Simulation of Multiphase Flows using Smooth Particle Hydrodynamics(SPH)

A Project Report
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by

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The project report entitled "Simulation of Multiphase Flows using Smooth Particle Hydrodynamics(SPH)" submitted by Vikas Kurapati (Roll No. 130010058) may be accepted for being evaluated.

Date: 23 October 2017

Prof. Prabhu Ramachandran

Declaration

I declare that this written submission represents my ideas in my own words and where others' ideas or words have been included, I have adequately cited and referenced the original sources. I declare that I have properly and accurately acknowledged all sources used in the production of this report. I also declare that I have adhered to all principles of academic honesty and integrity and have not misrepresented or fabricated or falsified any idea/data/fact/source in my submission. I understand that any violation of the above will be a cause for disciplinary action by the Institute and can also evoke penal action from the sources which have thus not been properly cited or from whom proper permission has not been taken when needed.

Vikas Kurapati

Date: 23 October 2017 (Roll No. 130010058)

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Abstract

Multiphase flows are encountered often in day-to-day life like mixing of two liquids etc., For many such flows, the interaction at the surface is important. In this work, multiphase flows' interaction is studies with emphasis of surface tension in SPH.

Smoothed-Particle Hydrodynamics(SPH) is a mesh-free Lagrangian particle method which is now used in various fields like astrophysics, fluid mechanics and solid dynamics. This SPH method has been used to solve the problems of surface tension. To do this, the important issue to be addressed is the calculation of interface accurately. Grid based schemes which interfacial tracking or interface capturing techniques cause issues in mass conservation, curvature capturing and interface diffusion. So, this work tries to overcome these using a grid-free scheme in Smoothed-Particle Hydronamics.

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Chapter 1

Introduction

There are 4 states of matter i.e., gas, liquid, solid and plasma. If a flow consists of at least two phases, it is called a Multiphase flow. Multiphase flows are often encountered in real life, like mixing of oil in water etc.,

Numerical modelling of the entire Multiphase flows can be performed using grid-based techniques. But, these grid based techniques are not so efficient due to the enormous amount of required computational resources. There are some common grid based codes in Eulerian frames which use interface tracking techniques like the volume of fluid(VoF) or the level set method for simulating multiphase flows. But, they have some disadvantages like the costly restructuring of interfaces, failure to conserve mass in coarse regions. But, these are required to calculate surface tension force which is one of the main driving forces in multiphase flows.

To solve the above discussed issues, a Lagrangian particle based technique using the concept of Smoothed Particle Hydrodynamics(SPH) has been developed. In this technique, the spacially discretized points, called the particles move with the local fluid velocity and belong to the phase they were assigned initially. For the above reason, there is no requirement for capturing of the phase change or reconstuction of the grid. As the surface tension can now be correctly applied on the interface, a more accurate modelling of the surfaces can be done.

1.1 Methodology

The SPH method was introduced in 1977 to solve the problems in astrophysics. There is no need of underlying grid for spatial discretization. As the SPH simulation is based on Lagrangian frame of reference, the fluid is discretized by movable spatial discretization points called particles. Only the initial domain is to be discretized and then these particles are moved according to their interactions. The physical propeerties like mass, density, velocity and internal energy are assigned to these particles. In accordance with the governing conservation equations, the fluid characteristics are calculated at each particle.

1.2 Objective

This work focuses on the applicability of SPH in the regime of multiphase fluid flows. The main objective is to simulate multiphase flows accurately using SPH.

SPH formulations using different schemes are to formulated. These formulations are to be applied on problems already simulated and validated against the available results. Later, this scheme can be used to simulate new problems.

