasion by the non-wetting phase. The throat-scale LBM simulation provides us with a relation between the normalized capillary pressure p_c^* and the position of the meniscus, the maximul value p_c^* during the drainage defines the entry capillary pressure p_c^{e*}. The normalized capillary pressure is defined with respect to the reference

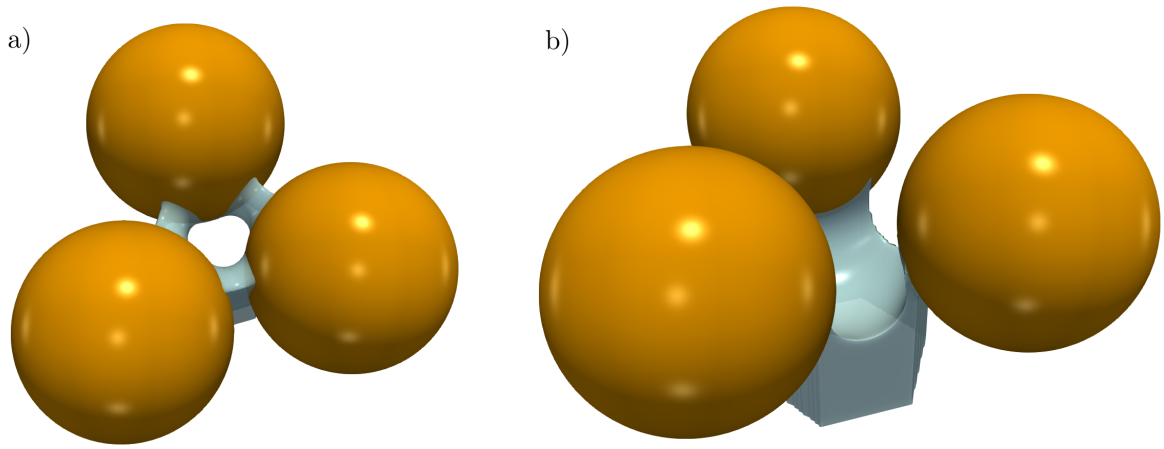

Figure 3: Wetting phase adopts different shapes for each pore throat after the invasion of the non-wetting phase. a) Pendular regime observed after the drainage of a pore throat with small interparticle-distance. b) Fluid interface passes through the pore throat without wetting phase trapping for wider pore throats.

particle size R and the surface tension γ, as $p_c^* = \dfrac{p_c R}{\gamma}$ (with p_c the absolute surface tension). All simulations are set to approach conditions of quasi-static drainage, in other words the viscous effects are negligibly small, and of perfect wetting of the solid (the contact angle of the interfaces approach zero).

Independently of that pore space decomposition into throats the drainage of the entire packing is also simulated in the entire box by prescribing mass source/sink on the top/bottom boundaries, starting from an initially saturated specimen. This reference solution is refered to as "full-LBM" hereafter. The two procedures are shown and compared on Fig. 2 for a specific value of capillary pressure.

3 LIQUID MORPHOLOGY

Fig. 1 reveals that the invasion by the non-wetting phase does not happen as a stable piston-like front. Instead, some remarquable fingering is observed. A very similar pattern is obtained with both the full-LBM and the pore-network method.

It is to be noted that the receding wetting phase may leave pendular bridges behind after the main invasion event. Those bridges can be captured by the throat-scale simulation, as shown on Fig. 3, even though they don not fit completely in the cross section. This entrapment of disconnected wetting phase by the formation of pendular bridges depend on ambiant capillary pressure and local geometry, the smaller the distance between the particles the more likely it is to form bridges.

In Figs. 4 and 5 we compare details of interfaces geometry as obtained from the full LBM and from the throat-scale simulations for a given p_c^*. It is shown that the meniscii from the two methods are nearly identical, which validates the choice of regular triangulation to map the pore space.

