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# An efficient mass-preserving interface-correction level set/ghost fluid method for droplet suspensions under depletion forces

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ABSTRACT

Aiming for the simulation of colloidal droplets in microfluidic devices, we present here a numerical method for two-fluid systems subject to surface tension and depletion forces among the suspended droplets. The algorithm is based on an efficient solver for the incompressible two-phase Navier–Stokes equations, and uses a mass-conserving level set method to capture the fluid interface. The four novel ingredients proposed here are, firstly, an interface-correction level set (ICLS) method; global mass conservation is achieved by performing an additional advection near the interface, with a correction velocity obtained by locally solving an algebraic equation, which is easy to implement in both 2D and 3D. Secondly, we report a second-order accurate geometric estimation of the curvature at the interface and, thirdly, the combination of the ghost fluid method with the fast pressure-correction approach enabling an accurate and fast computation even for large density contrasts. Finally, we derive a hydrodynamic model for the interaction forces induced by depletion of surfactant micelles and combine it with a multiple level set approach to study short-range interactions among droplets in the presence of attracting forces.



## 1. Introduction

In the field of colloidal science, much progress has been made on the synthesis of elementary building blocks (Fig. 1) mimicking molecular structures to elaborate innovative materials, *e.g.* materials with complete three dimensional band gaps [1–4]. The basic elements of such colloidal molecules are particles or droplets less than one millimeter in size, and their self-assembly relies on either lengthy brownian motion or careful microfludic designs, on top of typical colloidal interactions, *e.g.* depletion attraction and electrostatic repulsion [5–7]. Regardless of the approach, however, questions remain why the colloidal particles/droplets undergo certain path to organize themselves and how such process can be controlled and optimized. Since full data are not yet accurately accessible from experiments in such miniature systems, computer simulations will be useful to provide supplemental information.

Scaling down to microscale appears first to be a convenience for the numerical simulations of multicomponent and multiphase systems as the non-linear Navier–Stokes (NS) equations can be reduced to the linear Stokes equations. This allows

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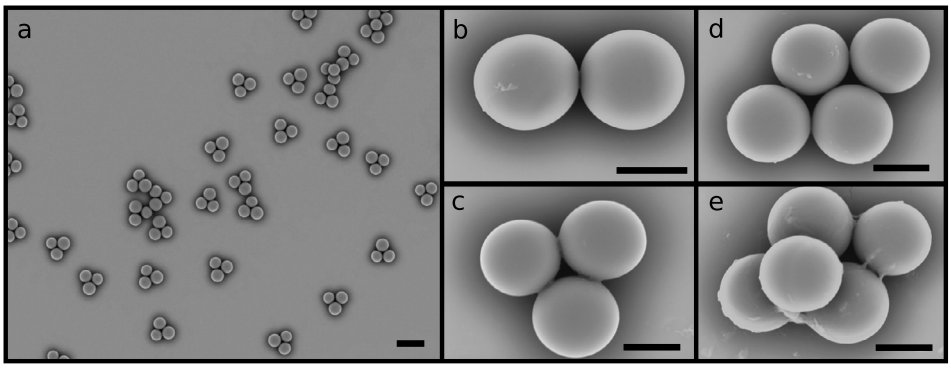


**Fig. 1.** Self-assembled colloidal clusters. a) Electron micrograph of a suspension of triplet clusters. Scale bar, 30 $\mu$m. b–e) Close up of doublet, triplet, quadruplet, and quintuplet clusters. Scale bars, 10 $\mu$m. Further details are available in [7], photograph courtesy of Dr. Joshua Ricouvier.

the use of boundary integral methods (BIM) [8], *e.g.* most recently the GGEM-based BIM [9,10] solving the Stokes equations in general geometries. However, it is also possible to use the conventional unsteady, fractional-step/projection-method NS solver at low Reynolds number, combined with an interface description method [11,12]. The latter approach is more versatile, probably less difficult to implement, and enjoys a rich literature of standard numerical techniques. Here, in view of a rich range of possible applications and considering also the rapid development of inertial microfluidics (where inertial effects are used to better control the flow behavior) we take the approach of simulating the incompressible, two-fluid NS as outlined in [13]. The splitting procedure proposed in [13] enables the use of fast solvers for the pressure Poisson equation also for large density and viscosity contrasts. The remaining choice then is to be made among the available interface-description methods.

Generally, there are two categories of methods to resolve an interface in a NS solver, *i.e.* front-tracking methods and front-capturing methods. An example of the front-tracking method is the immersed boundary method (IBM) [14,15]. Using Lagrangian points in a moving frame, IBM can offer a high interface resolution without the need to deform the underlying mesh in the fixed frame. However, the coupling of the two meshes relies on a regularized delta function, which introduces certain degrees of smearing. Moreover, large interface deformation requires frequent mesh rearrangement; and topology changes may have to be handled manually. These constraints make IBM typically more expensive and less appealing for droplet simulations.

Front-capturing methods, on the other hand, are Eulerian and handle topology changes automatically; they are therefore easier to parallelize to achieve higher efficiency. One of such methods is the volume-of-fluid (VOF) method [16], which defines different fluids with a discontinuous color function. The main advantage of VOF is its intrinsic mass conservation. It suffers however from inaccurate computations of the interface properties, *e.g.* normals and curvatures. This makes it less favorable for simulations of microfluidic systems where surface tension is the dominant effect and requires accurate modelling.

Another popular front-capturing method is the level set (LS) method [17,18]. Contrary to VOF, LS prescribes the interface through a (Lipschitz-)continuous function which usually takes the form of the signed distance to the interface. Under this definition, normals and curvatures of the interface can be readily and accurately computed. However, the problem when simulating incompressible flows is that mass loss/gain may occur and accumulate because the LS function embeds no volume information. In addition, errors can also arise from solving the LS advection equation and/or the reinitialization equation, a procedure commonly required to reshape the LS into a distance function. Therefore, additional measures have to be taken to ensure mass conservation.

Many different approaches have been proposed to make LS mass-conserving, which can be classified into the following four methodologies. The first approach is to improve the LS discretization and reinitialization so that numerical errors are reduced. In practice, one can increase the order of LS fluxes [19], minimize the displacement of the zero LS during reinitialization [20,19], or employ local mesh refinement [21–23]. By doing so, mass loss can be greatly reduced, although the LS function is still inherently non-conservative. The second remedy couples the LS with a conservative description (*e.g.* VOF) or Lagrangian particles. For example, the hybrid particle level set method [24], the coupled level set volume-of-fluid (CLSVOF) method [25], the mass-conserving level set (MCLS) method [26], or the recent curvature-based mass-redistribution method [27]. With varying level of coupling, these methods can usually preserve mass really well; the drawback is that the complexity and some inaccuracy (due to interpolation, reconstruction, *etc.*) of the other method will be imported. The third approach improves mass conservation by adding a volume-constraint in the LS or NS formulation. Examples of this kind include the interface-preserving LS redistancing algorithm [28] and the mass-preserving NS projection method [29]. Finally, one can also smartly modify the definition of the LS, such as the hyperbolic-tangent level set [30], to reduce the overall mass loss.

With the physical application of colloidal droplets in mind, and using ideas from some of the above-mentioned methods, we heuristically propose an interface-correction level set (ICLS) method. The essential idea of ICLS is to construct a normal