Chapter 2

Basics of SPH Formulations

In the following sections, the derivation and formulations of SPH methodology will be explained. In SPH, we interpolate any function to be expressed in terms of its values at a set of disordered points called as the particles. Every physical property of a fluid is regarded as a spatial function f(r). The ideas are given in (Monaghan and Gingold, 1977) and (Lucy and Leon, 1977). Each function in space be exactly represented by a convolution of the function f(r) itself with the Diract function $\delta(r)$.

$$f(r) = \int f(r')\delta(r - r')dr' \tag{2.1}$$

In SPH, the Dirac function $\delta(r)$ is replaced by a so called interpolating kernel function W(r-r', h), which resembles a Gauss distribution with compact support. Hence, in SPH, the integral approximation of any function f(r) is defined by

$$F_1(r) = \int F(r')W(r - r', h)dr', \tag{2.2}$$

where the integration is over the entire space, and W is an interpolating kernel which has the following two properties.

$$\int W(r - r', h)dr' = 1 \tag{2.3}$$

and

$$\lim_{h\to 0} W(r - r', h) = \delta(r - r') \tag{2.4}$$

where the limited is to be interpreted as the limit of the corresponding integral interpolants. The smoothing length 'h', determines the radius of influence of the kernel function.

For numerical work, the integral representation is approximated by a summation interpolant as below.

$$F_s(r) = \sum_j F_j \frac{m_j}{\rho_j} W(r - r_j, h) \tag{2.5}$$

where the summation index j is used to denote a particle label, the summation is performed over all the particles. Particle j carries mass m_j, position r_j, density ρ_j and velocity v_j. The value of any quantity A at position r_j is written as A_j.

And the differentials and gradients are written as

$$\nabla F(r) = \sum_j \frac{m_j}{\rho_j} F_j \nabla W(r - r_j, h) \tag{2.6}$$

2.1 SPH formulation of basic Navier Stokes Equations

To simulate a fluid flow, the Navier Stokes Equations are to be formulated into SPH. For this, equations 2.5 and 2.6 are used. These give us the approximations for the differentials of density, velocity and energy.

2.1.1 Continuity Equation

Continuity Equation gives the evolution of density. The formulations are as given below:

$$\rho_i = \sum_j m_j W_{ij} \tag{2.7}$$

This form of equation for density is called the Summation Density which uses SPH formulation of 2.5.

Density can also be evolved by using $\frac{d\rho}{dt} + \rho \nabla . \mathbf{v} = 0$

$$\frac{d\rho_i}{dt} = \sum_j m_j \mathbf{v_{ij}} \nabla_i W_{ij} \tag{2.8}$$

where $\mathbf{v_{ij}} = \mathbf{v_i} - \mathbf{v_j}$.

2.1.2 Momentum Equation

The momentum Equation generally contains pressure and viscous terms which are discussed here. Any extra forces like stress, surface tension forces are to be dealt separately and added to the momentum equation.

Pressure Force

The force per unit mass due to pressure is given as -$\frac{\nabla P}{\rho}$. The gradient of the pressure can be estimated as:

$$\rho_i \nabla P_i = \sum_j m_j (P_j - P_i) \nabla_i W_{ij} \tag{2.9}$$

This equation gives zero forces for constant pressures but doesn't conserve linear and angular momentum. Hence, a different SPH formulation is required.

For the same reason, a different formulation of the pressure gradient is used as follows:

$$\frac{\nabla P}{\rho} = \nabla \left(\frac{P}{\rho} \right) + \frac{P}{\rho^2} \nabla P \tag{2.10}$$

This when written in SPH form gives pressure to be as:

$$\frac{d\mathbf{v_i^p}}{dt} = - \sum_j m_j \left(\frac{P_j}{\rho_j^2} + \frac{P_i}{\rho_i^2} \right) \nabla_i W_{ij} \tag{2.11}$$

This form of pressure force conserves momentum as it is anti-symmetric.

Viscous Force

If there is no Physical Laminar viscosity in the flow, in general an artificial viscosity is used in SPH to improve the numerical stability.