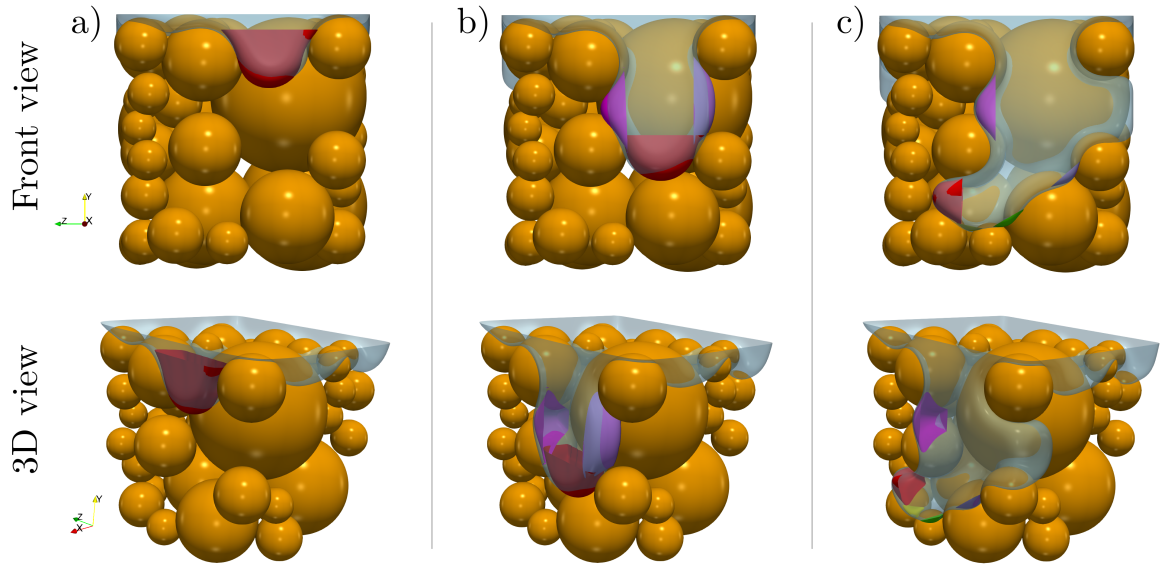

Figure 4: Superposition of the interfaces obtained with the fully resolved LBM solution and the Hybrid method during the first intrusion of the non-wetting phase. a) $p_c^* = 2.8$, b) $p_c^* = 3.5$ and c) $p_c^* = 4.0$.

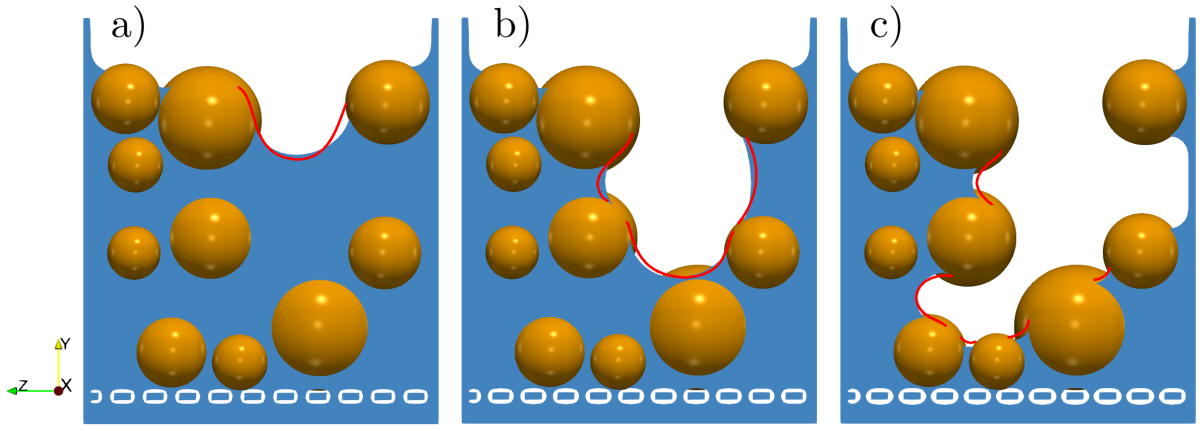

Figure 5: Fully resolved LBM and Hybrid interface porfiles generated by a vertical slicing plane. a) $p_c^* = 2.8$, b) $p_c^* = 3.5$ and c) $p_c^* = 4.0$.

