Application of Smooth Particle Hydrodynamics to Solid-Liquid Flows

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ABSTRACT

The work reported in this thesis represents research aimed at developing a macroscale simulation method for the determination of effective properties of multi-particle solid-liquid systems at low Reynolds number without resort to laboratory experiment. It is often possible to regard these systems as pseudo-homogenous fluids represented by effective properties obtained in a mean-field manner from the knowledge of fluid and solid properties including the shape, size distribution of the solid particles in the fluid. The simulation method involves explicit modeling of the moving solid particles and the interstitial fluid dynamics. The motion of the solid particles are integrated through time and space using equations of motion for solid bodies and the dynamics of intermediate fluid is modeled using Navier-Stokes equation. The continuum fluid phase is discretised using Smooth Particle Hydrodynamics (SPH). SPH, unlike other Lagrangian methods, does not use a mesh, a characteristic that makes it more suitable for massively deforming systems such as the solid-liquid suspensions under consideration.

The SPH formulation in the present work includes surface integrals that naturally arise during the derivation of the SPH equations but which are usually omitted by others in favour of applying boundary conditions using boundary particles. Retention of these integrals for imposing non-trivial boundary conditions was first suggested by Campbell (1989) but there is no work in the literature that demonstrates the usefulness of such approach. After slight modifications proposed in the present work, the implementation of these surface integrals to model no-slip boundary condition has demonstrated the stability, robustness, accuracy, and above all, the elegance of the SPH method in simulating incompressible, single-phase fluid flow under isothermal condition. Several benchmark tests including Couette flow, Poiseuille flow, lid driven cavity flow and flow past stationary cylinder in two-dimension carried out in this work and amply demonstrate the usefulness of surface integrals over the use of “boundary particles” in defining physical boundaries and boundary conditions.

The work shows that random placement of fluid particles in the domain achieves a more stable and faster progress of simulations towards steady state compared to regular placement, a configuration recommended by many. In SPH, the hydrostatic pressure is an explicit function of the local fluid density. Due to this, slight fluctuation in the estimation of fluid density causes large variation of fluid pressure. Moreover, representing liquid with finite and relatively smaller number of “SPH particles” requires the speed of sound in the liquid be moderated in a numerical simulation to capture the flow hydrodynamics. For the range of Reynolds numbers investigated in the present
study \((10^2 - 10^3)\), the value of the Mach number that gave good simulations was found to lie between 0.1 and 4.

Simulations of the coupled motion of fluid and one/two neutrally buoyant solid particles (of cylindrical shape) in a shear field have yielded encouraging results. Obtaining steady state estimates of the effective viscosity at higher solids concentrations was difficult due to the complexities required to deal with nearly touching solid particles. However, dynamic simulations of several solid particles within a fluid produced values of effective viscosity that agree reasonably well with Einstein’s (1956) model for low solids concentrations.
I would like to express my sincere gratitude to my thesis supervisors, Prof. Ugur Tüzün and Dr. Mark Biggs for allowing me the opportunity to work on an exciting new way of understanding and simulating physical phenomena. Prof. Tüzün’s capacity for physical insight has helped me immensely in shaping up the thesis. I would like to sincerely thank him for steering the work to completion. Thanks to Dr. Biggs for generously sharing his valuable time with me for the numerous discussions we had while he was at Surrey and also for his endeavour in pursuing the discussions through e-mails over last one year subsequent to his relocation to Edinburgh.

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Common sense is the collection of prejudices acquired by age eighteen
- Albert Einstein
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Chapter 1

INTRODUCTION

*Prediction is difficult, especially of the future.*

-Niels Bohr
CHAPTER 1: INTRODUCTION

Solid-liquid suspensions occur in a large number of industrial applications. Some of the examples include manufacturing of chemicals, plastics, pharmaceuticals, cosmetics, paints and food products (Yoo and Rao, 1994). Their occurrences in wastewater treatment, oil recovery from sludge, mineral processing industry (Turian et al., 1992; Bhattacharya et al., 1998), transport of slurries (Leighton and Acrivos, 1986) or processing of solid-rocket propellants (Husband, 1989) are also well known. The operations in such industrial applications could consist of various flow processes including pumping, handling, milling, agitation, mixing etc. In the past, applications involving solid-liquid systems in these processes drew heavily upon the experience of engineers to assess the flow behavior but as the applications grow increasingly complex, better understanding of the behavior the systems from fundamental perspective become a necessity to meet various stringent design and control specifications.

When dealing with solid-liquid systems, it is not always necessary to acknowledge that they are mixtures of particles and fluid; instead, it is often possible to regard them as pseudo-homogenous fluids and to ascribe to them certain "effective" fluid properties. This is particularly true when the length scales describing the motion of the suspension as a whole are much larger than the average particle size or the average particle separation. Under such conditions, one may not be interested in the response of any given individual particle but rather in the bulk response, that is, averaged properties.

The effective properties of a solid-liquid suspension such as viscosity, surface tension, suspension microstructure, thermal conductivity etc. manifest through a combination of several parameters such as particle size and its distribution (Chong et al., 1971), particle shape, volume fraction of the particles, temperature, shear rate (Metzner and Whitlock,
1958; Krieger, 1972; Hoffman, 1972), aging, inter-particle forces and the fluid properties. The dependence of the rheological properties of suspensions on some of these variables is widely available in literature (Batchelor, 1977; Jones et al., 1991; van der Werff and de Krief, 1989; Zaman et al., 1996).

The complex multi-dimensional nature of the suspension rheology arises out of the various interactive forces between particle-particle and particle-fluid as illustrated in Fig. 1.1. It shows that except for the long-range hydrodynamic forces, there are three major contributions to the forces, namely, Brownian forces, the London-Van der Waals forces, the electrostatic double-layer potential. The relative importance of these forces depends on the particle size. Furthermore, with the increase in particle concentration, the effect of neighboring particles becomes too large to be ignored. In the following section a brief outline of various approaches available for estimation of effective properties of suspensions is given.

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Fig. 1.1: Forces acting on particles in laminar flow (Liu and Masliyah, 1996)
1.1 Experimental Approach

The traditional approach to determine effective suspension properties such as viscosity is through laboratory experiments in viscometers covering a wide range of parameters influencing the viscosity. Working knowledge of the suspension fabric can be obtained from visual observations of samples using Transmission / Scanning Electron Microscope.

The simplest technique to measure relative viscosity for a homogenous fluid is by using a capillary viscometer. Ease of measurements and sophistication vary within different models such as: Ostwald viscometer, Ubbelohde viscometer, Cannon-Manning semimicro viscometer (Whorlow, 1980). While the results from these measurements are accurate, they suffer from the disadvantage that the rate of shear varies from zero at the center of the capillary to a maximum at the wall. Rotational type instruments such as cone and plate viscometer or concentric cylinder viscometer offers a more accurate measurement for suspensions as they employ uniform stress resulting in uniform deformation throughout the sample (Zaman and Moudgil, 1998). Numerous instruments (pastometers, penetrometers, extensiometers, etc.) are also available for measuring suspension rheology which show non-Newtonian characteristics (Ferry, 1980).

Over last four decades or so, tremendous effort has been directed towards measuring viscosity of solid-liquid systems and this has enriched our understanding of non-Newtonian behavior of suspensions. Measurements using classical rheometer/viscometer remain the basis for validation of any new theory that might be advanced towards understanding the complex world of suspension rheology. The review articles by Jeffrey and Acrivos (1976) and Davis (1993) offer excellent accounts of various attempts in this area.

Quite often, accurate determination of various dynamic rheological parameters from experiment is difficult due to the complex and coupled nature of the phenomena observed in a solid-liquid suspension. Even if rheological parameters are determined accurately in
the laboratory, they are often not applicable to the real problem at hand due to issues surrounding scale-up and inaccuracies resulting from extrapolation over a wide range. Though the availability of sophisticated instruments and rapid-assessing techniques have made process control easier, laboratory experiments still offer very limited scope when it comes to designing a new suspension.

On the basis of experimental data taken over a wide range of suspension parameters, some (Rutgers, 1962; Kreiger, 1972) attempted to develop simple empirical equations to correlate the parameters. Unfortunately, these correlations are usually applicable within the range of parameters investigated and any attempt of extrapolation will always involve inaccuracies that are likely to be significant and, further more, difficult to assess.

1.2 Theoretical Approach

Recognizing the limitations associated with experiment and correlation based approaches, vast efforts have been made to develop mathematical methods for prediction of closure model parameters knowing details of the suspension. Some very early attempts were based on theories having a restricted range of applicability but which, in principle, can be used to perform rigorous calculations. For example, the celebrated equation of Einstein (1956) for very dilute suspension of non-interacting spheres, developed based on energy dissipation approach, has been one of the fundamental relationships that relates the effective viscosity of a monodispersed non-interacting solid-liquid suspension with the solids volume fraction. The relationship is

\[ \mu^* = \mu_0 \left( 1 + \frac{5}{2} \phi \right) \]  

(1.1)

where \( \mu^* \) is the effective viscosity of the suspension at a volume fraction of particles \( \phi \) and \( \mu_0 \) is the fluid viscosity. The assumptions made in derivation of this equation are that the particles are near to neutrally buoyant and are far enough apart to be treated
independently of each other (i.e., the suspension is dilute, $\phi<0.15$) and that the flow around each particle is described by the Stokes law i.e., Reynolds number of the flow is extremely small ($Re<<1$). At relatively higher concentration, due to the complex nature of forces, no unified model to relate effective viscosity with particle shape, size, concentration is available till date.

However, several semi-empirical models, based on simplified assumptions and experimental results, are available in the literature (Krieger and Dougherty, 1959; Graham et. al., 1981, 1982; Liu and Masliyah, 1996). Good empirical formulas generally contain one or more adjustable parameters determined by experiments, and until these parameters can be predicted for any suspension, such formulas will be more useful for correlating data rather predicting them.

### 1.2.1 Mathematical Modeling Approach

With the availability of faster computer at affordable expense over the last decade and the rapid development of efficient algorithms to deal with mechanics of particulate suspensions, much of the focus has shifted to the predictive approach of numerical simulations for estimating these effective properties. The advantages of such a predictive approach are manifold. One of them is the ability to control a single parameter and thus isolate its specific effect, which, often is a very difficult task to accomplish experimentally. Simulations of physical processes also provide a rigorous testing ground for theories. It also plays a profound role in providing insights, often of qualitative nature, into a system's behavior and can therefore be used to design "real" experiments.

The fact that solid-liquid suspensions occur in various length scales (see Fig 1.1) means, there is no universal approach capable of spanning over the entire range of length and time scales of importance for determination of material properties and dynamic behavior of the system. Bearing this in mind, researchers have now come up with the idea of connecting the physics occurring at various length scales. The focus is on three
Chapter 1: Introduction

constituent length scales, namely the atomic/individual elemental level (microscale), the functional level (macroscale) and the collective level (mesoscale). What sets this approach apart from the previous ones is that fundamental physical and mathematical principles are rigorously applied to the modeling at each length scale and the data are then passed onto the next scale up. By combining a multi-scale link up strategy, scientists and engineers are now more capable of shedding lights on the fundamental mechanisms involved in the dynamics of solid-liquid systems.

A brief review of different numerical techniques available in the literature for simulating suspensions of varying solids concentration is discussed in the next chapter. The advantage of adopting Smooth Particle Hydrodynamics as an alternative technique in this context will also be addressed in the same chapter.

In Chapter 3, the essence of the Smooth Particle Hydrodynamics is presented first. This is followed by the derivation of governing equations, namely the mass and momentum balance equations, for the fluid phase where the surface integral term is included to model the solid surfaces, an important component of multi-particle suspensions.

Chapter 4 deals with some of the discretisation issues with regard to the accuracy of SPH simulations. Effect of initial particle distribution, an issue that lies in core of SPH methodology and particularly important for fluid flow at low and medium Reynolds numbers, on the performance of the SPH simulations is investigated. An attempt to understand the issue of flow Mach number, a key parameter in defining the 'relatively incompressible' nature of SPH fluid has also been made in Chapter 4.

The accuracy and elegance of including the surface integrals in the SPH governing equations has been addressed in Chapter 5 through a series of benchmarks on single phase flows. The geometry of the surfaces considered in the study includes straight lines and circles and tests include Couette flow, Poiseuille flow, lid driven cavity flow and flow past stationary cylinder in two-dimensional domain.
Simulations of the coupled motion of the fluid along with single, pair and multi-particles have been carried out in Chapter 6. In case of a single-particle-fluid coupled motion, the sedimentation experiments is considered for the evaluation of terminal velocity of a cylinder whilst the dynamic simulations of monodispersed multi-particle systems are carried out to estimate the steady state effective viscosity of such systems under various shear rates.

The final chapter, Chapter 7, presents the conclusions derived from the current work and indicates some possible future direction along which this work may be continued.
Chapter 2

LITERATURE SURVEY

Imagination is more important than knowledge.
-Albert Einstein
CHAPTER 2: LITERATURE SURVEY

As mentioned in the previous chapter, there are three broad classes of methods on the basis of the particle size and the corresponding inter-particle and fluid-particle forces, suitable for simulations of particulate solid-liquid systems. Smooth Particle Hydrodynamics, the technique adopted in this thesis represents the efforts aimed at developing a macroscale simulation method for the determination of effective equilibrium and transport properties of solid-liquid suspensions systems without resort to extensive laboratory experiments. Thus, SPH competes with its peer techniques at the largest length scale. In the following section, brief outlines of various techniques available in these three length scales are presented with particular emphasis on the suitability of SPH as an alternative technique for dynamic modeling of suspensions at the highest length scale.

At the lowest length scale, the Molecular Dynamics (MD) technique pioneered by Alder and Wainwright (1958) is suitable for dynamic simulations at the atomic or molecular scale. In this technique, the motion of atoms or molecules of solute and solvent are simulated by Newton's equation of motion where the interaction forces are modeled using Lennard-Jones, hard sphere, electrostatic, Van der Waals forces etc. The objective of simulations at this length scale is to understand the fundamental philosophy of evolution of transport coefficients and to seek explanation of many complex phenomena observed in fine particle suspensions. While this method is well developed and provide direct connection between the details of solid / fluid molecules and relevant rheological properties, they are restricted to small systems ($10^3 - 10^6$ atoms/molecules) and for a very short time scale ($10^{-6} - 10^{-3}$ sec).
In the next larger length scale, taking the lead from MD, Stokesian Dynamics (SD) (Brady and Bossis, 1988) and Brownian Dynamics (BD) (Ermak and McCammon (1978) techniques are developed to address the large difference in size and time scales of solid-liquid suspensions. At this length scale, the solid particles are relatively large and are dispersed in a continuum of solvent or fluid medium where they interact via continuum-scale interparticle forces including the hydrodynamic force, London-Van der Waals, Derjaguin-Verwey-Overbeck (DLVO), electrostatic forces. In case of sufficiently small particles the fluctuating thermal force from the surrounding fluid induces random motion, known as Brownian movement, to the suspending particles. This is the central idea of Brownian Dynamics. Unlike MD, instead of modeling the fluid explicitly, the effect of fluid is added to the solid particles in a mean-field manner in Brownian Dynamics. Owing to this incomplete treatment of the hydrodynamic forces, BD is only capable of simulating suspended particles at the very low shear rates (<0.1s⁻¹) with very dilute suspension (<1% w/w) or at very high shear rates (>100s⁻¹) with higher concentrations (>10% w/w), when interparticle hydrodynamics is neglected.

The effect of fluctuations in fluid temperature on the particle is neglected in Stokesian Dynamics. Instead, the hydrodynamic forces play a dominant role in SD for the kind of Reynolds numbers (defined by Stokes law regime) considered which also means that the particle size is slightly larger than that in BD. Besides the forces described earlier, SD also includes short range lubricating force and many-body interactions to reflect the hydrodynamic interactions at high solids fractions. However, it may be noted that in any given situation, it may not be necessary for all these forces to be present. The method was originally developed and tested for monodispersed sphere assemblies and extension to systems having a distribution of particle sizes (Laun et al., 1992) or rod/disk-shaped particles (Shelley and Ueda, 2000) or aggregated flocs (Chen et al., 1984; Adler, 1987) are also found in the literature. From the computational point of view, the presence of extremely small particle separation necessitates the use of a very small time step and thus rendering the simulation time extensive. The technique also falls far short of a full-fledged fluid dynamics technique required to address suspension hydrodynamics at finite
Chapter 2: Literature Survey

Reynolds number since it does not address any nonlinear inertia mechanism which governs effects such as translation and rotation of particles.

In the next higher length scale, the hydrodynamic forces along with the particle inertia become the major players in dictating suspension dynamics and microstructure, see Fig. 1.1. The continuum fluid is usually discretised based on some discretisation technique and the solid particles are considered having well defined surfaces where the viscous and hydrodynamic effects are evaluated. The essence of all the techniques lies in that, the solid particles move under the influence of local hydrodynamics, the particle-particle interactions and the particle-boundary surface (if any) while the dynamics of the fluid is governed by particle-fluid interaction and any other externally imposed force on the fluid. This is probably the most difficult yet interesting length scale at which the behavior of the fluid cannot be neglected. Traditionally, this length scale enjoys the maximum attention of researchers and consequently, there are quite a few well-established and mutually competing discretisation techniques available for modeling the liquid phase. In the following section a brief outline of some of these techniques are outlined.

The key techniques for modeling the liquid phase can be broadly categorized depending on what kind of constitutive model is used to represent the fluid phase. They include Lattice-Gas Automata and allied techniques, Dissipative Particle Dynamics (DPD) and Navier-Stokes equation based approach. The Smooth Particle Hydrodynamics (SPH) belongs to the last category of technique where it competes with Finite Difference, Finite Element and Direct Numerical Simulation.

In its early development, Lattice Gas Automata (LGA) was introduced by Frisch and coworkers (Frisch et al., 1986; d'Humières et al., 1986a, b) as a tool for studying single phase hydrodynamics and has been extensively reviewed in recent years (Biggs and Humby, 1998; Rothman and Zaleski, 1997). In the simplest of LGA models, the computational domain is divided into several triangular/hexagonal/octagonal lattices with particles of unit mass and speed occupying the vertices of the lattices. They move from
Lattice-Boltzmann Method grew out of LGA method (Chen et al., 1992). Not only does it retain the parallel nature of LGA, but also it provides an elegant way of regaining Galilean invariance and thermodynamically correct equation of state. However, it terms of the computer memory, it is much more expensive than LGA since it replaces boolean...
operations of LGA by floating points. With regard to its application in suspension
dynamics, solid particles move according to Newtonian dynamics in a continuous space
and the fluid 'particles' are treated as Lattice-Boltzman fluid. At the solid-liquid
interface, interactions are generated through new collision rules. The work of Audin and
Lu (1995) and Ladd (1993, 1994) in establishing LBM as an alternative technique for
studying suspension dynamics is commendable. The problem of exact resolution of
complicated boundaries makes LBM unsuitable for situations where hydrodynamic
interaction mainly originating at the interface is important, such as at highly concentrated
suspensions.

Recently an off-lattice technique has been proposed with the name of Dissipative
Particle Dynamics (Hoogerbrugge and Koelman, 1992; Español, 1995; Español and
Warren, 1995). The technique introduces the concept of dissipative particles (DP), which
are fluid molecules grouped together and are able to move in continuous space and
discrete time. In a two-phase system, some of these DPs belong to the other phase.
While conventional DPs are spherical, Flekkoy and Coveney (1999) introduced variable
sized Voronoi lattice DPs which offer the flexibility of choosing particle size according
to local resolution requirement. Among the DPs of fluid phase evolution equations are
established on the basis of the kinetic theory and between the fluid and solid DPs, one
can use relevant hydrodynamic forces. The overall solution technique is similar to
Molecular Dynamics type simulation. Applications of this technique include colloidal
suspensions (Boek et al., 1997), polymer solutions (Schlijper et al., 1995), and binary
immiscible fluids (Coveney and Novik, 1996).

If one assumes the suspension as an effective single-phase continuum, one can apply the
celebrated Navier-Stokes equation for predicting its hydrodynamical behavior:

\[
\frac{DV}{Dt} = -\frac{\nabla p}{\rho} - \frac{1}{\rho} \nabla \cdot \tau + b
\]  

(2.1)
where \( \rho \) is the effective density of the suspension, \( V \) is velocity vector, \( p \) is the hydrostatic pressure, \( \tau \) the viscous stress, \( b \) the body force per unit mass of the suspension. In that case, the closure parameters such as effective suspension density, viscosity, diffusion coefficient, stress-strain relationship need to be estimated in a mean-field manner from the microscopic interactions of a particular configuration of suspension and then be used as the bulk properties in the above equation. It is interesting to note that the Navier-Stokes equation, in a sense, is capable of connecting two consecutive length scales, namely,

- at the level of individual particle and surrounding fluid when the fluid and the solid particle are treated as separate phases;
- at the level of multi-particle and interstitial fluid under the assumption of homogeneity of the system.

Thus, it is seen that the Navier-Stokes equation based techniques offer more comprehensive way of dealing with solid-liquid suspensions. In this method the continuum fluid domain is discretised into very small elemental volumes; conservation of mass, momentum and energy is applied along with necessary initial and boundary conditions on each of these volumes. The resulting equations are solved to obtain the hydrodynamic behavior of the fluid by adopting various numerical schemes. The solid particles are moved by Newton's equations of motion. Together, they yield information on spatial and temporal distributions of the fluid and solid particles. The accuracy of the result would depend on how well one provides the information at the individual particle level. The variety of numerical schemes available differs among themselves in the way discretisation of the fluid phase is carried and boundary conditions are imposed for a specific problem.

The discretisation of the space domain is usually done by Finite Element (FEM) or Finite Difference (FDM) technique, and the time domain by any suitable time stepping scheme. Surfaces of the particles are also discretised to elemental length (in 2D) or elemental area (in 3D). These discretisation techniques being very well established and
applied to extremely wide range of engineering problems, presentation of any basic
details of the techniques is felt redundant.

Using FEM, Tezduyar et al. (1992a, b) developed a DSD/ST (Deforming-Spatial-
Domain/Space-Time) procedure to tackle moving boundaries and interfaces of a drifting
cylinder. This is probably one of the earliest work to demonstrate the ability of FEM to
model a moving interface. However, the procedure was unable to tackle three
dimensional problems and situations where the spatial domain changed strongly with
time. Around the same time, Hu et al. (1992) simulated two-dimensional motion of a
few sedimenting circular and elliptic cylinders confined in a channel as a first step to
simulate suspension dynamics. They observed instability near the particle surface while
applying the simplest fully explicit scheme, particularly at Reynolds numbers large
enough for the inertia effect to become significant. Subsequently the model was
modified to an explicit-implicit scheme to overcome the problem. Feng et al. (1994a, b)
used the same technique to study interaction of particles suspended in a Newtonian fluid
under Couette and Poiseuille flow conditions. Hu (1996) incorporated moving
unstructured grids by using an Arbitrary Lagrangian-Eulerian (ALE) technique to
simulate about 100 particles in a 2D domain with periodic boundary conditions. In order
to prevent particles from colliding, he maintained a minimum gap between close-by
particles and between the particles and the boundary walls filled with the fluid medium.
While the tests qualitatively demonstrated the particle migration phenomena, it lacked
quantification and comparison with experimental results. Johnson et al. (1996, 1997)
addressed the instability arising due to the proximity between two solid particles in multi-
particle systems. They allowed the particles to undergo perfectly elastic collisions. This
is a novel idea and the occurrence of collisions in their 3D simulations with 2-5 particles
was also reported. The idea was also implemented by Patankar (1997) to study the effect
of the inertia on the rheology of a suspension of rigid particles in a Newtonian fluid.
However, the situation when the particles did not collide but were very close to each
other, was hardly being addressed by such simplistic collision strategy of Johnson et al.
(1997). By improving collision strategy and adopting a fictitious domain method to
simplify the geometrical complications between two nearly-touching particles, Glowinski et al. (1999) and Patankar et al. (2000) eliminated the need for remeshing of the domain after every time step. The results of their 2D sedimentation experiments with up to 512 particles and 3D experiments with two particles (to show drafting, kissing and tumbling) were quite encouraging.

Two of the most important computational issues associated with this approach are discretisation and remeshing. In order to capture the solid-liquid interaction at the solid surface, the fluid medium should preferably be discretised at an order of magnitude below the size of solid particles. This results in prohibitively high number of elements and the time scale becomes extremely small. Theoretically, this method is capable of dealing with any type of force that may exist in the fluid-particle system, at any practicable Reynolds number and in any fluid medium. However, in practice, prediction of microstructural behavior of a dense suspension through FEM/FDM would require extensive computational resources at enormous cost. These techniques suffer in two accounts:

- **Remeshing**: Simulation of single-phase flow can be efficiently carried out in a fixed grid domain without undertaking any remeshing of the domain. But, in the flow of solid-liquid suspension, the discretely placed particles move continuously in the fluid continuum and to capture the new positions of particles, the domain needs to be remeshed after every time step. This is computationally very expensive. Ideally, a meshfree technique would be more suitable to deal with such Lagrangian type problem.

- **Instability**: At high strain rate due to higher degree of deformation, remeshing techniques become highly unstable thereby rendering it inefficient.

There has been much interest in meshfree Lagrangian methods because such techniques can do away with the mesh tangling problems common to Lagrangian calculations of a traditional Finite Difference or Finite Element technique, as mentioned above. Particularly, in the context of evolution of effective suspension properties as well as
dynamic modeling of a multi-particle system characterised by massive deformation at the solid-fluid interfaces, a Lagrangian method becomes an obvious choice. The **Smoothed Particle Hydrodynamics (SPH)** is a three-dimensional Lagrangian method that is truly grid free. SPH discretises the fluid by an ensemble of interacting point masses that move according to the local fluid dynamics and which carry a set of problem-specific quantities such as density and velocity that change with time according to equations derived from the relevant equations (i.e., Navier-Stokes equation) of continuum mechanics. As SPH follows the behaviour of moving lumps of fluid rather than fixed points in space, it belongs to the Lagrangian class of methods. However, unlike other Lagrangian methods [Trease et al., 1991], SPH does not use a mesh, a characteristic that makes it more suitable for problems where the shape and connectivity of the domain evolves significantly during the simulation. SPH particles being conceived as cloud, it has the adaptability to offer high resolution in case of dense suspension and low resolution in dilute solution, thus keeping the computational load at its optimum. Through SPH, the development of three-dimensional CFD code is as easy as a one-dimensional one and in modern day distributed computing environment, SPH fits very well as it can be parallelised with very little effort. Therefore, SPH offers great potential to explicitly simulate suspension hydrodynamics more efficiently compared to other traditional but well developed techniques, and warrants a closer look.

The earliest attempt at such a method was the particle-and-force (PAF) technique (Harlow and Meixner, 1961; Harlow, 1962). A method more like modern SPH was originally developed by Lucy (1977) and Gingold & Monaghan (1977). It was originally developed to tackle the wide variation of density over a large domain in astrophysical problems including formation of protostar from a dense interstellar cloud (Hernquist & Katz, 1989), fission of a rotating star etc, more efficiently. The formalism found success in dealing with such situations involving a compressible fluid. Since then, this technique has been applied to a variety of scientific and engineering problems including Magnetohydrodynamics (Morris, 1996), solid mechanics (Benz and Asphaug, 1994), viscous fluid flow at low Reynolds number (Morris et al. 1997), heat transfer & fluid
flow in industrial processes such as die casting, resin transfer (Cleary and Monaghan, 1999; Sawley et al., 1999) moulding, flow of cohesive granular material (Oger and Savage, 1999) etc. Several reviews have been published in the literature including Benz (1990) and Monaghan (1992). Over the past decade, SPH has acquired high degree of attention from scientific community as a possible alternative to deal with the Lagrangian type flow in an efficient grid-free manner.

The method was initially developed for the study of astrophysical systems where solid surfaces are rarely involved and the fluids are compressible. Whilst the method has been applied to problems involving solid surfaces, a more elegant way of imposing solid surface boundary conditions by means of surface integral is adopted in the present study. The surface integral naturally arises during the derivation of SPH constitutive equations for the fluid phase. Retention of these integrals for the purposes of imposing non-trivial boundary conditions was first suggested by Campbell (1989) in an unpublished report, but never implemented in hydrodynamic simulations. In the next chapter, apart from presenting the essence of the technique, the SPH form of Navier-Stokes equation for incompressible fluid is also developed that includes the surface integrals for the first time. The method will be tested using several benchmark problems of single-phase flow in two-dimension. The test problems are chosen in such a way that it demonstrate the rigor and capability of the surface integrals to accurately model various solid surfaces including simple straight line surfaces and more complex circular surfaces.

Navier-Stokes equation, applicable for incompressible fluid, is the starting point of present SPH formulation. However, since finite number of fluid particles represent the fluid domain, it implies that the “incompressible” behavior of the “SPH liquid” cannot be observed in strict sense. Though it is a common practice to assume slightly compressible fluids, little has been published on the behavior of SPH when this is the case. This issue is, therefore, addressed in some detail in Chapters 3 and 4, before considering suspension systems in Chapter 6.
One of the primary justifications for using SPH to simulate suspensions with many solid particles is its ability to handle large deformations of the simulation domain, something that obviously results in disordered particle positions during any simulation even if the fluid particles are positioned in regular grids at the beginning of the simulations. This has prompted the present study to assess the effect of initial SPH fluid particle positions on simulation results. This issue is addressed in Chapter 4 and Chapter 5.
Chapter 3

SMOOTH PARTICLE
HYDRODYNAMICS

An expert is a man who has made all the mistakes, which can be made, in a very narrow field.
-Niels Bohr
The aim of this chapter is to capture the main features of Smooth Particle Hydrodynamics method and establish the governing hydrodynamic equations to be used later for the analyses presented in the following chapters. We develop the SPH form of hydrodynamic equations, namely, the Equation of Continuity (EOC) and Equation of Motion (EOM) for the fluid phase. Furthermore, the following two important aspects of the present work require special attention and novel treatment:

- Implementation of various types of boundary conditions through adoption of surface integrals in EOC and EOM.
- Use of 'relatively incompressible' equation of state to model hydrostatic pressure of a liquid and its implication in the context of SPH.

The above computational framework is followed by a detailed discussion on various issues surrounding the implementation of SPH including choice of kernels, stability etc.

### 3.1 Key Features of SPH

This section is intended to introduce the reader to the concept of SPH which are fundamental to the method. Similar accounts may be found in Monaghan (1992) and Benz (1989), though each author has adopted a slightly different approach to obtain very similar equations.

#### 3.1.1 Particle Representation of Fluid

SPH is essentially a discretisation technique where a continuous domain of fluid is conceived as an ensemble of discrete clouds of matter with their mass located at their centers of mass and these centers of mass move according to the conservation laws of
fluid mechanics. The motion of these ‘fluid particles’ produced by various hydrodynamic forces may be seen in the same eye as the motion of solid particles in particle mechanics. The concept is schematically described in Fig. 3.1. The figure also indicates various possibilities on the shape of the particle clouds, though a spherical cloud is much easier to conceive, and to translate into realistic mathematical representation. These ‘fluid particles’ discretely move from one point to another within the flow domain, physically carrying (velocity, temperature etc.), and locally exchanging all the relevant information (i.e., various hydrodynamic quantities e.g., mass, momentum, energy etc.). This typically resembles phenomena such as convection/diffusion prevalent in fluids. These ‘fluid particles’ should not be viewed as real solid particles; they are mere coordinates in space, which store the local fluid properties. An ensemble of these particles would resemble a small fluid volume and the deformation of this fluid volume is obtained from the contour formed by the space created by joining the center of the particles at the boundary of the fluid element. From this chapter onwards, any mention of the word ‘particle’ will always refer to the SPH particles of the fluid medium, and in a solid-liquid system, described in Chapter 6, the solid particles or bodies would be described specifically as ‘solid particles’ to differentiate them from the fluid particles.

![Fig. 3.1: Schematic diagram showing the concept of discretisation of a continuous domain in SPH. The continuous phase is turned into a discrete assembly of particles.](image-url)
The idea of evaluating any physical property pertaining to a particle using an interpolating function is the central theme of SPH. It states that, any property of these 'fluid elements' is obtained by interpolating the same property over the neighboring particles using some kind of weighted function. In SPH terminology, this interpolating function is called kernel function (or smoothing function) and the value of the property obtained after interpolation (also known as smoothing operation) is known as "smoothed" value of the property. It is this smoothing operation coupled with the adoption of moving particles of fluid that give the method its name. The accurate evaluation of the fluid property at any particle location depends on how accurately these smoothing functions can reproduce the fluid property based on the values of the property of the neighboring particles. The kernel function may be viewed as the building block of SPH much the same way an 'element' in Finite Element Method. In the following section, the mathematical representation of the kernel function is described.

3.1.2 Kernel Function

Let us consider a continuous domain of fluid enclosed within an irregular boundary as shown in Fig. 3.2.
Let us now imagine that the domain is divided into \( N \) small, possibly overlapping volumes each with a certain mass where the masses are concentrated at their respective centers of mass. The volume elements are labeled by the coordinates of the centers of mass. According to kernel approximation in SPH, the smoothed value of any physical quantity \( f(r) \) (for example, fluid density or pressure), at any location \( r \), can be obtained by interpolating or integrating the quantity over the entire fluid domain. In mathematical terms, we can describe this as (see Appendix 1)

\[
\langle f(r) \rangle = \int_{\Omega} W(r - r', h) f(r) \, dr' 
\]  

(3.1)

where \( W(r - r', h) \) is the kernel function, \( h \) is a measure of influence of the kernel function, also known as the measure of compact support length or smoothing length, \( r \) is the position vector of the fluid volume of our interest with reference to the origin of any frame of reference, \( r' \) is position vector of any other volume element within the domain of integration, \( \Omega \). In case of three-dimensional domain, the integration is over the entire volume of the domain while for two-dimensional problem the integration is carried out over the domain area. Accordingly, the term \( dr' \) represents elemental volume and area for three and two-dimensional problems. Therefore, the term \( dr' \) is not a vector quantity.