The commonly used artificial viscosity used term as given in (Monaghan and Gingold, 1983):

$$\frac{d\mathbf{v_i^\nu}}{dt} = - \sum_j m_j \Pi_{ij} \nabla_i W_{ij} \tag{2.12}$$

where the viscosity term is:

$$\Pi_{ij} = -\nu\left(\frac{min(\mathbf{v_{ij}}, \mathbf{x_{ij}}, 0)}{(\mathbf{x_{ij}}^2 + \epsilon h_{ij}^2)}\right), \tag{2.13}$$

where the viscous factor is:

$$\nu = \frac{\alpha h_{ij} c_s}{\rho_{ij}} \tag{2.14}$$

where α is the viscosity constant, c_s is the artificial speed of sound, $\mathbf{v_{ij}} = \mathbf{v_i} - \mathbf{v_j}$ and $\mathbf{x_{ij}} = \mathbf{x_i} - \mathbf{x_j}$. In equation 2.13, $\epsilon \sim 0.01$ is used to avoid blowing up when $x_{ij} = 0$ and average smoothing length is given by $h_{ij} = 0.5 * (h_i + h_j)$. This viscous force basically gives a repulsive force between approaching particles.

2.1.3 The Energy Equation

The equation for the rate of change of thermal energy per unit mass is given by:

$$\frac{du}{dt} = -\left(\frac{P}{\rho}\right)\nabla.\mathbf{v} \tag{2.15}$$

which when written in SPH form gives:

$$\frac{du_i}{dt} = \left(\frac{P_i}{\rho_i^2}\right)\sum_j m_j \mathbf{v_{ij}}.\nabla_i W_{ij} \tag{2.16}$$

or by transforming the equation to:

$$\frac{du}{dt} = -\nabla\left(\frac{P\mathbf{v}}{\rho}\right) + \mathbf{v}.\nabla\left(\frac{P}{\rho}\right) \tag{2.17}$$

the equation can be rewritten as:

$$\frac{du_i}{dt} = \sum_j \left(\frac{P_j}{\rho_j^2}\right)\mathbf{v_i j}.\nabla_i W_{ij} \tag{2.18}$$

By taking the average of the above two representations, we find:

$$\frac{du_i}{dt} = \frac{1}{2}\sum_j m_j \left(\frac{P_j}{\rho_j^2} + \frac{P_i}{\rho_j^2}\right)\mathbf{v_{ij}}.\nabla_i W_{ij} \tag{2.19}$$

note that this has symmetric factors.

2.2 Moving the Particles

There are two ways to move the particles. One way is:

$$\frac{d\mathbf{r_i}}{dt} = \mathbf{v_i} \tag{2.20}$$

or the XSPH variant as given in (Monaghan and Gingold, 1983):

$$\frac{d\mathbf{r_i}}{dt} = \hat{\mathbf{v}}_\mathbf{i} = \mathbf{v_i} + \epsilon \sum_j m_j \left(\frac{\mathbf{v_{ji}}}{\rho_{ij}}\right) W_{ij} \tag{2.21}$$

where $\rho_{ij} = 0.5 * (\rho_i + \rho_j)$ and $\epsilon(0 \leq \epsilon \leq 1)$ as a constant. This XSPH correction helps in moving the particles with a velocity that is closer to the average velocity in its neighbourhood. XSPH is found to increase dispersion instead of introducing dissipation. The XSPH correction is useful in simulating nearly incompressible fluids like water, which keeps particles' motion orderly in the absence of viscosity.

2.3 Equation of State

For a closed system of equations, we need an Equation of State(EOS) which evaluates pressure. Generally, an equation of state provides a direct coupling of density and pressure. An incompressible fluid can be thought of as a weakly compressible fluid. This can be done by using a stiff EOS. Hence, pressure variations are high for small variations of density also. A numerical speed of sound $c_0 = \sqrt{\left(\frac{dP}{d\rho}\right)_s}$ is used in the EOS.

The Suitable equation as given by Tait is given by :

$$\Delta P = \frac{c_0^2 \rho_0}{\gamma} \left[\left(\frac{\rho}{\rho_0}\right)^\gamma - 1\right] \tag{2.22}$$

Using this equation, the pressure can be computed and used in the momentum equations.

Chapter 3

Physical Foundations of Multiphase flows

3.1 Introduction

Three main forces are considered in the regime of multiphase flows: Pressure, Viscous and Surface Tension forces.
In the following sections we discuss the calculations of Surface tension forces.
To calculate the surface tension force, we will need to calculate the interface curvature of different phases.