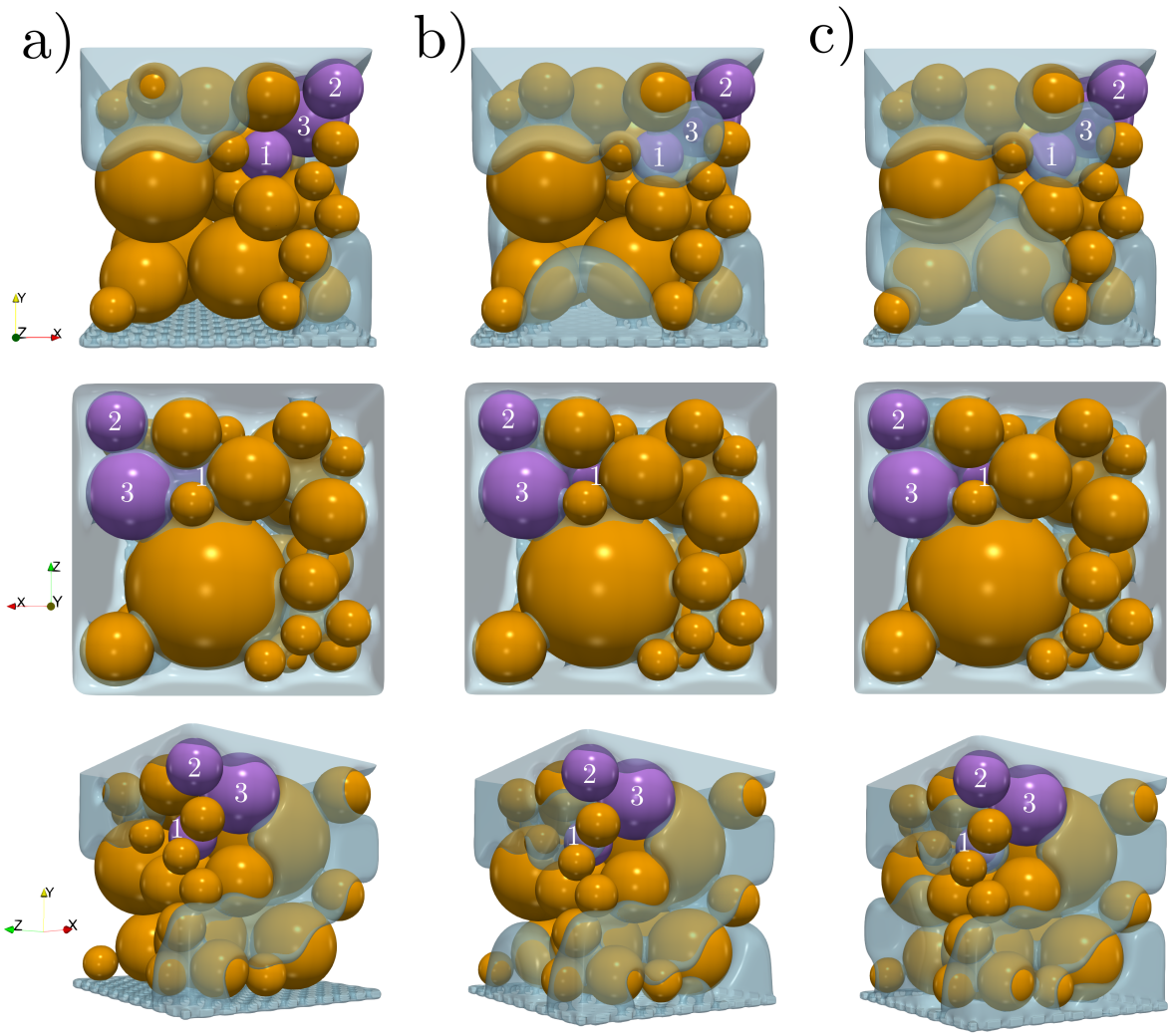

Figure 6: Capillary forces exterted on the purple spheres are examined during the drainage. a) $V^* = \frac{V^w}{\frac{4}{3}\pi R^3} = 45.6$, where V^w is the volume of the wetting phase. b) V^*=25.9 and c) V^*=12.8 .