It may be worthwhile to mention here that for kernels having compact support, the limit of the above integration changes to the kernel volume (in three-dimensional domain) or kernel area (in two-dimensional domain) instead of the entire domain volume or domain area of the system.

The kernel function is a weighting parameter that has a positive fractional numerical value with units of \( \text{cm}^{-1} \), \( \text{cm}^{-2} \) and \( \text{cm}^{-3} \) in case of one, two and three-dimensional problems, respectively. The function usually returns a higher value for locations closer to the point of evaluation. The smoothing length determines the extent of space to be included while evaluating the smoothed value, \( \langle f(r) \rangle \) of the function \( f(r) \). By varying the smoothing length, we can include or exclude fluid elements that are further away.
from the point of our interest. The actual value of smoothing length and the number of fluid elements to be included is generally a function of how accurately one would like to evaluate these smoothing properties in a particular simulation. This is discussed in detail in § 3.7, and demonstrated with examples in § 4.3. The discreteness of SPH means the integral form of Eqn. (3.1) is not convenient for implementation and it is, therefore, replaced by a summation over all particles within the domain. In three-dimensions:

\[
\langle f(r) \rangle_i = \sum_{j=1}^{N} W(r_i - r_j, h) f(r_j) \Delta \omega_j
\]

\[
= \sum_{j=1}^{N} \frac{W(r_i - r_j, h) f(r_j) m_j}{\rho_j}
\]

\[
= \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(r_j) W(r_i - r_j, h)
\]

(3.2)

where the suffix \( j \) is for all the particles in the domain \( \Omega \), \( m_j \) is the mass, \( \rho_j \) is the density and \( \Delta \omega_j \) is the volume of particle \( j \). \( N \) is the total number of particles in the kernel volume and \( i \) is the index of the fluid particle we are interested in to evaluate the smoothed function. If we choose, for example, to evaluate the smoothed density of particle \( i \), then replacing \( f(r) \) in Eqn. (3.2) by \( \rho(r) \), we obtain

\[
\langle \rho(r) \rangle_i = \sum_{j=1}^{N} m_j W(r_i - r_j, h)
\]

(3.2a)

where \( \langle \rho(r) \rangle_i \) is the smoothed density of fluid particle \( i \). It may be noted that, in order to estimate the smoothed density at any fluid particle location, knowledge of all fluid particle locations within its kernel and their masses is necessary.

It is also possible to obtain an estimate of the smoothed gradient of the property \( f(r) \), simply by differentiating Eqn. (3.2). After minor manipulation, the smoothed gradient can be expressed as (see Appendix 3):
Chapter 3: Smooth Particle Hydrodynamics

\[ \nabla \langle f(r) \rangle_i = \sum_{j=1}^{N} \frac{m_j}{\rho_j} \nabla_i W(r_i - r_j, h) \]  

(3.3)

where \( \nabla_i \) is the 'del' operator of any particle \( j \) within the kernel with respect to the position of particle \( i \). Here, the kernel function is assumed to be differentiable over space. It is interesting to note that the gradient of the function \( f(r) \) comes from the cumulative effect of the positions of the particles-\( j \) in the field of the kernel of particle-\( i \).

Thus, the gradient of the property \( f(r) \), apart from being a function of the same property of its neighbors, it also depends on the spatial gradient of the kernel function used. Unlike other discretisation schemes (e.g., Finite Difference or Finite Element Method) where the gradient of any property is explicitly evaluated, the aforementioned characteristic of SPH necessitates one to study the properties of kernel gradient. This is discussed in § 3.6 and § 3.7. The relative locations of the 'fluid particles', as observed in Eqn. (3.3), also significantly contribute to the evaluation of the smoothed property of the function which is demonstrated with some examples in Chapter 4.

### 3.1.3 Characteristics of Kernel Function

The previous section has established that the kernel is the basic building block in SPH. In many ways, the significance of kernel in SPH is similar to that of elements and nodes in Finite Element method or grids in the Finite Difference technique. Some of the most important properties a kernel should exhibit include the following:

- It should resemble a Dirac-Delta function i.e., \( W(r-r', h) \) should be a function strongly peaked at \( r'=r \).
- The volume integral of the kernel function over the domain should be unity, i.e., \( \int_{\Omega} W(r-r', h) dr' = 1 \). This is a property of Dirac-Delta function as well.
- The function \( W(r-r', h) \) should be symmetric about position \( r \).
- For computational economy, the kernel should have a compact support (\( h \) or its multiple) to limit the number of particles contributing to the smoothing
operation. Beyond this compact support length, the value of the kernel function should be zero. Here, the underlying assumption is that, any two fluid particles separated by a distance more than the compact support distance should not influence each other’s hydrodynamic property directly.

- It should be continuous within its compact support length and its first derivative should exist.
- $h \to 0$ for closest approximation of a continuum.

To some extent, the choice of the kernel is not very critical as long as the above criteria are met. This is particularly true in the limit of $h$ and $\Delta r$ (the inter-particle distance) being infinitely small. Beside that, the value of the integral $\int W(r - r', h) dr'$ will be unity in the limiting case when there are infinite number of particle positions within the kernel itself. That means, each kernel should have large number of ‘fluid particles’ and simultaneously, the size of the kernels (i.e., the length, area or volume of each ‘fluid particle’ in case of one, two or three dimensional simulations) should be extremely small. However, in practice, the computational economics dictate the values of $h$ and $\Delta r$ to be finite and the kernel to have a limited number of neighbors. This means that the criteria of $\int _{\Omega} W(r - r', h) dr' = 1$ cannot be met in the strictest sense in any practical simulation having finite compact support length and finite number of neighbors. Thus, by carrying out kernel approximation, we do introduce some degree of loss of numerical accuracy.

### 3.2 Standard SPH Model for Isothermal, Compressible, Single-phase Fluid

In the preceding sections, the reader was introduced to with the fundamentals of SPH. In this section it is aimed to develop the SPH formalism of hydrodynamic equations as applicable to viscous, incompressible fluid flow under isothermal conditions. In a two-phase system like solid-liquid suspension, the hydrodynamic equations are developed for the continuum fluid phase where the interactions of the fluid with the solid particles
appear as an integral part of the governing equations of the fluid phase. The equations include:

- Equation of Continuity, derived on the principle of conservation of mass within the system.
- Equation of Motion, derived on the principle of conservation of momentum in the system.
- Equation of State, which relates hydrostatic pressure to the density or volume of the fluid.

A complete description of the fluid system also requires specification of the initial and boundary conditions.

The motion of solid particles follows the principle of particle mechanics, where the net force on each particle is calculated by summing up the force contributions from the surrounding fluid and neighboring solid particles. Thus, in modeling suspension flows, the overall dynamics of the solid-liquid system is coupled at the individual solid particle level. Coupling of forces between solid and liquid phase forces is discussed separately in Chapter 6.

SPH being a particle based technique, the Lagrangian frame of reference becomes an automatic choice for developing all the governing equations, particularly when the primary interest is to simulate the motion of both solid and liquid phases in a suspension. In the Lagrangian approach, one tracks the properties including the position of each discrete fluid element as the flow progresses. In contrast to the Eulerian frame of reference, where one follows the evolution of hydrodynamics at certain fixed locations in space, tracing the history of an individual particle is often cumbersome. Lagrangian approach offers us a much more efficient choice when dealing with dynamic simulations of solid-liquid systems. In order to avoid tedious details, the SPH formulations are developed below from the standard differential forms of the equations of continuity and motion.
Special attention should also be paid here to the way various hydrodynamic interactions between the fluid phase and the domain boundary or any other phase, present within the system enter in the model equations through the surface integral terms. Campbell (1989) showed in a rarely cited internal report that surface integrals arise as a matter of course in the derivation of the SPH equations. These surface integrals provide a direct means of applying non-trivial boundary conditions, whilst they may also remove boundary-induced instabilities which is an important concern in particle-based techniques (Belytschko et al., 1996). Standard SPH formalism ignores these surface integrals. In this work, we demonstrate the validity and utility of retaining the surface integrals by applying it in all our simulations. It should be mentioned here that Campbell only considered inviscid fluids, and he neither implemented nor tested his model.

### 3.2.1 Equation of Continuity (EOC)

The main application of the SPH technique lies in hydrodynamic situations where there is no mass source or sinks. That means if one deals with a fixed number of 'smooth particles' in a given system, the total mass of the system remains constant and thus the conservation of mass is automatically satisfied. However, the density as well as the volume of each SPH fluid particle may still vary. This necessitates the use of the Equation of Continuity as a tool to examine the variation of density in the system. As would be noticed while deriving Equation of Motion in § 3.2.2, a density-based technique like SPH is very sensitive to the fluid density and accurate estimation of density remains an important part of the SPH formulation.

The smoothed density of the fluid particles can be estimated directly from the knowledge of particle distribution (i.e., coordinates of the particles in the domain) and their masses. Using Eqn. (3.2a), one can write:

\[
\langle \rho \rangle_i = \sum_{j=1}^{N} m_j W_{ij} \tag{3.8}
\]
where \( \langle \rho \rangle_i \) is the smoothed density of particle \( i \), \( m_j \) is the mass of a neighboring particle \( j \). For brevity, \( W(r_i-r_j,h) \) is written as \( W_i \). The summing operation is performed over all \( N \) particles within the kernel of particle \( i \). For cases where the kernel does not intersect with the domain boundary, the above equation may be used to estimate the smoothed density as accurately as we want. But, inaccuracy in estimation of smoothed density occurs near the boundaries due to lack of particles since the fluid density falls to zero and there are no fluid particle on the other side of the domain boundary for the smoothing operation. This is further discussed in § 3.3.1.

The other approach of estimating the temporal evolution of density is from Equation of Continuity. As suggested by Monaghan (1994), the use of Equation of Continuity with an initial density distribution to calculate the evolution of density has two significant advantages:

- Firstly, if the system is initialized with an accurate density distribution, the density will only change if there is finite difference in relative movements among the neighboring fluid particles. Otherwise, it will remain the same.
- Secondly, some type of boundary conditions can be conveniently implemented through the Equation of Continuity by use of surface integrals as will be explained in the following paragraphs.

![Fig. 3.3: Control volume in SPH is the volume of the kernel.](image)
In the Lagrangian frame of reference, the differential form of Equation of Continuity, applicable to an infinitesimally small fluid element \( P \) (see Fig. 3.3) may be written as:

\[
\frac{d\rho}{dt} = -\rho \nabla \cdot V \tag{3.9}
\]

where \( \rho \) is the density of the fluid element, \( V \) is the velocity vector and \( \nabla \) is the divergence. To conserve linear and angular momentum, and to reflect the relatively incompressible nature of SPH fluid, Monaghan (1992) suggested to include the density parameter inside the divergence operator. Thus, Eqn. (3.9) can be rearranged as:

\[
\frac{d\rho}{dt} = -\nabla \cdot (\rho V) + V \cdot \nabla \rho \tag{3.10}
\]

Multiplying Eqn. (3.10) by the kernel function \( W(r - r', h) \) and integrating over the kernel volume \( \Omega \), one is essentially carrying out conservation of mass over fluid volume at position \( P \). The integration yields:

\[
\int_{\Omega} \frac{d\rho}{dt} W(r - r', h)dr' = -\int_{\Omega} \nabla \cdot (\rho V) W(r - r', h)dr' + \int_{\Omega} V \cdot \nabla \rho W(r - r', h)dr' \tag{3.11}
\]

Here \( r \) is the position vector of the fluid element at point \( P \) and \( r' \) is position vector of any other infinitesimally small fluid element in the domain \( \Omega \). Now applying Leibnitz's rule (Appendix 2) and simplifying it further by smoothed expression for a function given in Eqn. (3.2), one can rewrite the fluid particle expression for the left hand side of Eqn. (3.11) as:

\[
\int_{\Omega} \frac{d\rho}{dt} W(r - r', h)dr' = \frac{d}{dt} \int_{\Omega} \rho W(r - r', h)dr' = \frac{d}{dt} \langle \rho \rangle, \tag{3.12}
\]
Eqn. (3.12) is the expression for time derivative of smoothed density for particle $i$. Here $\rho'$ is the density at any point within the kernel volume. Both terms in the right hand side of Eqn. (3.11) have spatial derivatives associated with them. If the kernel does not intersect with any physical boundary, then the derivatives can be cast in the form of Eqn. (3.12) quite easily. However, for the sake of completeness, let us assume that the kernel intersects with a boundary as shown in Fig. 3.4.

\[ \int_{\Omega} \nabla \cdot (\rho V) W(r - r', h) \, dr' = -\int_{\Omega} (\rho V) \cdot \nabla W(r - r', h) \, dr' + \int_{S} (\rho V) \cdot n W(r - r', h) \, dS \]

(3.13)

In the second term of above expression, we introduce the mass flux term in the form of surface integral. This takes care of any mass added or removed from the kernel volume $\Omega$, whose surface is $S$. This term will appear if the control volume, $\Omega$, intersects with the domain boundary. In the case of simulating solid-liquid system, this term will appear when the liquid volume intersects with any solid particle surface. In case of a two-dimensional domain, while the region of integration for the first two terms is over the kernel area, the third term, the so called 'surface integral', reduces to a line integral along
the portion of the boundary line that intersects with the kernel. Applying similar treatment to the second part of the right hand side of Eqn. (3.11) results in:

$$\int_{\Omega} V \cdot \nabla \rho W (r - r', h) \, dr' = -\int_{\Omega} V \cdot \rho \nabla W (r - r', h) \, dr' + \int_{S} V \cdot n \rho W (r - r', h) \, dS$$

(3.14)

After minor manipulation and using Eqn. (3.2) to cast Eqns. (3.13) and (3.14) in particle form and then combining it with Eqn. (3.12), one can obtain the final particle approximation of Equation of Continuity as:

$$\frac{d}{dt} \langle \rho \rangle_i = -\sum_{j=1}^{N} m_j (V_j - V_i) \cdot \nabla_i W_{ij} - \rho_i (V_s - V_i) \cdot \int_{S} n W_{is} \, dS$$

(3.15)

where

- $V_s$ is velocity of the surface $S$ at position $r_s$
- $V_i$ and $\rho_i$ are velocity and density of particle $i$
- $V_j$ and $m_i$ are velocity and mass of any particle $j$, in the neighborhood of particle $i$
- $\nabla_i$ is the divergent of any particle with respect to the position of particle $i$
- $W_{is} = W (r_i - r_s, h)$
- $r_i$ is position vector of particle $i$
- $r_s$ is the position vector of any point on the surface $S$
- $n$ is unit vector directing away from the surface $S$, normal to the surface at $r_s$

Fig. 3.5 shows schematically that for particles belonging to the core of the fluid domain, $W_{is}$ is identically zero and hence the surface integral vanishes for those fluid particles. However, it is interesting to note that if the particle is close to a boundary having a non-trivial boundary condition, then the effect of such a boundary can be introduced to the continuity equation by the surface integral. Introduction of this surface integral term is clearly a step forward in implementing fluid-particle and fluid-domain boundary interactions in the hydrodynamic equations for modeling solid-liquid systems.
3.2.2 Equation of Motion (EOM)

The second evolution equation required for isothermal flows is that of the fluid particle velocity, obtained from a balance of forces on the fluid element. The vast majority of SPH models to date including that of Campbell (1989), are valid for inviscid fluids only. The few that have included physical viscosity do so by a number of different ways. Some (Monaghan, 1994; Reichl et al., 1998; Monaghan and Kocharyan, 1995; Nagasawa and Kuwahara, 1993) use an artificial viscosity term first developed to better handle shocks in inviscid SPH (Monaghan and Gingold, 1983), but which has since been shown (Meglicki et al., 1993; Morris and Monaghan, 1997) to be equivalent to a Newtonian constitutive model as the number of fluid particles, $N \to \infty$. Moreover, the use of artificial viscosity does not have any basis for modeling real viscosity of a fluid and it produced inaccurate velocity profiles in attempts to do so (Morris et al., 1997). Apart from that, the approach cannot be extended to non-Newtonian fluids, it provides no basis for recovering surface integrals, and it has been found to be inaccurate when viscous effects are dominant (Morris et al., 1997). Morris et al. (1997) used a combined SPH/Finite Difference approach to derive the SPH viscous stress. Once again, this approach does not permit recovery of the surface integrals which means one has to resort to the conventional method of using ghost particles / boundary particles (described in § 3.4.2). This defeats one of the important purpose of the present work where it is intended to utilize surface integrals as a means of introducing various boundary surface conditions. A third
Chapter 3: Smooth Particle Hydrodynamics

approach (Takeda et al., 1994) substitutes the stress tensor directly into the momentum equation. However, this approach introduces second order derivatives of the kernel into the SPH evolution equation for the velocity, making it sensitive to particle maldistribution. The final method calculates the stress tensor for each particle, by applying the SPH formalism directly to the stress model, and then uses these particle stresses in the momentum equation (Watkins et al., 1996; Flebbe et al., 1994). Whilst computationally more expensive, this approach provides a formal basis for recovering the required surface integrals, and it is flexible in that it permits treatment of any constitutive stress model for the fluid. The current work adopts and extends this last approach.

In the Lagrangian frame of reference, the differential form of the Equation of Motion, applicable to an infinitesimally small fluid element may be written as:

\[
\frac{dV}{dt} = -\frac{\nabla p}{\rho} - \frac{1}{\rho} \nabla \cdot \tau + b \tag{3.16}
\]

where \( \rho \) is the density of the fluid element, \( V \) is velocity of the fluid element, \( p \) is the hydrostatic pressure, \( \tau \) is the viscous stress tensor and \( b \), the body force per unit mass of the fluid. As before, using the symmetric form advocated by Monaghan (1992) to conserve linear momentum, we can rewrite the above equation as:

\[
\frac{dV}{dt} = -\nabla \left( \frac{p}{\rho} \right) - \nabla \rho \frac{p}{\rho} - \nabla \cdot \left( \frac{\tau}{\rho} \right) - \nabla \rho \cdot \left( \frac{\tau}{\rho^2} \right) + b \tag{3.17}
\]

Multiplying Eqn. (3.17) by kernel function, integrating by parts over the kernel volume \( \Omega \) using Gauss's Divergence theorem and replacing the integrals by particle summation we get SPH form of Equation of Motion as:
\[
\frac{d}{dt} \langle V \rangle_i = - \sum_{j=1}^{N} m_j \nabla_i W_0 \left[ \left( \frac{p}{\rho^2} \right)_j + \left( \frac{p}{\rho^2} \right)_i \right] - \sum_{j=1}^{N} m_j \nabla_i W_0 \cdot \left[ \left( \frac{\tau}{\rho^2} \right)_j + \left( \frac{\tau}{\rho^2} \right)_i \right] - \int_S \rho_i W_{is} n \left[ \left( \frac{p}{\rho^2} \right)_j + \left( \frac{p}{\rho^2} \right)_s \right] dS - \int_S \rho_i W_{is} n \cdot \left[ \left( \frac{\tau}{\rho^2} \right)_j + \left( \frac{\tau}{\rho^2} \right)_s \right] dS + \langle b \rangle_i \quad (3.18)
\]

where \( \frac{d}{dt} \langle V \rangle_i \) is the smoothed acceleration of particle \( i \)

\( \langle b \rangle_i \) is the smoothed body force acting on particle \( i \)

\( \rho_i, \rho_j \) are densities of particle \( i, j \)

\( \rho_s \) is density of the fluid at the boundary

\( \tau_i, \tau_j \) are viscous stress tensors for particle \( i, j \)

\( p_i, p_j \) are hydrostatic pressures of particle \( i, j \)

\( \nabla_i \) is the divergence of any particle within the kernel of particle \( i \) with respect its position

\( n \) is the unit vector directing from particle \( i \) to the surface \( S \), normal to the surface

\( W_{is} = W(r_i - r_s, \rho) \)

\( W_0 = W(r_i - r_j, \rho) \)

\( r_i \) is position vector of particle \( i \)

\( r_s \) is the position vector of any point on the surface \( S \)

Eqn. (3.18) is the most general form of SPH evolution equation of motion. It does not assume any particular form of viscous stress model or pressure-density relationship.

Now, without loss of generality, it is possible to restrict attention to Newtonian fluids and in that case, the viscous stress tensor may be expressed as:

\[
\frac{\tau}{\rho^2} = -\frac{\eta}{\rho} \left[ \nabla V + (\nabla V)^T \right] + \frac{2\eta}{3\rho} (\nabla \cdot V) I \quad (3.19)
\]
where $\eta$ is the kinematic viscosity of the fluid, and $I$ the rank 2 unit tensor. The following symmetric forms of velocity gradient

\[
\nabla \frac{V}{\rho} = \nabla \left( \frac{V}{\rho} \right) + \nabla \rho \left( \frac{V}{\rho^2} \right)
\]

(3.20a)

and divergence

\[
\frac{\nabla \cdot V}{\rho} = \nabla \cdot \left( \frac{V}{\rho} \right) + \nabla \rho \cdot \left( \frac{V}{\rho^2} \right)
\]

(3.20b)

can be used in Eqn. (3.19). Treating Eqn. (3.19) and (3.20) in the same way as we have done to Equations of Continuity and Motion, we obtain the smoothed viscous stress of the fluid particle $i$ as:

\[
\left\langle \frac{\tau}{\rho^2} \right\rangle_i = -\eta_i \left[ \left\langle \frac{\nabla V}{\rho} \right\rangle_i + \left\langle \frac{\nabla V}{\rho} \right\rangle_i^T \right] + \frac{2\eta_i}{3} \left\langle \frac{\nabla \cdot V}{\rho} \right\rangle_i I
\]

(3.21)

where

\[
\left\langle \frac{\nabla V}{\rho} \right\rangle_i = \sum_{j=1,N} m_j \nabla_i W_{ij} \left[ \left( \frac{V}{\rho^2} \right)_i + \left( \frac{V}{\rho^2} \right)_j \right] + \int_{S} \rho_x W_{ij} \cdot \left[ \left( \frac{V}{\rho^2} \right)_i + \left( \frac{V}{\rho^2} \right)_k \right] dS
\]

(3.22a)

\[
\left\langle \frac{\nabla \cdot V}{\rho} \right\rangle_i = \sum_{j=1,N} m_j \nabla_i W_{ij} \cdot \left[ \left( \frac{V}{\rho^2} \right)_i + \left( \frac{V}{\rho^2} \right)_j \right] + \int_{S} \rho_x W_{ij} \cdot \left[ \left( \frac{V}{\rho^2} \right)_i + \left( \frac{V}{\rho^2} \right)_k \right] dS
\]

(3.22b)

where $k$ is the index of the surface segment if the surface is irregular and represented by more than straight line segment (see § 3.3). Here the first term on the right hand side represents the kernel contribution describing internal shear whilst the second term is the surface integral taking into account the flow boundary condition.
3.2.3 Equation of State

In SPH, the hydrostatic force is an explicit function of the local fluid pressure. While in traditional grid-based methods (Finite Element or Finite Difference) the knowledge of pressure difference between any two points is sufficient to solve the EOM, in SPH, the evaluation fluid pressure for each particle is essential. This makes the treatment of the pressure term in the SPH governing equation more difficult and unique.

In the case of a compressible fluid, the pressure is replaced by a function of density using an equation of state of the form \( p = f(\rho) \). However such an equation of state is not available for incompressible fluids. This is probably one of the reasons why the initial developments in SPH mainly focussed on compressible fluids. One of the common pressure-density relationship being used in SPH to represent incompressible flow is:

\[
p = c^2 \rho
\]

(3.23)

where \( c \) is the speed of sound wave in the fluid. The value of \( c \) being very high for an incompressible fluid, it makes the absolute fluid pressure \( p \), an overriding component in the overall momentum balance equation, whilst at the same time the hydrostatic pressure becomes overly sensitive to the density. Monaghan (1994) argued that for typical smoothing lengths used in SPH, the kernel interpolation is generally accurate within 1% and thus, the best achievable density estimation would have an error of 1% contributed from the smoothing operation. Density estimation error of 1%, in turn, would cause 1% fluctuation in pressure which is large enough to cause force imbalance in the equation of motion.

The way forward lies in choosing a value of sound speed that preserves the physics of the flow and reduces the sensitivity of pressure on the liquid density. It is not uncommon also to find a similar approach being adopted in other numerical techniques. In grid-based techniques such as Artificial Compressibility Method (ACM) used by many researchers (Chorin, 1967; Turkel, 1987; Tamamidis et al., 1996) to solve incompressible
viscous flow uses an arbitrary artificial compressibility factor, $\beta$. The value of this factor has been found to be extremely problem dependent (Kwak, 1986; Rogers and Kwak, 1991; Pentaris et al., 1994). A detailed discussion on the choice of sound speed in the context of SPH and its effect on the physics of the fluid may be found in § 4.5.

### 3.2.4 Final Form of SPH Equations

The dimensionless form of SPH governing equations in two-dimensional Cartesian coordinate system are given below. As mentioned in § 3.2.1 while introducing the surface integrals, the surface integral reduces to line integral when the flow domain is two-dimensional. Accordingly, the limit of integration is changed to $\zeta$ in place of $S$ in all surface integration expressions where $\zeta$ signifies the portion of the solid boundary that intersects with the SPH fluid kernel. These equations will be frequently referred to during the case studies in next three chapters.

#### Equation of Continuity

$$\frac{d}{dt^*} \langle \rho \rangle_j = - \sum_{j=1,N} m_j \left( u_j - u_i \right) \frac{\partial W_{ij}^*}{\partial x_i} - \sum_{j=1,N} m_j \left( v_j - v_i \right) \frac{\partial W_{ij}^*}{\partial y_i}$$

$$- \rho_i \left( u_i - u_i \right) \int_{\zeta} W_{ii}^* \, dx^* - \rho_i \left( v_i - v_i \right) \int_{\zeta} W_{ii}^* \, dy^*$$

(3.24)

#### Equation of Motion: x-component

$$\frac{d}{dt^*} \langle u \rangle_j = - \frac{1}{M^2} \left[ \sum_{j=1,N} \left( \frac{1}{\rho_j} + \frac{1}{\rho_i} \right) m_j \frac{\partial W_{ij}^*}{\partial x_i} + \left[ W_{ii}^* dx^* + \frac{\rho_i}{\zeta} \left[ W_{ii}^* dx^* \right] \right] + \frac{1}{Fr} \left[ \sum_{j=1,N} m_j \right] \right]$$

$$- \frac{1}{Re} \left[ \sum_{j=1,N} m_j \left( \frac{\partial W_{ij}^*}{\partial x_i} \frac{\tau_{xx}}{\rho^2} \right) + \frac{\partial W_{ij}^*}{\partial y_i} \frac{\tau_{xy}}{\rho^2} \right] + \sum_{j=1,N} \left[ \frac{\partial W_{ij}^*}{\partial x_i} \frac{\tau_{xx}}{\rho^2} \right] + \frac{\partial W_{ij}^*}{\partial y_i} \frac{\tau_{xy}}{\rho^2} \right]$$

$$+ \rho_i \left( \frac{\tau_{xx}}{\rho} \zeta_x^* + \frac{\tau_{xy}}{\rho} \zeta_y^* \right) + \rho_i \left( \frac{\tau_{xy}}{\rho} \zeta_x^* + \frac{\tau_{xx}}{\rho} \zeta_y^* \right)$$

(3.25)
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Equation of Motion: y-component

\[
\frac{d}{dt^*}(v_i^*) = -\frac{1}{M^*} \left[ \sum_{j=1,N} \left( \frac{1}{\rho_j} \mathbf{v}_j - \mathbf{v}_i \right) m_j \frac{\partial W_{ij}^*}{\partial v_j} + \frac{1}{Fr} \sum_{j=1,N} W_{ij}^* \right] - \frac{1}{Re} \sum_{j=1,N} \left[ m_j \left( \frac{\partial W_{ij}^*}{\partial x} \frac{\tau_{ijx}^*}{\rho_j^2} + \frac{\partial W_{ij}^*}{\partial y} \frac{\tau_{ijy}^*}{\rho_j^2} \right) \right] + \rho_i \left( \frac{\tau_{ix}^*}{\rho_i^2} \zeta_x^* + \frac{\tau_{iy}^*}{\rho_i^2} \zeta_y^* \right)
\]

(3.26)

where

\[
\frac{\tau_{xx}^*}{\rho^2} = -2 \frac{\partial u^*}{\partial x} + \frac{2}{3} \left( \frac{\partial u^*}{\partial x} + \frac{\partial v^*}{\partial y} \right)
\]

\[
\frac{\tau_{yy}^*}{\rho^2} = -2 \frac{\partial v^*}{\partial y} + \frac{2}{3} \left( \frac{\partial u^*}{\partial x} + \frac{\partial v^*}{\partial y} \right)
\]

(3.27)

\[
\frac{\tau_{xy}^*}{\rho^2} = \frac{\tau_{yx}^*}{\rho^2} = \left( \frac{\partial u^*}{\partial y} + \frac{\partial v^*}{\partial x} \right)
\]

All starred (*) quantities appearing in the above equations are dimensionless. \( \tau_{xx}, \tau_{yy}, \tau_{yx}, \tau_{xy} \) are the four components of viscous stress in two-dimensional domain. The suffix I stands for the boundary line or the phase boundary in a two-dimensional simulation. \( \zeta_x \) and \( \zeta_y \) are the line integrals along \( x \) and \( y \)-directions. The length, velocity and density scales used for non-dimensionalisation are \( L_0, V_0 \) and \( \rho_0 \) respectively. The relationships between dimensional and non-dimensional quantities are as follows:

\[
\begin{align*}
 x^* &= x/L_0 & y^* &= y/L_0 & r^* &= \sqrt{x^2 + y^2} & t^* &= t/(L_0/V_0) \\
 u^* &= u/V_0 & v^* &= v/V_0 & h^* &= h/L_0 & W^* &= L_0^2 W \\
 \tau^* &= \tau/(\rho_0 V_0/L_0) & \rho^* &= \rho/\rho_0 & Re &= L_0 V_0/\nu & M &= \nu/\rho c \\
 Fr &= V_0^2/bL_0
\end{align*}
\]
where \( u \) and \( v \) are \( x \) and \( y \) components of velocity vector \( V \), \( x \) and \( y \) are the two components of the position of the fluid particles; \( c \) is the speed of sound in the fluid medium and \( b \) is the magnitude of body force per unit mass of the fluid medium.

### 3.3 Surface Integral

Campbell (1989) attempted to introduce the surface integral term \( \int W_{is} dS \), where \( W_{is} = W(r_i - r_s, h) \), in the most simplistic way. In a two dimensional Cartesian co-ordinate system, he deduced the integral as \( W_{il} \Delta \zeta \), where \( \Delta \zeta \) is the arc length intercepted by the surface and kernel, and \( W_{il} \) is evaluated based on the normal distance, \( R \) of the particle from the surface as shown in Fig. 3.6. In this two-dimensional example, the solid surface reduces to a line belonging to either the domain boundary or another phase within the fluid; consequently, the surface integral becomes a line integral along the domain boundary or phase boundary. But this simplistic approach of Campbell has been found to overestimate the integral compared to the integral obtained by actually carrying out (analytically or numerically) the required integration, \( \int W_{il} d \zeta \). The reason is obvious: Campbell's estimate of \( W_{il} \) is based on \( R \), the normal distance of the solid boundary line from the SPH particle (see Fig. 3.6). The normal distance being the minimum distance of the surface from the particle, the value of the kernel function, \( W_{il} \) is the maximum for this value of \( R \) (indicated by the blue dotted line, which is longer than the black line in the \( W_{il} \) vs. \( (r_i - r_i) \) plot). Thus, the product \( W_{il} \Delta \zeta \) becomes maximum when \( R \) is taken as the representative distance between the SPH particle and the solid surface. It is clear from Fig. 3.6 that \( (r_i - r_i) \) varies along the solid boundary line, and a proper integration taking into account the variation of \( W_{il} \) along the boundary line would be anything but less than \( W_{il} \Delta \zeta \). Moreover, the inaccuracy in the estimation of \( W_{il} \Delta \zeta \) increases as the SPH particle approaches the solid line.
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Fig. 3.6: Schematic diagram showing how \( (r_f-r_l) \) varies along the solid line/domain boundary when the kernel of the SPH fluid particle intersects with it. The value of \( (r_f-r_l) \) is minimum when it is normal to the solid line. The figure also shows how \( W_\alpha \) varies with \( (r_f-r_l) \) indicating a maximum value of \( W_\alpha \) when \( (r_f-r_l) \) is normal to the solid line.

In Fig. 3.7a, a quantitative comparison of the surface integral between the present approach and Campbell’s approach using a two-dimensional cubic spline kernel (this kernel will actually be introduced in § 3.6) shows that Campbell’s approach overestimates the surface integral by as much as three times compared to the value obtained by carrying proper integration along the surface. The difference between the two approaches is particularly prominent when the fluid and the surface are separated by a distance less than 0.5h. At larger separating distance though, there is not much difference between the two methods probably because of the nature of the kernel function. Fig. (3.7b) shows similar comparison of line integrals using the centrally peaked kernel (to be introduced in § 3.7) proposed by Chaubal et. al. (1997). The figure indicates that irrespective of the normal distance of the SPH fluid particle from the solid line, the line integral is always more in case one uses Campbell’s approach. The primary difference between Campbell’s approach and present approach lies in recognizing the
variation of the value of $W_{ij}$ along the solid line. In all our subsequent simulations the surface integrals are evaluated in their entirety.