3.2 Interface Tracking Techniques

In the case of immiscible fluids, each corresponding to a different 'color', c, interface tracking can be achieved by simulating the advection of the color function. (Morris, 2000)

$$\frac{\partial c}{\partial t} + \mathbf{v}.\nabla c = 0 \tag{3.1}$$

The color function may be evolved in a Lagrangian fashion by assigning it as a physical property to 'particles', which are then advected through the computational domain. In genral, this may be achieved using particles on the interface alone(surface-marker methods) or by employing particles which fill the entire computational domain(volume-marker methods). Surface markers have been used extensively to track the location of interface with high accuracy. This approach may be exploited by fully Lagrangian Techniques like SPH. With SPH, each extra phase is modelled simply by introducing an extra species of a particle of different color property.

3.3 The Continuum Surface Force Method

The Continuum surface force(CSF) method (Brackbill *et al.*, 1992) permits numerical simulation of surface tension without placing restrictions upon the flow geometry. The CSF approach models process localized to a fluid interface by applying them to fluid elements in the transition region of the interface. Interfacial phenomena, such as surface tension and phase change, are translated into volume processes having a net effect that emulates the desired physics. In the CSF model, surface tension is translated into a force per unit volume $\mathbf{F_s}$, by

$$\mathbf{F_s} = \mathbf{f_s}\delta_s \tag{3.2}$$

where δ_s is a normalized surface delta function, which peaks at the interface and $\mathbf{f_s}$ is the force per unit area given by

$$\mathbf{f_s} = \sigma\kappa\hat{\mathbf{n}} + \nabla_s\sigma \tag{3.3}$$

where σ is the surface tension coefficient, $\hat{\mathbf{n}}$ is the unit normal to the interface, κ is the curvature to the interface and ∇_s is the surface gradient. The second term in 3.3 acts tangentially to the interface, forcing fluid from regions of low surface tension to higher surface tension. In this work surface tension is assumed constant throughout the fluid and hence that part is neglected. The first term in 3.3 acts normal to the interface corresponding to the net surface tension force due to the local curvature. This force acts to smooth regions of high curvature, in an attempt to reduce the total surface energy. The normal in 3.3 can be obtained using

$$\mathbf{n} = \frac{\nabla c}{[c]} \tag{3.4}$$

where c is the color function identifying each fluid in the simultion and [c] is the jump in c across the interface. The curvature can be calculated as

$$\kappa = \nabla.\hat{\mathbf{n}} \tag{3.5}$$

There are many possible choices for δ_s however, it should be normalized such that its integral through the boundary is one. This is necessary for the correct physics of the interface to be recovered as the resolution is increased. The function should also be non-zero only in those fluid elements that correspond to the transition regions in the numerical method. The surface delta function employed in this work is

$$\delta_s = |\mathbf{n}| \tag{3.6}$$

Chapter 4

SPH formulations

Using SPH, the fluid is represented by particles, generally of fixed mass, which follow the fluid motion according to their governing differential equations. These governing equations become expressions for interparticle forces and fluxes when written in SPH form. Using the standard approach of SPH, the particles move with the local fluid velocity carrying a mass m. Each particle has it's own velocity **v** and other fluid quantities specific to the given problem.

4.1 Density

Density is evaluated for every particle at the beginning of the time step using the following equation called as Summation Density.

$$\rho_a = \sum_b m_b W_{ab} \tag{4.1}$$

where W_{ab} denotes

$$W_{ab} = W(\mathbf{r_{ab}}, h) \tag{4.2}$$

and

$$\mathbf{r_{ab}} = \mathbf{r_a} - \mathbf{r_b} \tag{4.3}$$

where $\mathbf{r_a}$ denotes the position of particle a. The kernel typically takes the form

$$W(\mathbf{r_{ab}}, h) = \frac{1}{h^N} f\left(\frac{|\mathbf{r_{ab}}|}{h}\right) \tag{4.4}$$

where N is the number of dimensions and the function f is typically either a Gaussian or a spline approximating a Gaussian. The smoothing length is generally between 1-1.5 times the shortest particle separation.

