***Proteus*[1]: a new computational method for multiphase flow**

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Keywords: Particles, deformable, computational method, Lattice Boltzmann

Extended summary

Proteus is a new computational scheme that combines several desired components of the Lattice Boltzmann Method (LBM) the Immersed Boundary Method (IBM) and the Direct Forcing Method (DFM) in order to solve fluid-particle interaction problems, including problems with deformable boundaries. The method uses a regular Eulerian grid for the flow domain and a Lagrangian grid to follow particles in the flow field. The velocity field of the fluid and particles is solved by adding a force density term into the LBM. The no-slip condition on the boundary of a moving particle is enforced by adding a forcing term in the momentum equations as in the case of the IBM (Feng and Michaelides, 2004). *Proteus* applies the direct forcing scheme and eliminates the need for the determination of the stiffness coefficient, a free parameter that requires trial and testing to select. This allows the enforcement of the rigid body motion of a particle in a more direct and efficient way. This novel method preserves the advantages of LBM in tracking a group of particles and, at the same time, provides an alternative and more efficient approach to treating the solid-fluid boundary conditions. *Proteus* enables one to simulate problems with particle deformation and fluid-structure deformation.

The computational method and the parameters used have been validated by comparing its results with experimental results on the flow of one particle in an enclosure and the on the drop of a single particle in a small finite box given by ten Cate et al. (2002) (acceleration and deceleration processes). Here we present results on the validation of the method as well as the solution to a problem with 1234 spheres in an enclosure. The initial setup of this problem is that the group of particles is initially packed in a closed three-dimensional box, 3.125 cm long, 3.125 cm high and 0.09375 cm wide. The diameter of the particles is d=0.0625 cm and, hence, the width of the box is 1.5d. As in the previous case, the fluid density is ρ_f=1000 kg/m^3, and the particle/fluid density ratio is 1.01. The kinematic viscosity of the fluid is 0.001 kg/ms. The "safe zone" between particles for these simulations was chosen to be equal to d/8. The stiffness parameters for the collisions are ε_P=0.25, E_P=0.02 and ε_W=0.5ε_P.

Initially, both the fluid and particles are stationary in an arrangement similar to closely-packed spheres, with the heavier particles on top of the fluid. There are 28 lines of particles with each horizontal line having 44 particles. The initial gap between two neighboring particles is d/8. The gap between the upper wall and the first line of particles (line 1) is 3d/8. The gap between the left wall and the left-most particle of the odd horizontal lines (lines 1, 3, 5, …) is 3d/8. The gap between the left wall to the left-most particle of the even horizontal lines (lines 2, 4, 5, …) is 2d/8. The gaps at the right side are 2d/8 and 3d/8, respectively, for the odd and even lines.

The numerical simulation box is 400X12X400 in lattice units, and the diameter of each particle is equal to 8 lattice units. Two boundary conditions were examined in the width direction: a) solid walls with no-slip boundary condition and b) periodic boundary conditions, which imply an infinite array of identical particles. The boundaries in all the other directions are solid boundaries with no-slip velocity conditions. The relaxation time for the first case is τ=0.9915 and each lattice time step corresponds to a physical time of 0.001 s; the relaxation time for the second case τ=0.74576 and each lattice time step corresponds to a physical time of 0.0005 s. Figures 1 and 2 show the state of the system of the 1232 particles in two times from the commencement of the process with the no-slip boundary condition applied at the sidewalls.

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[1] In the Greek mythology *Proteus* is a hero, the son of Poseidon. In addition to his ability to change shapes and take different forms at will, Zeus granted him the power to correctly predict the future.

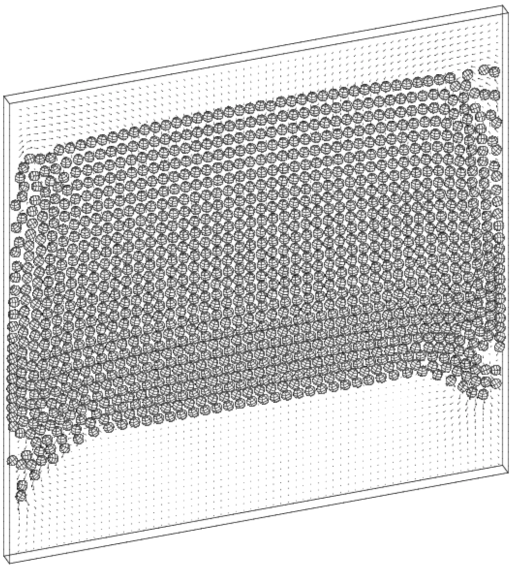

Figure 1: Particle positions at t=10s

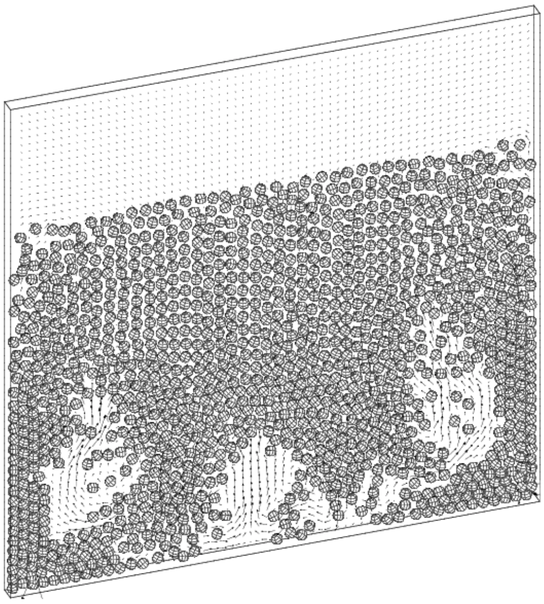

Figure 2: Particle positions at t=25 s

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