![Graph](image)

**Fig. 3.7:** Comparison of surface integrals between Campbell's approach and the current approach near a straight surface in two-dimensional domain using (a) cubic spline kernel, (b) using the kernel proposed by Chabal et al. (1997). The sketches below the plot in (a) schematically indicate the relative positions of the solid line and the fluid particle under two extreme cases i.e., when the fluid particle is on the surface and when it's kernel just touches the surface. All dimensions are non-dimensionised with respect to $h$. 
According to the present approach, the situation slightly differs when the solid surface is curved, for example, if the solid line is of circular shape in case of a two dimensional domain. In the expression for surface integral in 2D, \( \int W_{il} d\zeta \), the line element \( d\zeta \) is replaced by the differential form of equation of the arc. According to Campbell’s approach, the surface integral would still be computed based on the straight line segment joining the two points of intersection of the solid circle and the kernel as shown by the dotted red line in Fig. 3.8a. Fig. 3.8b shows the variation of the surface integral as a function of the normal distance of the SPH particle from the solid circle. The figure also shows the difference in the line integral when it is calculated using the present approach along the lines AB and ACB for \( R_c = 3h \), where \( R_c \) is the radius of the solid circle. Since the distance is measured from the SPH particle, the distance of the solid circle will always be less than that of the straight line. Thus, for the same position of the SPH particle, the value of the integral will be always less when the integration is done along the straight line AB, compared to the curved line ACB. In the limiting case, when the radius of the circle is very large compared to the kernel compact support length, the two curves will eventually merge and follow the blue curve in Fig. 3.7b. However, it should be noted that the estimation of surface integral (or line integral in case of two-dimensional domain) will be same irrespective of the curvature of the solid surface according to Campbell approach since he used a straight line.

However, for the purpose of recovering the no-slip boundary condition at the solid circular surface accurately the size of the SPH kernel for the fluid particles near the solid surface should always be much smaller than the radius of curvature of the solid boundary.
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Fig. 3.8: (a): In case of curved boundaries, evaluation of surface integrals should be done along the surface; (b) Comparison of line integrals (surface integral, in case of 3D domain) when the integral is carried out along the straight line AB and along the curved line ACB using present approach; (c) Irregular boundaries can be approximated by several straight line segments as shown in (d).

Evaluation of the surface integral, particularly for complex curved boundaries, is greatly eased by assuming that the boundaries can be represented by $N_b$ number of straight line...
segments, as shown in Fig. 3.8(c), where the density and velocity are constant over each segment. In case the boundary curves are simple in form the surface integral can be evaluated analytically making its numerical implementation simple and cheap. In such case, the surface integral term can be replaced by a summation over all the constituent line segments. Thus, for example, the EOC of Eqn. (3.15) becomes (in two-dimensions):

\[
\frac{d}{dt} \langle \rho \rangle_i = - \sum_{j=1,N} m_j \left( V_j - V_i \right) \cdot \nabla_i W_{i'k} - \rho_i \sum_{k=1,N} \left( V_{s_k} - V_i \right) \int n W_{i\zeta_k} d\zeta_k
\]

where \( k \) is the index of the line segment.

### 3.3.1 Lack of Particles Near Domain Boundary

While discussing the properties of the kernel function in § 3.1.2 it was mentioned that when symmetrical kernels are used, SPH suffers from lack of fluid particles near the domain boundary or near any solid surface within the fluid. This is schematically shown in Fig. 3.9. The value of the integral \( \int_{\Omega} W(r-r',h)dr' \) is generally close to 1. In the limiting case, for a particle sitting on the domain boundary the value of the integral becomes \( \frac{1}{2} \). This makes the density estimation erroneous near the domain boundary, and error also creeps in the estimation of hydrostatic pressure (since hydrostatic pressure is obtained from Equation of State), thereby degrading the calculation. Lack of particles becomes important only when the domain is finite or there is more than one phase.

There are a number of ways to get around this problem. One apparently easy way to reduce the error is to increase the number density of particles near the boundary and use smaller compact support length \( (h) \) near the boundary. In other words, the use of variable compact support length, similar to mesh refinements in FEM, can improve the accuracy near the boundaries. While this approach is expected to produce more accurate results, the complication involved in estimating variable smoothing length and maintaining symmetry in the system simultaneously sometimes overtakes the advantage derived from
such method. The Reproducing Kernel Method (RPKM) (Liu et al., 1995; Chen et al., 1996; Jun et al., 1998; Aluru, 1999) overcomes particle deficiency at the boundary with some success by introducing a correction function for particles near the boundary. However, such technique fails to describe the essential boundary conditions correctly. Chen et al. (1999) developed a Corrective Smooth Particle Method (CPSM) by combining a kernel estimate with the Taylor series expansion and solved the boundary value heat conduction problem with high accuracy but hydrodynamic problems with actual movement of fluid particles were not attempted.

![Fig. 3.9: Particles away from domain boundary has access to the full kernel volume where as, particles closer to a boundary can have access to as low as half the kernel volume.](image)

### 3.3.2 Advantage of Surface Integrals

In the derivation of Equation of Continuity and Equation of Motion it was noticed that the surface integral term appeared naturally in the SPH formulation. It would be demonstrated in Chapter 5 that the introduction of surface integral term in the SPH evolution equations helps in overcoming the deficiency of particles near domain boundaries. This is particularly the case where the particles interact with the boundary conditions such as externally applied pressure, temperature or velocity. It may also be noted that the surface integrals assume non-zero values only when a particle is near a boundary i.e., within \( h \), else they can be excluded from the SPH equations because they are redundant. In typical fluid dynamic problems, it is the boundary that imposes certain conditions onto the system and the response of the system changes as per the changes in
the boundary condition. In SPH, the particles near any boundary have the pivotal role of carrying the information to neighboring particles through smoothing operation.

Thus, the surface integral serves two purposes in the current formalism:

- It helps in imposing certain types of boundary conditions.
- Eliminates the need for "boundary particles" which is traditionally used to identify the boundary of a domain. This also reduces the complication in programming, as one does not need to store these 'boundary particles' and treat them separately.

3.4 Boundary Conditions

3.4.1 Periodic Boundaries

Periodic boundary condition (PBC) is the most common type of boundary condition implemented in SPH. It is quite easy to implement, as it does not require interaction with any solid boundary. This type of boundary conditions are characteristics of any particle based technique such as Molecular Dynamics simulations where one is interested in studying the development of inter-particle forces rather than the particle-surface interactions. In MD, studies are carried out with a fewer number of particles in a unit cell to simulate the dynamic behavior of the ensemble. Like MD, SPH is also Lagrangian in nature where, movement of the particles in and out of the system becomes an integral part of the technique. Moreover, our interest lies in studying the evolution of effective viscosity and other similar solid-liquid suspension properties, which can be estimated best by studying the ensemble behavior in a periodic cell.

Typically, under the periodic boundary condition, particles leaving through any of the cell faces are replaced by an exact number of particles entering the system through its image boundary surface with the exact velocity components with which they left the system. This is schematically shown in Fig. 3.10. The three particles in Fig. 3.10a,
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possessing net velocities in the direction shown by the arrows, have been replaced by three particles at the corresponding image locations in Fig. 3.10b. The velocities of the particles remain unchanged; only the positions change. In SPH implementations under PBC, all particles near a periodic boundary must consider particles close to its image boundary for estimating the smoothed value. For example, particles near the right boundary of the periodic lattice ABCD, shown in Fig. 3.11, will interact with some of the particles close to the left boundary of the cell.

Despite the usefulness of PBC, care must be taken to apply such boundary condition, as this is applicable only when the upstream boundary condition is same as the downstream one. In a situation where fluid leaving the system is expected to have velocity or pressure different from the fluid entering, periodic boundary condition cannot be applied. Periodic boundary condition is also not applicable where the boundary is solid or impermeable or a non-trivial boundary condition exists at the boundary. They are being discussed in the following section.
3.4.2 Solid Boundaries

Solid boundaries or solid surfaces are implemented in SPH in a variety of ways. They include imaginary particles, repulsive forces, immobile particles and boundary modification in the equation of motion.

Libersky and Petschek (1990) used imaginary particles to model the impact of an iron rod with a rigid wall. The scheme works by placing extra particles along the outside edge of the boundary. For every 'real' particle within the distance of $2h$ of the boundary, an extra particle is placed symmetrically on the opposite side of the boundary. These particles have the same density and pressure, and a velocity opposite that of their corresponding real particle counterpart. This procedure works well for straight boundaries but introduces density errors in curved surfaces. Because the imaginary particles must be included in the computation, this technique requires extra CPU time and memory. Extension to multidimensional situations may cause particle tracking problems.

Slight modifications of this approach were found in Takeda et al. (1994) and Morris et al. (1997). Takeda achieved no-slip boundary condition using special boundary terms which mimic a half-space filled with SPH image particles. The method overcomes the problem of...
near a curved surface. While this approach proved useful for compressible and moderate Reynolds number flows, stability was reported to be unsatisfactory (Morris et al., 1997). Morris et al. further modified this approach to include a preset numerical constant $\beta$ to calculate relative velocity between fluid and boundary particles, thus preventing the fluid particle from approaching a curved boundary.

In the repulsive force technique, boundary particles are placed along the boundary and an inter-particle force is introduced between boundary particles and the approaching fluid particles. If a particle moves within a preset distance of the boundary, a repulsive force is added to the momentum summation. The force can be modeled by Lennard-Jones type of intermolecular force (Nagasawa and Kuwahara, 1993; Monaghan, 1994):

$$F(r) = \kappa L J \left[ \frac{(r_b^2 - r^2)}{R_b^2} \right] \quad \text{if } r < R_b \quad \text{else } F(r) = 0 \quad (3.29)$$

where $r$ is usually set equal to initial particle separation distance, $R_b$ is the distance to the boundary, and $\kappa L J$ is determined by the initial conditions. Alternatively, the repulsive force can be modeled by a simple spring force:

$$F(r) = \kappa_S [r - R_b]^2 \quad \text{if } r < R_b \quad \text{else } F(r) = 0 \quad (3.30)$$

where $r$ is usually set equal to initial particle separation distance, and $\kappa_S$, the spring constant, is determined by initial condition. Compared to the imaginary particle method, this method does not require extra particles except the ones to designate the outline of the boundary.

The immobile particle (or infinite inertia) boundary treatment involves placing stationary particles along the boundary. They are included in the smoothing operation and after every time step their velocities are brought back to zero.
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The last approach is to modify the equation of motion to introduce the effect of the solid boundary in an analytical way. In the present work, this approach has been followed and the presence of the surface integrals may be gainfully exploited to model the solid boundaries. The usefulness of such a technique will be demonstrated in Chapter 5.

3.4.3 Other Boundary Conditions

**No-slip Boundary:**
The implementation of no-slip boundary condition according to our present SPH formalism is fairly straightforward. Boundary velocity appears in EOC explicitly as $V_b$. By assigning a value of zero to this vector, one can implement no-slip boundary condition. Unlike imaginary particle method, it does not require any extra memory to implement no-slip boundary condition. Moreover such an approach can deal with any shape of boundary as long as it can be described by a mathematical equation.

**Constant Velocity Shear Boundary:**
Constant velocity shear boundaries are also implemented in the same way as no-slip boundaries. In this case, the boundary velocity $V_b$ is assigned the desired value instead of a null.

**Boundary Density and pressure:**
Boundary density $\rho_i$ appears in the terms associated with surface integrals of hydrostatic and viscous force. In all the present simulations a boundary density value equal to the the fluid density is used. This is true in all our simulations since there is only one fluid phase present in the systems we will be considering. But, for cases where two fluid phases are present, SPH becomes unable to resolve the fluid-fluid interface correctly if the density difference is very high because of its inherent inability to estimate the smoothed density very accurately. Since boundary pressure appears in the equation of motion implicitly in the form of boundary density, the hydrostatic pressure at the solid boundaries becomes a function of fluid density at the solid surface.
3.5 Choice of Time Stepping Algorithm and Stability Criteria

Numerical integration of Equation of Motion is typically done step by step using methods that are called Finite Difference methods. These methods are explicit and use the information available at time $t$ to predict the system's coordinates, velocities, and also the density in the present approach since the Equation of Continuity is invoked to measure the density variation, at a time $t + dt$, where $dt$ is a short time interval. These methods are based on a Taylor expansion of the position of the fluid particle at time $t + dt$. There are various methods available that differ amongst each other the way they implement the Taylor expansion; they include: predictor-corrector scheme (Welton and Pope, 1997), Runge-Kutta-Gill method (Takeda et al., 1994), leap-frog method (Lattanzio et al. 1985, Libersky and Petschek, 1990; Libersky et al., 1993; Schussler & Schmitt, 1981; Simpson & Wood, 1996), Velocity Verlet (Swope et al., 1982) algorithm. Among these, the last one is the most accurate for velocity evaluation though it is computationally more expensive than the other two. For all simulations in the present work, the Velocity Verlet algorithm is used where each time integration cycle includes four steps:

a) \[ r_i^n = r_i^{n-1} + \Delta t \cdot V_i^{n-1/2} \]

b) \[ V_i^{n+1/2} = V_i^{n-1/2} + \frac{\Delta t}{2} \cdot f_i^n \]

c) Calculate $f_i^{n+1}$ and $(d\rho/dt)_i^{n+1}$ based on $r_i^n$ and $V_i^{n+1/2}$

d) \[ V_i^{n+1} = V_i^{n+1/2} + \frac{\Delta t}{2} \cdot f_i^{n+1}, \quad \rho_i^{n+1} = \rho_i^n + \Delta t \left( \frac{d\rho}{dt} \right)_i^{n+1} \]

where $r_i$ is the position vector for particle $i$, $V_i$ is the velocity and $f_i$ is the acceleration vectors for the same particle; the integer superscripts $n$, $n+1/2$ and $n+1$ represent indices of three consecutive half time steps and $\Delta t$ is the value of each time step, assumed constant for the whole duration of the experiments. The method has error of $O(\Delta t)^2$. 


Often, computational instability due to the choice of too large a time step will arise. For an unsteady state simulation in SPH, it is sufficient to satisfy the following three criteria to calculate the maximum value of the time step size, $\Delta t$, which will maintain stability:

- Courant-Friedrichs-Levy (CFL) condition (Courant et al., 1928), due to hydrostatic pressure, $\Delta t \leq \frac{h}{c}$
- Due to viscous diffusion, $\Delta t \leq 0.125 \frac{h^2}{\nu}$
- Due to body force, $\Delta t \leq 0.25 \left(\frac{b}{h}\right)^{1/2}$

where, $h$ is the measure of kernel compact support length, $c$ is the velocity of sound in the fluid, $\nu$ is the kinematic viscosity of the fluid and $b$ is the body force per unit mass of the fluid. Stability of the system also depends on the choice of kernel function. This has been discussed in greater details in § 3.6. Generally, higher order spline interpolant kernels are used to improve stability property. The early applications of SPH, (Lucy, 1977) and (Gingold and Monaghan, 1977), were to problems involving compressible gas which always had a positive gas pressure. When applied to different problems where stress can become negative, particles are seen to attract each other, instead of repulsion. It is sometimes possible for the particles to pair up under such situation, causing "clumping" and subsequently disruption of solution. The nature of this type of instability is quite different from the instabilities observed when large time step is used. Instability is also induced by domain boundaries. However, implementation of the surface integral advanced in the present work, is expected to reduce such instabilities arising out of solid boundaries.

### 3.6 Various Forms of Kernel Function

Mathematically, one can write several forms of kernel function that may satisfy the criteria mentioned in § 3.1.2 within an acceptable error limit. For the reason of symmetry, kernels are generally spherical (in 3D) or circular (in 2D) in shape though spheroidal kernel has also been found in literature (Fulbright et al., 1995). Fulk and
Quinn (1996) reviewed some of the commonly used kernels in SPH applications along with mathematically possible kernels (after satisfying criteria in § 3.1.2) and classified them in four groups depending on their shapes. They are (in one dimension):

**Bell shaped kernels (example 1: Cubic spline kernel)**

\[ f(r, h) = \frac{2}{3} \left( 1 - 1.5 \frac{r}{h} + 0.75 \frac{r^3}{h^3} \right) \]

if \( 0 \leq \frac{r}{h} < 1 \)

\[ \frac{1}{6} \left( 2 - \frac{r}{h} \right)^3 \]

if \( 1 \leq \frac{r}{h} < 2 \)  \hspace{1cm} (3.32)

0

if \( 2 \leq \frac{r}{h} \)

**Bell shaped kernels (example 2: Exponential kernel)**

\[ f(r, h) = \frac{1}{\sqrt{\pi}} \left( e^{\frac{-r^2}{h^2}} \right) \]

for \( \frac{r}{h} > 0 \)  \hspace{1cm} (3.33)

**Hyperbolic shaped kernels**

\[ f(r, h) = 7.337 \left( \frac{1}{2 + |r/h|} + \frac{|r/h| - 6}{16} \right) \]

if \( 2 \leq \frac{r}{h} \)  \hspace{1cm} (3.34)

**Double hump kernels**

\[ f(r, h) = 0.1025 \left( \frac{r}{h} \right)^2 \left( 2 + 3 \frac{r}{h} \right) \left( 2 - \frac{r}{h} \right)^3 \]

if \( 2 \leq \frac{r}{h} \)  \hspace{1cm} (3.35)

**Parabolic shaped kernels**

\[ f(r, h) = 0.09375 \left( 8 - \frac{r^3}{h^3} \right) \]

if \( 2 \leq \frac{r}{h} \)  \hspace{1cm} (3.36)

Plots of the kernel function \( f(r,h) \) vs. \( r \), along with their gradients may be found in Fig. 3.12.
Chapter 3: Smooth Particle Hydrodynamics

3.7 Choice of Kernel

Theoretically, the choice of kernel is arbitrary, provided it satisfies the conditions set out in § 3.1.2. In practice, there are many, sometimes competing factors to be considered when choosing kernel for a particular SPH application and there is no kernel that is suitable for all types of problems. The main considerations are:

- Order of interpolation
- Number of nearest neighbors
- Symmetry of the kernel
- Behavior of kernel gradient
- Stability properties of the kernel

Fig. 3.12(a,b,c,d): Kernel function $f(r)$, its first and second derivatives $\text{der1}(r)$ and $\text{der2}(r)$ respectively, for (a) Bell shaped (cubic spline), (b) Hyperbolic shaped, (c) Double hump and (d) Parabolic shaped kernels. $r$ is non-dimensionalised with respect to 'h'.

r is non-dimensionlised with respect to 'h'.
Chapter 3: Smooth Particle Hydrodynamics

The order of interpolation is an important consideration while choosing a particular kernel. Higher the order, better is the approximation. However, this accuracy doesn’t come cheap, computationally, as the kernel now has to include more particles within its fold. The order of the kernel also depends on the type of application. In hydrodynamics, generally forces depend on spatial gradients up to second order (e.g., the viscous force is a function of second spatial derivative of fluid velocity) a kernel of second or third order in space is considered sufficient.

Theoretically speaking, the kernel interpolation function does not restrict us from considering all the particles in a domain to evaluate the smoothed value of a function. This would, however, mean that for a kernel such as the exponential kernel (see Eqn. (3.33)), which does not have compact support, must include the contributions from all $N$ particles in the flow domain to calculate the smoothed value at each particle position. This would result in $N^2$ smoothing operations for updating any physical quantity in each time step, thereby, rendering the numerical implementation with this type of kernel extremely slow, particularly when one has to deal with a very large number of particles. On the other hand, kernel such as cubic spline kernel (see Eqn. (3.32)) has a compact support length of $2h$, which means particles within $2h$ distance from the point of interest are the ones to be considered for smoothing operations. For example, if there are about 400 particles in a domain with about 20 particles within the close neighborhood of each particle, one needs to carry out only 8000 smoothing operation as opposed to 160000 operations with the exponential kernel. This gives a clear advantage of using spline kernels. It is because of this advantage of fewer neighbors that Monaghan and Lattanzio (1985) introduced the cubic spline kernel. However, it suffers from some instability problem under compressive force that is discussed later in this section. The quartic spline (Schoenberg, 1946) and quintic kernel kernels have progressively better stability since they include higher order terms of the Taylor series, but the computational cost increases. The parabolic kernel function is not generally used in SPH applications probably because it is not as much centrally peaked as the bell-shaped or hyperbolic kernels. Through a series of measurements of errors arising from the consistency analysis, Fulk and Quinn
(1996) indicated that the bell shaped kernels perform better than the other three shapes in the context of SPH. Within the bell shaped kernels, the cubic spline kernel family is believed to be an optimum choice for most SPH applications.

Out of the three basic forces responsible for particle motion in SPH, hydrostatic and viscous force depend on gradients of density and velocity, respectively. While deriving the fluid flow equations in SPH form in § 3.3, it was noticed that smoothed gradient of any quantity largely depends on the gradient of the kernel function. Therefore, the behavior of the particles under various types of forces would depend on the properties of their kernel gradients and the primary consideration for a stable SPH system lies choosing the right kernel for right type of application.

Fig. 3.12 shows first and second spatial derivatives of the four types of kernels described in § 3.7. Cubic spline kernel being the most commonly used kernel in SPH, let us analyze the behavior of cubic spline kernel’s stability. A close look at the first derivative of the cubic spline kernel (Fig. 3.12a) reveals that the spatial gradient between two mutually approaching particles monotonically increases until the distance between them reduces to \( \frac{2}{3} \), below which the gradient starts reducing and eventually comes to zero when their positions coincide. This means, forces that depend on the spatial gradients such as Brownian or hydrodynamic force would become weaker if two particles get any closer than \( \frac{2}{3} \) distance. Though, the idea of having such numerical constraint is good because it prevents SPH particles from colliding with each other under a compressive force, such phenomena should ideally happen when particles nearly touch each other. Thus, the location of a maximum/minimum at a distance of \( \frac{2}{3} \) implicitly introduces some numerical error and stability problem as we have to ensure that the minimum distance between neighboring particles does not become less than the critical distance, \( \frac{2}{3} \). One way of getting around this stability problem in cubic spine kernel is to shift the critical distance close to zero, i.e., to the center of the kernel. Chaubal et al. (1997) made such an attempt to modify the cubic spline kernel as shown below (in one dimension):
While both the kernels (Chaubal *et al.* and cubic spline kernel) are of third order, the absence of the first order term (*i.e.*, \( r/h \)) and the presence of different coefficients in the above kernel (Eqn. 3.37) changes the shape along with the behavior of the kernel. The above kernel function and its gradients as a function of distance are plotted in Fig. 3.13. Compared to the cubic spline kernel, this function is centrally peaked and more akin to an impulse function. It may be observed from Fig. 3.13 that the first derivative of Chaubal's kernel is a monotonic function of distance, having discontinuity at the center (*i.e.*, at \( r=0 \)). However, this doesn't invalidate the convergence result for the derivative of the kernel function at the center if we externally impose it to be zero only at \( r=0 \). By comparing the first derivative with cubic spline kernel (Fig. 3.12a) one observes the gradient of the kernel monotonically increases (or decreases) until the two mutually approaching particles actually coincide, when the force between them ceases to exist. This not only causes some error in force estimation but also the mass at that point continues to increase. Despite the fact that it might bring in some unphysical artifact in the system, one can justify by saying that as the sample size increases, the number of neighbors contributing significantly towards evaluating the force at the point in question keeps increasing, and so an error in the contribution made by a single particle (whose coordinate is same as the coordinate where the property is being estimated) becomes insignificant. The other way to overcome this problem is to remove the particle from the system altogether.

\[
f(r,h) = \begin{cases} 
 1 - \frac{3}{2} \left[ \frac{r}{h} - \frac{1}{2} \left( \frac{r}{h} \right)^2 + \frac{1}{12} \left( \frac{r}{h} \right)^3 \right] & \text{if } 0 \leq \frac{r}{h} < 2 \\
 0 & \text{if } 2 \leq \frac{r}{h} 
\end{cases}
\]
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3.8 Summary

In this chapter, a brief introduction on the particle nature of SPH was given. Many of the inaccuracies and instabilities in SPH simulations arise due to improper choice of kernel function, the building block of SPH. Though higher order kernels are better equipped to mimic any arbitrary function, cubic spline kernel is a popular choice as it has second accuracy and compact support. The smoothing operation also depends on the relative positions of the SPH particles. The impact of kernel function and many other discretisation parameters including distribution of particles on the smoothing operations are discussed in the next chapter.

The hydrostatic pressure appears explicitly in the Equation of Motion. For incompressible fluids the pressure-density relationship is extremely sensitive to any fluctuation in density. Care must be taken to make sure that the density fluctuations remain at its minimum. Moreover, modeling incompressible liquids with finite number of particles has certain disadvantages in recovering the hydrodynamics accurately. A further appreciation on the issues surrounding incompressibility of liquid in the context of SPH may be found in the next chapter.
In this chapter, we have developed the SPH form of governing equations that describe the flow of incompressible liquids under isothermal condition. The formalism includes surface integral terms which were usually dropped from all previous SPH formulations, excepting Campbell, 1989. The surface integral terms are believed to capture certain types of boundary conditions more easily than the past practice of using 'boundary particles'. This will be demonstrated in great details for single-phase flow in Chapter 5 and for two-phase flow in Chapter 6.
Chapter 4

UNDERSTANDING FUNDAMENTALS OF SPH

“Obvious” is the most dangerous word in mathematics
-Eric Temple Bell
In the previous chapter an introduction was provided to the concept of particle approximation in SPH that is developed on the basis of reproducibility of any fluid property using kernel function. The SPH form of the hydrodynamic equations was developed starting from conservation laws where the surface integral terms were included. These formulations now provide the tools necessary to investigate some of the fundamental aspects of SPH in this chapter.

Decisions made in implementing numerical methods like finite differences and elements including the nature of the interpolation scheme (i.e. the kernel in the SPH context) and level of discretisation can have a profound effect on the solutions obtained; this is true also of SPH. Despite this fact, remarkably little has been said in the literature regarding SPH implementation, particularly with respect to the kernel type, particle number density, particle configurations (i.e. regular vs. random) etc.

SPH being an approximation technique, special emphasis is placed on estimating and minimizing errors that arise from the smoothing operations. It was specifically noticeable in deriving the SPH formulation that the gradient of any fluid property depends on the gradient of the kernel function (Eqn. 3.3, 3.24-3.27). In other words, estimation of the smoothed gradients of fluid properties such as pressure and viscous force not only depends on the individual density and velocity of the particles within a kernel, but also they depend on the spatial gradients of the kernel function being used. Thus, apart from studying the smoothing property of the kernel function, study of the smoothed gradient of the kernel function also becomes necessary.
According to SPH formulation, the hydrostatic pressure of the liquid at any particle location is obtained from its density. Slightest fluctuations in density due to computational errors are likely to cause enormous pressure differences between neighboring particles in the liquid. This means that density estimation needs to be very accurate. Implementation of accurate pressure-density relation in SPH is only possible at extremely high level of time and space discretisation. This, in turn, makes it almost impossible to obtain sufficiently accurate density estimation from the simulations within reasonable time and resources. Thus, the option remains one of living with an amount of inaccuracy that is permissible in any engineering analysis. Moreover, representing a liquid with fewer particles, as we do in SPH may be viewed as simulating a 'relatively incompressible' fluid. In that case, the implication of the error in density estimation is nothing but representation of a fluid whose density is varying due to hydrodynamic forces. The extent of such 'compressibility' would largely depend on the discretisation and hydrodynamic parameters one uses to solve the SPH equations. A further discussion on the interdependency of physics of the fluid in the context of SPH has been presented in later part of this chapter.

4.1 Initial Particle Positions

The initial particle positions can influence the stability of the system and hence, the overall behavior of the fluid to a great extent. Thus, it is necessary to explore the different possibilities of initial placement of particles in the computational domain and understand how the smoothing operation is influenced by particle positions. The two possible schemes of inserting particles in the computational domain include regular and random distributions. Again, particles placed in regular manner can be arranged in linear or hexagonal structures. These three schemes of initial particle distributions are schematically shown in Fig. 4.1. If the domain geometry is regular, it is very easy to place the particles in linear or lattice structure. Apart from that, most of the applications in SPH reported in the literature, particularly with incompressible fluids, use linear or hexagonal lattice structure as it is understood that these regular structures do not have too
much of internal energy and the simulation can have a ‘quiet’ start. However, there are a few concerns when particles are placed in regular lattice-like structure. Some of them are:

- Such regular lattices will have directions along which particles form straight lines.
- Forces along these lines are artificially large and under the slightest misalignment, the lines would buckle.
- Use of cubic spline kernel indicates that the internal energy of the system will be zero only if all the particles are placed symmetrical to each other. This is only possible with hexagonal lattice structure.
- It is impossible to have a quiet start at contact discontinuities, such as near a boundary, where the smoothed density of the particles change.

Thus, it is almost certain that even if the particles are placed in regular fashion, there will be ample opportunities during simulations when the particles would not be able to maintain such geometric structures. This will eventually lead to collapse of the structure and particles get randomly orientated. Apart from this, for complex domain geometry such as in solid-liquid suspensions, placing the particles in regular grid may require substantial care and effort. In such cases, random placement of particles becomes a natural choice. Placing particles in purely random manner has been discouraged by Morris (1996) as it results in a great deal of noise and hence, internal energy. In spite of that, the present work focuses on random insertion of particles, as it is more realistic,
takes into account the robustness of the model and represents the inherent stochastic nature of SPH. For developing better understanding and for the purpose of comparison, we shall use regular insertion scheme from time to time during the initial stage of development. The behavior of the linear and hexagonal structures in SPH is found to be very much similar due to their spatial similarity. In order to restrict the number of numerical experiments as well as to capture the essence of regular distribution of particles, only the linear structure is considered in the present work.

4.2 Controlling the Number Density

In a typical SPH fluid flow experiment, once the details of domain geometry are identified, the next step is to decide on the level of discretisation. The level of discretisation in SPH depends on the number of locations (i.e., number of SPH particles) to which we would like to apply the fluid flow equations, which obviously depends on the inter-particle distance. At high level of discretisation, the inter-particle distance is small signifying the presence of large number of fluid particles in a small volume of fluid. While introducing the fluid particles in a given domain, it is essential to decide, a priori, the minimum inter-particle distance one would like to maintain. Once the inter-particle distance is decided, one can follow one of the three schemes described in the preceding section to introduce the fluid particles.

It is natural that the inter-particle distance be a function of the characteristic length ($L_o$) of the domain. However, the kernel being the fundamental building block of SPH, it is generally preferred to relate the inter-particle distance with the measure of kernel compact support length, $h$. This is particularly the case when one uses a kernel having compact support. Since in all the simulations in the present work kernels having compact support is chosen, the choice of $h$ as the fundamental discretisation parameter is more convenient. Moreover, the efficient neighbor searching scheme adopted in the present work (to be described in § 4.6) also dictates us to use $h$ as a fundamental parameter.
Having decided on a value of $h$, the next obvious issue that needs to be addressed is the average number of neighbors for each SPH particle one would like to have in a particular simulation. The accuracy of the smoothing operation in a discrete domain of particles improves as the number of particles within the kernel (known as neighbors) increases. However, the accuracy due to higher number of neighbors comes at a significantly higher computational cost. Thus, it is essential to have an optimum number of neighbors depending on the computational resource. Apart from this, many a times the decision of number of neighbors also depends on the kernel function (including its gradient) and the type of problem being solved. For example, it was mentioned in § 3.7 that for cases where the inter-particle distance is less than $2h/3$, the cubic spline kernel gives rise to 'particle clumping' under the influence of compressive force such as hydrostatic pressure.

Since we have chosen cubic spline kernel for most of our numerical experiments and we are aware of the behavior of its gradient, controlling inter-particle distance while placing the fluid particles in the domain becomes important. For this purpose, we introduce a parameter, $IPDF$ (Inter-Particle Distance Fraction) such that

**Minimum Inter-particle Distance** = $IPDF \times h$ \hspace{1cm} (4.1)

Thus, Eqn. (4.1) provides us a relationship between the fundamental parameter $h$ and the inter-particle distance. By varying the value of $IPDF$ for a given value of $h$ one can control the average number of neighbors for each particle. Moreover, in the context of cubic spline kernel function, a value of $IPDF$ less than $\frac{1}{3}$ will straight away indicate that the particles have been placed closer than the distance required for them to maintain stability under any compressive force field (for details, please refer to § 3.7). $IPDF$ approaching 2 is too large because a value in excess of 2 means on average no other particle takes part in the averaging process. Independent of $h$, smaller value of $IPDF$ means more neighbors.
Typical SPH simulations in two-dimensions have 23-25 neighbors (Villa, 1999), which also corresponds to the number of particles in a cubic spline kernel using $IPDF = \frac{\lambda}{3}$. Fig. 4.2 shows how the number of neighbors in a two-dimensional domain varies with the parameter $IPDF$ in case a cubic spline kernel is used. $IPDF$ can be viewed as a smoothing parameter while $h$, a discretisation parameter. Since most of our simulations are based on random insertion of particles, it was found more convenient to use parameters like $h$ and $IPDF$ rather than total number of particles, $N$, as discretisation controlling parameters.

Fig. 4.2: Variation of number of neighbors with $IPDF$ for randomly distributed particles using cubic spline kernel.

### 4.3 Effect of Discretisation Parameters on Smoothing

So far we have learnt about the properties of various smoothing kernels, variety of initial particle distributions, implementation of periodic boundary conditions etc. in SPH, independent of each other. However, before carrying out the actual simulations of solid-liquid flows, it was felt necessary to gain further insight into the interplay among all these parameters with particular reference to the behaviour of the smoothed value of a function.
and its gradient as we vary discretisation level. While, evaluation of smoothing properties of any function assumes special importance in dealing with body force that appears in Equation of Motion (refer Eqns. 3.25, 3.26), understanding the smoothing properties of kernel gradient becomes important where the force appears as surface force (e.g., pressure, viscous force).

In this section, we will consider a static fluid of uniform density and assess the level of errors in estimating the smoothed value of density and its gradient under various discretisation schemes. Density is taken only as a representative property and the study is equally applicable for other fluid properties as well. Some of the aspects of discretisation being investigated include:

- Type of initial particle distribution.
- Nature of smoothing kernel used.
- Total number of particles in the domain.
- Average number of neighbors for each particle.