4.2 Equation of State

In SPH, pressure is an explicit function of local fluid density and a quasi-incompressible equation of state is used. For this work, the isothermal EOS as follows is used.

$$p_a = c_s^2(\rho_a - \rho_0) \tag{4.5}$$

where ρ_0 is the reference density of the fluid and c_s is the artificial speed of sound. Subtracting the reference density was found to lead to more accurate simulations. The reason for this is that subtracting the reference density removes a zeroth-order term associated with conservative forms of SPH pressure gradients. The speed of sound is chosen to be generally 10 times the maximum velocity of the particles.

4.3 Forces

The forces in the simulations are divided into three parts:

- Pressure forces
- Viscous forces
- Surface Tension forces

4.3.1 Pressure Forces

The pressure forces are caused due to pressure gradients. The SPH expression used to approximate the pressure gradient term in this work is:

$$-\left(\frac{1}{\rho}\nabla p\right)_a = -\sum_b m_b \left(\frac{p_a + p_b}{\rho_a \rho_b}\right) \nabla_a W_{ab} \tag{4.6}$$

where p_a is the pressure at particle a and ∇_a denotes the gradient with respect to the coordinates of particle a. This form of pressure gradient conserves momentum exactly, since forces acting between individual particles are antisymmetric.

4.3.2 Viscous Forces

Viscous forces were calculated using a formulation recently applied to low Reynolds Number flow. (Morris *et al.*, 1997) The SPH momentum equation may be written as (Morris *et al.*, 1997):

$$\left(\frac{d\mathbf{v_v}}{dt}\right)_a = \sum_b \frac{m_b(\nu_a + \nu_b)\mathbf{v_{ab}}}{\rho_a \rho_b}\left(\frac{1}{r_{ab}}\frac{\partial W_{ab}}{\partial r_a}\right) \tag{4.7}$$

4.3.3 Surface Tension Forces

Calculating Interfacial Curvature

In order to obtain the surface tension forces, the curvature κ should be calculated. This requires calculation of surface normals and their divergence.(Morris, 2000)

The simplest SPH expression for $\mathbf{n}$ is given by

$$\mathbf{n_a} = \sum_b \frac{m_b}{\rho_b} c_b^i \nabla_a W_{ab} \tag{4.8}$$

where c_b^i is the color index of particle b.
More accurace estimates of the surface normal are obtained when the color field is smoothed by convolution with the kernel. With SPH, this smoothing is done using SPH approximation of the color function.

$$c_a = \sum_b \frac{m_b}{\rho_b} c_b^i W_{ab} \tag{4.9}$$

Additional improvements in normals is done using:

$$\mathbf{n_a} = \sum_b \frac{m_b}{\rho_b}(c_b - c_a)\nabla_a W_{ab} \tag{4.10}$$

The simplest SPH expression for the divergence of $\hat{\mathbf{n}}$ is:

$$(\nabla.\hat{\mathbf{n}})_a = \sum_b \frac{m_b}{\rho_b}\hat{\mathbf{n}}_\mathbf{b}.\nabla_a W_{ab} \tag{4.11}$$

A more accurate estimation of divergence is obtained using (Monaghan, 1992)

$$(\nabla.\hat{\mathbf{n}}_\mathbf{a}) = \sum_b \frac{m_b}{\rho_b}(\hat{\mathbf{n}}_\mathbf{b} - \hat{\mathbf{n}}_\mathbf{a}).\nabla_a W_{ab} \tag{4.12}$$

If equations 4.10 and 4.12 are used to evaluate the curvature, large errors occur at the transition region's edges. The main issue is the requirement of normalized normals

$\hat{\mathbf{n}}$. Some distance away from the interface, $\mathbf{n}$ will be small and may have a random direction. So, any curvature using these normals would be inaccurate. Hence, for a more accurate calculation, we used only 'reliable' normals to do the divergence calculations. The following were used to do it:

$$N_a = \begin{cases} 1, & if\ |\mathbf{n_a}| > \epsilon \\ 0, & otherwise \end{cases} \tag{4.13}$$

and

$$\hat{\mathbf{n}}_\mathbf{a} = \begin{cases} \frac{\mathbf{n_a}}{|\mathbf{n_a}|}, & if N_a = 1 \\ 0, & otherwise \end{cases} \tag{4.14}$$

