1 Abstract

In previous homework on MD simulation, we implemented periodic boundary conditions, which is commonly chosen for estimating a infinite system by using a small unit cell. The goal of this project is to implement a free-surface boundary condition on fluid dynamics simulation. Fluid dynamics simulation with explicit Smoothed Particle Hydrodynamics (SPH) method is the main part of my current research, which coincides with MD simulation in many aspects, including time integration scheme and enforcement of boundary conditions. In addition, they are both lagrangian grid based method that keeps track of particles instead of mesh cells (as far as I know). The difference of them would be MD simulation concerns more about energy conservation and thermal properties, whereas fluid dynamics simulation only cares about the advancement of position and velocity, or to say how they are impacted by the pressure term and viscous term in Navier-Stokes equation.

As a result of its neighbor search nature, SPH method requires a full support domain [1], even at the free-surface of fluid flow, which makes it necessary to include surface tension force term for an accurate solution at the free-surface. The formulation of surface curvature based on a sharp color function implemented in [2] will be used to simulate a cube of fluid particles without gravity force in a vacuum space, which will evolve in time and form a sphere under the effect of surface tension force.

I will write my own code, which is based on a current working CUDA code for parallel GPU computing (kind of stable but still in progress) on weakly compressible SPH. I will first implement the surface tension force term according to [2] and try to achieve similar plots as Fig. 4 in [2] for a demonstration of pressure and velocity field. Further, I will try to set up a simulation showing the animation of particle movements.

References

[1] Joe J Monaghan. Smoothed particle hydrodynamics. *Annual review of astronomy and astrophysics*, 30(1):543–574, 1992.

[2] S Adami, XY Hu, and NA Adams. A new surface-tension formulation for multi-phase sph using a reproducing divergence approximation. *Journal of Computational Physics*, 229(13):5011–5021, 2010.