### 4.3.1 Smoothing of Properties

The smoothed density of any particle \(i\), can be obtained from

\[
\langle \rho(r) \rangle_i = \int_{\Omega} W(r - r', h) \rho(r') dr' = \sum_{j=1,N} m_j W(r_i - r_j, h)
\]

where \(m_j\) is the mass of particle \(j\); for the sake of simplicity, let the mass of all particles be same. Unless otherwise mentioned, cubic spline kernel is considered for all smoothing operations and in two-dimension, the equation of the kernel is given by,

\[
W(r, h) = \begin{cases} 
\frac{10}{7\pi h^2} \left( 1 - 1.5 \frac{r}{h} + 0.75 \left( \frac{r}{h} \right)^3 \right) & \text{if } 0 \leq \frac{r}{h} < 1 \\
\frac{10}{28\pi h^2} \left( 2 - \frac{r}{h} \right)^3 & \text{if } 1 \leq \frac{r}{h} < 2 \\
0 & \text{if } 2 \leq \frac{r}{h}
\end{cases}
\]
where $r = r_i - r_j$.

For all the cases described in this section, particles were inserted in a doubly periodic square cell (Fig. 4.3) of 0.1 cm in each side and the fluid had density of 1 gm/cm$^3$. The number of particles inserted would depend on $h$ and $IPDF$. As long as $IPDF$ remained same, the average number of neighbors to a particle remained unchanged. The density of the fluid in dimensionless form was unity and the smoothed density of each fluid particle was estimated using Eqn. (4.2) under various discretisation schemes described in Table 4.1, where all distances are nondimensionalised with respect to the cell width (i.e., $L_0$=cell width). There could be several ways of representing the smoothed density of the particles. One of them is to plot the variation of the dimensionless smoothed density of each of the fluid particles with respect to their $y$-coordinates. This gives a gross idea about the variation of the smoothed density of all the particles in the domain. Another way is to divide the periodic cell into a number of horizontal bins of equal width and obtain the (arithmetic) average of the smoothed density of all the particles within each bin, together with the average of their $y$-coordinates. Apart from estimating the average smoothed density in each bin, the standard deviation of the smoothed density of the group of particles within each bin from the bin average smoothed density also estimated. A smaller standard deviation would indicate more homogeneity of the smoothed densities within each bin. This is thought to be a more compact way of representing the smoothed results.

Fig. 4.3: Schematic diagram of a cell with doubly periodic boundary condition.
Table 4.1: Discretisation parameters for experiments on smoothing of property

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Initial Positions</th>
<th>( h )</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Random</td>
<td>0.04</td>
</tr>
<tr>
<td>B</td>
<td>&quot;</td>
<td>0.01</td>
</tr>
<tr>
<td>C</td>
<td>Regular</td>
<td>0.04</td>
</tr>
<tr>
<td>D</td>
<td>Random</td>
<td>0.04</td>
</tr>
<tr>
<td>E</td>
<td>&quot;</td>
<td>0.01</td>
</tr>
</tbody>
</table>

\( IPDF \) and \( N \)

4.3.1.1 Effect of \( h \) on Smoothing

Random placement of particles:

Fig. 4.4 shows distribution of particles for scheme A of Table 4.1. Smoothed density of each of these fluid particles depends on the spatial distribution of its neighbors. The particles being distributed randomly in space, the smoothed density computed using Eqn. (4.2) also showed variation. The variation of the dimensionless smoothed density along the width (i.e., \( y \)-axis) of the periodic cell is plotted for schemes A and B in Figs. 4.5 and Fig. 4.6. The average number of neighbors for each particle in both the schemes (have same \( IPDF \) of 0.7) was approximately 19. The variation of smoothed density of each particle in the domain and the average smoothed density for groups of particles (as described in the previous paragraph) are reported in the figures. For estimating average smoothed densities, the periodic cell was divided into 20 horizontal bins of equal width. Each error bar in the plots indicates the standard deviation of smoothed density of the particles within the same bin.

From the density plots, we observe:

- Though the actual dimensionless density of the fluid is unity, after applying the smoothing function, the smoothed density of the system is found to be significantly deviating from unity. Ideally, the red lines in Figs. (4.5b) and (4.6b) should be horizontal, passing through a density value of unity and the
error bars should vanish. This would not only mean that the kernel function is able to approximate the density distribution accurately but also mean that the smoothing operation is independent of spatial distribution of the particles.

- However, due to random distribution of the particles in space, there is a spread in the smoothed density with the density values on either side of unity (which is the actual fluid density). The standard deviation of the spread is about 8% (Figs. 4.5b and 4.6b), which does not seem to significantly depend on the level of discretisation (i.e., on the value of $h$).

- The spread in the smoothed density arises due to the randomness in the spatial distribution of the particles. Random particle position means particles will not have the same number of neighbors and even if some of the particles have the same number of neighbors the relative positions of the neighbors will be different. Thus, the spread (or standard deviation) will disappear when each particle will have same number of neighbors at the same relative locations within its kernel. This contradicts the very nature of random insertion scheme where the inter-particle distances between two neighboring particles are never same. If they were same, the distribution will cease to be random. This means that in case of random distribution, there will be some amount of standard deviation, which will depend on how well the kernel function being approximated by the discrete particles. In other words, more number of neighbors within each kernel would reduce the standard deviation. This is the reason why no significant change in the standard deviation was observed when $h$ was reduced.

- By reducing $h$, there seems to be no apparent improvement in the accuracy (measured by the deviation of the red line in (b) from a horizontal line at avg. smoothed density =1) or the standard deviation of the average particle density.

- The density fluctuations even out at very low value of $h$. This is indicated by a rather smooth red line (obtained by joining the averages from the bins) in Fig. 4.6b and may be attributed to the presence of a large number of particles in each bin while estimating the average smoothed density in each bin.
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Fig. 4.4: Typical example of random distribution of particles in a doubly periodic square cell. There are 888 particles in the cell.

Fig. 4.5: Variation of (a) dimensionless smoothed density of all particles in the cell and (b) average dimensionless smoothed density, along y direction for $h=0.04$, $IPDF=0.7$ and $N=888$. For averaging, the cells are divided into 20 horizontal bins of equal width. Average of smoothed density of all particles in each bin is plotted in (b). The blue error bars indicate the standard deviations within each bin.
Fig. 4.6: Variation of (a) dimensionless smoothed density of all particles in the cell and (b) average dimensionless smoothed density, along y direction for \( h=0.01, \) \( IPDF=0.7 \) and \( N=14041. \)

**Regular placement of particles:**

Fig. 4.7 shows distribution of particles for scheme C. The smoothed density variation for this configuration is plotted in Fig. 4.8. The nature of the variations at other values of \( h \) is exactly same and hence not shown separately. From Fig. 4.8, we observe:

- The smoothed density is same for all the particles and hence, the standard deviation is zero.
- Due to symmetry of the particle positions, each particle has equal number of neighbors at exactly same relative locations. This makes the smoothed density uniform for all the particles.
- The difference between the smoothed density and the actual density is due to very few numbers of neighbors of the particles. It also depends on the ability of the spline kernel to reproduce a function.
Conclusions: The spatial distribution of smoothed value of any property in SPH arises due to spatial randomness of the particle positions. If the particles are not randomly distributed, the smoothed value of a uniform field will be the same everywhere.

4.3.1.2 Effect of IPDF on Smoothing

In order to understand the effect of IPDF, the two experiments described in § 4.3.1 (i.e., schemes A and B) were repeated with a smaller value of IPDF as indicated in the schemes D and E of Table 4.1. The average number of neighbors for each particle in
these experiments increased to 35. The smoothed density and the errors are plotted in Figs. 4.9 and 4.10. The important observations are as follows:

- By increasing number of neighbors, a reduction in the standard deviation of smoothed density is observed. This is because the kernel function at each particle location is being more accurately represented due to a larger sample size for each kernel.
- The accuracy of the average smoothed value of density has improved. Since there are more particles within each kernel over which the summation of Eqn. (4.2) is carried out, the smoothed density for each particle becomes closer to the actual density of the fluid and hence the improvement in the accuracy of the average smoothed density in each bin.

Experiments were further carried out to observe the effect of number of neighbors on the smoothed value of density in a more extensive manner where the average number of neighbors were varied by two orders of magnitude. Experiments were conducted for random as well as regular initial positions of the particles using slightly different approach where a large number of fluid particles in a doubly periodic domain were introduced using small value of $h (=0.01)$ and $IPDF (=0.5)$ and was used as the database for the particle positions. The average number of neighbors for each particle, $N_b$, was changed by changing the value of $h$ with higher value of $h$ giving more neighbors. Based on the results from experiments at various levels of $h$ and initial particle distribution, their effect on the smoothed value of particle density is summarized in Fig. 4.11(a&b). In these figures, the average smoothed densities were obtained by averaging the smoothed densities of all the particles in the domain. Similar approach was followed for evaluating the standard deviations of the smoothed density, reported in these figures. The figures show that for any given number of neighbors, the smoothed density obtained from a regular distribution of particles is more accurate than that obtained from a random distribution of particles though the difference between the two distribution systems becomes insignificant for large values of $N_b (>200)$. Moreover, the standard deviation in smoothing doesn’t exist in case of regular distribution of SPH particles. With random
distribution, the smoothed density can be estimated within 2% error with as few as 35 neighbors. However, it may be interesting to note that, in order to have 35 neighbors the value of $IPDF$ should be about 0.5 (refer Fig. 4.2). This has particular significance in the context of numerical stability when we use cubic spline kernel (refer § 3.8) since $IPDF \leq \frac{2}{3}$ is found to cause 'clumping'. It may also be interesting to note that the average smoothed value of the dimensionless density for all configurations approaches unity (i.e., the actual value of the dimensionless fluid density), irrespective of the distribution scheme (i.e., regular or random) from values greater than unity. When estimating smoothed density for a particle the contribution of the particle itself was included. This has probably resulted in having the average smoothed density always greater than unity.

![Figure 4.9](image)

**Fig. 4.9:** Variation of (a) dimensionless smoothed density of all particles in the cell and (b) average dimensionless smoothed density along $y$ direction for $h=0.04$, $IPDF=0.5$ and $N=1713$. 
Fig. 4.10: Variation of (a) dimensionless smoothed density of all particles in the cell and (b) average dimensionless smoothed density along y direction for $h=0.01$, IPDF=0.5 and $N=27279$.

Fig. 4.11: Variation of average dimensionless smoothed density as a function of average number of neighbors for (a) random and (b) regular particle distributions using cubic spline kernel. The average smoothed densities represent the average of all the particles in the periodic cell. The blue lines indicate standard deviations of smoothed densities. For the sake of clarity, only one side of the standard deviations has been shown. For regularly placed particles, the standard deviation is zero.

**Conclusions:** If we want to reduce the error in estimation of the smooth value of any property, the only way to do is by increasing the average number of neighbors. As long as the particles are positioned in a regular grid, the spread of the smoothed value ceases to exist. Random particle positions will always give rise to a spread in the smoothed values, which can be reduced by increasing the number of neighbors alone. More
neighbors in turn minimize the "randomness" of the particle positions and bring the system closer to the "isentropic" state.

4.3.1.3 Effect of Kernel Function on Smoothing

The study in the previous section was restricted to only cubic spline kernel. It would be interesting to investigate the response of smoothing properties of some other kernel, particularly one with better stability properties. Despite having 2nd order accuracy (same as cubic spline kernel), the kernel proposed by Chaubal et al. (1997) is chosen as it was designed to be more stable than the cubic spline kernel under compressive force. The equation of the kernel in two-dimension is:

\[
W(r, h) = \frac{5}{2\pi h^2} \left[ 1 - \frac{3}{2} \left( 1 - \frac{r^2}{h^2} + \frac{r^2}{2h^2} + \frac{r^2}{12h^2} \right)^2 \right] \quad \text{if} \quad \frac{r}{h} < 2
\]

\[
0 \quad \text{if} \quad \frac{2}{h} \leq \frac{r}{h}
\]

(4.4)

Using this kernel, we studied its smoothing properties at various levels of discretisation and initial particle positions. The results are summarized in Fig. 4.12. Some of the important observations made from these plots include:

- Performance of this kernel is inferior to cubic spline kernel at all levels of discretisation. For example, at \( N_b = 35 \), the smoothed density is approximately 7% higher than the fluid density when particles are distributed randomly, while with cubic spline kernel, the error is about 2%. Moreover, the standard deviations of the smoothed density are also higher if we use this kernel.

- Compared to cubic spline kernel, the errors in smoothed density estimation when the particles are placed in regular grid, is significantly higher. Compared to the cubic spline kernel, Chaubal’s kernel is more centrally peaked (see Fig. 3.13) and more akin to a Dirac-Delta function. The high error probably implies that a Dirac-Delta function may not be an ideal
smoothing function for SPH application. Another possibility of large error in case of Chaubal’s kernel may be the large contribution from the particle itself for evaluating smoothed property. In all cases of evaluation of smoothed properties for any particle, the contribution of the particle itself has been considered and the self contribution is larger for Chaubal’s kernel than for cubic spline kernel.

![Graph](image)

**Fig. 4.12:** Variation of average dimensionless smoothed density as a function of number of neighbors for (a) random and (b) regular particle distributions using the kernel proposed by Chaubal et al. (1997).

**Conclusion:** On the basis of smoothing property, the kernel proposed by Chaubal et al. appears to be inferior to the cubic spline kernel (refer Eqn. 4.3).

### 4.3.2 Smoothing of Gradient of any Property

The smoothed gradient of density, $\rho(r)$, can be expressed as:

$$\nabla \left< \rho(r) \right>_i = \sum_{j=1}^{N} m_j \nabla_i W(r_i - r_j, h)$$

The above expression shows that the spatial gradient of density (or any other property) is a function of the spatial gradient of the kernel we choose. Kernel gradient being a
function of the relative positions of the neighboring particles, the smoothed gradient of density, thus, depends on the particle distribution. This shows that, particles with the same density should have a smoothed density gradient if they are randomly placed while this should vanish if they are placed in regular grid (i.e., lattice structures shown in Fig. 4.1) and if the kernel is symmetric! For any particle \(i\) in a regular grid of particles, there will always be two particles \(j\) and \(j'\) located symmetrically on either side of \(i\) along the line joining \(j, i\) and \(j'\). With a symmetric kernel such as cubic spline, the gradient of particle \(j\) with respect to a particle \(i\) will be exactly same in value but opposite in sign to that of particle \(j'\). This renders the smoothed gradient zero. The observation has far reaching consequences in the current study, since the present work uses random distribution of particles in all the simulations presented in Chapters 5 and 6. In this section, a quantitative appreciation is provided of the effect of discretisation on the smoothed density gradient when particles are placed randomly.

The study was carried out at same two configurations described in § 4.3.1.1 (i.e., schemes \(A\) and \(B\)) and the results are reported in Figs. 4.13 & 4.14. The figures show the variation of the average smoothed density gradient and standard deviation of the smoothed density gradients in each of the 20 bins, calculated in a manner described in § 4.3.1.1. It may be worth mentioning that the general features of these gradients are similar in both the axial directions, and to avoid repetition, only the \(x\)-component of the smoothed density gradients along \(y\)-direction has been plotted. The plots show:

- The average smoothed density gradients in each bin (i.e., the red line), irrespective of \(h\), is very close to zero. This indicates that a large assembly of particles (in each bin) having the same value of property (say, density), would not exhibit gradient in any preferred direction.
- The spread of the standard deviation of the smoothed density gradient increases as the inter-particle distance decreases. The smoothed gradient is proportional to the mass of each particle (particle mass is proportional to \(h^2\)) and the kernel gradient (proportional to \(h^3\)). This explains why the spread of the smoothed gradient increases as \(h\) decreases.
Fig. 4.13: Variation of dimensionless average smoothed density gradient of particles along the width of the periodic cell when the particles are placed randomly. The blue lines indicate the standard deviations within the particles in each bin. \( h=0.04, \text{IPDF}=0.7 \) and \( N=888 \).

Fig. 4.14: Variation of dimensionless average smoothed density gradient of particles along the width of the periodic cell when the particles are placed randomly. The blue lines indicate the standard deviations within the particles in each bin. \( h=0.01, \text{IPDF}=0.7 \) and \( N=14041 \).

In Fig. 4.15, we have cited another example of smoothed density gradient using scheme \( D \) of Table 4.1. The average number of neighbors, \( N_b \), is increased to 35 in this example. A comparison with Fig. 4.13 indicates that the standard deviation of the smoothed gradient of any property decreases with an increase in the number of neighbors.
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Fig. 4.15: Variation of dimensionless average smoothed density gradient of particles along the width of the cell when they are placed randomly in a doubly periodic square lattice. The blue lines indicate the standard deviations within the particles in each bin. Here, $h=0.04$, $IPDF=0.5$ and $N=1713$.

Results of a series of experiments at different levels of discretisation for cubic spline kernel and Chaubal's kernel are summarized in Figs. 4.16 and 4.17. The experiments were carried out with fixed number of SPH particles, namely $N=42774$ and $14041$ (obtained by using $h=0.01$ & $IPDF=0.5$ and $h=0.01$ & $IPDF=0.7$ respectively), and the kernel compact lengths were varied to vary the number of neighbors. The standard deviations reported in these figures were obtained by averaging the standard deviations of all 20 bins in the periodic cell. Following observations are made from these figures:

- There is no discerning difference in the fluctuations of smoothed gradients (measured by average standard deviation) between cubic spline kernel and the kernel proposed by Chaubal et al.
- For randomly distributed particles, there will always be some fluctuations in the smoothed gradient (i.e., non-zero standard deviation).
- The fluctuations of the gradient monotonically decrease with increasing number of neighbors for a given number of particles in the domain. However, it is very intriguing to note that the average standard deviation of the smoothed density gradient decreases as the number of particles in the domain decreases. The reason is as follows. In all the experiments in this section, the domain dimensions and the density of the actual system were same. Thus, larger number of particles in the system means the inter-particle distance
decreases. In order to have the same number of neighbors, the value of $h$ needs to be higher when total number of particles is smaller. The smoothed density gradient being inversely proportional to the inter-particle distance (see Eqn. 4.5) and hence $h$, it decreases as $h$ increases or the total number of particles decreases. Along with the value of the smoothed density gradient, its fluctuation also decreases as the total number of particles in the system decreases. Thus, in the limiting case of a domain with extremely few particles, the average standard deviation of the density gradient would be very small.

Study of the fluctuations of any property is an important part of SPH, particularly if the property is density and the fluid is incompressible. Fluctuations in density can be viewed as a measure of compressibility of the fluid. In general, one can say that by increasing the number density in the computational domain, one can get a step closer in representing an incompressible fluid because incompressible fluids are characterized by orders of magnitude higher number density than a compressible fluid. The analysis in this section reveals that fluctuations in smoothed density would also increase for an incompressible fluid. A detailed analysis on modeling of incompressible fluid physics using SPH follows in the next section.

![Graph](image)

**Fig. 4.16:** Variation of average standard deviation of smoothed density gradient (in dimensionless form) with number of neighbors in a doubly periodic cell when particles are placed randomly. Average value of the standard deviation obtained by averaging over all the particles within the domain. Cubic spline kernel has been used.
Fig. 4.17: Variation of average standard deviation of smoothed density gradient (in dimensionless form) with number of neighbors in a doubly periodic cell when particles are placed randomly. Average value of the standard deviation obtained by averaging over all the particles within the domain. The kernel proposed by Chaubal et al. (1997) has been used here.

4.4 Modeling Incompressible Fluid Physics with SPH

When the pressure in some point of a fluid is changed, it takes a finite time to propagate to another point in the medium because the state of each intervening fluid element has to be changed. The speed of propagation of the pressure wave depends on the compressibility of the fluid; with a more compressible fluid, it takes more time to travel between any two points compared to the time it takes for a relatively less compressible fluid. This directly relates to the number of molecules in a given volume of fluid or the inter-atomic/inter-molecular distance in the fluid. Higher the number density of molecules in a given volume of fluid, faster is the transmission of the pressure wave. Thus, the argument may be extended to state that in an incompressible fluid, the propagation of the pressure wave takes significantly less time. As a consequence, the time step required to capture the state of each intermediate fluid element accurately in a numerical simulation needs to be extremely small. Not only that, the number of fluid elements required to represent the liquid is several orders of magnitude more than the fastest supercomputer would be able to handle! This poses some practical difficulties in
numerical simulations such as in SPH, where the fluid is simulated with a finite number of 'SPH particles' which are separated by much larger distance than in the real fluid and use a time step that is always constrained by the limited availability of computing resources. Some of these properties that make a fluid behave as liquid or as gas has been outlined on a relative scale in Fig. 4.18. From the diagram and from the discussion above, it may be qualitatively inferred that the simulated liquid deviates from the real liquid mainly in four accounts. These are as follows:

- We represent the liquid with fewer particles,
- Each particle interacts with a relatively small, finite number of neighbors,
- Inter-particle distance is much larger than the intermolecular distance that exists in real liquids,
- For reasons of computational economy, the time step chosen for the simulation needs to be much larger than that dictated by the actual speed of propagation of pressure wave in a real liquid.

In an attempt to simulate an incompressible fluid (i.e., liquid), SPH still constraints us to simulate a “relatively” incompressible fluid. The extent of incompressibility that we can build in the model fluid remains entirely a practical constraint. In general, one can say that if one increases the number of SPH particles in a given fluid volume and decreases the time step, \( \Delta t \), one would get closer to simulating a real incompressible fluid. In that case, the system would exhibit a speed of propagation of pressure wave closer to the actual value.

It may be mathematically derived that the speed of propagation of pressure wave in any fluid medium obeys the following relation:

\[
\omega = \sqrt{\frac{\kappa}{\rho}}
\]

(4.6a)

where \( \kappa \) is the bulk modulus of elasticity and \( \rho \) is the specific volume of the fluid. Incidentally, the value of \( \omega \) is found to correspond closely to the velocity of sound in the...
fluid. For example, the bulk modulus of elasticity for air and water are $1.5 \times 10^6$ and $2.068 \times 10^{10}$ gm/cm.s$^2$ respectively and they yield the velocity of propagation of pressure wave in the above mediums as $3.41 \times 10^4$ cm/s and $1.44 \times 10^5$ cm/s respectively. These velocities are same as the velocity of sound wave in the corresponding medium. It can also be shown (see Appendix 6) that for an incompressible fluid, the fluid pressure is approximately related to its velocity (under isentropic conditions) according to:

$$u_w = \sqrt{P/\rho}$$

(4.6b)

---

**Fig. 4.18**: Qualitative relationships among various properties of fluid in the context of modeling.
This means, under isentropic conditions, the pressure wave in an incompressible fluid moves at the speed of sound. Mach number of any fluid flow is defined as the ratio of fluid velocity to the velocity of sound wave within the fluid. Velocity of sound wave being very close to the speed of transmission of pressure wave in any fluid, one can define Mach number as the ratio of fluid velocity to the speed of pressure transmission wave as well. Thus, we can write,

\[ M = \frac{V_o}{c} \]

where, \( M \) is the Mach number, \( V_o \) is the characteristic velocity of the fluid and \( c \) is the speed of propagation of sound wave or the sonic speed in the fluid medium. For low Reynolds number flows, this ratio in Eqn. (4.6c) is extremely small, and even for most practical turbulent flows of liquids the ratio remains relatively small (under no practical circumstances, would a liquid, say water, flow at a speed of \( 1.440\times10^5 \) cm/s to make the Mach number \( =1 \)). Thus, theoretically, the Mach number for any real liquid flow irrespective of the flow conditions is quite small and is always less than unity.

Now let us look at the situation when numerical simulations are performed of these incompressible fluids. Here, the fluid is simulated using a compressible equation for pressure (i.e., hydrostatic pressure lower than actual), while the viscosity of the fluid remains that of the actual incompressible fluid (i.e., correct viscous force is used). By virtue of having relatively higher viscosity, the viscous force of the incompressible fluid remains a dominant component particularly at low Reynolds number flows. Thus, incompressible SPH flow generally remains a viscous force dominated phenomenon and under all situations, the hydrostatic force remains under-evaluated due to the relatively small, finite number density of fluid particles. Now let us look at various situations as the Reynolds number is altered.

At low Reynolds numbers, the velocity of the liquid being naturally low, the flow Mach number would also be much less than unity. Artificially increasing the Mach number
(i.e., by decreasing the speed of pressure wave) would imply that the fluid is going to exhibit a hydrostatic behavior that corresponds to a more compressible regime; i.e., the pressure transmission speed will be low. This will cause further imbalance between hydrostatic and viscous forces and should be avoided. Hence, we should artificially try to reduce the Mach number or increase the speed of pressure wave propagation.

With the same particle configuration as above, at higher Reynolds numbers, the system is aimed to have relatively higher pressure wave speed. But, if we don’t increase the pressure wave speed (i.e., reduce Mach number), the system becomes too ‘soft’ or too compressible where the pressure wave can hardly propagate. In such a case, care should be taken such that the system does not become excessively compressible, as this will make the system behave like a highly viscous fluid since we impose a real value of liquid viscosity on the fluid, which is high. If too high a value of the Mach number is chosen, this will further widen the difference between these forces quite unrealistically. Hence, a reduction in the value of the Mach number becomes necessary. Hence, from the above discussion, one can derive the following conclusions:

- Mach numbers much in excess of unity are not desirable as the flow will be overly compressible and hence, viscous dominated without appreciable contribution from the hydrostatic force component.
- Mach numbers much smaller than unity are desirable but not achievable since time stepping has to be very slow.
- At low Reynolds number, we need to choose a pressure wave propagation speed that will result in Mach numbers less than unity.
- At high Reynolds number, for the same configuration, computational Mach number must be greater than unity since the pressure wave propagation velocity in the SPH domain will always remain less than the speed of sound wave. However, the Mach number cannot be unity, as this would tend to eliminate the hydrostatic pressure contribution and the flow becomes almost exclusively viscous dominated which is not applicable with a real liquid.
It may be worthwhile to mention that from the thermodynamic point view, under isentropic condition, the velocity of propagation of pressure wave in air is about 20% ($\sqrt{\gamma_{\text{air}}} \approx 1.2$) more than that under isothermal condition. Isentropic condition implies that the system is thermodynamically in the most stable configuration. Increase in randomness in the system, indicated by isothermal condition, thus increases the velocity of pressure wave propagation. This means that the fluid flow under two different thermodynamic conditions offers a small window of variation of pressure wave propagation speed and hence, the Mach number in real fluid systems. By applying similar logic in the present formulation of relatively incompressible ‘SPH liquid’ using randomly placed particles, it is justified to use Mach numbers higher than unity.

4.5 Study of Bulk Flow

Study of the bulk motion of SPH liquid, in absence of any domain boundary, under various numerical and hydrodynamic conditions can help us in understanding the fundamentals of evolution of incompressible liquid physics from both numerical as well as physical point of view. For this reason, the “unbound flow” case is focussed upon in this section. In unbound flow, due to absence of any solid boundary, all quantities in the hydrodynamic equations involving surface integrals do not participate in any significant manner, the reason being explained in § 3.2.1.

Eqns. (3.24 - 3.27) describe the fluid flow in an unbound domain once the surface integral terms are removed (for ease in representation, the stars have been deleted from the equations presented earlier, but they still represent dimensionless quantities):

**Equation of Continuity:**

$$\frac{d}{dt} \langle \rho \rangle_i = - \sum_{j=1,N} m_j (u_j - u_i) \frac{\partial W_{ij}}{\partial x_i} - \sum_{j=1,N} m_j (v_j - v_i) \frac{\partial W_{ij}}{\partial y_i}$$ (4.7)
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**x-component of acceleration:**

\[
\frac{d}{dt} \langle u \rangle_i = -\frac{1}{M^2} \left[ \sum_{j=1}^{N} \left( \frac{1}{\rho_j} + \frac{1}{\rho_i} \right) m_j \frac{\partial W_y}{\partial x_i} \right] + \frac{1}{Fr} \left[ \sum_{j=1}^{N} W_{ij} m_j \right] \frac{1}{\rho_j} \frac{d (u_j)}{dt} + \frac{1}{Re} \sum_{j=1}^{N} m_j \left( \frac{\partial W_y}{\partial x_j} \frac{\tau_{xy}}{\rho_j^2} + \frac{\partial W_y}{\partial y_j} \frac{\tau_{yx}}{\rho_j^2} \right) \]

\[ (4.8) \]

**y component of acceleration:**

\[
\frac{d}{dt} \langle v \rangle_i = -\frac{1}{M^2} \left[ \sum_{j=1}^{N} \left( \frac{1}{\rho_j} + \frac{1}{\rho_i} \right) m_j \frac{\partial W_y}{\partial y_i} \right] + \frac{1}{Fr} \left[ \sum_{j=1}^{N} W_{ij} m_j \right] \frac{1}{\rho_j} \frac{d (v_j)}{dt} + \frac{1}{Re} \sum_{j=1}^{N} m_j \left( \frac{\partial W_y}{\partial x_j} \frac{\tau_{xy}}{\rho_j^2} + \frac{\partial W_y}{\partial y_j} \frac{\tau_{yx}}{\rho_j^2} \right) \]

\[ (4.9) \]

Let us consider flow of liquid along x-direction, in a doubly periodic domain under the influence of body force. Let the liquid be stationary at \( t=0 \). Since there is no boundary, there will be no resistance to the flow due to the fluid viscosity. The fluid would move as a block under acceleration due to the body force and its velocity should be predicted from particle kinematics. The x-component of velocity should follow:

\[
u^{t+1} = u^t + b_x t \]

\[ (4.10) \]

where \( u \) is the x-component of velocity, \( b_x \) is the x-component of body force, \( t \) is any time after start of simulation and the superscripts indicate the time step.

When the particles are introduced in the domain in a regular fashion (see Fig. 4.1) the smoothed gradients in Eqns. (4.7-4.9) do not play any role until such a stage reaches when, due to accumulation of error that arises in the smoothing operations, the particles lose symmetry with respect to each other. This has been demonstrated by carrying out an experiment using 5041 particles; IPDF was 0.7 and there were about 20 neighbors for
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The dimensionless body force was 1.0 at $Re=1.0$ and $M=0.1$. x-component of velocity of all the SPH particles are plotted against their y-positions, for this experiment in Fig. 4.19. It shows that once the symmetry is lost, the ensemble of particles behave just the way a randomly distributed ensemble of particles would have behaved. Until this point, the regular assembly of particles would behave in a very predictable and regular manner. Hence, we should bear in mind that, be it regular or random distribution, SPH is an approximation method and there will be an element of error in estimating any smoothed property. It is this error that would turn the ordered particles into disorder even in such simple experiment.

![Graph of x-component of velocity of all the particles in a bulk flow experiment plotted against their y-coordinates. The domain is doubly periodic and the particles were initially placed in a regular grid. The figure shows that after some time, the particles lose their symmetry. All quantities are in dimensionless form. The dimensionless velocity exceeds unity because the particles are under constant acceleration.](image)

Fig. 4.19: x-component of velocity of all the particles in a bulk flow experiment is plotted against their y-coordinates. The domain is doubly periodic and the particles were initially placed in a regular grid. The figure shows that after some time, the particles lose their symmetry. All quantities are in dimensionless form. The dimensionless velocity exceeds unity because the particles are under constant acceleration.

Now, we will demonstrate the effect of compressibility and hence, density, on such simple flow by changing the Mach numbers or the speed of propagation of sound in the 'SPH liquid'. For this, two experiments were carried out, the details of which are shown in Table 4.2. In the absence of any surface, and hence any retarding force, the velocity of
the fluid is supposed to increase continuously with time under the influence of a constant body force, $b_x$. In such a situation, the velocity scale, $V_0$ is obtained from the following relationship:

$$V_0 = \frac{\rho b_x L_0}{8 \mu}$$

which is obtained assuming the flow is occurring along the positive $x$-direction within a two-dimensional channel. The width of the cell, $W$ is used as the length scale, $L_0$. The two experiments differ only in Mach number. The Mach numbers are 0.1 and 1.0 respectively. The $x$-component velocity profiles at three different times for both experiments are shown in Fig. 4.20, while the density has been reported in Fig. 4.21. From the figures, it is clear that the variations in the properties are wider at lower Mach number though the average values remain same at corresponding times. The fluid behaves as a bulk and the average velocity obtained from the SPH simulations was found to match very well (not shown here) with the velocity predicted from particle mechanics described in Eqn. (4.10).

### Table 4.2: Various parameters used for the bulk flow experiments

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cell width, $W$</td>
<td>0.1 cm</td>
</tr>
<tr>
<td>Cell length, $L$</td>
<td>0.1 cm</td>
</tr>
<tr>
<td>Body force/mass of fluid, along $x$ direction, $b_x$</td>
<td>$8 \times 10^{-3}$ cm$^2$/s</td>
</tr>
<tr>
<td>Fluid viscosity, $\mu$</td>
<td>0.01 gm/cm.s</td>
</tr>
<tr>
<td>Fluid density, $\rho$</td>
<td>1 gm/cm$^3$</td>
</tr>
<tr>
<td>Reynolds number based on cell width, $Re_z$</td>
<td>0.01</td>
</tr>
<tr>
<td>Time step, $\Delta t$</td>
<td>$5 \times 10^{-5}$ s</td>
</tr>
<tr>
<td>Compact support length, $h$</td>
<td>$2 \times 10^{-3}$ cm</td>
</tr>
<tr>
<td>Number of SPH particles, $N$</td>
<td>2966</td>
</tr>
<tr>
<td>IPDF</td>
<td>0.7</td>
</tr>
</tbody>
</table>
At High Mach, the fluid becomes more compressible and, with the fluid being represented by these few particles, density fluctuation becomes very low. On the other hand, by decreasing the Mach number, the SPH fluid actually represents a fluid that is less compressible where density fluctuations at such low Reynolds number should indeed be high since the density estimation is not very accurate. Despite the compressibility effect and the fluctuations therein, it is interesting to note that both the fluids move at an average velocity that matches closely with the velocity predicted from particle kinematics.