ϵ is generally taken to be $\frac{0.01}{h}$ in this work. An intermediate estimate of curvature is done to correct 4.12 for absence of some of the normals in the neighbourhood of particle a.

$$(\nabla.\hat{\mathbf{n}})^*_a = \sum_b min(N_a, N_b)\frac{m_b}{\rho_b}(\hat{\mathbf{n}}_\mathbf{b} - \hat{\mathbf{n}}_\mathbf{a}).\nabla_a W_{ab} \tag{4.15}$$

This estimate can be corrected by a factor of f_a

$$(\nabla.\hat{\mathbf{n}})_a = \frac{(\nabla.\hat{\mathbf{n}})^*_a}{f_a} \tag{4.16}$$

where

$$f_a = \sum_b min(N_a, N_b)\frac{m_b}{\rho_b}W_{ab} \tag{4.17}$$

reflects the local number density of particles with 'reliable' normals.

The surface tension is then calculated as:

$$(\mathbf{a_s})_a = -\frac{\sigma_a}{\rho_a}(\nabla.\hat{\mathbf{n}})_a\mathbf{n_a} \tag{4.18}$$

Momentum Conserving Form

The method explained above does not guarantee exact conservation of momentum. We now discuss one method which conserves momentum. Surface tension force can be expressed as the gradient of the tensor. (Lafaurie *et al.*, 1994)

$$\kappa\hat{\mathbf{n}}\delta_s = \nabla[(\mathbf{I} - \hat{\mathbf{n}} \times \hat{\mathbf{n}})\delta_s] \tag{4.19}$$

The given expression can be approximated in SPH by (Morris, 2000):

$$(\mathbf{a_s})_a = \left(\frac{1}{\rho}\frac{\partial S_{ij}}{\partial x_j}\right) = \sum_b m_b \frac{(S_{ij})_a + (S_{ij})_b}{\rho_a \rho_b} \nabla_{a,j} W_{ab} \tag{4.20}$$

where

$$S_{ij} = \delta_s(\delta_{ij} - \hat{\mathbf{n}}_\mathbf{i}\hat{\mathbf{n}}_\mathbf{j}) \tag{4.21}$$

Where, δ_{ij} is the Kronecker delta, $\nabla_{a,j} W_{ab}$ is the j^{th} component of the gradient of W_{ab} with respect to $\mathbf{r_a}$ and the repitition of j means summation. To improve accuracy, only those normals satisfying 4.13 are used in summation. Since, the reciprocal particle summations are anti-symmetric, this conserves the momentum.

This method is potentially unstable as attractive forces when momentum conserving formulations are used are unstable when SPH particles are considered.
As the resolution is increased, the maximum of δ_s will increase and at some point, the method will blow up. A solution to this issue is to replace S_{ij} with a modified tensor as follow:

$$S^*_{ij} = S_{ij} - \delta_{ij} \times max(\delta_s) \tag{4.22}$$

Removing the Singularity

A disadvantage of the momentum conserving formulation explained above is that the delta function introduces a singularity in the pressure field as the resolution is increased. A work around for this is the following(taking [c] = 1)

$$\mathbf{F_s} = \sigma\kappa\nabla c = \nabla(\sigma\kappa c) - \sigma c \nabla\kappa \tag{4.23}$$

The first term of 4.23 will be incorporated into the pressure term of the momentum equations by introducing new pressure and surface tension forces as follows:

$$p^* = p - \sigma\kappa c \tag{4.24}$$

$$\mathbf{F^*_s} = -\sigma c \nabla\kappa \tag{4.25}$$

So, the same momentum equation will be used with 4.25 replacing surface tension forces and with modified pressure boundary conditions which accommodate the new definition of pressure. This formulation of surface tension doesn't have a dependance on surface delta function and hence doesn't have a singularity as the resolution is increased.

To improve the stability of this technique, only the curvature of those particles which satisfy $|\mathbf{n_a}| > \epsilon$ are used in the calculations. The same value of ϵ can be used as used before.

This method is expected to exhibit better stability numerically as the resolution is increased.

