HIGH ORDER SMOOTHED PARTICLE HYDRODYNAMIC
METHODS FOR SLIGHTLY COMPRESSIBLE BOUNDED FLOW

by

Zhenyu He

A dissertation submitted to the Faculty of the University of Delaware in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Applied Mathematics

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ABSTRACT

This thesis investigates the accuracy and the implementation of solid wall boundary conditions for Smoothed Particle Hydrodynamics (SPH) for the simulation of slightly compressible fluid flows. The accuracy of SPH is affected by two key parameters: the smoothing length and the overlap. Investigation of the convergence of SPH is conducted on a two-dimensional doubly periodic flow. The result shows that the standard SPH formulation does not converge with a fixed rate and the overall error is limited by the discretization error with a fixed overlap value. New algorithms are developed for the approximations of gradient operator and laplacian operator that have third order convergence rate with a fixed overlap value. In order to generate the model efficiently and maintain accuracy an appropriate boundary treatment is important. Two existing boundary treatments are investigated: the ghost particle method and the boundary force method. Those methods have their advantage and disadvantage. The ghost particle method works well for boundaries with straight lines or flat plane but it is difficult to implement for boundaries with complex geometry. The boundary force method is easy to handle boundaries with complex geometry but one of the parameters is application dependent. A new boundary technique is developed based on the new SPH approximation algorithms. The new boundary treatment adopts the ability to handle curved boundaries from the boundary force method without any free parameters. The algorithms were tested through SPH simulations of doubly periodic flow, plane Couette Flow and circular Couette flow. The determined velocity profiles agree well with theoretical results. The results of the convergence study show that the new algorithms are high-order methods and better than currently existing techniques.
1.1 Motivation

Computational Fluid Dynamics (CFD) is a well established area in applied mathematics and CFD has been a powerful tool in many fields of industry and science. At the core of CFD, numerical methods pose many mathematical challenges. Broadly speaking, according to discretization methods, numerical methods may be categorized into two classes: mesh-based methods and mesh-free methods. In mesh-based methods, the computational domain is discretized into a finite number of grid points connected by a mesh. Grid points are the locations where variables are evaluated. Different mesh-based methods define different connectivities, and hence, different meshes. On the other hand, in mesh-free methods, the continuous domain is discretized by a set of nodes, or particles, without any connectivity or mesh.

Traditional mesh-based methods such as Finite Elements Methods, Finite Differences Methods and Finite Volume Methods have been implemented in various area of CFD by investigators. Mesh-based methods are more popular in academic and industrial researches and many commercial softwares used by industrial companies are based on mesh-based methods. However, mesh-based methods have certain limitations and they are not always preferred in applications.

- The grid-mesh discretization is an approximation of the physical continuum. In some applications, it is not an efficient approximation or an accurate approximation. For example, for problems with fragmentation or explosion, one may encounter mesh deformation or mesh distortion, which can affect the accuracy of the numerical simulation.
• Traditional mesh-based methods require very fine resolution when large gradient of the field variable occurs. It can be computationally very expensive for simulations to use a fine mesh on the entire domain. Hence adaptive refinement is crucial to the efficiency of the simulation. However, for problems with complex geometries, refinement in mesh-based methods may be limited by the amount of local refinement. For example, applications involving solid impaction or penetration raise many numerical instabilities for mesh-based numerical methods. In those cases, researchers intend to remesh the domain and to map the field variables from the old mesh to the new mesh. This procedure introduces computation complexity and pollutes the accuracy of the simulation.

• It is computationally very expensive for many mesh-based methods to achieve high order of accuracy for problems with complex geometries in higher dimensions. For example, in traditional FEM, construction of a cubic polynomial on an element in three dimension is prohibitively expensive and cubic elements are seldom used.

At a certain point, many numerical analysts believe that the numerical simulation is more efficient and more accurate using a set of arbitrarily distributed particles without the constraint of a mesh. Examples of mesh-free methods are: Smoothed particle hydrodynamics (SPH) ([23, 35]), Vortex Method ([10, 28, 51]), Finite Point Methods ([31]), Diffuse Element Method (DEM) ([48]), Element Free Galerkin (EFG) method ([5]), Particle-in-Cell (PIC) ([20, 24]), HP-cloud method ([17]), Meshless local Petrov-Galerkin (MLPG) method ([3]), and the Reproduced kernel particle method (RKPM) ([33]). Smoothed particle hydrodynamics (SPH) methods are mesh-free technique for obtaining approximate solutions of the equations of the fluid dynamics by replacing the fluid with a set of particles. The advantages of SPH over traditional mesh-based methods can be summarized as follows:

• Applications with fracture or large deformation can be handled easily. Chen et al. [8] study bonded rubber deformations that usually exist in bearing applications using RKPM, a variation of SPH. The behavior of rubber is studied in the bonded rubber under an interlaminar compression. Due to excessive mesh distortion occurring near the edges on the rubber-metal interfaces, the finite element simulation of the bonded rubber usually fails [9]. RKPM demonstrates improved performance for larger magnitude of compression or tension where the finite element analysis fails without experiencing the difficulty of mesh distortion. Maurel and Combescure [37] study the fracture of a cracked plate. A bar is pre-cracked halfway through its width and subjected to traction forces at both ends.
For conventional mesh-based methods, the difficulties raised from the cracking of the solid often lead to complexly and costly remeshing problems. Remeshing allows the problem to continue for a short time, but the large distortions result in remeshing repeatedly. More complete treatment of the problem is given by the SPH method to predict the fracture behavior of the solid.

- The refinement procedure is much more flexible for SPH due to its inherently adaptivity. In conventional mesh-based CFD, techniques for choosing locations of mesh refinement are quite sophisticated. Kitsionas and Whitworth [27] describe a particle splitting algorithm to meet the requirement of high local resolution for an SPH simulation of self-gravitating collapse. The simulation is accomplished efficiently with the On-The-Fly particle splitting implementation. Lastiwka et al. [29] present a robust and flexible framework for SPH in which particles can be inserted and removed according to any constraint. They applied the adaptive scheme to compressible flow with a Riemann shock tube problem. The method improved the shock front resolution as well as the post-shock solution while keeping the same total number of particles used in non-adaptive cases.

- Discretization of complex geometry is trivial. Marongiu et al. [36] implement a parallel SPH algorithm to study the flow in a Pelton turbine. A Pelton turbine is an impulse type water turbine which consists of Pelton buckets. The geometry of a real Pelton bucket is very complex. But, the authors can discretize the bucket simply by placing particles on the surface of the bucket.

- It is easy to track the deformation of the domain. Since the materials or boundaries are represented by particles in a Lagrangian reference frame, interface problems, free surface problems and applications with deforming boundaries are no longer difficult. Antoci et al.[2] performed simulations of the deformation of an elastic plate subjected to time-dependent water pressure using the SPH method. A rubber plate gate is clamped only along the upper side, and it is free to deform when subjected to the pressure of the fluid. In conventional approach, structures are usually described in Lagrangian frames, whereas fluids are often described by Eulerian formulations. The Lagrangian nature of SPH makes it very effective to study applications with moving and deforming boundaries. Ferrari et al. [22] propose a three-dimensional parallel SPH scheme to correctly track complex three-dimensional non-hydrostatic free surface flows, as well as to compute an accurate pressure field with little oscillation using a monotone upwind flux for the density equation. Their algorithm is implemented in three-dimensional dam break simulations with triangular obstacles in the domain.

1.2 Problems addressed

Among many fluid dynamics applications, viscosity plays an important role and the capability and the accuracy of SPH in handling viscous momentum transfer are of
concern. Monaghan and Gingold [42] employ artificial viscosity to model the flow with
shocks. Their scheme conserves linear and angular momenta. The artificial viscosity
term vanishes for rigid rotations, and is Galilean invariant. These are important prop-
erties for problems involving large fluid velocities, but it has been reported that the
artificial viscosity gives an inaccurate velocity profile at very small Reynolds number
flow [47]. Morris et al. [47] introduce a more realistic form of viscosity to model low
Reynolds number incompressible flows. The formulation conserves linear momentum
exactly, but it does not conserve angular momentum. The Laplacian is approximated
using a hybrid expression combining an SPH first derivative with a finite difference ap-
proximation of the first derivative. The authors show that the new formulation gives
stable and accurate velocity for the problem where flow passes a cylinder with very
term by modifying Morris’ formulation to ensure the continuity of the stress across
material interfaces and the conservation of angular momentum for flow problems in
a casting process. Alternative approaches have been used to calculate the derivatives
in the viscous term using SPH methods. Takeda et al. [55] solve the Navier-Stokes
equations with a viscous term based on direct evaluation of the second derivatives of
a Gaussian kernel. Wathins [57] calculates the SPH viscous diffusion term based on
nested standard SPH expressions for the first derivative.