At High Mach, the fluid becomes more compressible and, with the fluid being represented by these few particles, density fluctuation becomes very low. On the other hand, by decreasing the Mach number, the SPH fluid actually represents a fluid that is less compressible where density fluctuations at such low Reynolds number should indeed be high since the density estimation is not very accurate. Despite the compressibility effect and the fluctuations therein, it is interesting to note that both the fluids move at an average velocity that matches closely with the velocity predicted from particle kinematics.

Fig. 4.20 (a, b): x-component of velocity profiles for a bulk flow experiment at two Mach numbers. (a) At $M=0.1$, (b) at $M=1.0$. Each figure shows three different plots of velocity profiles at different times during the experiment. Though the average velocities (at corresponding time) are very similar in both the figures, there is wider variation of the property at lower Mach number when an incompressible fluid is simulated using very few particles. All quantities are dimensionless.
average velocity that matches closely with the velocity predicted from particle kinematics.

![Graph](image)

4.21 (a,b): Dimensionless smoothed density profiles of all the particles in the bulk flow experiment at two Mach numbers: (a) At M=0.1, (b) at M=1.0 at t=0.0025. The plots show that at higher Mach number due to compressibility effect, the fluctuations in density is extremely small compared to the fluctuations observed at M=0. It shows that an attempt to simulate incompressible fluid with very few particles results in high fluctuations in density in SPH.

### 4.6 Development of Computer Code

In any particle-based technique, the neighbor searching procedure takes up a considerable proportion of the computational time; in order to increase computational efficiency, design of an efficient neighbor-searching algorithm becomes essential. This is particularly true when one uses kernels having finite compact support length.

In case we use Gaussian or exponential kernel, all fluid particles in the domain are neighbors to each particle. Under such situation, the question of neighbor searching does not arise but the computation time for each smoothing operation would vary with \( N^2 \), where \( N \) is the total number of fluid particles in the domain. On the other hand, by using kernels with compact support, one would be required to perform a much smaller number of calculations. Despite that, extensive searching needs to be carried out for suitable...
neighbors from all the particles unless an efficient way is found to restrict the search to within very few particles.

In this technique, the domain is divided into small square cells of $2h$ (if we use a spline kernel whose compact support length is $2h$) in each axial direction as schematically shown in Fig. 4.22. By doing so, particles belonging to any cell (indicated as the clear cell at the center) would have neighbors within the nine cells around it (the shaded cells) including the cell in question. This will reduce the load on neighbor searching procedure and the computational speed would enhance by:

- Maintaining a list of particles in each cell and updating the list, as particle(s) move to some other cell,
- Maintaining a list of neighboring cells for each cell in the domain. This will help identify which cells are to be ‘looked at’ for neighbors of a specific particle.

![Fig. 4.22: The computational domain has been divided into small squares of length 2h.](image)

For example, if each of these cells contains about 20 particles and the domain has 2500 cells (i.e., 50,000 particles in total), then the smoothing operation of each particle would involve only $9 \times 20 = 180$ neighbor searching operations as opposed to 50,000. The benefit of such a technique increases as the number of particles in the domain increases.
In spite of adoption of the cell method described above, computation of $r_{ij}$, the inter-particle distance between particle $i$ and $j$ can become laborious if periodic boundary condition exists. Because in that case, not only does one need to check the actual distance between $i$ and $j$, but also one has to calculate the distance between $i$ and $j'$, the image of $j$. Indiscriminate use of checking the periodic distances for all particle-particle combinations within the neighborhood cells would inevitably becomes significantly time consuming as the number of particles in each cell or in the whole domain increases. One way of decreasing the computational load is to identify the cells that are near the periodic boundaries as shown in Fig. 4.23 and mark them as ‘periodic cells’ while the rest of the cells may be marked as ‘core cells’. Subsequently, one needs to perform the check for the image particles only if the particle $i$ belongs to one of these periodic cells. The current work has derived substantial benefit from this scheme.

![Fig. 4.23: Schematic diagram showing periodic and core cells used in the present work to optimize neighbor searching procedure.](image)

### 4.7 Summary

In this chapter, some basic aspects of the SPH discretisation technique have been explored including the properties of kernels and the choice of initial particle distributions. Appreciation is developed of interweave between SPH technique as applied to the
incompressible fluid flow and the flow hydrodynamics. Some of the salient points emerging from this chapter include:

**Discretisation issues:**

- Cubic spline kernel is has been chosen as the main kernel for this work as it has compact support and is accurate up to second order.
- Though Chaubal's kernel, a modified version of cubic spline kernel, was designed to remove the instability the later suffers under compressive force, the former was found having superior smoothing property.
- Higher order spline kernels, though more accurate, are more expensive in terms of computational time since their neighborhood extends beyond $2h$ and different spline function needs to be applied in different zones.
- Based on a compromise between computational economy and numerical accuracy, an IPDF of 0.677-0.70 for cubic spline kernel may be a reasonable choice. This means the SPH particles will have about 18-24 neighbors.
- It is easier to insert particles in a regular fashion in a domain, particularly when the domain is of regular shape and, such initial positions offer a quiet start to the SPH fluid system.
- However, when the relative motion of the particles is high, such regularly placed particles cannot maintain the regular lattice-like structures and eventually collapse. They become randomly oriented.
- Random insertion has been chosen as the main scheme of inserting particles. This is expected to make the system flexible and robust. The system is also expected to be more stable than regularly inserted particles as the later might go through dynamic instability due to particle rearrangements as the flow develops.

**Hydrodynamic issues:**

- SPH is a density based discretisation technique where fluid pressure is estimated from its density.
- For incompressible flow, density needs to be estimated very accurately. Typically, smoothing operation is accurate to within 1% (Monaghan, 1994), this makes the liquid pressure fluctuate at a very high level.

- The other reason for such high fluctuation is that in SPH, we try to simulate a liquid that has extremely high particle density, with very few particles that makes it a 'relatively incompressible fluid' rather than a liquid.

- Speed of propagation of pressure wave in liquid being very high, the Mach number of flow at low to medium Reynolds number liquid flows is very small. Such low Mach number means the time step in simulations has to extremely low and SPH particle density needs to be very high. This necessitates a high power computer that doesn’t exist, to solve any simulation within reasonable time.

- The solution lies in softening the 'incompressibility' of the liquid by slightly modifying the Mach number, the value of which is expected to depend on factors including the hydrodynamics and domain discretisation.

- Mach numbers much in excess of unity are not desirable as the flow will be overly compressible and hence, viscous dominated without appreciable contribution from hydrostatic force.

All numerical experiments in this chapter were carried out in doubly periodic domains without any presence of boundary conditions. In Chapters 5 and 6, the presence of various types of boundaries is investigated using the surface integrals.
On two occasions I have been asked, “Pray, Mr. Babbage, if you put into the machine wrong figures, will the right answers come out?” I am not able rightly to apprehend the kind of confusion of ideas that could provoke such a question.

-Charles Babbage
In Chapter 4, various fundamental implementation issues in SPH including the kernel function, particle number density, particle configurations and modeling slightly-compressible flows were studied in doubly periodic domains having no boundary. Study of fluid flow remains incomplete without acknowledging the presence of boundaries in a system as the boundary conditions, and sometimes the initial conditions dictate the solutions to be obtained from the governing equations. This necessitates one to examine the role of the surface integrals introduced in the Equations of Continuity and Motion in the present formulation of SPH as many physical boundary conditions are captured through these surface integrals.

Due to the presence of solid surfaces in the isothermal viscous flow of solid-liquid suspensions, correct implementation of boundary conditions such as 'no-slip' along the surfaces and 'no-flow' normal to the surfaces are considered essential. This is particularly the case since the present formulation imposes boundary conditions in a way (i.e., using surface integrals) that is not demonstrated in the literature. Therefore, a few test cases of isothermal, incompressible single-phase flow in the presence of surfaces of varying complexity are considered here. The cases primarily vary in the way the fluid is imparted motion from a state of rest. This includes application of shear from moving walls and use of body force. The later part of this chapter deals with flow around stationary objects where the objects of circular geometry are considered only.

5.1 Couette flow

The first test case is on two-dimensional unidirectional unsteady flow of liquid between two infinitely long parallel rigid walls with one of the walls moving at constant velocity,
known as Couette flow. A continuous supply of energy to the fluid by tangential stresses from the wall raises the momentum of the stationary fluid, initially at rest, and balances the viscous dissipation after reaching steady state. Being one of the simplest flow configurations, Couette flow is regarded as an obvious choice to test the validity and accuracy of any numerical model.

The schematic diagram along with the boundary conditions for the Couette flow is shown in Fig. 5.1. The liquid and the walls are at rest for \( t \leq 0 \) and at \( t=0 \), the upper wall starts moving along positive \( x \)-direction with constant velocity, \( U \). While the SPH form of the Equation of Continuity for the fluid remains same as Eqn. (3.24), the Equation of Motion [Eqns. (3.25-3.27)] can be simplified if we neglect the effect of gravity. The equations, along with the boundary conditions are rewritten (all in dimensionless form) below for ease of reference where, the velocity of the moving wall and the width of the cell are taken as the parameters for non-dimensionalisation (i.e., \( V_0=U, L_0=W \)):

**Equation of Continuity:**

\[
\frac{d}{dt}(\rho_i) = - \sum_{j=1,N} m_j (u_j - u_i) \frac{\partial W_{ij}}{\partial x_i} - \sum_{j=1,N} m_j (v_j - v_i) \frac{\partial W_{ij}}{\partial y_i} \\
- \rho_i (u_s - u_i) \int_{S_i} W_{is} \, dx - \rho_i (v_s - v_i) \int_{S_i} W_{is} \, dy \tag{5.1}
\]


**Equation of Motion, x-component:**

\[
\frac{d}{dt}(u)_i = - \frac{1}{M^2} \left[ \sum_{j=1,N} \left( \frac{1}{\rho_j} + \frac{1}{\rho_i} \right) m_j \frac{\partial W_j}{\partial x_j} + \int_{\Omega} \frac{W_{ij} \partial \rho_i}{\partial x_j} \right] + \frac{1}{Re} \left[ \sum_{j=1,N} m_j \left( \frac{\partial W_{ij}}{\partial x_i} \frac{\tau_{xx}}{\rho_j} + \frac{\partial W_{ij}}{\partial y_j} \frac{\tau_{xy}}{\rho_j} \right) + m_j \left( \frac{\partial W_{ij}}{\partial x_i} \frac{\tau_{xx}}{\rho_j} + \frac{\partial W_{ij}}{\partial y_j} \frac{\tau_{xy}}{\rho_j} \right) \right] + \rho_i \left( \frac{\tau_{xx}}{\rho_i^2} \zeta_x + \frac{\tau_{xy}}{\rho_i^2} \zeta_y \right) + \rho_i \left( \frac{\tau_{xy}}{\rho_i^2} \zeta_x + \frac{\tau_{xx}}{\rho_i^2} \zeta_y \right)
\]

(5.2)

**Equation of Motion, y-component:**

\[
\frac{d}{dt}(v)_i = - \frac{1}{M^2} \left[ \sum_{j=1,N} \left( \frac{1}{\rho_j} + \frac{1}{\rho_i} \right) m_j \frac{\partial W_j}{\partial y_j} + \int_{\Omega} \frac{W_{ij} \partial \rho_i}{\partial y_j} \right] + \frac{1}{Re} \left[ \sum_{j=1,N} m_j \left( \frac{\partial W_{ij}}{\partial x_i} \frac{\tau_{xx}}{\rho_j} + \frac{\partial W_{ij}}{\partial y_j} \frac{\tau_{xy}}{\rho_j} \right) + m_j \left( \frac{\partial W_{ij}}{\partial x_i} \frac{\tau_{xx}}{\rho_j} + \frac{\partial W_{ij}}{\partial y_j} \frac{\tau_{xy}}{\rho_j} \right) \right] + \rho_i \left( \frac{\tau_{xx}}{\rho_i^2} \zeta_x + \frac{\tau_{xy}}{\rho_i^2} \zeta_y \right) + \rho_i \left( \frac{\tau_{xy}}{\rho_i^2} \zeta_x + \frac{\tau_{xx}}{\rho_i^2} \zeta_y \right)
\]

(5.3)

**Initial conditions:**

at \( t=0 \), \( u = 0 \) and \( v = 0 \) for all particles in the domain

(5.4)

**Boundary conditions:**

at upper wall, i.e. at \( y=1 \), \( u_i = 1 \ \ \ v_i = 0 \)

at lower wall, i.e., at \( y=0 \), \( u_i = 0 \ \ \ v_i = 0 \)

(5.5)

For a Newtonian and incompressible liquid, the SPH form of viscous stress is:

\[
\frac{\tau_{xx}}{\rho^2} = -2 \frac{\partial u}{\partial x} + \frac{2}{3} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right), \quad \frac{\tau_{xy}}{\rho^2} = -2 \frac{\partial v}{\partial y} + \frac{2}{3} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right), \quad \frac{\tau_{yy}}{\rho^2} = \frac{\tau_{yx}}{\rho^2} = - \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)
\]

(5.6)

Eqns. (5.1 - 5.6) define the system completely and are solved for each fluid particle in the domain employing a suitable kernel function and using the time integration scheme described in § 3.5. The simulation is continued until the acceleration of the fluid particles
become negligibly small, which signifies steady state. While the $y$-component of velocity of the particles should be zero, the analytical expression for the $x$-component of velocity of any particle, having its $y$-coordinate at $y_j$ is given by:

$$u(y_i, t) = y_i + \sum_{n=1}^{\infty} \frac{2}{n\pi} (-1)^n \sin(n\pi y_i) \exp \left(-\frac{n^2 \pi^2}{Re} t\right)$$

(5.7)

Table 5.1: Various Couette flow configurations used for experiments

<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>3525</td>
<td>0.04</td>
<td>0.02</td>
<td>0.01</td>
<td>Rand</td>
<td>0.01 1 100 0.01 0.1</td>
</tr>
<tr>
<td>B</td>
<td>5041</td>
<td>0.04</td>
<td>0.02</td>
<td>0.01</td>
<td>Reg</td>
<td>0.01 1 100 0.01 0.1</td>
</tr>
<tr>
<td>C</td>
<td>4764</td>
<td>0.04</td>
<td>0.02</td>
<td>0.01</td>
<td>Cub</td>
<td>0.01 1 100 0.01 0.1</td>
</tr>
<tr>
<td>D</td>
<td>4764</td>
<td>0.04</td>
<td>0.02</td>
<td>0.01</td>
<td>Chb</td>
<td>0.01 1 100 0.01 0.1</td>
</tr>
<tr>
<td>E</td>
<td>1208</td>
<td>0.04</td>
<td>0.02</td>
<td>0.01</td>
<td>Rand</td>
<td>0.04 0.02 0.01 0.7 0.6</td>
</tr>
<tr>
<td>F</td>
<td>19020</td>
<td>0.04</td>
<td>0.02</td>
<td>0.01</td>
<td>Reg</td>
<td>0.04 0.02 0.01 0.7 0.6</td>
</tr>
<tr>
<td>G</td>
<td>19020</td>
<td>0.04</td>
<td>0.02</td>
<td>0.01</td>
<td>Cub</td>
<td>0.04 0.02 0.01 0.7 0.6</td>
</tr>
<tr>
<td>H</td>
<td>19020</td>
<td>0.04</td>
<td>0.02</td>
<td>0.01</td>
<td>Chb</td>
<td>0.04 0.02 0.01 0.7 0.6</td>
</tr>
<tr>
<td>I</td>
<td>27300</td>
<td>0.04</td>
<td>0.02</td>
<td>0.01</td>
<td>Rand</td>
<td>0.04 0.02 0.01 0.7 0.6</td>
</tr>
<tr>
<td>J</td>
<td>19020</td>
<td>0.04</td>
<td>0.02</td>
<td>0.01</td>
<td>Reg</td>
<td>0.04 0.02 0.01 0.7 0.6</td>
</tr>
<tr>
<td>K</td>
<td>19020</td>
<td>0.04</td>
<td>0.02</td>
<td>0.01</td>
<td>Cub</td>
<td>0.04 0.02 0.01 0.7 0.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Chb</td>
<td>0.04 0.02 0.01 0.7 0.6</td>
</tr>
</tbody>
</table>

- For an experiment to be properly defined, one set of data from each block of parameters (in yellow) is required.
- Blocks filled in turquoise color indicate the set of data used for the configuration.
- Number of particles is not an independent parameter; it depends on all the parameters under the heading 'Discretisation parameters'.
- Cub – Cubic Spline Kernel; Chb – kernel proposed by Chaubal et al. (1997).
- Rand – random distribution of particles; Reg – regular distribution of particles

Numerical experiments were systematically performed in a periodic cell (periodic along $x$-axis) to understand the effect of particle positions, discretisation parameters and properties of kernel. Input data for various experiments are shown in Table 5.1. Simulation results are compared with the analytical solutions during the progress of the experiments. To present the SPH results in a more meaningful way, the periodic cell was divided into 40 horizontal bins of equal width and smooth properties of each bin was evaluated by arithmetic average amongst the particles within the bin. The standard deviation within each bin is also calculated. The standard deviation may be regarded as a
measure of fluctuations of the properties, a characteristic of SPH. All results are reported in dimensionless form.

5.1.1 Initial Particle Positions

The influence of initial particle position on stability and accuracy of the results is demonstrated by considering two modes of particle placements, e.g., random and regular. (Configurations A and B, Table 5.1). Due to symmetry of particle positions, the number of particles placed in regular insertion (5041) was more than that with random insertion (3525). The initial and final particle positions for the two experiments are shown in Fig. 5.2. It is interesting to note that in spite of choosing an IPDF>$2/3$, particles were found to form ‘clusters’ when they were initially placed in regular grids. On the other hand, particles initially placed in random manner under the same conditions didn’t form any cluster.

Fig. 5.3 shows the x-component velocity profile with respect to the y-coordinates of the fluid particles for both the simulations at three different times during the progress of the simulations. In order to assess the stability of the simulations, the simulations were continued for a time much beyond the flow attained steady state; and the third temporal velocity profiles in the figures are plotted to indicate that the simulations are quite stable. Whether the simulations attained steady state were tested by observing no further change in the analytical velocity profiles. Some of the important observations made from these plots include:

- The agreement between the analytical results and the average SPH velocities are found to be good in general and in particular, the agreement gets even better as the flow approaches steady state. The maximum error observed in velocity estimation was about 2%.

- When the particles were placed in regular order, the fluctuations in $u$ were almost absent at the initial stages of simulation. As the simulation progressed, the relative movements of the particles caused the ‘stable’ lines of force to
buckle and release huge amount of energy in the form of 'local disorder'. The situation is schematically shown in Fig. 5.4. Due to unidirectional motion of the particles, the number of particles contributing to the smoothing operations makes discrete jumps causing discrete changes in the mass and momentum transferred to or from a specific kernel. This results in fluctuations of all smoothed properties and the extent of such fluctuations will depend on the mass of each particle as well as the number of particles in each kernel. The fluctuations are captured through the large standard deviations in Fig. 5.3a2.

- The fluctuations are essentially caused by discretisation errors in SPH and remain a part of this numerical scheme like any other discretisation scheme. Moreover, in a Lagrangian scheme like SPH, when particles move from one point to another errors in estimation of the forces also cause two particles to get too close to each other. This is exactly what we observe with regularly distributed particles.

- For regularly placed particles, though the axial inter-particle distance is 0.7h, the distance between two diagonal neighbors is \( \sqrt{2} \) times the inter-particle distance. Thus, the smoothing operation in a kernel operates under two distinct and different length scales. Subsequent to slight misalignment to particle positions, while the axial neighbors try to get closer to the center of the kernel, the diagonal particles recede from the center to conserve mass and momentum. The result is formation of 'clusters' or 'clumps'. It is understood that irrespective of the value of IPDF, such phenomena will always occur when particles are placed in linear grids. This kind of instability is quite different from the instabilities observed in explicit scheme such as SPH when time step size is large (Swegle et al., 1995). Even if the time integration is exact, such clumping will occur (Morris, 1996).

- However, once the particle rearrangements through 'clumping' are over, the system gradually returns to stability. Obviously though, it would take a longer time to dissipate the high level of energy the system acquires due to large relative displacement of the particles. This is indicated in Fig. 5.3a3, where a
considerable amount of standard deviation is present even after steady state is attained. Further continuation of the experiment indicates (not shown in the figure) gradual reduction of the velocity fluctuation.

- Random particle distribution, on the other hand, starts with some amount of 'internal energy' as is indicated by the standard deviation in Fig. 5.3b1. Addition or removal of another particle to/from the kernel for the smoothing operation does not cause any significant jumps in its smoothed value. Similarly, the kernel gradient always possess some residual gradient (see § 4.3.2) due to random position of the particles and any further error in the estimation of the smoothed gradient does not make the situation unstable until the particles are placed too close together ignoring the criteria of IPDF<2/3 (refer § 4.3.1.2). This means, the system monotonically reaches steady state and the smoothed standard deviations become extremely small as the flow progresses towards steady state, Figs. 5.3b2 and 5.3b3. On the other hand, particles initially placed in regular fashion goes through particle rearrangement after which the system behaves as if the particles were placed randomly.

The formation of 'clumps' in a system of randomly inserted particles for IPDF=0.6 (i.e., <2/3) is demonstrated in Fig. 5.5a. This experiment was carried out using configuration C of Table 5.1. The trend of the standard deviations shown in Fig. 5.5b is similar to the experiment with IPDF of 0.7 (see Fig. 5.3b), but the deviations are in general higher due to 'particle clumping'. The fluctuations are observed since the fluid particles were initially placed with IPDF<2/3 and cubic spline kernel was used. It is needless to say that under similar dynamic conditions with regularly placed particles for IPDF<2/3, the particles would obviously form 'clumps'.
Fig. 5.2: Effect of initial particle positions in Couette flow for IPDF = 0.7 using cubic spline kernel – (a&b) Initial and final (at t=0.5) positions of the particles when the particles were initially placed in linear structure showing most of the particles pair up and form 'clumps'; (c&d) Initial and final (at t=0.5) particle positions when the particles were placed randomly, showing absence of 'clumping' if IPDF > 2/3.
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Fig. 5.3: Comparison of analytical results (pink lines) vs. SPH simulations (blue points) for Couette flow at \( Re=1.0 \). x-component of dimensionless velocity of the particles are plotted against their y coordinates. For the SPH results, the periodic cell is divided into 40 bins of equal width and the average of particle velocities in each cell along with the standard deviations among the particles within the cells are reported here. (a1-a3) for regular distribution; (b1-b3) for random distribution. The velocity plots are at \( t=0.05, 0.375 \) and 0.5 (non-dimensional time).

Fig. 5.4: Schematic representation of the asymmetry that arises during unidirectional shear flow of regularly arranged layers of particles. (a) The kernel for the particle in black has all its neighbors located symmetrically when the relative displacement is small making its smoothed gradient insignificant, (b) As the relative displacements of the layers increase, the same black particle is found to lose its symmetry with respect to its neighbors. Moreover, the number of particles in the kernel volume also changes in a discrete manner leading to large fluctuations in the smoothed quantities.
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5.1.2 Effect of Kernel Function

The fact that the nature of the gradient of cubic spline kernel is responsible for ‘particle clumping’ with random particles at $IPDF<2/3$, can be demonstrated by carrying out an experiment using configuration $D$ (Chaubal’s kernel used) and comparing the results with configuration $C$. Fig. 5.6a clearly demonstrates the absence of any ‘clumping’ in contrast to Fig. 5.5a, where cubic spline kernel was used for the same particle and flow configurations. Though the graphs show that the initial fluctuations in smoothed values using Chaubal’s kernel is much less than that with cubic spline kernel, there is hardly any difference in fluctuations between the two kernels at steady state. Added to this, the
benefit of a more stable simulation using Chaubal's kernel can only be realized when $IPDF$ is less than $2/3$ which means more neighbors and more computing time per particle. Moreover, from § 4.3.1.3 it may be noted that the smoothing property of Chaubal's kernel is less accurate than the cubic spline kernel for same number of neighbors. From all the above analyses, it may be concluded that despite having better stability, Chaubal's kernel is not of great benefit compared to cubic spline.

5.1.3 Effect of Discretisation

Like any other numerical method, the accuracy of the results in SPH depends on the level of space discretisation. Higher level of discretisation, achieved by smaller inter-particle distance monotonically improves the accuracy of results. This is demonstrated by comparing the results of configurations $E$, $C$ and $F$, where the non-dimensional compact support length, $h$, was varied between $0.04$ to $0.01$, Fig. 5.7. The figure shows the presence of enormous fluctuation in velocity when the inter-particle distance is large, though, the steady state velocity profiles have significantly less fluctuations for all the three cases cited. When the system has as few particles as 1208 (Fig. 5.7a1,a2), the mass of each particle is comparatively high and any discrete movement of these particles would automatically cause large exchange of mass and momentum between the locations they move from and to. Since a decrease in inter-particle distance is always associated with smaller values of time step and longer execution time, one needs to weigh the gain in accuracy against the execution time while deciding the discretisation level in a particular simulation. Particle number density, as we will see later, is also important to evolve the right physics under a given hydrodynamic condition.
Chapter 5: Single-Phase Flow

Fig. 5.6: Couette flow results with same configuration as Fig. 5.5 but the kernel proposed by Chaubal et al. (1997) is used. (a) Particle positions at \( t = 0.5 \). Use of this kernel shows absence of 'particle clumping' even though \( \text{IPDF} < 2/3 \). (b1-b3) Comparison of analytical and SPH velocity profiles at \( t = 0.05, 0.375 \) and 0.5 units of dimensionless time. The trend of standard deviations is similar to that with \( \text{IPDF} = 0.7 \) (Fig. 5.3).
Fig. 5.7: Effect of discretisation on accuracy of results in Couette flow experiments at \( Re=1, M=0.1 \). Plots of \( x \)-component of velocity against \( y \)-position of the particles at \( t=0.05 \) and \( t=0.5 \). (a1&a2) \( h=0.04, IPDF=0.6, N=1208 \); (b1&b2) \( h=0.02, IPDF=0.6, N=4764 \) and (c1&c2) \( h=0.01, IPDF=0.6, N=19020 \).

### 5.1.4 Density and \( y \)-Component of Velocity Distribution

The steady state density and \( y \)-component velocity profiles at \( Re=1 \) and \( M=0.1 \) are plotted in Fig. 5.8 for the same set of configurations described in Fig. 5.7 (i.e., configurations E, C and F). Beside the average velocities being close to zero, the velocity fluctuations are also seen to be very small even at moderate discretisation level (\( h=0.02 \)). It is interesting
to note that the density fluctuation is rather high (8%) and remains nearly same for all the three cases.

![Graphs showing variation of steady state dimensionless density and y-component of dimensionless velocity with y-position of particles for Couette flow at Re=1, M=0.1. Particle configurations: (a) h=0.04, IPDF=0.6, N=1208; (b) h=0.02, IPDF=0.6, N=4764 and (c) h=0.01, IPDF=0.6, N=19020.](image)

Though Couette flow is a unidirectional phenomena where the y-component of velocity should be zero, initial randomness in particle position causes the system to possess some amount of 'residual' kernel gradients (demonstrated in § 4.3.2) along y-direction. This means that the viscous and hydrostatic forces which depend on velocity and density gradients respectively, will be non-trivial even if the particle starts with zero velocity. The physics of Couette flow requires the y-component of hydrostatic force should be annihilated by the dissipative mechanism generated by the viscous force. In other words, in a properly defined Couette flow simulation, the rate of viscous momentum transfer along y-axis should be as much as the y-component of hydrostatic force.

The variation of density, an essential part of incompressible SPH where one actually adopts a 'relatively incompressible' equation of state, is obtained from the conservation of mass. Initial randomness in particle position also means existence of a certain amount of density variation within the system inherently. Considering these facts, a standard deviation of 8% in density estimation may be accepted.
5.1.5 Couette Flow at Different Reynolds Numbers

All the results presented so far are at $Re=1$ where the viscous force and inertial force are of the same order of magnitude. The issue of discretisation becomes an overriding factor when the ratio of these two forces becomes either very small or very high. At low Reynolds number, the hydrodynamics is dominated by the presence of large viscous force. An accurate resolution of the viscous term becomes essential and it is usually done by ensuring the viscous momentum does not propagate more than one inter-particle distance in any time step. This kind of stability criteria severely limits the size of time steps at low Reynolds number flows. Thus, the simulations at very low Reynolds number such as 0.01 require high degree of space and time discretisation. The results of Couette flow simulation at $Re=0.01$ are shown in Figs. 5.9 and 5.10 where configuration $G$ is used. Severe fluctuations in smoothed property feature at such low Reynolds number. Fig. 5.9 indicates that even at high number density of 19020 particles in the system, the steady state $x$-component velocity profile has about 16% fluctuation! Velocity fluctuations eventually die down to 2.3% if the experiment continues long enough, Fig. 5.10. However, the figure shows that the density fluctuation continued to increase until it reached a steady value of about 12% standard deviation for the Mach number of 0.01. The reason for such an increase is not clear.

Following the discussion on Mach number and compressibility of SPH liquid mentioned in § 4.4, it is understood that for a low Reynolds number of 0.01, a Mach number of 0.01 would only make the 'SPH liquid' too incompressible. At high level of incompressibility, a very small fluctuation in density causes large fluctuation in the hydrostatic pressure and as well as in the overall momentum balance for the SPH particles, and random initial distribution only adds to this maze of high fluctuations. Reynolds number being very small, the overall displacement of the particles in these simulations are extremely small. This means that the fluctuations observed in these experiments using an $IPDF<2/3$ may not be due to the formation of 'particle clumping'. Though the average smoothed properties show good agreements with the actual values,
the undesirable effects of fluctuations remain too high. In situations where the actual
displacements of the particles are extremely small (due to small Reynolds number),
regularly placed particles are expected to do much better since the gradient of properties
such as velocity, density etc. remain close to zero for all the particles in the domain.

Fig. 5.9: At very low or high Reynolds number, the level of discretisation needs to be high. Couette flow
results for $Re=0.01, M=0.01$. Here, $h=0.01, PPDF=0.6$ and $N=19020$. (a) Comparison of x-component of
velocity profiles with analytical solutions at $t=0.0005, 0.00375, 0.005$. (b) Steady state y-component
velocity (green) profile shows high fluctuations as well as large deviation from the expected profile i.e.,
zero; the smoothed density (red) profile shows the average value is very close to the actual value of fluid
density of unity (in dimensionless form).

Fig. 5.10: The exact experiment described in Fig. 5.9, but continued for very long time up to $t=0.05$. It
shows very good match between analytical and SPH simulations. (a) x-component of velocity profile,
matches very well with the analytical results and the standard deviations are insignificantly small; (b)
smoothed density and y-component velocity profiles showing that the curvy nature of $v$, caused due to very
small value of Mach number, eventually vanishes but density fluctuation increases.
Reduction in the speed of propagation of pressure wave (i.e., increase in Mach number) would logically reduce the fluctuations as shown in Fig. 5.11 (configuration $H$), where the fluctuations of all the parameters are significantly smaller than those in Fig. 5.9 though they are at same level of particle discretisation. However, the number of neighbors being very small, the viscous force does not get accurately estimated at this value of $IPDF$. This is indicated by poor agreement between the SPH and analytical results; particularly at the initial stage of the experiment. The way forward lies in increasing the number of neighbors since the cubic spline kernel has about 2% error in smoothing at $IPDF=0.7$ (from Fig. 4.2, we find the average number of neighbors to be 18-20 for this value of $IPDF$, and from Fig. 4.11a, we can find the error in average smoothed density to be about 2% for this value of number of neighbors) and the accuracy improves as the number of neighbors increases. The results of configuration I, plotted in Fig. 5.12 indicates the improvement in the agreement between SPH results and the analytical velocity profile at larger number of neighbors ($IPDF=0.5$).

Fig. 5.11: Density fluctuation is less since the fluid behaves as a relatively more compressible liquid due to increase in Mach number to 0.1 at $Re=0.01$. Here, $h=0.01, IPDF=0.6$ and $N=19020$. Though the match of all the properties are very good at steady state, the initial velocity profiles are far from accurate. At such small Reynolds number, the viscous force needs to be calculated more accurately. An $IPDF$ of 0.7 is not sufficient as it has about 2% error in smoothing when cubic kernel is used; on the other hand, more neighbors means instability and inaccuracy due to ‘clumping’.
As the Reynolds number increases, the nature of the flow gradually shifts from a viscous driven to inertia dominant. In other words, fluid viscosity becomes important at low Reynolds number while the fluid particle mass is more responsible for the overall motion of the fluid at higher Reynolds number. If we keep the mass of the system same, then the mass of each SPH particle becomes inversely proportional to the number of particles in the system. Larger number of particles in the domain means a reduction in the mass of each fluid particle. For an inertia dominated flow, the error due to convection of the particles from one point to the other reduces as the mass of each particle reduces. Associated with it, the time steps in an explicit scheme such as SPH also needs to be very small when the inter-particle distance is small. In Fig. 5.13a, the velocity and density profiles for Couette flow at Re=100 (configuration K) is plotted. The standard deviations for both u and v are extremely small (<2.5%) signifying that the very small value of time step used in the simulation indeed restricted the convective error. However, the density fluctuation remained high with standard deviation of about 12%. 