Chapter 5

Implementation

All the simulations which are performed in this project are done in PySPH, a python environment built to solve problems using the framework of SPH. (Ramachandran, 2016). It is an open source framework which uses Python and Cython for fast performance.

PySPH is implemented in a user friendly where a user can specify the entire simulation in Python using SPH. A high performance code is generated from the code written, compiled and executed. PySPH has options to use multi-cores using OpenMP and MPI for parallelizations.

The following is the flow of PySPH and how it works (Sethy, 2017):

- First we create particles in the domain. We discretize the domain into different particles and assign them the initial properties required according to the problem description. PySPH stores all these in an array called particle array where every array has a unique name and id.
- Next, we choose a kernel for SPH approximations. There are many kernels available already in PySPH. A new kernel class can be implemented in case a new kernel is required.
- Next, equations have to be created based on the governing equations of the flow and their SPH approximations. Care is to be taken the summations are written properly as the sequence of the particles in the arrays are not known.
- The last step of the simulation process is to specify the integrator to be used and the stepper for the integration. There are many integrators and steppers already implemented in PySPH. Different steppers for different materials or arrays can also be specified.

The data generated by the simulations can be viewed using the mayavi viewer tool built for PySPH which reads in the numpy files and displays them.

Chapter 6

Results and Discussions

The following test case was implemented in PySPH using the method of Interface curvature described in the above sections.

6.1 Stability of an Interface: Problem Statement

Previous studies using the CSF formulation have reported a numerical instability at the fluid-fluid interface. (Rudman, 1998; Lafaurie *et al.*, 1994). This instability leads to parasitic currents(non-zero velocities) at the interfaces. Using SPH, these currents could lead to particle disorder at the fluid-fluid interface, showing the effect of the diffusing at the interface.

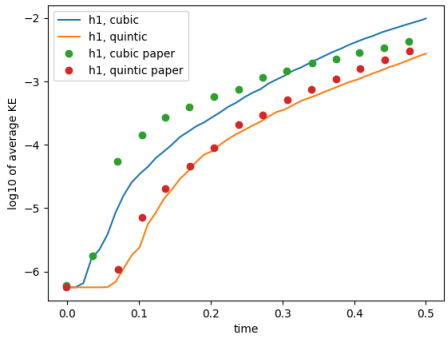
This phenomena is studied here: A simple static case in a periodic domain spanning 0.5 units in x-direction and 1 unit in y-direction with upper half with fluid of color 1 and lower half with fluid of color 0 is simulated. The fluid densities were considered constant of 1, the surface tension coefficient to be 1 and inviscid flow is considered. The speed of sound for this simulation is set to 20 units (Morris, 2000). At t=0, a constant velocity in both directions is set so as the KE of each particle is 6 orders less than their internal energy. The evolution of Kinetic Energy with time is recorded for different SPH parameters like smoothing length and spline. The smoothing length hdx = 1.0 and 1.5 are considered and varied smoothing length for different equations is considered where hdx = 1.0 is used all through except when calculating the surface delta function. In this way, by using a larger smoothing length for curvature calculation, more reliable estimates of curvature are obtained in the region where surface normals are non-zero.

6.2 Results

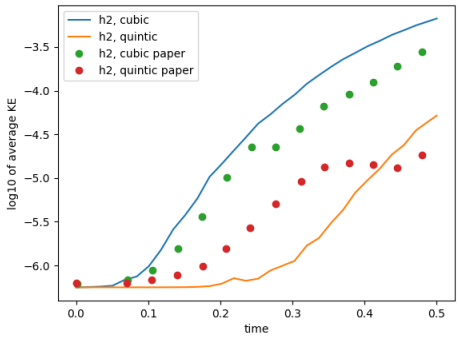
The following section shows comparision of smoothing lengths and kernels for this simulation.