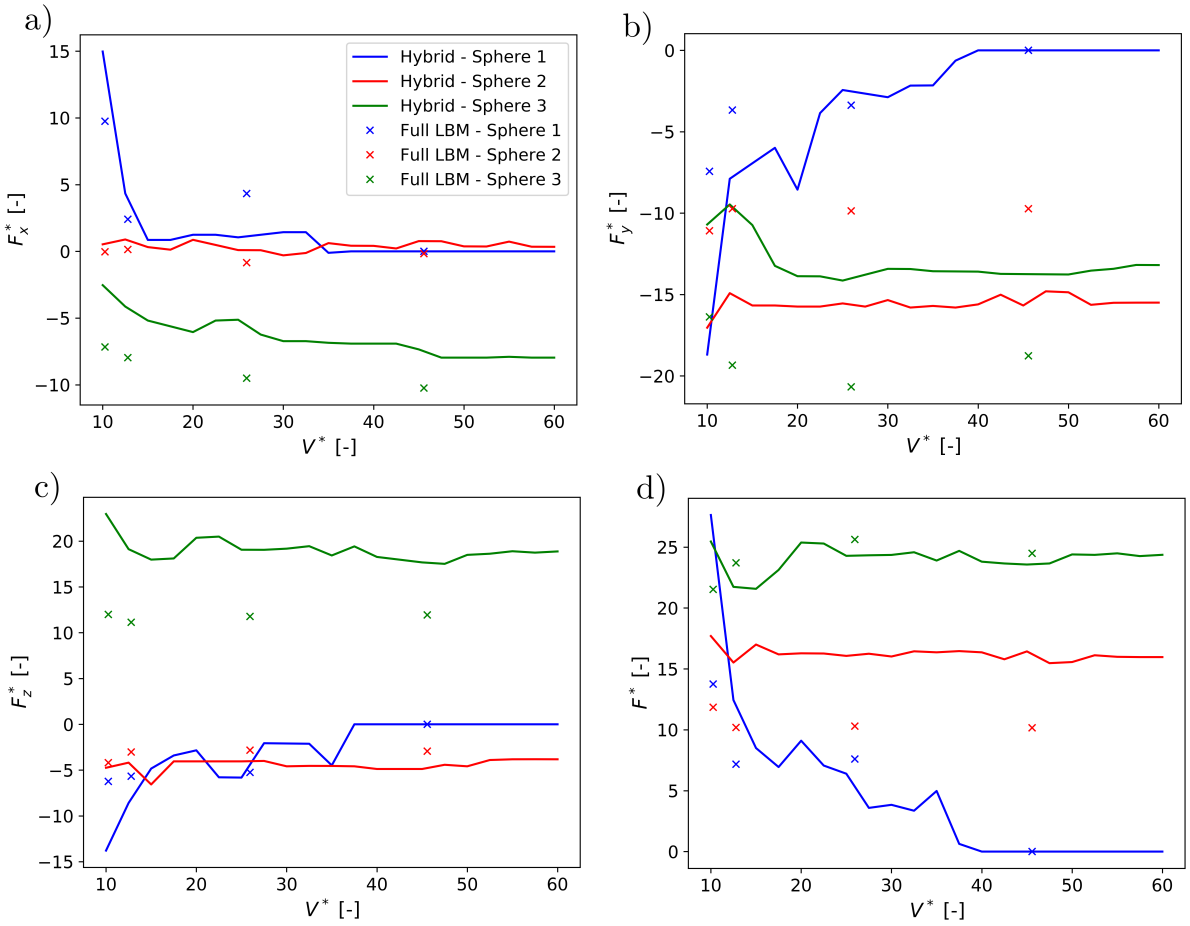

Figure 7: Force analysis on the purple grains of figure 6. The evolution of capillary forces with the liquid content is evaluated under drainage conditions. Forces have been decomposed into x, y and z contributions.

4 CAPILLARY FORCES

Finally, we examine the evolution of the capillary forces on selected particles (Fig. 6). The evolution of the forces magnitude and cartesian components with drainage are given by Fig. 7. The main trends given by the full-LBM results are captured very well by the hybrid PN-LBM approach. Maximum errors of about 50% are found on the force magnitude, which can be partly explained by the fact that not all details of the true 3D meniscii geometry can be accessed via the throat decomposition. Indeed, the cylindrical domains (like green domain in Fig. 1) associated to the throat do not define a partition of the pore space: some regions of the pore space are covered multiple times (intersecting cylinders) while others are not covered, in the later case the geometry of the meniscus has to be extrapolated.

5 CONCLUSION

A hybrid model combining the decomposition of the pore space as a network of throats and the Lattice-Boltzman method in each throat has been presented. Results from the hybrid method have been compared to results of a full-LBM simulation. Even though improvements of the force determination are still needed for a fully quantitative agreement, the results are encouraging. The hybrid method captures the movement of interfaces at increasing capillary pressure rather accurately, and the force estimations are in semi-quantitative agreement.

On the basis of that proof of concept one may envision the replacement of LBM in the pore throats by empirical or semi-empirical approximations to provide pressure-volume relationships. Indeed, the resolution of one LBM problem per pore-throat makes the current method computationally demanding still, even if it is potentially much faster than a full-LBM resolution.

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