Fig 5.12: Couette flow results at Re=0.01, M=0.1, IPDF=0.5, h=0.01, N=27300. Because of more neighbors, evaluation of viscous force becomes more accurate and the agreement between analytical and SPH velocity is better than that in Fig 5.11. However, an IPDF<2/3 has resulted in 'particle clumping'.
In order to understand the effect of Mach number at higher Reynolds number, the results of another experiment at \( M = 0.1 \) is shown in Fig. 5.13b (configuration J). It is clear that at such low Mach number, slip occurs near the walls where apparently no-slip conditions were enforced. While the velocity fluctuations are less, the agreement of SPH velocity profiles with the analytical results are very poor. The velocity profiles for all three plots show waviness which might be arising due to large amount of hydrostatic pressure caused by the small Mach number. Comparison of the analytical velocity profile with that of the SPH result at the initial stage of the simulation probably indicates that the progress of the SPH simulation reached dynamic equilibrium earlier than predicted by the analytical results. If we draw a vertical line at \( \gamma = 0.5 \), then the velocity profiles in the two sections at all three temporal plots seem qualitatively symmetrical about this line. This probably indicates that the loss in momentum in the upper half of the periodic cell is compensated by the gain in momentum by the fluid in the lower half of the cell, thereby conserving the overall momentum of the system. Detailed explanation of SPH hydrodynamics at Mach numbers greater than unity at high Reynolds number may be found in § 4.4 and § 5.2.

5.1.6 Summary of Couette Flow Experiments

Results of Couette flow experiment at Reynolds number ranging from \( 10^2 \) to \( 10^2 \) has been reported in this section. The effect of various SPH parameters including number of particles, number of neighbors, levels of discretisation on stability of the fluid particles and accuracy of results have been systematically studied. Although in most of the cases the steady state solution matches the analytical solution rather well, the temporal behavior of the SPH particles is somewhat different for different configurations. Some of the points emerging from the experiments described above are:

- The constant velocities of the two boundary walls in Couette flow enter the hydrodynamic equations through surface integrals. In the absence of surface integrals, such boundary conditions in SPH are implemented by using
boundary particles, ghost particles etc. Thus, the treatments of boundary conditions are different in the present work.

- The usefulness of surface integral in the conservation equations to model constant velocity and pressure boundary conditions has been successfully demonstrated for a simple surface geometry.

- Regular positioning of particles is inherently an unstable scheme except when the relative displacements of particles are insignificant.

- Usually higher resolution of space at very small $Re$ and higher resolution in time at high $Re$ is essential for obtaining less error in incompressible hydrodynamics.

- Cubic spline kernel produces significant 'particle clumping' for $IPDF<2/3$ irrespective of initial particle positions.

- In order to represent the "relatively incompressible" nature of SPH liquid, the Mach number of the liquid must be varied with the Reynolds number. The findings from the present work corroborates with the views of Monaghan (1992) and Morris et al. (1997) at lower Reynolds numbers ($<1$) where the later suggested that a Mach number of 0.1 would be sufficient to model the low Reynolds number hydrodynamics correctly. At higher Reynolds number ($\approx 55$), use of higher Mach number ($M=0.5$) is not uncommon in SPH literature (Takeda et al., 1994) though no clear explanation was given. At moderate Reynolds numbers with finite number of particles often a Mach number greater than unity is necessary. In the following section, a specific example of single-phase flow at $Re=100$ elaborates further on the effect of Mach number in SPH liquids as viewed in the present work.
Fig. 5.13: (a) Couette flow at $Re=100$, $M=1.0$, IPDF=0.6, $h=0.01$, $N=19020$. The $x$-component velocity profiles are at $t=5$, 37.5 and 50 (in dimensionless unit), the dimensionless density and $y$-component dimensionless velocity profiles are $t=50$. The smoothed standard deviations for both $u$ and $v$ are strikingly small (<2.5%) but the match of $u$ is poor at initial stages when the predictions from SPH is generally more than the analytical solution. (b) Same configuration as (a) except $M=0.1$. The velocity profiles are wavy and show that the shear stress from the walls is not accurately transferred to the fluid.
5.2 Study on the Effect of Mach Number on Fluid Flow

No material is truly incompressible but it is often a good assumption for liquids. When using this assumption in connection with any numerical simulation it is necessary to devise some way to impose the physical mechanism that is responsible for the incompressibility. The underlying mechanism lies in the assumption that propagation of pressure wave in an incompressible fluid is much faster than the fluid itself. However, the question remains ‘how much faster?’. The answer probably lies in devising a Mach number that can bring out the physics of the flow, rendering the problem ‘solvable’ within a reasonable time and numerical accuracy. This means there could exists a small window of Mach number that would characterize certain flow, with the width of the window signifying ‘relatively incompressible’ nature of the liquid being modeled. In this section, an attempt is made to understand the physics and find such a window of Mach number for Couette flow at $Re=100$ where the motion of the fluid kept within a periodic cell was studied. Fig. 5.14 shows the details of periodic and wall boundary conditions for the experiment. The wall velocity ($U$) and the width of the cell ($W$) were used as length ($L_0$) and velocity scale ($V_0$) for non-dimensinalisation.

Simulations were carried out at five different Mach numbers of 0.1, 1, 2, 4 and 8. All parameters except the time step size were kept constant for these experiments. In Fig 5.15, the $x$-component velocities of all the particles in the periodic cell are plotted against their $y$-positions at $t=4$ and $t=16$. The particle positions long after the system attained steady state are shown in the same figure.
The plots clearly indicate that between $M=1$ and $M=4$, the overall behavior of the liquid does not change, but marked difference in the velocity profile as well as the particle positions may be observed once the Mach number falls outside this range.

The particles are found to arrange themselves in an ordered lattice-like structure, more akin to a high density fluid, at smaller values of Mach numbers (say, $M=0.1$) which indicates that the hydrostatic pressure in the system resembles relatively closer to that in an incompressible system. This also means that the viscous stress transferred from the wall needs to be resolved with high accuracy, i.e., large number of neighbors and very high number density and not to mention, a very small time step become obvious requirements for maintaining stability. At this stage, the choice of kernel function becomes critical and a higher order kernel with good stability property is required to accurately resolve the viscous momentum transfer from the walls. Use of higher order kernel further adds to the computational demand of the simulation. All these are required for the simulations to represent the behavior of an incompressible fluid more accurately, but the fact remains - however much we try to get closer to representing an incompressible fluid, there will still be considerable gap between our ability to numerically represent a liquid and the liquid itself. Thus, one may infer that there is a lower limit of Mach number for a given Reynolds number below which it is impractical to attempt any SPH simulation and this limit varies with the Reynolds number.

At higher Mach number, the fluid becomes too compressible and overly viscous as may be seen from the velocity profile at $M=8$ where the few fluid particles very close to the walls stick to them. The speed of propagation of pressure wave being very small at this Mach number, bulk of the fluid remains relatively less mobile and more compressible. A very high level of discretisation near the wall through employment of variable smoothing length is believed to improve the transfer of viscous stress from the wall. In real liquid, though a Mach number greater than unity cannot be conceived, the computational Mach number for the SPH liquid can, thus, be greater than unity under higher Reynolds number in order to recover the hydrodynamics accurately.
Chapter 5: Single-Phase Flow

(a) $y$

(b) $x$

$M=0.1$

$M=1$

$M=2$

$M=4$

$M=8$
5.3 Lid Driven Cavity Flow

Lid driven cavity flow is often used to test numerical methods where a fluid enclosed within four solid impermeable walls (in two-dimension), initially at rest, is set in motion by maintaining one of the walls at constant velocity. It differs from Couette flow only in terms of boundary conditions - presence of four walls means periodic boundary condition is not required. In stead of unidirectional flow found in the Couette flow, the fluid in cavity flow develops two-dimensional circulation. Accuracy of the method can be measured by the location of epicenter of circulation. The schematic of the boundary conditions for fluid flow in a square cavity is shown in Fig. 5.16. The wall moves at a constant velocity, $U$. The wall velocity and the width of the cavity are used as the representative velocity ($V_0$) and length ($L_0$) scales for non-dimensionalisation. All the hydrodynamic equations are exactly same as Couette flow. Two experiments at $Re=1$ and $Re=100$ were carried out to estimate the accuracy of the present SPH technique in inducing circulation through shear stress from the boundary. Figs. 5.17 and 5.18 show the comparison between SPH results and the result obtained using commercial software package, FLUENT at steady state. For the SPH results, the cavity was divided into 400 cells of equal size and average of the velocities of all the fluid particles within each cell was calculated.

Fig. 5.16: Schematic diagram showing boundary conditions in lid driven flow in a square cavity.
Fig. 5.17: Comparison of velocity vectors obtained from SPH simulation with the streamlines from FLUENT at $Re=1$, $M=0.1$, $N=3464$. The velocity vectors are obtained from SPH experiments while the streamlines are obtained from FLUENT simulations.

Fig. 5.18: Comparison of velocity vectors obtained from SPH simulation with the streamlines from FLUENT at $Re=100$, $M=1.0$, $N=13918$. The velocity vectors are obtained from SPH experiments while the streamlines are obtained from FLUENT simulations.
It is evident from the above comparisons that the centers for zero circulation match quite well between the two methods of solution, particularly at $Re=1$. However, at higher $Re (=100)$, there is slight deviation in the position of the main ‘zero recirculation’ point. The smaller recirculation zone near the dead zone (lower right corner of the cavity) could not be obtained in SPH experiment at $Re=100$ cited here, due to poor resolution of the domain. Proper circulation of the fluid also means that the two surfaces normal to the main direction of input velocity were able to stop the fluid particles from going out of the domain by developing the reaction force in the form of normal pressure that resisted the particles.

### 5.4 Poiseuille Flow

In the previous three sections, the concept surface integrals in the SPH constitutive equations to recover the hydrodynamic stresses from moving boundaries of very simple geometry was verified. Implementation of stationary boundary may be examined by carrying out numerical simulations of two-dimensional Poiseuille flow. In Poiseuille flow the fluid is usually set in motion by maintaining constant pressure difference between the inlet and outlet of a channel separated by two infinitely long stationary walls. The infinitely long channel is simulated in SPH by maintaining periodic boundary condition between the inlet and outlet of a finite length of the channel, Fig. 5.19. The fluid develops a parabolic velocity profile at steady state under laminar condition.

![Schematic diagram of two-dimensional Poiseuille flow.](image)

*Fig. 5.19: Schematic diagram of two-dimensional Poiseuille flow.*
In SPH, fluid pressure being an explicit function of density through the equation of state maintaining an accurate pressure gradient across the domain becomes quite tricky. For many applications, it may be simpler to use the dynamic pressure, \( p_d \), defined as

\[
p_d = p_t - p_h
\]  
(5.8)

where \( p_t \) and \( p_h \) are the total and hydrostatic pressures, respectively. Thus, the gradient of total pressure that appears in the Navier-Stokes equation may be expressed as

\[
-\frac{1}{\rho} \nabla p_t = -\frac{1}{\rho} \nabla p_d + \frac{1}{\rho} \nabla p_h = -\frac{1}{\rho} \nabla p_d + b
\]  
(5.9)

where \( b \) is force per unit mass. This shows that the effect of pressure gradient can be modeled by equivalent amount of body force. This approach (Morris et al., 1997) is used here to drive the fluid in Poiseuille flow. Use of body force means the SPH equations derived in § 3.1.2 need to be solved in their entirety without dropping the body force term. It may be noted that the body force, which accelerates the volumetric flow is not the acceleration due to gravity. Instead, an externally imposed force is applied that can be manipulated to obtain the desired pressure drop across the periodic cell.

In two-dimensional Poiseuille flow, the length scale \( L_0 \) is taken as the width \( W \) of the channel while the velocity scale \( V_0 \) is taken as the velocity at the center of the channel. For a given value of Reynolds number, the value of \( V_0 \) is obtained from Eqn. (5.). The body force required to achieve this Reynolds number is estimated from the Eqn. (5.) (Morris et. al., 1997):

\[
V_0 = \frac{Re \mu}{\rho L_0}
\]  
(5.10a)

\[
b_x = \frac{\rho V_o L_0^2}{8 \mu}
\]  
(5.10b)
where \( \mu \) and \( \rho \) are the density and viscosity of the fluid, \( b_x \) is the x-component of body force per unit mass of the fluid (the y-component is zero since the flow is along x-direction). Thus, as we change the Reynolds number, the body force per unit mass (may be termed as acceleration due to body force) also changes. The initial and boundary conditions for the two-dimensional Poiseuille flow are (in dimensionless form):

Initial conditions:

at \( t=0 \), \( u = 0 \) and \( v = 0 \) for all particles in the domain

at \( t \geq 0 \), the fluid is imposed with only x-component of body force

\[(5.11a)\]

Boundary conditions:

at upper wall, i.e., at \( y = 1 \), \( u_i = 0 \) and \( v_i = 0 \)

at lower wall, i.e., at \( y = 0 \), \( u_i = 0 \) and \( v_i = 0 \)

Periodic boundary condition along x-axis

\[(5.11b)\]

While the y-component of velocity of the particles should be zero, the series solution for the transient x-component velocity of any fluid particle \( i \) having its vertical position at \( y_i \) (measured from the lower wall) may be expressed as:

\[
   u(y_i, t) = 4y_i(y_i - 1) + \sum_{n=0}^{\infty} \frac{32}{\pi^3 (2n + 1)^3} \sin(ny_i(2n + 1)) \exp\left(\frac{(2n + 1)^2 \pi^2 t}{Re}\right)
\]

\[(5.12)\]

Eqns. (3.26-3.29) and (5.10-5.12) describe the transient hydrodynamics of isothermal flow of an incompressible fluid in Poiseuille flow. Numerical experiments were carried out at various Reynolds numbers and particle density. Results of some of the experiments are presented in Figs. 5.20-5.24.

In Fig. 5.20, x and y-component velocities and densities are plotted for Poiseuille flow at \( Re = 0.01 \) and \( M = 0.1 \). The SPH particles were initially placed in linear structure. Extremely small standard deviations in all smoothed properties are typical characteristic...
of a flow at such small Reynolds number. Since the effective movements of the particles are extremely low, the smoothed gradients of all quantities remain uninfluenced and the 'clustering' of particles usually prevalent in regularly placed system remains dormant. This is indicated by the small value of standard deviations (<1% for $u$). The results also show very good agreement with the analytical solutions both in space and time.

Fig. 5.20: Dimensionless velocity and density profiles for Poiseuille flow at $Re=0.01$, $M=0.1$ when the particles were placed in regular linear structure. (a) The $x$-component of SPH velocities (in blue color) are compared against the analytical solutions (pink color) at $t=0.0005$, $0.00375$ and $0.005$ units of dimensionless time. $IPDF=0.7$, $h=0.02$, $N=5041$. For the SPH results, the periodic cell is divided into 40 bins of equal width and the average of the particle velocities in each cell along with the standard deviations among the particles within the cells are reported here. The standard deviation is less than 1% and the agreement in velocity is very good. (b) $y$-component of velocity profile (in green) and density profile (in red) after reaching steady state, at $t=0.005$.

However, once the particles are initially placed randomly, the simulations show high level of fluctuations similar to what was observed in Couette flow. Fig. 5.21 shows the velocities and density at a very small Reynolds number, $Re=0.01$. The accuracy of the results, particularly of the $x$-component of velocity is found to deteriorate as the flow
progresses. It may be noted that unlike the other two forces (i.e., hydrostatic and viscous), the body force is not a surface force and consequently, it appears in the equation of motion without any surface integral. This means that the smoothing operation now becomes equally important if not more, since the body force is the main driving force in the present formulation of Poiseuille flow. A simulation with a large number of neighbors (IPDF=0.25), as shown in Fig. 5.22, would obviously be more accurate in terms of the average properties. This is also associated with large amount of fluctuations since the value of IPDF is less than 2/3.

Fig. 5.21: Poiseuille flow with randomly inserted particles at Re=0.01, M=0.1. N=15309, IPDF=0.5, h=0.02. (a) dimensionless x-component of SPH velocities (in blue color) are compared against the analytical solutions (pink color) at t=0.0005, 0.00375 and 0.005 units of dimensionless time. (b) y-component of velocity profile (in green) and density profile at steady state, at t=0.005. High degree of fluctuations (15% in u and v) in the properties mark the simulation at low Reynolds number. The average values of u are about 10% more than analytically obtained velocities.
At higher Reynolds number, such as at $Re=1$ (Fig. 5.23) and $Re=125$ (Fig. 5.24), the agreement between SPH results and analytical solution is generally very good. It may be noted that in these experiments rather large values of kernel compact support length were used. The computational time is directly proportional to the number of neighbors of each particle has. This makes the Poiseuille flow simulations extremely computer intensive and in order to reduce the execution time the discretisation levels were generally kept low.

![Graphs](image)

**Fig. 5.22:** Steady state (at $t=0.005$) (a) dimensionless velocity and (b) dimensional density distribution for Poiseuille flow at $Re=0.01$, $M=0.1$. $N=6676$, $IPDF=0.25$, $h=0.04$. More number of neighbors has improved the smoothing of body force that drives the flow.

![Graphs](image)

**Fig. 5.23:** The body force in Poiseuille flow needs better smoothing at all times. Results of Poiseuille flow at $Re=1$, $M=0.4$, $N=6676$, $IPDF=0.25$, $h=0.04$. (a&b) $x$-component velocity profiles at $t=0.3$ and $t=6$. Though there is about 10% fluctuations, the average velocity matches very well with the analytical solutions. (c) $y$-component velocity and density profiles at steady state, $t=6$. 

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5. Flow Past a Circular Cylinder

Flow past solid bodies has been the subject of great interest to the fluid dynamics community for many years. Numerical simulation of flow around a solid body forms the basis for subsequent developments that eventually lead to the complex hydrodynamics of multi-particle solid-liquid suspensions. By varying the fluid and solid properties including the nature of solid-solid interactions in a two-phase system at different length scales, one can cover a wide range of substance which, albeit two-phase system, remarkably differ in their rheological properties. Almost every form of non-Newtonian behavior including shear thinning and thickening, yield stress, normal stress differences, etc. has been observed (Bagnold 1954; Russel 1980; Gadala-Maria and Acrivos 1980; Kreiger, 1972) in solid-liquid flows. Accurate modeling of flow around a single cylinder, presented in this section, naturally becomes the stepping stone for estimating effective suspension properties as will be seen in the next chapter.
Relative motion between a fluid and any solid object inevitably produces drag, the value of which depends on the flow Reynolds number, the shape of the body and most importantly on accurate implementation of the boundary conditions. In this part of the work, the focus is primarily restricted to liquid flow around a stationary body in two-dimension. For ease of verification of the results, all the experiments were performed using a rigid neutrally buoyant cylinder placed across the flow which, in two-dimensions, reduces to flow around a cylinder. The code being developed in the present work, however, can take up any other – regular or irregular shape of the object.

The main difference between the developments presented in previous sections and in this part of the work is in the presence of a solid boundary or solid-liquid interface within the fluid, and this makes the problem more complex and challenging. Though physically challenging, it is found to be rather trivial to set up such a boundary in the current formulation of SPH. In the most generalized sense all that is required is a mathematical definition of the surface contour and in this particular case it happens to be the equation of a circle. While the mass and momentum conservation equations for the liquid phase essentially remain the same the hydrodynamics of the liquid phase greatly changes under the influence of the solid cylinder.

The stationary fluid in the system can be imparted motion either by shear stress from two parallel walls or by the exertion of a body force. The overall effect on the fluid hydrodynamics greatly differs resulting in different drag coefficients. These two schemes of imparting fluid motion separately dealt with separately in the following sections.

### 5.5.1 Imparting Fluid Motion by Exerting Body Force

Let us first consider a two-dimensional doubly periodic cell (i.e., periodic boundaries along $x$ and $y$-axes) of fluid of certain density, as shown in Fig. 5.25 without the cylinder therein. Employing body force on this volume of fluid (considering cell is of unit length in the third dimension) means that the fluid will keep moving at the same acceleration as
long as the force is imposed. The viscous resistance to the flow, which only arises if there is any relative movement of the fluid phase with respect to any other phase present in the system, is absent. The fluid would move as a block and its temporal velocity can be analytically obtained from simple particle mechanics i.e., Newton’s second law of motion. Tests with present SPH code showed excellent match of the temporal velocity of the system with that obtained from particle mechanics.

![Periodic boundary applied along X and Y direction of a two-dimensional domain](image)

**Fig. 5.25:** Periodic boundary applied along X and Y direction of a two-dimensional domain

![Cylinder within periodic cell](image)

**Fig. 5.26:** (a) The cylinder occupies a significant portion of the periodic cell; (b) the cylinder occupies extremely small portion of the periodic cell. The dotted circle schematically shows the region of the fluid that may come under the influence of the body.

Now, as soon as an object is introduced, say a cylinder, the drag is generated around the cylinder. Within a close proximity of the cylinder the fluid will decelerate and a velocity gradient will be established as time goes by. If the cylinder is relatively large compared to the periodic cell (Fig. 5.26a), then the entire fluid domain might experience the influence of drag force and the system might eventually come to equilibrium. On the other hand, if the cylinder is too small compared to the size of the periodic cell (Fig. 5.26b) the effect of drag may not reach the fluid elements far away from the cylinder wall.
and these fluid elements will keep moving under the influence of the body force. This means, the free stream velocity or the ‘undisturbed velocity’ (i.e., velocity of the fluid elements far away from the cylinder) will keep increasing as long as the simulation continues and estimation of drag under such condition would be of no great value. This explains the importance of the relative size of the cylinder with respect to the flow domain. Examples of situations where symmetry exists along as well as perpendicular to the direction of main flow includes fluid flow across banks of tubes in a heat exchanger as shown in Fig. 5.27.

Fig. 5.27: Application of periodic boundary condition along both the axes resembles flow around tube banks. The dotted region may be ideally considered as a periodic cell.

Various studies (Humby 1999; d’Humières and Lallemand 1986a, b) have shown that in case of channel flow around a cylinder, the ratio of $W/D_c > 6-8$ is large enough not to influence the estimation of drag force. Here, $W$ is the width of the periodic channel and $D_c$ is the cylinder diameter. This means that a square lattice of periodic length of up to $8D_c$, see Fig. 5.28, approximately guarantees that the body force applied on the fluid and the drag force generated thereupon would bring the system to equilibrium.

Fig. 5.28: A square lattice of up to $8D_c$ ($D_c = \text{diameter of the cylinder}$) is expected to bring the flow to equilibrium at the Reynolds numbers investigated.
In a typical experiment, schematically shown in Fig. 5.29, the fluid and the cylinder were initially at rest and a constant body force was applied at time $t \geq 0$. Unsteady state SPH equations were solved until the change in flow parameters such as velocity, drag force etc. became significantly small. The drag coefficient was calculated by summing up the contributions from the form drag (due to hydrostatic pressure) per unit length of the cylinder and the viscous drag (due to fluid viscosity) per unit length of the cylinder as:

$$C_d = \frac{P_c + V_c}{\frac{1}{2} D_c}$$

(5.13)

where $D_c$ is the diameter of the solid cylinder, $P_c$ is the summation of the surface integral component of the hydrostatic force per unit length for all the particles within $2h$ distance from the cylinder surface and $V_c$ is the summation of the surface integral component of the viscous force per unit length for the same set of particles. As body force is not a surface force, it does not contribute to the drag force around the cylinder. The SPH expressions for the various components of drag force are (in dimensionless form):

**x-component of Pressure drag:**

$$- \frac{1}{M^2} \left[ \sum_{j=1}^{N} \left[ W_{ij} \delta x + \frac{\rho_i}{\rho_j} \int W_{ij} \delta x \right] \right]$$

(5.14)

**x-component of Viscous drag:**

$$- \frac{1}{\text{Re}} \left[ \sum_{j=1}^{N} \rho_i \left( \frac{\tau_{xx}}{\rho_j^2} \right)_i \delta x + \left( \frac{\tau_{yx}}{\rho_j^2} \right)_i \delta y \right] + \rho_i \left( \frac{\tau_{xx}}{\rho_j^2} \right)_i \delta x + \left( \frac{\tau_{yx}}{\rho_j^2} \right)_i \delta y$$

**y-component of Pressure drag:**

$$- \frac{1}{M^2} \left[ \sum_{j=1}^{N} \left[ W_{ij} \delta y + \frac{\rho_i}{\rho_j} \int W_{ij} \delta y \right] \right]$$

**y-component of Viscous drag:**

$$- \frac{1}{\text{Re}} \left[ \sum_{j=1}^{N} \rho_i \left( \frac{\tau_{xy}}{\rho_j^2} \right)_i \delta x + \left( \frac{\tau_{yy}}{\rho_j^2} \right)_i \delta y \right] + \rho_i \left( \frac{\tau_{xy}}{\rho_j^2} \right)_i \delta x + \left( \frac{\tau_{yy}}{\rho_j^2} \right)_i \delta y$$
In order to compare the simulation results, exactly similar experiments were carried out using the commercial software package ‘FLUENT’. In FLUENT, while choosing the option of periodic cell, the software requires the value of pressure drop or average mass flow rate across the cell as input. The time average mass flow rate of the fluid through the periodic cell, estimated from the fluid velocity profile (along line $B$ in Fig. 5.29) of the SPH simulations was used as the input in FLUENT. The objective of such comparison is to estimate the drag coefficients using two different techniques when same mass of fluid flows through the same periodic cell. It may be noted that in case of ‘FLUENT’ the incompressible code was executed. Comparison of velocity profiles along various cross sections (Morris et. al., 1997) of the cell would provide qualitative indication of the performance of the present SPH algorithm. Experiments were carried out at various Reynolds numbers. In Table 5.2, some of the numerical details of the three experiments to be presented here are given. The term ‘solid fraction’ in two-dimensional system defines the ratio of the area of the solid cylinder to the area of the periodic cell. In solid-liquid suspensions with many solid particles, the concentration of the suspension is generally represented by this term.

The results of three experiments with the same configuration but with different Reynolds number are presented below. In all cases, the width of the lattice ($W$) was used as the characteristic length ($L_0$). In absence of any prior estimation of the steady state
maximum velocity in the system where there is no domain boundary, the velocity obtained from Eqn. (5.10a) was used to calculate the maximum velocity. This was duly used as the measure for velocity scale \((V_o)\). The Reynolds number used in Eqn. (5.10a) was subsequently used for calculating \(Re_c\), the Reynolds number based on the cylinder diameter. For estimation of body force, Eqn. (5.10b) was used. The Mach numbers for the flow were changed in each experiment to reflect the 'relatively incompressible' nature of SPH liquid.

Table 5.2: Input data for experiments on flow around cylinder using body force

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cylinder dia, (D_c) =</td>
<td>4 cm</td>
</tr>
<tr>
<td>Lattice width, (W) =</td>
<td>10 cm</td>
</tr>
<tr>
<td>Lattice length, (L) =</td>
<td>10 cm</td>
</tr>
<tr>
<td>Compact support length, (h) =</td>
<td>0.1 cm</td>
</tr>
<tr>
<td>Number of SPH particles, (N) =</td>
<td>12135</td>
</tr>
<tr>
<td>Liquid viscosity, (\mu) =</td>
<td>0.01 gm/cm.s</td>
</tr>
<tr>
<td>Liquid density, (\rho) =</td>
<td>1 gm/cm³</td>
</tr>
<tr>
<td>Solid fraction = 12.6%</td>
<td></td>
</tr>
</tbody>
</table>

Case 1: \(Re_c = 0.5\)

It was mentioned in Chapter 4 that for any flow Reynolds number, there is a small window of Mach number within which the hydrodynamics of the flow is accurately represented. In order to demonstrate that, a Mach number of 0.4, slightly higher than 0.1 was chosen for this Reynolds number. In Fig. 5.30(a, b), the \(x\)-component velocity of the SPH particles as a function of their vertical positions at planes \(A\) and \(B\) (shown in Fig. 5.29) have been plotted along with the velocity profiles obtained from repeating the experiment using FLUENT. The figure shows very good agreement between the two techniques. Comparison of \(y\)-component of velocity distribution for all the SPH particles with the nodal values from FLUENT may be found in Fig. 5.31. At such low Reynolds...
number, though the symmetry of $y$-component of velocity observed in 'FLUENT' result is very obvious, there is slight lack of symmetry in the SPH results. The skewness in the $y$-component velocity profile obtained from SPH simulation is also reflected in the velocity contour plots in Fig. 5.32. Both are instantaneous velocity plots and since it is known that velocity fluctuations are usually present in SPH simulations, an average of the velocity over several time steps might even out the asymmetry in SPH results. It would also be interesting to see whether slight variation in Mach number could bring in the symmetry in the velocity contour. Due to paucity of time, such experiment was not attempted. The figures qualitatively demonstrate good agreement between the standard method of CFD with SPH in simulating flow around cylinder at this low Reynolds number. The extent of agreement can further be quantified by estimating the components of the drag coefficient using both the techniques.

In Table 5.3 the drag coefficients separately obtained from the viscous and pressure force using the above two techniques are compared. The results show that the overall drag coefficient obtained from SPH is lower by about 10% from the corresponding FLUENT
results. However, the difference in the viscous drag coefficient between the two techniques is much less. Relatively large difference in the hydrostatic drag coefficient may possibly be due to the use of a high Mach number.

Fig. 5.31: Comparison of y-component of velocity for the entire domain at various x-location in the domain; a) from FLUENT; b) from present SPH calculations at Re = 0.5.

Fig. 5.32: Velocity contours obtained from (a) FLUENT (velocity in m/s) and (b) from present study (velocity in cm/s) for flow around cylinder at Re = 0.5.
Table 5.3: Comparison of drag coefficients at $Re_{c}=0.5$

<table>
<thead>
<tr>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>SPH</td>
<td>FLUENT</td>
<td>SPH</td>
</tr>
<tr>
<td>$x$-component</td>
<td>40.07</td>
<td>38.71</td>
<td>25.9</td>
</tr>
<tr>
<td>$y$-component</td>
<td>0.95</td>
<td>0</td>
<td>0.79</td>
</tr>
<tr>
<td>$y$-component</td>
<td>0</td>
<td>0.79</td>
<td>1.74</td>
</tr>
</tbody>
</table>

**Case 2: $Re_{c}=7.5$**

A Mach number of 1 was used for this experiment. Fig. 5.33 shows the $x$-component of velocity along the two locations of the periodic cell indicated in Fig. 5.29. Fig. 5.34 compares the $y$-component of velocity profile along the length of the cell for all the particles in SPH simulation with similar experiment using ‘FLUENT’. It is interesting to note that the symmetry in the $y$-component of velocity profile observed at lower Reynolds number (Fig.5.31a) using ‘FLUENT’ not any more present at the current Reynolds number. It compares very well with the results from FLUENT, Fig. 5.34(a). An overall idea of the velocity contours for the entire domain for both the techniques are shown in Fig. 5.35. It may be interesting to note from Fig. 5.36, how the $x$ and $y$-components of viscous drag (presented in the form of coefficient using Eqn. 5.13) dynamically converge to the steady state value. The following table summarizes the drag coefficients for $Re_{c}=7.5$.

![Fig. 5.33: Comparison of x-component of velocity profiles (a) along path B, (b) along path A indicated in Fig. 5.29 after steady state is reached. The pink points are the data points from similar experiments using FLUENT; the blue points are from the present SPH simulations at $Re_{c}=7.5$.](image-url)
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Fig. 5.34: Comparison of y-component of velocity for the entire domain at various x-location in the domain; a) from FLUENT; b) from present SPH calculations at Reₜ=7.5.

Fig. 5.35: Comparison of velocity contours obtained from FLUENT (velocity in m/s) and from present study (velocity in cm/s) at Reₜ=7.5.

Table 5.4: Comparison of drag coefficients at Reₜ=7.5

<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td></td>
<td>SPH</td>
<td>FLUENT</td>
<td>SPH</td>
</tr>
<tr>
<td>x-component</td>
<td>2.1</td>
<td>2.7</td>
<td>2.34</td>
</tr>
<tr>
<td>y-component</td>
<td>0.04</td>
<td>0</td>
<td>0.18</td>
</tr>
</tbody>
</table>
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Fig. 5.36: Temporal profile of x (blue) and y (violet)-components of viscous drag force for flow around a periodic lattice. Each point in the curves is an instantaneous estimation of the drag coefficient.

**Case 3: \( Re_c = 75 \)**

The experiment described above was repeated with a higher Reynolds number of 75. The Mach number used for this experiment was 2. Comparison of velocity magnitudes may be found in Fig. 5.37 while the velocity contours obtained from the SPH experiment and from FLUENT are reported in Fig. 5.39. Fig. 5.38 shows a comparison of the y-component of fluid velocity as a function of the length of the periodic cell. Though the nature of the velocity profiles are similar, SPH results are typically marked by larger fluctuations in the y-component of velocity. The fluctuations can possibly be reduced by improving the discretisation level of the fluid particles. The qualitative agreement between the two techniques is excellent. The quantitative comparison of drag coefficients at \( Re_c = 75 \) is made in the following table.
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Fig. 5.37: Comparison of x-component of velocity profiles (a) along path B, (b) along path A indicated in Fig. 5.29 after steady state is reached. The pink points are the data points from similar experiments using FLUENT; the blue points are from the present SPH simulations at Reₚ = 75.

Fig. 5.38: Comparison of y-component of velocity for the entire domain at various x-location in the domain; (a) from FLUENT; (b) from present SPH calculations at Reₚ = 75.
8.39a-04
7.55o-04
6.719-04
5.87e-04
5.030-04
4.1 ge-04
3.36e-04
2.52o-04
1.680-04
8.390-05
0.000+00
0.006
0.066

Fig. 5.39: Comparison of velocity contours obtained from FLUENT (velocity in m/s) and from present study (velocity in cm/s) at Re, = 75.

