Simulation of Multiphase Flows using Smooth Particle Hydrodynamics(SPH)

A Project Report
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the requirements for the degree of
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by

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Prof. Prabhu Ramachandran

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Abstract

A method of simulating multi phase flows including surface tension is presented. The approach uses the concept of Smooth Particle Hydrodynamics(SPH). Several possible implementations of surface tension forces are studied. The methods presented here apply to problems involving arbitrary shape undergoing deformations within a two-phase system and readily extended to three dimensional problems.

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Chapter 1

Introduction

The three main forces involved in multi phase flows are the pressure forces, viscous forces and surface tension foces. Many techniques have been developed to simulate multiphase flows with surface tension. Smoothed Particle Hydrodynamics is a computational technique which was originally developed to model astrophysical problems Monaghan and Gingold (1977), which was later extended to model a wide variety of problems in computational physics. Monaghan (1992, 1994). SPH is a fully Lagrangian technique where fluid interfaces are advected with very little numerical diffusion. The SPH formalism readily accomodates extra physical effects and highly irregular, mobile or even deformable boundaries. However, SPH can often be more computationally expensive than competing methods for idealized problems. In this work we simulate surface tension acting on an interface between two fluids.

1.1 Methodology

The SPH method was introduced in the late 1970's 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 moval 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.

Chapter 2

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). 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

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

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 differenct '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 unti 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 funciton 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 shortes 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 **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

$\mathbf{\hat{n}}$. 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 inaccuracte. 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

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

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.

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

This estimate can be corrected by a factor of f_a

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

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:

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

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)

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

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

$$S_{ij} = \delta_s(\delta_{ij} - \mathbf{\hat{n}_i \hat{n}_j}) \tag{4.21}$$

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 formulaitons 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 accomodate the new definition of pressure. This formulation of surface tension doesn't have a dependance on surface delta function and hences doesn't have a singularity as the resolution is increased.

To improve the stability of this technique, only the curvaturs of those particles which satisy $|\mathbf{n_a}| > \epsilon$ 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.

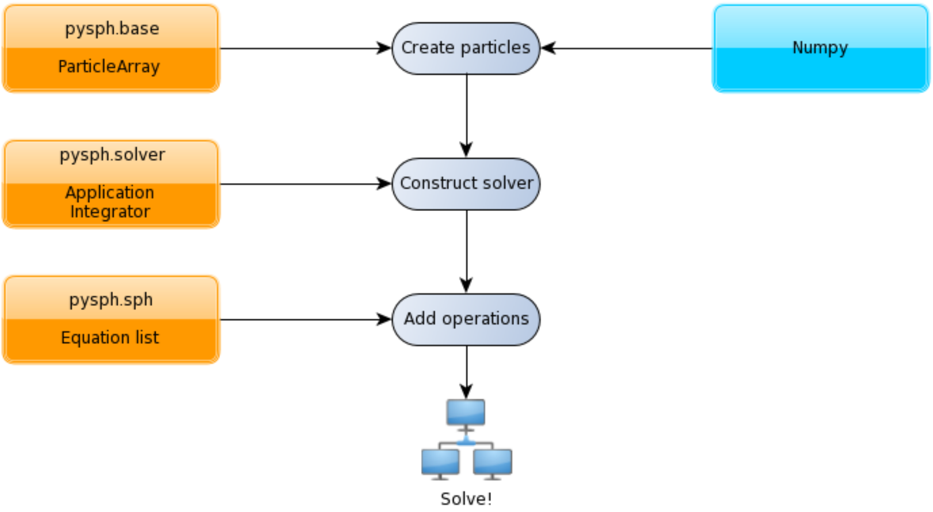

Figure 5.1: Block Diagram of PySPH

The image above is picked from `http://pysph.readthedocs.io/en/latest/tutorial/circular_patch_simple.html`

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

Appendix A

Supporting Material

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Sethy, J., 2017, *Simulating Sprays with Smoothed Particle Hydrodynamics(SPH)*, Master’s thesis (Aerospace Engineering, Indian Institute of Technology Bombay, Mumbai, India).

List of Publications

Put your publications from the thesis here. The packages `multibib` or `bibtopic` or `biblatex` or enumerate environment or thebibliography environment etc. can be used to handle multiple different bibliographies in the document.

Acknowledgements

This section is for the acknowledgments. Please keep this brief and resist the temptation of writing flowery prose! Do include all those who helped you, e.g. other faculty/staff you consulted, colleagues who assisted etc.

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