6.2.1 Kernels' Comparisions

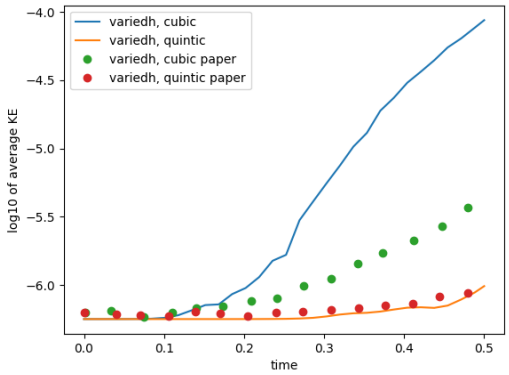
The following plots show the comparision of the solutions for different kernels for various smoothing lengths: h1 = 1.0, h2 = 1.5 and variedh case where different smoothing length is used for different parts of the simulation.



(a) h=h1=1.0



(b) h=h2=1.5



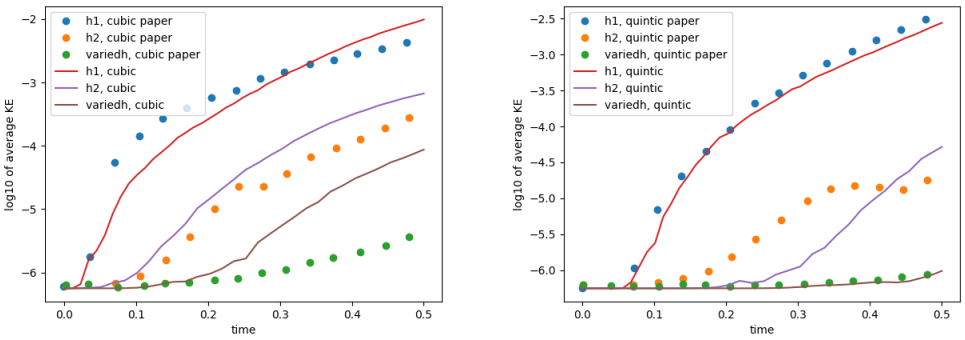
(c) Varied smoothing length

Figure 6.1: Variation of KE for different smoothing lengths

In all the cases it can be clearly seen that the Quintic spline has better stability with lower diffusion and KE than the cubic spline. The variations in results when compared to (Morris, 2000) as the initializations used are not exactly random(as it was not explained in the paper how the initializations were done), we used a constant velocity in both the dimensions and the magnitude was used so as to match, the initial KE.

6.2.2 Smoothing Lengths' Comparisions

The following plots show the comparisions of the solutions for different smoothing lengths for various kernels: Cubic spline and Quintic Spline



(a) Cubic Spline

(b) Quintic Spline

Figure 6.2: Variation of KE for different Kernels

In all the cases, it can be noted that the varied smoothing lengths when used give the best solution preventing diffusion, then h2=1.5 and h1=1.0 has the worst simulation.

6.3 Discussions

It can be seen from the plot that the variableh case has better stability of the interface preventing much diffusion of the particles into each other.

It is seen that, for the same parameters, the quintic spline is more stable than the cubic spline.

Also, the increased smoothing length caused to a considerable amount of stability in the interface. The best stability properties are however exhibited when the smoothing length for curvature is higher than that of delta function calculation.

Chapter 7

Conclusion

Implementation of surface tension forces in the regime of Smoothed Particle Hydrodynamics(SPH) was discused in this work. Specialized expressions for curvature between two species of particles are formulated. The most straightforward method which calculates the SPH estimate of curvature and applying it directly to get surface tension force is discussed. The issue of not conserving momentum is tackled by a tensor form which might have singularities. A corrected form of pressure and surface tension forces are discussed to tackle that issue.

Chapter 8

Future Work

The following are to be implemented in the second phase of this project:

- The already simulated problem using surface tension is to be implemented in the other two methods which were explained using the momentum conserved form and the form which removes the singularities.
- Other benchmark problems which include Equilibrium rod, Oscillating rod (Morris, 2000), Capillary Wave, Three Phase interaction etc., (X.Y.Hu and N.A.Adams, 2006) will be implemented using different schemes.
- These implementations can be extended to three dimensional problems
- A volume density based method where the ratio of mass and density will be replaced by the volume of the particle. This implementation will be useful for problems with high density variations.
- All these equations put together can be made into a new scheme which can be readily used by a user in PySPH.

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