Table 5.5: Comparison of drag coefficients at Re, = 75

<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td></td>
<td>SPH</td>
<td>FLUENT</td>
<td>SPH</td>
</tr>
<tr>
<td>x-component</td>
<td>0.2955</td>
<td>0.3611</td>
<td>0.4187</td>
</tr>
<tr>
<td>y-component</td>
<td>0.0044</td>
<td>0</td>
<td>0.09</td>
</tr>
</tbody>
</table>

5.5.1.1 Effect of Discretisation

In the above experiments, the discretisation parameter, \( h \), was kept unchanged. A flavor of qualitative as well as quantitative variation of the results may be obtained by repeating one of the above experiments described above, namely for \( Re = 7.5 \), with a coarser particle density i.e., larger value of \( h \). In this experiment the value of \( h \) was doubled; as a result there were only 3007 particles in the system. In Fig. 5.40 a comparison is made of the smoothed velocities for the two situations. The excellent agreement between the velocity profiles seen in these plots is also reflected in the velocity vector plots shown in Fig. 5.41. Thus, for the overall drag coefficient, it is not surprising to obtain a value of 4.47 at a relatively small level of discretisation as opposed to 4.44 with 12135 particles.
Fig. 5.40: Comparison of particle positions, $x$ and $y$-component of velocity distribution at steady state at two levels of discretisation for flow around cylinder at $Re_c = 7.5$. a, c and e are for $N=3007$; b, d and f are for $N=12135$. Average number of neighbors kept constant for the experiments.
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(a)

(b)

Fig. 5.41: Velocity contours for $Re_c = 7.5$ at two different discretisation levels: a) $N=3007$ and b) $N=12135$. The plots are very similar except, in case of (b), due to lack of particles in the system, the contours are not as smooth as seen in (a). Velocity is in cm/s

Finally, the variation of drag coefficient with Reynolds number is plotted in Fig. 5.42. The plot also indicates the values of drag coefficient from similar experiments using FLUENT. In some of the cases, the agreement of results is so good that the data points are practically indistinguishable in the plot.

Fig. 5.42: Comparison of overall drag coefficients for flow around cylinder between SPH results and the results obtained from FLUENT.
5.5.2 Imparting Fluid Motion by Shear Stress From Walls

Imparting fluid motion by shear stress from moving walls has already been dealt with in great details in Couette flow. In the event that both walls move in the same direction, the fluid will eventually come to steady state and all the SPH particles would move at the same velocity as that of the moving walls. Once a cylinder is placed at the center of the periodic cell and held firmly in position, the fluid starts experiencing the drag. A further verification of the present method of estimating drag coefficient is attempted in this part of the work. The situation is schematically shown in Fig. 5.43.

![Schematic diagram of flow around a stationary cylinder when the fluid is imparted motion by moving walls.](image)

Experiments were carried out for the same three configurations described in the preceding section. The diameter of the cylinder and the velocity of the moving walls ($U$) are $L_0$ and $V_0$ respectively, for these simulations. Due to the presence of the walls the number of particles in the current simulations reduced to 11980 instead of 12135 as indicated in Table 5.2 for the previous set of experiments. In each case, the experiment was carried out until the system reached steady state. The velocity contours from the SPH experiments are shown in Fig. 5.44. The figure also contains the velocity contour plots of similar experiments using FLUENT. The plots qualitatively indicate good agreement between the two methods. The drag coefficients calculated from these experiments are plotted in Fig. 5.45. There is about 20% difference between the two methods.
Fig. 5.44: Velocity contour plots for flow around a stationary cylinder placed between two parallel plates moving in the same direction: (a-c) using FLUENT at $Re_c = 0.5, 7.5$ and 75 respectively, velocity in m/s; (d-f) using SPH at $Re_c = 0.5, 7.5$ and 75 respectively, velocity in cm/s.
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5.5.3 Summary of Flow Past Circular Cylinder

Study of flow past stationary cylinder is of great importance in engineering hydrodynamics because of various reasons. In this preceding section, the study of liquid flow around a stationary solid cylinder at various Reynolds numbers and different values of particle density is reported. The fluid was imparted motion either by body force or by shear stress from moving walls. The drag force was measured and compared with results obtained from similar experiment using the conventional software FLUENT. The conclusions from these experiments are as follows:

- By examining the velocity profiles, one can say that the current method of solving Navier-Stokes equation by SPH technique produces qualitatively satisfactory results.

- The overall drag coefficients obtained from the SPH experiments are about 10% lower than those obtained using FLUENT when body force was used; the difference was about 20% in the other configuration. It may be possible to

Fig. 5.45: Comparison between SPH and FLUENT estimates of overall drag coefficients for flow around cylinder when the motion is imparted by moving walls.
improve upon the accuracy of SPH results by using higher level of discretisation, or a higher order smoothing function with better stability properties.

- Considering the random nature of the initial placement of particles and the inherent approximations therein, the results of the above experiments are considered to be very encouraging.

5.6 Summary

In this chapter, isothermal viscous flow of liquid was studied to show that the present method of surface integral could be implemented for simple as well as complex shaped boundary using numerical integration. Imposition of boundary condition required the knowledge of the equation of the surface. The method is more convenient and efficient to model solid surfaces as opposed to some of the currently available methods where boundary particles are required to model solid surfaces or solid objects. As a consequence, there is substantial reduction in computational load both in terms of memory and speed. The method was tested extensively using a number of benchmark problems including Couette and Poiseuille flow, flow in a lid driven cavity and flow around cylinder. The test cases differed in the complexity of the shape and kinematic conditions of the boundaries they included. The tests all showed that under optimal conditions, the method for imposing boundary conditions is robust, stable and capable of yielding accurate results both in space and time.

During the tests it became clear that initial particle distribution (regular or random) plays an important role in SPH. For very low Reynolds number flow, since the actual displacements of the fluid particles were very small, particles may be placed in regular grids. However, at moderate and high Reynolds numbers, initial position of particles in regular grids must be avoided as it causes instability and delay in reaching steady state due to particle clumping. Like other discretisation schemes, accuracy of the simulations
depended on time and space discretisation particularly at very low and high Reynolds numbers.

The formulation developed in the later part of this chapter to estimate fluid-solid hydrodynamic interaction at the individual solid surface level will now be utilized in the next chapter to assess the motion of single and multi-particle solid-liquid systems when both the phases move.
Chapter 6

TWO-PHASE SOLID-LIQUID FLOW EXPERIMENTS

Logic is invincible, because in order to combat logic it is necessary to use logic.
-Pierre Leon Boutroux
In Chapter 5 a detailed study of single-phase flow was carried out where the fluid was imparted motion either by the body force or by the shear stress from moving walls. Fluid flow experiments around a stationary solid cylinder were also reported in the same chapter. From the latter studies the drag force around a stationary solid cylinder was estimated at various Reynolds numbers. While the outputs from such ‘static’ simulations are useful in developing a better understanding of some fundamental aspects of hydrodynamic interactions, they serve very little in assessing the complex behavior of a multi-solid particle-fluid system when both phases are moving. If we imagine a situation where the solid particles are suspended in a fluid medium and move due to some external force, there will be occasions when some of these solid particles come close to each other posing greater complexity in the hydrodynamics of the system. The situation would be even more complex when variations of shape and size of these particles are taken into consideration. The presence of various inter-particle and particle-fluid forces makes a remarkable difference in the overall system behavior between the ‘static’ and the ‘dynamic’ simulations in a solid-liquid suspension. It may also be said that by performing dynamic simulations of a solid-liquid suspension, one can estimate effective suspension properties that characterize the system in a mean-field manner. This chapter exclusively deals with experiments and issues related to the coupled motion of solid particle(s) and the surrounding fluid medium.

It is obvious that the first stage in the dynamic simulation of a multi-particle fluid system is to develop and test the model with only one particle, which can then be refined to include various forces such as the lubrication force, solid-solid interactions, etc. to simulate a multi-particle suspension. Since SPH is a Lagrangian and particle-based technique where all hydrodynamic quantities are associated with the fluid and solid
particles, modification of such a code either to include more of solid particles or to include various force models is a rather trivial exercise.

The SPH model for the fluid phase developed and verified in the last three chapters is now to be integrated with another particle-based model of similar type that describes the motion of the solid particles. Being solid objects, the conservation of mass for the solid particle phase is satisfied as long as the number of solid particles in the system remains the same. The conservation of momentum for each of the solid particles is obtained in exactly the same way as with SPH fluid particles; i.e., by using Newton's second law of motion. The rotational motion of the solid particles are neglected to keep the simulations simple; and only translational motion is considered for the development of the formulation. In that case the time rate of change of velocity and displacement for each particle is obtained from:

\[ M_c \frac{dU}{dt} = F \]  \hspace{1cm} (6.1)

and

\[ \frac{dx}{dt} = U \]  \hspace{1cm} (6.2)

where \( M_c, U \) and \( x \) are the mass, the instantaneous velocity and the position vector of the solid particle respectively. The net force, \( F \), on the particle depends on a wide range of issues. It includes forces arising out of the local fluid dynamics, Brownian forces, electrostatic forces and particle-particle interactions. The relative importance of the various forces on a particle varies with the particle size, fluid flow rates, surface and fluid chemistries, and other factors such as the local solid particle distribution. In principle, all of these forces and dependencies can be incorporated within the model developed in the present work; the main constraint on the amount of detail included is the level of discretisation relative to the range of the forces in question. To keep matters simple, the current study only includes hydrodynamic forces for single-particle-fluid case. Force considerations for multi-particle systems, where the solid particles are too close to
neglect each other's presence will be discussed separately in § 6.2. The value of $F$ in the present study is obtained from the fluid drag (see Eqn. 5.14) when there is only one solid particle in the fluid domain. The velocity and displacement of the solid particle are obtained from Eqns. (6.1) and (6.2) by performing time integration. Techniques such as the Velocity Verlet method described in § 3.5 can be used for the time integration.

This completes the definition of the coupling of the motion of the solid and the liquid in a two-phase flow. The validation of such coupled models can be performed in many ways. In the next two sections (§ 6.1 and § 6.2) a few test cases for coupled motion of one solid object are considered while experiments with two or more particles will be discussed in § 6.3 and § 6.4. Estimation of the effective viscosity of dilute multi-particle systems will also be addressed in § 6.4. The chapter is concluded with the summary of observations and comments on the simulation test case results.

6.1 Coupled Motion of Single Particle and Fluid

Tests considered in this part of the work include:

- Two-dimensional study of the motion of a solid cylinder heavier than the surrounding liquid, through a channel of stationary liquid.
- Motion of a neutrally buoyant cylinder within a two-dimensional channel where the motion of the liquid is imparted by shear stress from the walls.

For all the experiments described in this section, the fluid particles were introduced randomly in a two-dimensional channel with periodic boundary condition along x-axis. The periodic channel was bounded by two walls placed $W$ distance apart. Cubic spline kernel with $IPDF=0.7$ was used for all smoothing operations. The longitudinal axis of the cylinder is along the normal to the paper. Thus, in a 2D simulation, the cylinder was represented by a circle the surface of which was approximated by a polygon of 100 straight line segments. The fluid was considered incompressible and Newtonian. The system was initially at rest and only the translational motion of the cylinder was
considered. The motion of the cylinder and the fluid developed depending on the specific boundary conditions mentioned in each section.

### 6.1.1 Sedimentation Experiment

When a heavier body is dropped into a stationary viscous liquid placed within a channel between two parallel stationary solid walls, the interactions of the two forces e.g., force due to the body's own weight (including fluid buoyancy) and the fluid drag generated owing to the body's motion bring the body to dynamic equilibrium. As a consequence, the body moves at constant velocity known as terminal settling velocity. Measurement of terminal settling velocity has been the subject of experimental and theoretical studies for many decades. Apart from numerically measuring the terminal velocity, mathematical modeling of this system has also been gainfully utilized to observe complex phenomena such as particle migration, drifting, kissing, tumbling etc. in single and multi-particle sedimentation experiments (Hu et al., 1992; Feng et al., 1994; Johnson and Tezduyar, 1996). Due to such involved nature of the problem, it is usually considered as separate a topic of research in its own right. Since the stress in the present work is more on demonstrating the ability of the novel SPH formulation to capture the basic philosophy of such complex phenomena rather than investigating the details of one particular situation, the current study is restricted to estimating the terminal velocity of a falling cylinder only. In this case, the SPH model is developed to measure the terminal velocity of a cylinder falling perpendicular to its longitudinal axis.

A channel of width $W$ and infinite length is simulated by applying periodic boundary conditions to a cell of length $L$ as shown in Fig. 6.1. The periodic boundary condition is applied to the fluid as well as the cylinder which means the cylinder is repositioned at $x=0$ once it reaches the end of the channel at $x=L$, keeping the velocity of the cylinder unchanged. The ratio of the length of the periodic cell to the diameter of the cylinder should be kept high to ensure that the fluid motion behind the cylinder does not influence the stationary fluid in front of the moving cylinder.
Fig. 6.1 also shows a schematic of the various forces that act on the cylinder. The net resultant force per unit length of the cylinder along positive x and y directions, acting on the cylinder due to its own weight, buoyancy and the surface forces due to the surrounding fluid is:

\[ F_x = \left( \rho_c - \rho_f \right) f \frac{\pi}{4} D_c^2 - F_{sx} \]
\[ F_y = F_{sy} \tag{6.3} \]

where \( \rho_f \) is the fluid density, \( \rho_c \) is the cylinder density, \( f \) is the acceleration due to gravity acting along positive x direction and \( D_c \) is the cylinder diameter. Generally, \( F_{sx} \) is known as drag force per unit length of the cylinder and \( F_{sy} \) is known as lift force per unit length of the cylinder. The drag force, \( F_{sx} \), imparted by the surrounding fluid onto the cylinder surface at steady state is given by:

\[ F_{sx} = C_d \frac{1}{2} \rho_f V_i^2 D_c \tag{6.4} \]
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where $V_t$ is the terminal settling velocity of the cylinder and $C_d$ is the drag coefficient. The net force along $x$ direction acting on the cylinder at steady state being zero, from Eqns. 6.3 and 6.4, the expression for the drag coefficient is obtained as:

$$C_d = \frac{(\rho_c - \rho_f) \frac{\pi}{4} D_c}{\frac{1}{2} \rho_f V_t^2}$$  \hspace{1cm} (6.5)

The corresponding Reynolds number is:

$$Re_c = \frac{D_c V_t \rho_f}{\mu}$$  \hspace{1cm} (6.6)

where $\mu$ is the fluid viscosity. In the right hand side of Eqn. (6.5), all quantities except $V_t$ are known beforehand and the value of $V_t$ is known only after the cylinder reaches steady state. Once $V_t$ is known, the drag coefficient and Reynolds number can be calculated using Eqns. (6.5) and (6.6). The input data used for the experiment are as follows:

<table>
<thead>
<tr>
<th>Table 6.1: Input data for sedimentation experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluid density, $\rho_f = 1 \text{ gm/cm}^3$</td>
</tr>
<tr>
<td>Cylinder density, $\rho_c = 1.02 \text{ gm/cm}^3$</td>
</tr>
<tr>
<td>Cylinder diameter, $D_c = 1.2 \text{ cm}$</td>
</tr>
<tr>
<td>Kernel compact support length, $h = 0.1$</td>
</tr>
<tr>
<td>Number of SPH particles, $N = 38290$</td>
</tr>
<tr>
<td>Channel width, $W = 10 \text{ cm} = 8.33D_c$</td>
</tr>
<tr>
<td>Periodic length, $L = 30 \text{ cm} = 25D_c$</td>
</tr>
<tr>
<td>External acceleration on the cylinder, $f = 98 \text{ cm/s}^2$</td>
</tr>
<tr>
<td>Fluid viscosity, $\mu = 0.01 \text{ gm/cm.s}$</td>
</tr>
<tr>
<td>Mach number, $M = 2$</td>
</tr>
</tbody>
</table>

The value of externally imposed acceleration on the cylinder is taken much less than acceleration due to gravity. The idea of acceleration is to generate some driving force and it is not important to the final results. In case of using the actual value of acceleration due to gravity, the time steps had to be extremely small and a large number of SPH fluid particles had to be considered. This would have made the simulation computationally more intensive. Hence a smaller value of the acceleration on the solid cylinder was used.
In Fig. 6.2, the x and y-components of the cylinder velocity have been plotted. The figure shows that the steady state reached within six seconds after releasing the cylinder and the experiment was continued well beyond the steady state. The terminal velocity obtained from the figure was 1.64 cm/s. Using Eqns. (6.5 and 6.6) the drag coefficient and Reynolds number were calculated and compared with values reported in the literature. For easy reference, one such $C_d$ vs. $Re$ curve from literature is reproduced here, Fig. 6.3. The comparison of the drag coefficient in the following table shows very good agreement with previous literature.

**Table 6.2: Comparison of drag coefficient for the sedimentation experiment**

<table>
<thead>
<tr>
<th>$Re_c$</th>
<th>$C_d$ from SPH experiment</th>
<th>$C_d$ from Fig. 6.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>196.8</td>
<td>1.374</td>
<td>1.4</td>
</tr>
</tbody>
</table>

The trajectory of non-neutrally buoyant particles is rather complex and migration of the particle depends on density difference between the solid and the fluid. The driving force for the migration, as identified by Feng *et al.* (1994), are wall repulsion due to lubricating
force, an inertial lift related to shear slip, a lift due to particle rotation. Since the cylinder was released from the most stable and equilibrium position i.e., midway between the channel width, it was supposed to travel along the x-axis. However, once the cylinder drifts slightly from its equilibrium position it becomes more prone to further drift caused by the imbalance of the drag force, known as lift. The dynamic and complex interaction of the forces mentioned above eventually force the cylinder to move in a zigzag fashion along the equilibrium line (i.e., midway between the channel width). The amplitude of zigzag is a function of the location (across the width) of release of the cylinder (Hu et al., 1992). The present test case shows slight tendency of zigzag though it is not conclusive. For studying the transverse motion the experiment should have been continued for longer duration. Further improvement in the resolution of the fluid particles around the cylinder could improve the accuracy of estimation of lift force. This could be achieved by either increasing the ratio $D_c h$ or by employing variable kernel size.

Fig. 6.4 shows a few snap shots of velocity contours at different times during the experiment. It shows the development of wakes behind the cylinder.

![Velocity Contours](image)

Fig. 6.3: Reynolds number vs. Drag coefficient chart (Perry, 1984)
6.1.2 Coupled Motion of a Cylinder Between Two Parallel Plates

A conventional method to estimate the effective viscosity of a fluid-particle system in laboratory as well as in computer simulations is by conducting a shear cell or a "viscometer" experiment. In a viscometer cell, the suspension kept between two moving surfaces undergoes shearing action due to motion of one or both the walls and the measurements of fluid stresses on the walls are used to estimate the effective viscosity of the suspension under sustained shear. Depending on the physical properties of the fluid and solid particles including particle shape and size distributions, the stress on the wall varies and so does the viscosity. For detailed information on different techniques of rheological measurements, one may refer to Chhabra and Richardson, 1999.

Following the principles of a rheological shear cell, a few test cases on the motion of a neutrally buoyant cylinder have been investigated. In all the cases described in this section, the cylinder was initially positioned at the center of the periodic cell and the cylinder diameter and the width of the channel were kept constant, see Fig. 6.5. Since the cylinder was neutrally buoyant, the net force acting on the cylinder was due to the fluid drag. The value of net force on the cylinder, \( F \) in Eqn. (6.1) was directly estimated from Eqn. (5.14). Due to the geometrical symmetry of the system about the centerline along \( x \)-axis passing through the cylinder, the net \( y \)-component of force on the cylinder should be zero. Extensive study on lateral migration of neutrally buoyant cylinder in simple shear flow has shown that irrespective of its initial position, the cylinder will always try to migrate to the centerline (Feng et al., 1994). In case the cylinder is placed at the center of the periodic cell, the question of lateral migration of the cylinder does not arise since it is the most equilibrium and symmetric position in the periodic cell. This means, in all the three test cases considered below, there should not be any lateral migration and any migration observed will be primarily due to initial rearrangement of the fluid particles around the cylinder.
Fig. 6.4: Snap shots of velocity contours for the sedimentation experiment at different times during the experiment.
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Fig. 6.5: Schematic diagram showing boundary conditions and steady state fluid velocity profile for coupled motion of a cylinder and fluid where both the walls move in the same direction.

The base configuration used for all the shear flow experiments in this section is shown in Table 6.3. The value of \( \Delta t \), the time step was varied between \( 10^{-3} \) to \( 4 \times 10^{-3} \) s during the experiment with the higher value used at the beginning and the lower value towards the end. The width of the periodic cell and the velocity of the moving wall are taken as the length \( (L_0) \) and velocity \( (V_0) \) scale for the experiments. The Reynolds number, \( Re_p \) is calculated based on the cylinder diameter. As the velocity of the cylinder increased due to fluid motion, the velocity gradient that existed on the surface of the cylinder decreased. At this stage, unless the value of the time step was reduced the small velocity difference between the cylinder and the surrounding fluid might cause numerical instability at the cylinder surface.

Table 6.3: Input data for experiments on coupled motion of single cylinder and fluid

<table>
<thead>
<tr>
<th>( L ) =1 cm</th>
<th>( W ) =1 cm</th>
<th>( h ) =0.01 cm</th>
<th>( D_c ) =0.2</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V_{max} ) =1 cm/s</td>
<td>( W/D_c ) =5</td>
<td>( L/D_c ) =5</td>
<td>( \rho_f ) =1 gm/cm(^3)</td>
</tr>
<tr>
<td>( \mu_f ) =0.01 gm/cm.s</td>
<td>( Re_p ) =20</td>
<td>( M ) =4</td>
<td>( N ) =13258</td>
</tr>
</tbody>
</table>

6.1.2.1 Two Plates Moving in the Same Direction

Fig. 6.5 shows a schematic outline of the simulation experiment. In the model experiment, the cylinder was placed at the center of the computational cell that was periodic along \( x \) direction. SPH Particles were carefully placed within the cell excluding
the area covered by the cylinder. While the fluid and the cylinder started from rest, the two walls were maintained a constant velocity of $U$ along the positive $x$ direction.

![Image of velocity contours]

Fig. 6.6: Positions of the cylinder and velocity contours for the fluid at various times, indicated below each snapshot, for coupled motion of a cylinder in shear flow with both walls moving and the ratio of the length to width of the cell, $L/W=1$. The velocity scale is in cm/s and the cell is 1 cm in each side. Though not clear from the plots, the cylinder has made nearly 80 horizontal passes along the periodic cell during the experiment.

Fig. 6.6 shows six snap-shots of velocity contours for the fluid at various times, indicated against each contour plot, during the flow. Fig. 6.7 shows the $x$ and $y$-component velocity of the cylinder. The figure shows that the cylinder took about 40s to reach the steady state when its $x$-component of velocity became the same as that of the moving walls. The inset in Fig. 6.7 shows an enlarged view of the variation of $y$-component of the cylinder’s velocity indicating very small fluctuations (about 0.2% of the wall velocity) at the beginning of the simulation. Velocity fluctuations reduced significantly as the system approached steady state. Fig. 6.8 shows the $x$ and $y$-components of the
displacement of the cylinder. Due to the periodicity along the x-axis, the x-component displacement of the cylinder is plotted as the cumulative displacement from the beginning of the experiment. It is evident from the figure that the cylinder made about 80 passes across the length of the periodic cell during the experiment.

![Graph showing cylinder velocity over time](image)

**Fig. 6.7:** Velocity of the cylinder as a function of time. After about 40s from the start of the experiment, the cylinder reached steady state when its velocity became same as that of the moving walls. The inset shows small fluctuations in y-component of the cylinder’s velocity.

![Graph showing cylinder displacement over time](image)

**Fig. 6.8:** Displacement of the cylinder along x and y-axes as a function of time. The Cell being periodic along x-axis, the plot shows that the cylinder made nearly 80 passes along x-axis during the experiment.

The figure also shows that the cylinder has migrated in y-direction by about 10% of the width (0.1 cm) of the cell. The reason for the migration is believed to be purely due to the finite number of discrete fluid particles present in the SPH simulations. Though it
may appear to be a large displacement (10% of the channel width) along y-direction, a careful inspection reveals that the total migration of the cylinder took place by 0.1 cm during the same period when the cylinder also moved nearly 80 cm (=80 passes along the cell) along x-axis. This is equivalent to only 0.125% [(0.1/80)×100] shift along the y-direction. Moreover, the y-displacement curve in Fig. 6.8 also shows that most of this lateral shift had taken place before the cylinder attained steady state. The initial fluctuation in the y-component of the forces on the cylinder due to the geometric rearrangement of the fluid particles around the cylinder, Fig. 6.9, is primarily responsible for the cylinder’s migration.

The fluctuation is independent of the periodic length of the cell as is evidenced from Fig. 6.10 where velocity profiles for another experiment with double the periodic distance (i.e., $L/W=2$) compared to the previous experiment are plotted. The indistinguishable nature of the velocity profiles for the two experiments proves that for solid-liquid coupled motion the periodic length of the cell does not significantly alter the hydrodynamics. It is believed that the initial fluctuation of the forces on the cylinder can be reduced further by improving the discretisation of the SPH fluid particle in the immediate vicinity of the cylinder. Fig. 6.11 shows the velocity contour plots for the experiment with $L/W=2$. 

Fig. 6.9: Variation of x and y-components of the surface forces on the cylinder as a function of time.
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Fig. 6.10: Comparison of temporal velocity profiles for two different domain lengths showing that length of the periodic domain doesn’t influence the motion of the cylinder when its motion is coupled with fluid.

Fig. 6.11: Positions of the cylinder and velocity contours for the fluid at various times, indicated below each snapshot, for coupled motion of a cylinder in shear flow with both walls moving and \( L/W = 2 \).

It may be concluded from the above experiments that the two-phase coupling of the hydrodynamic forces is modeled successfully using SPH though the quantitative accuracy of the cylinder’s motion needs further assessment. For the purpose of a quantitative comparison of motion of a body under shear flow, another example of coupled flow of solid and fluid is presented in the following section.
6.1.2.2 One Plate Moving

Another simple experiment using the solid-fluid coupled forces can be devised where the solid cylinder is under the influence of asymmetric velocity gradient such as in Couette flow. The experiment is shown schematically in Fig. 6.12. The advantage of this experiment lies in the availability of an analytical solution particularly when the ratio of \( \frac{W}{D_c} \) is very large. In such cases, replacement of the cylinder with fluid reduces it to an experiment of single phase Couette flow for which analytical solution is available and extensive study using SPH approach has already been reported in Chapter 5.

The experiment is exactly same as the one described in § 6.1.2.1 except the boundary conditions. In the current experiment, the only difference is that the bottom wall is stationary. At steady state, a linear velocity profile is expected to develop. The velocity contours for the fluid phase at four different times during the experiment and velocity profiles for the solid cylinder are shown if Figs. 6.13 and 6.14 respectively. The \( x \)-component velocity of the cylinder is seen to rise continuously with time though the rate diminishes at later stage of the flow. The inset of Fig. 6.14 shows that small fluctuations were present in the \( y \)-component of the cylinder’s velocity, which is also reflected in the \( y \)-displacement of the cylinder, Fig. 6.15. It is important to note that due to the asymmetric wall boundary conditions seen in Fig. 6.12, the cylinder is placed across a considerable velocity gradient in the \( y \)-direction compared to the experiment described in
§ 6.1.1.1. This has resulted in a much larger drift upwards of the cylinder along the y-axis in the present case.

Fig. 6.13: Motion of a neutrally buoyant cylinder in Couette flow. The figures show velocity contours of the fluid at various times, indicated below each of the contours, during the experiment. It also shows that the cylinder has slightly shifted upward. Scale is in cm/s.

Fig. 6.14: x and y-component velocity of the cylinder as a function of time in Couette flow. The inset shows that the cylinder has small amount of y-component velocity.
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Fig. 6.15: Displacement of the cylinder along x and y-axes as a function of time in Couette flow. The Cell being periodic along x-axis, the plot shows that the cylinder has made nearly 80 passes along x-axis during the experiment.

The x-component of the fluid phase velocity is now compared with the analytical solution of single-phase Couette flow in Fig. 6.16. The comparisons are made at the same times as in the snapshots seen in Fig. 6.13. The Figure shows very good agreement between the analytical and SPH solution of the fluid phase at all three stages during the coupled motion. The distinct velocity band observed in all the plots indicate the presence of boundary layers around the solid cylinder surface and this will decrease as the ratio of channel width to the cylinder diameter, $W/D_c$, increases.

The final example on demonstrating the issue of accuracy in resolving the drag forces on the body is described in the next section where the body experiences very sharp shear rate gradients brought about by the movement of the boundaries in opposite directions.

Fig. 6.16: Comparison of dimensionless x-component of velocity profiles for the fluid phase with and without the cylinder. The red points are obtained from analytical solution of single-phase Couette flow; the blue points from SPH experiments for coupled motion of cylinder under Couette flow. The velocity and length scales for non-dimensionalisation are the moving wall velocity and width of the periodic cell.
6.1.2.3 Two Plates Moving in Opposite Directions

In this experiment, the periodic cell bounded by walls at \( y=0 \) and \( y=W \) that were moving at constant velocity \( U \) in opposite directions as shown in Fig. 6.17. Since the walls were moving in opposite directions and the cylinder was placed at the most symmetrical and equilibrium position, the cylinder must remain stationary at the same position as the flow developed. Slightest inaccuracy in estimation of the forces on the cylinder would displace the cylinder from its equilibrium position and, once it is displaced, the symmetry of the flow is lost and the body would tend to move further away from the equilibrium position. Thus, merely by tracking the motion of the cylinder one could obtain a very good indication of the ability and accuracy of the present SPH technique to deal with relatively less benign situation like this.

![Diagram of coupled motion of a cylinder in Couette flow](image)

Fig. 6.17: Schematic diagram of coupled motion of a cylinder in Couette flow where the two parallel boundaries are moving in opposite directions.

The test case presented here differs slightly from the base case mentioned in Table 6.3 at the beginning of § 6.1.3. Here, the particle number density was increased by four times compared to the base case. Naturally, the time step size was reduced to maintain stability as shown in Table 6.4. The velocity and length scales used were the plate velocity and the width of the cell respectively.

The simulation was carried out for 32000 time steps which was equivalent to 9.6s. Fig. 6.18 shows the velocity contour of the fluid at the end of the simulation. It is evident that the cylinder has migrated towards the lower wall. In Fig. 6.19, the \( x \)-component of fluid
velocity is plotted against y-position at two locations, A and B of the cell as indicated in Fig. 6.17. The slight deviation of the x-component of velocity profile around y=0.5 indicates the presence of boundary layer on either side of the cylinder along the direction of main flow. The deviation depends on the relative size of the cylinder to the channel width and it will decrease as the ratio decreases. In the limiting case of absence of any solid body within the fluid, these two protruding portion of the velocity profile would actually merge with the mainstream velocity profile. The imbalance of the drag forces on the cylinder is reflected in the plot of x and y-components of velocity of the cylinder shown in Fig. 6.20(b). It shows a gradual increase of the cylinder velocity, particularly of the x-component. Up to about 4s, the cylinder maintained its symmetric position beyond which point the accumulation of errors became significant enough to cause instability in the net force on the cylinder, particularly in the y-component of the drag force. Migration of the cylinder towards the lower wall was accompanied greater influence of the fluid below the cylinder on the cylinder’s motion. This caused the cylinder to move along the negative x-direction. The reason for the departure of the cylinder from the equilibrium position is believed to be due initial rearrangement of the fluid particles and also due to inaccuracy in estimation of forces on the cylinder surface for having fewer SPH particles around the cylinder.

Table 6.4: Discretisation details for shear flow experiments
(Other parameters same as in Table 6.3)

| Compact support length, $h=5\times10^{-3}$ cm |
| Number of SPH particles, $N=48649$ |
| Time step, $\Delta t=3\times10^{-4}$ s |

In other words, the result can be improved by improving the discretisation of the space and the time domain. By decreasing the value of $h$, the kernel compact support length, one can have more SPH particles around the cylinder to contribute to the evolution of the various surface forces. It may be important to note that due to random insertion of fluid particles, it is very unlikely to have exactly even distribution of fluid particles all around
the cylinder and the only way of reducing the degree of unevenness is by reducing inter-
particle distance and having more particles per unit area of the periodic cell.

In the experiment described above, the cylinder had about 353 neighbours. Now, another
two experiments were carried out at two different levels of discretisations, namely with
12488 and 76858 fluid particles in the periodic cell which resulted in about 191 and 455
neighbours to the cylinder, respectively. In Fig. 6.21 and 6.22, the velocity and
displacement of the cylinder against elapsed time for these two situations are plotted. As
one would expect, the experiment with 191 neighbors was found to have larger
fluctuations in both components of the cylinder’s velocity. On the other hand, with 455
neighbours, not only the net y-displacement of the cylinder was extremely low, the
velocity fluctuations were also insignificant during the duration of the experiment. Fig.
6.23 shows the final velocity contours along with the net displacements of the cylinder in
the two experiments described above. It may be concluded from the above experiments
that:

- The present formulation of SPH is capable of simulating the motion of a solid
  object even in higher shear rate gradient cases of Couette flow.
- There is further evidence that a significant quantitative improvement in the
  results can be brought about by increasing the number of particles in the
  domain; i.e., by reducing the inter-particle distance of the fluid particles.

![Velocity contour of the fluid at steady state, after 9.6s. The dotted cross indicates the original position of the cylinder before the start of the experiment. The velocity unit is cm/s.](image)
Fig. 6.19: x-component of velocity of the fluid across the width of the cell at two locations: red points along line A and blue points along line B of Fig. 6.17, at the end of the simulation.

(a) (b)

Fig. 6.20: (a) Plot of displacement of the centre of the cylinder against time for the experiment with 48649 particles. It shows insignificant displacement of the cylinder until 3s after which inequilibrium of forces develops. (b) x and y-components of velocity of the cylinder as a function of time showing gradual increase in u after about 3s.
Fig. 6.21: (a) Plot of displacement of the centre of the cylinder against time for the experiment with 12488 particles. It shows insignificant displacement of the cylinder until about 2s after which inequilibrium of forces develops. (b) x and y-components of velocity of the cylinder as a function of time showing gradual change in u before 2s.

