

## Lattice Boltzmann for Colloids in Binary Fluids

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The lattice Boltzmann (LB) method provides a very attractive approach to the study of mesoscopic systems which have complex geometry and/or constituents, of which a good example is that of solid particles (colloids) in a two-phase fluid mixture. Such two-phase fluid systems have been studied extensively using LB [1,2] without solid particles, and the approach is now extended to include them. This paper describes the implementation of spherical colloidal particles within the binary fluid LB framework and their parallelisation.

The LB approach for the binary fluid is based around two distributions: one for the density, and a second for an order parameter which describes the composition of the fluid. The general method for representing solid-fluid boundary conditions via bounce-back on links [3] is adopted for the density and extended to the order parameter distribution. Fluid is excluded from the interior of the particles to prevent unphysical transfers of fluid across the solid surface. Bounce-back on links must also ensure conservation of fluid composition when applied to particles moving freely across the lattice. A number of simple exercises are performed to check the behaviour of the simulated particles.

A numerical bottleneck associated with the close clustering of particles has been identified [4] when lubrication forces between particles which are unresolved by the fluid lattice are added back explicitly. Solid particles with neutral wetting (for which the solid-fluid surface tension is the same for both fluid phases) are surfactant and congregate strongly at the interface between the two fluid phases. This means that the problem of clustering rapidly becomes acute even for modest solid volume fractions in these systems. Two solutions to the clustering problem are described.

Parallelisation of the colloid-fluid problem is achieved relatively easily using shared memory, and scales well to a reasonable number of processors provided large clusters are avoided. The strategy for the more challenging problem of parallelisation using a domain decomposition and message passing, which will allow the study of very large systems with many particles, is also discussed.

### References

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