Fig. 6.22: (a) Plot of displacement of the centre of the cylinder against time for the experiment with 76858 particles. It shows insignificant displacement of the cylinder during the whole period of experiment. (b) x and y-components of velocity of the cylinder as a function of time showing minor fluctuations in the velocities.
6.2 Coupled Motion of Multi-Particle Systems

Modeling of a multi-particle fluid system differs from that of single-particle fluid system only in the way the force on each of the solid particles is evaluated while the SPH formulation for the fluid particles remains unchanged. As mentioned earlier in the introduction of this chapter, depending on the length scale of the solid-liquid system, various types of forces may arise in the multi-particle system.

One approach of evaluating the solid-solid forces independent of SPH is by using Discrete Element Modeling (DEM) (Potapov et al., 2001). By this, one can model the force, torque etc. due to particle-particle interactions which can then be added to the hydrodynamic components of the force on individual particles obtained from SPH analysis to obtain the total values of force and torque on each solid particles. While such a holistic approach of combining DEM and SPH is very much suitable for estimating effective suspension properties including suspension viscosity, density, microstructure etc., this is beyond the scope of present work due to time and resource constraints.

Fig. 6.23: Velocity contours (in cm/s) of the fluid at steady state, after 9.6s for (a) 12488 and (b) 76858 SPH particles respectively. The dotted cross in each figure indicates the original position of the cylinder before the start of the experiment.
However, the central theme of accurate modeling of inter-particle force lies in choosing the right interaction models from a host of available models (Langstone et al., 1994). Some of the particle-particle interaction models include:

**Hertzian model**

\[
F_{pp} = \frac{4}{3} E^* \sqrt{R(D_c - r)^3}
\]

where \( E \) is the elastic modulus, \( R \) the contact radius of curvature and \( r \) the separation distance.

**Continuous normal interaction model**

\[
F_{pp} = \frac{n}{r} \left( \frac{D_c}{r} \right)^n
\]

where \( n \) is an arbitrary index, \( \varepsilon = D_c mg/n \) (\( m = \) mass of the solid particle). The coefficients are chosen so that the force is equal to the gravitational force, \( mg \), when the particle center to center separation equals \( D_c \).

**Hookean spring interaction model**

\[
F_{pp} = k(D_c - r)
\]

where \( k \) denotes an effective value of bulk stiffness. These forces vary distinctly with the separation distance \( r \). The advantage of the continuous interaction model is that it becomes appreciably stiffer with greater overlap, \( (D_c - r) \), much more so than the other two models which manifest comparatively modest increase in stiffness in the same separation region. In case particles touch each other, the tangential frictional component that depends on the coefficient of friction needs to be considered along with the collision rules to conserve momentum (angular and translational). All these factors provide a flavor of the degree of complexity involved in the estimation of particle-particle forces. To keep matters simple only the continuous normal interaction model is included in the present
work with an aim to stop two mutually approaching particles from getting too close to each other. The exact equation used in the present work is:

\[ F_{pp} = -A \left( \frac{D_c}{r} \right)^{30} \]  

where \( D_c \) is the cylinder diameter assuming uniform particle size, \( r \) is the inter-particle distance measured center-to-center and \( A \) is a lump parameter that depends on the mass of the solid particles. In literature, the numerical value of the index ‘\( n \)’ of Eqn. (6.8) is usually ranges from 16 to 48.

The complexity of modeling multi-particle suspensions is not just restricted to the variety of force considerations only. There are important issues related to the stability of the system which, more than often, brings the numerical simulation to a halt. For example, in the course of motion, the particles may approach one another and stay close to each other forming long-standing resilient clusters. Under such situations, the system of equations governing the motion of the particles become extremely stiff that necessitates unaffordably small time steps to prevent overlapping of the particles. Though for smaller solid fractions it does not pose any serious threat to the stability of the system, methods such as geometrical exclusion (Pozrikidis, 2001) have been used at higher solids fractions (\( \phi=0.25 \)) with some success to impose arbitrary numerical criteria to prevent particles coming too close to each other.

Two test cases are considered here. In both cases, the neutrally buoyant solid particles (cylindrical in shape) were placed randomly within a two-dimensional periodic domain. This was followed by random introduction of the fluid particles. The system was initially at rest. Depending on the specific boundary conditions, the motion of the cylinders and the fluid were developed as appropriate.
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6.2.1 Motion of Two Cylinders Between Two Parallel Plates

The motion of two cylinders in a periodic cell between two parallel plates moving in the same direction was studied to probe the details of particle migration phenomena. The details of the parameters used in this experiment are shown in Table 6.5.

Table 6.5: Input data for coupled motion of two cylinders and fluid

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(L)</td>
<td>1 cm</td>
</tr>
<tr>
<td>(W)</td>
<td>1 cm</td>
</tr>
<tr>
<td>(h)</td>
<td>0.01 cm</td>
</tr>
<tr>
<td>(D_c)</td>
<td>0.12 cm</td>
</tr>
<tr>
<td>(V_{max})</td>
<td>1 cm/s</td>
</tr>
<tr>
<td>(W/D_c)</td>
<td>8.33</td>
</tr>
<tr>
<td>(\rho_f)</td>
<td>1 gm/cm³</td>
</tr>
<tr>
<td>(\mu_f)</td>
<td>0.01 gm/cm.s</td>
</tr>
<tr>
<td>(Re_f)</td>
<td>12</td>
</tr>
<tr>
<td>(M)</td>
<td>4</td>
</tr>
<tr>
<td>(N)</td>
<td>13408</td>
</tr>
<tr>
<td>No. of cylinders</td>
<td>2</td>
</tr>
</tbody>
</table>

Initial coordinate of Cylinder 1: \(x=0.57\) cm, \(y=0.52\) cm

Initial coordinate of Cylinder 2: \(x=0.10\) cm, \(y=0.73\) cm

Since there were only two cylinders in this experiment, Eqn. (6.10) practically had no role to play here as the cylinders never came within a distance of cylinder diameter of each other i.e., \(r >> D_c\). In spite of symmetric boundary conditions, since the initial position of the cylinders were asymmetric with respect to the their distances from the moving walls, one could expect to see migration of the cylinders to more stable positions. Fig. 6.24 shows velocity contours for the fluid and position of the cylinders at six different times during the experiment. Fig. 6.25 shows cumulative displacement and velocity of the cylinders. It is evident that both the cylinders started migrating once the fluid velocity field developed within 3s from the start of the experiment. However, the migration of cylinder 2 almost stopped quite early (after about 13s from the start) while the cylinder 1 continued its migration till very late though at a diminishing rate. The vertical positions of the cylinders at the end of experiment along with geometrically most stable positions are shown in Table 6.6.

The table clearly indicates why cylinder 2 stopped its migration much earlier than the other cylinder. It was initially placed very close to its expected equilibrium position \((y=0.67\) cm) and once it reached that position no further migration of cylinder 2 took.
place. On the other hand, the cylinder 1 was far off from its expected equilibrium position \((y=0.33 \text{ cm})\) and hence it continued to migrate to that position.

The experiment demonstrates that the present formulation of SPH can be applied to simulate relatively complex but interesting phenomena such as particle migration.

Fig. 6.24: Velocity contours (cm/s) for the fluid and positions of the cylinder at different times during the experiment of coupled motion of two cylinders in shear stress driven flow. The cylinders have made nearly thirty passes across the periodic length between the first and last snaps. The figures show migration of both the particles along y-axis.
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Fig. 6.25: (a&b) Displacement of the two cylinders along x and y-axes as a function of time; (c&d) x and y-components of the velocity of the cylinders as a function of time.

Table 6.6: Positions of the two cylinders when their motion is coupled with the fluid

<table>
<thead>
<tr>
<th></th>
<th>Initial</th>
<th>Final</th>
<th>Equilbm.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vertical position of Cylinder 1</td>
<td>0.52 cm</td>
<td>0.42 cm</td>
<td>0.33 cm</td>
</tr>
<tr>
<td>Vertical position of Cylinder 2</td>
<td>0.73 cm</td>
<td>0.68 cm</td>
<td>0.67 cm</td>
</tr>
</tbody>
</table>

6.2.2 Motion of Many Cylinders Between Two Parallel Plates

The final section of the present work is devoted to the study of the evolution of effective properties of multi-particle solid-liquid suspensions with particular emphasis on evaluation of suspension effective viscosity of a system consisting of a viscous liquid and multi-particle, neutrally buoyant and non-interacting cylinders. To keep the system
simple, factors such as size distribution, shape, orientation of the solid particles are not considered here. In order to calculate the effective viscosity of suspensions the following methodology, in line with the working principle of a shear cell, is being proposed.

If any fluid undergoes shear within a periodic cell with two of its parallel walls moving at constant velocity in opposite directions, the fluid develops a velocity gradient (known as shear strain). The gradient developed is a function of the viscosity of the fluid under shear. By carrying out a numerical experiment using suitable conservation laws one can estimate the fluid pressure (a combination of shear stress and normal stress) on the walls at steady state. For a Newtonian fluid under laminar flow condition, the ratio of the shear stress imparted by the fluid to the wall to the strain developed within the fluid is the viscosity of the fluid. For other fluids or for a multi-particle suspension, the same idea can be applied to recover what one may call the effective viscosity of the material under investigation. Estimation of bulk properties in such a mean-field manner from the microscopic interactions is highly desirable and useful in many engineering applications.

Before the actual measurements of effective viscosity of multi-particle suspensions by above-mentioned method, it was felt necessary to establish the validity of the approach by recovering the viscosity of a single-phase fluid. In the following section an attempt has been made to recover the viscosity of a reference liquid (water). While the single-phase SPH hydrodynamic equations described in Eqns. (3.24-3.27) were used to simulate the motion of the SPH particles, the shear stress on the walls was calculated from Eqn. (5.14). Fluid particles within $2h$ distance from the walls were considered for the summing up operations. In principle, the stresses on the walls were estimated exactly in the same way as the drag force on the cylinder was calculated in Chapter 5. The only difference between the two calculations is the surface geometry.
6.2.2.1 Recovery of Fluid Viscosity From Wall Shear Stress

The discretisation parameters and the fluid properties used for this experiment are described in Table 6.7. Let the relative viscosity, $\mu_r$, of the fluid be defined as the ratio of the viscosity obtained from wall stress measurement using SPH to the actual fluid viscosity. The evolution of relative viscosity of the single-phase liquid is plotted against time in Fig. 6.26. It is very interesting to see that after about 10s the effective viscosity reaches steady state and the value matches very well the actual liquid (water) viscosity. The technique is now extended to measure the effective viscosity of a multi-particle system.

Table 6.7: Input data for experiment on the recovery of single phase fluid viscosity

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
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<td>$L$</td>
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<td>$W$</td>
<td>10 cm</td>
</tr>
<tr>
<td>$h$</td>
<td>0.16 cm</td>
</tr>
<tr>
<td>$N$</td>
<td>5002</td>
</tr>
<tr>
<td>$V_{max}$</td>
<td>0.1 cm/s</td>
</tr>
<tr>
<td>$\rho_f$</td>
<td>1 gm/cm³</td>
</tr>
<tr>
<td>$\mu$</td>
<td>0.01 gm/cm.s</td>
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<tr>
<td>$Re_f$</td>
<td>100</td>
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<tr>
<td>$M$</td>
<td>4</td>
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</tbody>
</table>

Fig. 6.26: Estimation of single-phase fluid viscosity based on measurement of shear stress on the walls of the periodic cell in Couette flow experiment. The relative viscosity is the ratio of the viscosity measured by the current method to the actual viscosity of the fluid.
6.2.2.2 Estimation of Suspension Effective Viscosity

Subsequent to the establishment of the method to measure the effective viscosity, let the method be applied to measure viscosity of a multi-particle fluid system. For this purpose, three experiments were designed at 5.8%, 11.6% and 21.7% solid fractions (\(\phi\)), which were equivalent to 8, 16 and 30 cylinders in the present configurations. Experiments were also carried out at two shear rates (\(\gamma=\Delta U/W=2U/W\)). The detailed configurations for the experiments are given in Table 6.8.

<table>
<thead>
<tr>
<th>Table 6.8: Input data for experiments on multi-cylinder and fluid</th>
</tr>
</thead>
<tbody>
<tr>
<td>(L=10) cm</td>
</tr>
<tr>
<td>(U=1) cm/s</td>
</tr>
<tr>
<td>Expt1: (\gamma=0.02) s(^{-1})</td>
</tr>
<tr>
<td>Expt2: (\gamma=0.02) s(^{-1})</td>
</tr>
<tr>
<td>Expt3: (\gamma=0.02) s(^{-1})</td>
</tr>
<tr>
<td>Expt4: (\gamma=0.002) s(^{-1})</td>
</tr>
<tr>
<td>Expt5: (\gamma=0.002) s(^{-1})</td>
</tr>
<tr>
<td>Expt6: (\gamma=0.002) s(^{-1})</td>
</tr>
</tbody>
</table>

A value of 0.1 gm.cm/s\(^2\) was chosen for the constant \(A\) in Eqn. 6.10. The relative viscosity as a function of time for all the experiments is plotted in Fig. 6.27. It may be noted that except for the lowest solid fraction, all the other experiments could not be continued until they reached steady state due to instability problems. The problem was particularly prevalent around the cylinders that were closest to the moving walls due to poor resolution of SPH fluid particles around these areas. Due to lack of sufficient fluid particles the surface forces were not resolved accurately that lead to erroneous velocity vectors for the fluid particles near these cylinders. This resulted in inappropriate velocity for the fluid particles leading a premature termination of the simulations. It may be said that occurrence of such instability is a serious problem with all numerical methods applied to such severe conditions and SPH is no exception. However, once the particle-
particle interaction models are further refined by including contact force model and fine
tuning of the parameter A in Eqn. 6.10 and experiments were performed at higher level of
discretisation, it is believed that the model would be capable of simulating at higher solid
fractions.

![Image of graphs]

Fig. 6.27: Evolution of relative viscosity for multi-particle suspension at various solids fractions (\(\phi\)) and
shear rates (\(\gamma, \text{s}^{-1}\)). It may be noted that except for \(\phi=5.8\%\), no other experiment reached steady state.

The effective viscosity plot for \(\phi=5.8\%, \gamma=0.002 \text{ s}^{-1}\) is found to converge at a value of
1.21 (based on last 500 time steps towards steady state). The two profiles for the two
different shear rates considered for \(\phi=5.8\%\) are also seen to merge on each other
signifying that the model is capable of simulating suspension dynamics at smaller value
of solid fractions. Theory of infinitely dilute suspension (Einstein, 1956) for spherical
particles predicts a value of 1.145 [using \(\mu_{\text{eff}}=\mu(1+2.5\phi)\)] for the effective viscosity at
\(\phi=5.8\%\) while use of analytical solution for circular disks (Pozrikidis, 2001) yields a
value of 1.116 [using $\mu_{eff} = \mu(1+2\phi)$]. The present simulation result at $\phi=5.8\%$ is about 8% higher than the analytical solution which can be considered reasonable. The value of the effective viscosity at smaller values of $\phi$ is expected to improve by increasing the SPH particle density in the current approach. Fig. 6.28 shows the final velocity contour plots for various experiments carried out in this study.

Fig. 6.28: Fluid velocity contours in shear cell experiments at two different shear rates ($\gamma$, s$^{-1}$) and three different solids fractions ($\phi$) as indicated below each contour. It may be noted that except for $\phi=5.8\%$, no other experiment reached steady state.
6.3 Conclusions

In the last chapter, SPH methodology was developed to estimate the drag and lift force acting on stationary solid objects immersed in a moving fluid. As a follow up, in this chapter the dynamic interactions between the solid objects and fluid when both the phases in motion was taken up. The study was primarily divided into single and multi-particle fluid systems with an objective to develop the formulation for single particle first and extend the formulation for multi-particle systems.

Various cases including sedimentation of a cylinder in a stationary liquid and motion of a symmetrically placed cylinder under shear driven flow were considered to demonstrate the capability of the present SPH algorithm. In all cases, the exchange of momentum between the solid and the fluid took place through the use of surface integrals developed in this work. The presence of no-slip boundary condition at the solid surface meant time integration of both the phases were of utmost importance particularly in the immediate vicinity of the solid surface.

The value of the drag coefficient obtained from the sedimentation experiment matched closely with the literature value though lateral migration was present. The issue of lateral migration in this case and also for the subsequent cases of motion of the cylinder under shear flow were mostly viewed as an effect of uneven distribution of SPH fluid particles around the cylinder. The argument was subsequently corroborated by the results from a set of experiments at three levels of discretisation (§ 6.1.2.3). The extent of migration for the shear flow experiments greatly reduced when a large number of SPH particles contributed to the evaluation of drag force on the solid cylinder. Moreover, the other possible source of computational artifact, usually associated with the Lagrangian approach is the time integration. Use of smaller time step size was something not looked into.
Chapter 6: Two-Phase Solid-Liquid...

The motion of two asymmetrically placed cylinders in shear flow revealed some interesting phenomena of ‘particle migration’ purely due to hydrodynamic effects. The results qualitatively showed that for cases where solid particles are sparsely distributed in the fluid medium, SPH formulation along with the surface integral term is a convenient and easy to apply technique.

Recovery of artificial viscosity from wall shear stress measurements can be thought of a good approximation of estimating effective viscosity. The effective viscosity of a single-phase fluid, recovered by this method was found in very good agreement with the actual fluid viscosity. The idea was also implemented for a multi-particle system.

Due to the simplistic approach adopted to simulate complex phenomena observed in multi-particle suspensions, majority of the experiments presented in this work could not be continued until steady state. This means that the results of most of the experiments presented here are not conclusive. However, it may be said that the hydrodynamic interactions evaluated at the individual solid particle level were found to model the motion of the cylinders quite accurately. The kind of numerical artifacts experienced here is also a serious challenge in other numerical techniques and considered beyond the scope of the current work.
Chapter 7

CONCLUSIONS AND FUTURE WORK

In questions of science the authority of a thousand is not worth the humble reasoning of an individual
-Galileo Galilei
CHAPTER 7: CONCLUSIONS AND FUTURE WORK

7.1 Conclusions

Solid-liquid suspensions occur in a large number of industrial applications. The ability to predict the behaviour of such suspensions during processing is therefore extremely important. Process-level modelling of systems involving solid-liquid suspensions is often done by assuming the suspension may be modelled as a pseudo-homogenous fluid with "effective" properties. The work reported in this thesis represents initial efforts aimed at developing a macroscale simulation method for the determination of such effective properties without resort to laboratory experiment. This method involves the explicit modeling of the moving solid particles and the interstitial fluid dynamics. The motion of the solid particles are integrated through time using the equations of motion of solid bodies with the forces arising from the dynamics of the interstitial fluid, particle-particle interactions and body forces such as gravity. The dynamics of the interstitial fluid is integrated through space and time using the smoothed-particle hydrodynamics (SPH) method, which is ideal for handling the massively deforming fluid domain defined by the surfaces of the moving solid particles.

The SPH method was initially developed for the study of astrophysical systems where solid surfaces are rarely involved and the fluids compressible. Whilst it has been applied to problems involving solid surfaces, treatment of the former has been largely ad hoc and is unsuitable for the problem of interest here. It has also been used to consider the behaviour of slightly compressible fluids, but little has been published on the behaviour of SPH when this is the case. These issues were, therefore, addressed in some detail in Chapters 3 and 4, before considering suspension systems in Chapter 6.
Chapter 7: Conclusions and ...

The rigorous inclusion of boundary conditions has been done by retaining surface integrals that naturally arise during the derivation of the SPH equations but which are normally omitted. Retention of these integrals for the purposes of imposing non-trivial boundary conditions was first suggested by Campbell (1989) in an unpublished report, but never implemented. The surface integral approach has been implemented here for the first time and it was shown that the original method suggested by Campbell is inaccurate. The method used in the present work can be implemented for arbitrary shaped surfaces using numerical surface integration, and was tested extensively using a number of benchmarks including Couette and Poiseuille flow, flow in a driven cavity and flow around a stationary cylinder. The tests all showed that under optimal conditions, the method for imposing boundary conditions is robust, stable, and capable of yielding accurate results both in space and time.

A remarkable effect of particle disorder on fluid behaviour was found in the present study. The study showed that the use of initial randomness in particles' positions was better in terms of attaining a stable and steady state quicker as opposed to starting with ordered particles, which is the initial configuration recommended by some (Morris, 1996). In case of later arrangement, the particles eventually become disordered during the simulation in any case releasing large amounts of 'internal energy' that lead to poorer solutions. Moreover, one of the primary justifications for using SPH to simulate multiparticle suspensions is its ability to handle large deformations of the simulation domain, something that can only be done if we accept the presence of disordered particles. All these reasons prompted the use of random placement of particles in most of the benchmark problems in the present study.

The fact that SPH was originally developed for simulating compressible fluids means that the technique will have its fair share of problems in dealing with incompressible liquids where the hydrostatic pressure is an explicit function of the smoothed density of the liquid particles. Representing liquids with finite number of 'fluid particles' as we do in SPH has profound effect on the 'compressibility' of the fluid. Through a series of
arguments, it has been deduced in this work that SPH can model a ‘relatively incompressible’ liquid under all practical computational constraints. This means that the speed of pressure wave propagation in the model ‘SPH liquid’ cannot be as high as the sound speed in a real liquid. Mach number, the measure of compressibility would depend on the flow Reynolds number and, for the range of Reynolds number investigated in the present study (\(10^{-2} - 10^{2}\)), the value of the appropriate Mach number is found to lie between 0.1 and 4. Furthermore, for viscous dominated flow at \(Re<1\), the Mach number should be around 0.1 while for \(Re>1\), a Mach number greater 1 is required to accurately recover the hydrodynamics of viscous flow.

The final novel aspect of the work, reported in this thesis is the application of SPH to liquid-solid suspensions. In this case, single, pair and multiparticle systems were simulated with encouraging results. The drag coefficient recovered from a simulated sedimentation experiment appears to match published experimental data well. The effective viscosity of multiparticle systems was estimated by adopting a Couette flow configuration inline with that of traditional rheological viscometers and by summing the macroscopic wall shear stress calculated from the particles adjacent to the walls. This approach was validated for single phase homogenous flow and the effective viscosity satisfactorily compared with that obtained from Einstein’s model for low solids concentration (\(\phi=5.8\%\)). Obtaining steady state estimates of the effective viscosity at higher solids concentrations was difficult due to inadequate handling of the situation when particles come close together. A paper detailing the use of SPH to model multiparticle systems was recently published by Potapov et al. (2001). The approach adopted by this group differs from the work presented here in its use of a non-rheological viscous shear stress model coupled with the implementation of no-slip boundary condition, implemented by placing SPH particles in the interior of solid macroscopic particles similar to Morris et al. (1997).
Chapter 7: Conclusions and ...

7.2 Future Work

While the results of effective viscosity at small solids fractions are promising, there are many issues outstanding, which time has not permitted to deal with and any future work has to tackle these issues. Some possible future work is briefly outlined below.

Further modifications of the model developed in the present work to tackle the issues related to stability when the solid particle gets too close to the solid surface or to another solid particle would enhance the model’s capability to compute effective properties of densely packed suspensions. At the fluid-solid interface, lack of fluid particles was observed when the separation distance between two solid particles became smaller than the kernel width (also observed by Potapov et al., (2001)). Use of adaptive kernels, similar to the variable mesh technique in the Finite Element method may be a good option to reduce such inaccuracies and instabilities maintaining computational economy.

The solid-solid interaction forces must be estimated in a more comprehensive manner by considering various forces outlined in § 6.2. The present formulation did not consider rotational shear contributions that are likely to be important when dealing with the fabric and structure of dense suspensions.

In many cases suspending fluids are themselves complex fluids (e.g. polymers) – just one example is the suspension of carbon fibres in resin during extrusion to make high strength lightweight parts for automobiles and wind turbine blades. One of the strengths of SPH advanced by its proponents is the ease with which constitutive models may be added to SPH codes compared to the other traditional numerical methods. However, traditional ad hoc methods for imposing boundary conditions means adoption of non-Newtonian stress models, which has never been done in the fluid context, means extensive experimentation will be required. The use of the more formal surface integral approach adopted in the current work will make the inclusion of more complex constitutive models less fraught.

There are alternative ways of dealing with the incompressibility of liquid. One of them is to initialise the density of the fluid system using Eqn. (3.2a) instead of having the same
density of the fluid everywhere. By this, the density difference will only exist when there is relative motion of the fluid particles though the initial density will not be the same as the actual fluid density. Consequently, the background pressure of the system does not remain too sensitive to the Mach number. Though this approach has been adopted by some (Vila, 1999), the effect of the surface integral under such a scheme is not very clear. This method certainly deserves some attention for any future work to address the density or incompressibility issue.

In a slightly different note, the work on sedimentation of single particle can be extended to study the sedimentation of two and three particles to observe complex hydrodynamic effects such as drifting, kissing, tumbling. In order to do this, the angular momentum of the fluid and torque on the solid particles need to be considered. Validation of results from these experiments with available literature (Hu et al., 1992) that uses Finite Element would only establish the robustness of SPH and can be viewed as a step closer towards understanding the complex behaviour of solid-liquid systems.

In areas other than incompressible fluid, numerical simulations in the area of heat conduction and convection can also be attempted. Work has already begun in this area (Cleary, 1998) but the present formulation has the potential to model the thermal diffusion phenomena in a more elegant way than others. The added advantage of advancing the present formulation in this direction is the development of a combined heat transfer and fluid flow model for studies under non-isothermal conditions.

Future investigations of the effect of particle geometry including the shape and size will be rather straightforward in the present formulation. Use of surface the integrals to define solid boundary surfaces compared to traditional approach of using boundary particles to represent irregular geometry, is clearly a more flexible approach to adopt in dealing with polydispersed solid particle mixtures.
Chapter 8

REFERENCES

The real voyage of discovery consists not in seeking new landscapes, but in having new eyes
-Marcel Proust
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APPENDIX 1: EXPLANATION OF INTEGRAL SIGNS USED

The smoothed value of a function in three-dimensional space is obtained from the following equation:

\[
\langle f(r') \rangle = \int_{\Omega} W(r - r', h) f(r') dr'
\]  
(A.1)

where \( W(r - r', h) \) is the kernel function, \( h \) is a measure of influence of the kernel function, \( r \) is the position vector of the fluid volume of our interest with reference to the origin of any frame of reference, \( r' \) is position vector of any other volume element within the domain of integration, \( \Omega \).

The integration is over the entire volume of the domain denoted by \( \Omega \). The elemental volume is denoted by \( dr' \), which has a dimension of \([L^3]\) in three dimensions. The dimension of the kernel function in three-dimensional space is \([L^{-3}]\).

When the same Eqn. (A.1) is used to represent the smoothing operation in a two-dimensional problem, the domain of integration \( \Omega \) would represent a surface or plane and \( dr' \) would represent an elemental area having a dimension of \([L^2]\). The dimension of the kernel function accordingly changes to \([L^{-2}]\).

The surface integral term that arises at solid boundaries in three-dimensional space is represented by:

\[
\int_S nW_n dS
\]  
(A.2)
where \( n \) is a vector directed from the SPH fluid particle towards the boundary surface, but normal to that surface. \( dS \) is the elemental surface area with a dimension of \([L^2]\). \( W_{ss} \) is the abbreviation for the kernel function \( W(r_i - r_s, h) \). The integration is over the surface area intercepted between the kernel volume and the domain boundary, denoted by \( S \). \( W \) has a dimension of \([L^2]\).

In case of two-dimensional domain, the term \( dS \) denotes the elemental length intercepted between the kernel area and the domain boundary, having a dimension of \([L]\). The limit of integration denoted by \( S \) would also have the same dimension. Thus, in a two-dimensional domain Eqn. (A.2) actually represents a line integral.
APPENDIX 2: LEIBNITZ'S RULE

The differentiation of a definite integral whose limits are functions of differential variable can be achieved by using Leibnitz's rule described as follows:

\[
\frac{dI(t)}{dt} = \int_{a(t)}^{b(t)} \frac{\partial f(t, r)}{\partial t} \, dr + f\left(t, b(t)\right) \frac{db(t)}{dt} \left(\frac{a(t)}{f\left(t, a(t)\right)}\right) \frac{da(t)}{dt}
\]

where,

\[
I(t) = \int_{a(t)}^{b(t)} f(t, r) \, dr
\]

As a special case when the limits are not a function of the differential variable, i.e., \(a(t) = a\) and \(b(t) = b\) then

\[
\frac{dI(t)}{dt} = \int_{a}^{b} \frac{\partial f(t, r)}{\partial t} \, dr
\]

Application of the above relationship (in a reverse manner) in the left hand side of Eqn. (3.11) means,

\[
\frac{d}{dt} \langle \rho \rangle = \frac{d}{dt} \int_{\Omega} \rho W(r-r', h) dr' = \frac{d}{dt} \int_{\Omega} \rho W(r-r', h) dr'
\]

where \(f(t, r)\) is replaced by \(\rho W(r-r', h)\) and \(\rho\) is a function of \(r\) and \(t\). \(W(r-r', h)\) is not a function of \(t\).
APPENDIX 3: SPH REPRESENTATION OF GRADIENT OF A SCALAR FUNCTION

If \( f(\mathbf{r}) \) is a scalar function then its gradient is \( \nabla f(\mathbf{r}) \). The smoothed gradient of the function \( f(\mathbf{r}) \) expressed as

\[
\nabla \langle f(\mathbf{r}) \rangle_i = \langle \nabla f(\mathbf{r}) \rangle_i = \int_{\Omega} W(\mathbf{r} - \mathbf{r}', h) \nabla f(\mathbf{r}') d\mathbf{r}'
\]

From the following identity,

\[
\int_{\Omega} \nabla [f(\mathbf{r}') W(\mathbf{r} - \mathbf{r}', h)] d\mathbf{r}' = \int_{\Omega} f(\mathbf{r}') \nabla' W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}' + \int_{\Omega} W(\mathbf{r} - \mathbf{r}', h) \nabla' f(\mathbf{r}') d\mathbf{r}'
\]

or

\[
\int_{\Omega} W(\mathbf{r} - \mathbf{r}', h) \nabla f(\mathbf{r}') d\mathbf{r}' = \int_{\Omega} \nabla [f(\mathbf{r}') W(\mathbf{r} - \mathbf{r}', h)] d\mathbf{r}' - \int_{\Omega} f(\mathbf{r}') \nabla' W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}'
\]

we obtain, ignoring the surface term (i.e., the first term in the right hand side) and using the symmetric property of the kernel,

\[
\int_{\Omega} W(\mathbf{r} - \mathbf{r}', h) \nabla f(\mathbf{r}') d\mathbf{r}' = -\int_{\Omega} f(\mathbf{r}') \nabla' W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}' = \int_{\Omega} f(\mathbf{r}') \nabla' W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}'
\]

Thus, in particle form the gradient can be written as

\[
\nabla \langle f(\mathbf{r}) \rangle_i = \int_{\Omega} f(\mathbf{r}') \nabla' W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}' = \sum_{j=1,N} \frac{m_j}{\rho_j} f(\mathbf{r}_j) \nabla' W(\mathbf{r}_i - \mathbf{r}_j, h)
\]
The divergence theorem relates volume integrals to surface integrals of a vector field. According to this theorem, if a region $\Omega$ in space enclosed by a surface $S$, then

$$ \int_{\Omega} \nabla \cdot f(r') \, dr' = \oint_{S} f(r') \cdot ndS $$

where $f(r)$ is a vector and $n$ is a unit vector normal to the surface $S$ in the direction away from the surface. The theorem is also known as Gauss's theorem. In order to evaluate the smoothed expression of the divergence of any vector field, one can follow the same steps in Appendix 2 and, instead of dropping the surface term one can retain it to implement the divergence theorem. The underlying assumption in doing so is that the value of the function $f(r)$ doesn't vanish at the surface. Thus,

$$ \nabla \cdot \langle f(r) \rangle_i = \sum_{j=1,N} \frac{m_j}{\rho_j} f(r_j) \nabla W(r_i - r_j, h) + \oint_{S} f(r') \cdot ndS' $$

where the second term on the right hand side is the surface integral, extensively used in the present work.
In a two-dimensional domain, let us assume that an SPH particle is near the domain boundary or another phase the equation of which is given by a straight line (surface, in case of three-dimensional domain) as shown in the following figure. Let us also assume that a cubic spline kernel is used in Cartesian co-ordinate system whose origin coincides with the fluid particle position.

Let $h=1$ and the equation of the line is $y=1.5$. The arc length, $A\zeta=AB=2.6458$ (calculated after finding the coordinates of points $A$ and $B$). According to Campbell, the kernel function is evaluated for the point $C$ ($y=1.5$) for the purpose of estimating line integral (surface integral, in case of three-dimensional domain). Since the line is only intersecting with the outer kernel (i.e., $h>1$), the value of kernel function for $|r|=1.5$ is:

$$W_c = \frac{10}{7\pi(1^2)} \left( 2 - \frac{|r|}{h} \right)^3 = 0.05684$$

and the line integral is $SI_{Campbell} = W_c A\zeta = 0.1504$. 
According to the present method, the line integral is written as

\[
SI_{current} = \int_{\eta}^{\eta'} W(|r|, h) d\zeta = \frac{10}{7\pi(1^2)} \left(2 - \frac{|r|}{h}\right)^3 d\zeta
\]  

(A1)

The straight line being horizontal, the distance of any point on the line from the SPH particle is given by

\[|r| = \sqrt{x^2 + 1.5^2} = \sqrt{x^2 + 2.25}\]  

and \(d\zeta = dx\)

Substituting the above expression in Eqn. (A1), one obtains

\[
SI_{current} = \frac{10}{7\pi} \left(2 - \frac{\sqrt{x^2 + 2.25}}{h}\right)^3 dx
\]

\[= 0.065383\]  

(using Simpson's rule)

Thus, \(SI_{Cambell} > SI_{current}\)