Although the formulations of SPH viscous diffusion models have been studied for
decades, only a few of those studies address the order of accuracy of these viscous
schemes. Like any mesh-based method, the accuracy and rate of convergence of
mesh-free methods are of particular importance. Various numerical schemes have
been introduced to approximate the first derivative and the second derivative in SPH
[41, 25, 34, 6]. It is generally considered that the sources of the overall error of the
SPH derivative approximation are the error of the kernel approximation and the error
of the discretization of integrals. Monaghan[41] showed that the error of the kernel
approximation is second order in the smoothing length $h$. Higher order accuracy can
be achieved with higher order kernel functions. However, higher order kernel functions are negative in parts of the support domain, which may lead to negative density and energy during simulation. Quinlan et al. [50] performed error analysis for the standard SPH first derivative in one dimension for particles with regular and irregular arrangements. The authors discover that the accuracy of SPH methods is influenced by the particle separation $p_{sep}$ as well as the smoothing length $h$. The discretization error can increase as smoothing length is decreased to a critical value for a fixed ratio of $h/p_{sep}$ and convergence can be observed with a decreasing $h$ and an increasing $h/p_{sep}$. Amicarelli et al. [1] state that the error of a standard SPH derivative is limited by a constant due to the truncation error of the smoothing kernel function, by performing a error analysis in three dimension.

Based on [50], Fatehi et al. [21] performed error analysis for common SPH viscous schemes and developed a new viscous diffusion model for SPH. The authors replace the kernel in the standard SPH formulation with a corrected kernel to improve the consistency of the method. The kernel estimate of a function is $n$th order consistent if $n + 1$ terms are retained in the Taylor series expansion. The authors show through a thermal diffusion problem that their scheme has second order convergence rate for a uniform particle distribution, and it has first order convergence rate for a non-uniform particle distribution with a fixed $h/p_{sep}$ ratio. This important result encourages us to explore the nature on the convergence of the SPH method and to push the rate of convergence to higher order.

Another difficulty raised in the SPH method is the boundary condition. The treatment of boundary conditions was neglected in the conventional SPH method. Takeda et al. [55] makes an early attempt to introduce several layers of imaginary particles beyond the boundary to specify various physical boundary conditions. Libersky [30] introduces ghost particles as the mirrors of fluid particles beyond the boundary. The no-slip or free-slip boundary condition can be imposed depending on the velocity
assigned to ghost particles. However, the ghost particle method is limited to simple boundaries. The placement of ghost particles is not straightforward when the geometry of the boundary is complex, for instance, corners and curved boundaries. Morris et al. [47] use fixed virtual particles filling the solid wall domain to impose boundary conditions on curved boundaries. Fixed virtual particles can be considered as extrapolation points placed outside the boundary. The velocity of those fixed virtual particles at each time step is calculated using a linear extrapolation of the velocity of fluid particles, based on the ratio of shortest distances from the tangent line to the fluid particle and from the tangent line to the virtual particle. But for complex boundary geometries, there may be different ways to calculate normal vectors which results in difficulties in implementation. An alternative approach is the boundary force method proposed by [44, 45, 43]. Particles are placed on the boundary with the desired boundary velocity, and also, the boundary particles exert certain normal forces to keep fluid particles from penetrating the solid wall boundary. The boundary force method can easily handle boundaries with complex geometries. All of those boundary methods have advantages and disadvantages. A more general and efficient boundary method needs to be developed.

1.3 Thesis outline

This thesis is organized as follows. The current chapter discusses a comparison between mesh-based and mesh-free methods and the motivation for the current research. The second chapter describes the basic concepts and formulations of the Smoothed Particle Hydrodynamics method. The third chapter begins with the details of common methods for boundary conditions, followed by new designed boundary condition treatment. The error analysis of the SPH approximations and the new algorithm designed for higher order consistency are presented in Chapter 4. In the fifth chapter these new algorithms are applied to some test cases. The algorithms have been tested through comparison of fluid velocities on plane Couette Flow and circular Couette flow.
Chapter 2

SMOOTHED PARTICLE HYDRODYNAMICS

2.1 Introduction

SPH was developed to solve fluid dynamics problems in the form of a system of partial differential equations (PDEs). The method was first introduced by Gingold and Monaghan [23] and Lucy [35] to study gas dynamical problems in astrophysics. It is a fully Lagrangian, mesh-free numerical method. The fluid or gas in the physical system is represented by a set of finite number of particles, which follow the fluid motion and carry the mass, pressure, velocity and other material properties. The governing equations of continuum fluid are then expressed by particle-particle interactions and forces. This chapter reviews the essential theory of SPH and explains the details of using SPH to solve the equation of interest.

2.2 Notations

To clearly express the multi-dimensional Taylor expansion and the multi-dimensional error analysis, for the rest of the thesis, the Einstein summation convention is used. An index variable that appears twice in a single term implies summation of that term over all the values of the index. The Greek alphabet \((\alpha, \beta, \cdots)\) in the superscript is used for spatial components, where indices take values 1,2,3. The Latin alphabet \((i,j,\cdots)\) is used as an index of particles. The Einstein summation convention is only applied to the spatial components index, i.e. the Greek letters. For example,

\[
(r_i - r_j)\alpha \frac{\partial f(r_i)}{\partial r^\alpha} = (x_i - x_j) \frac{\partial f}{\partial x}(r_i) + (y_i - y_j) \frac{\partial f}{\partial y}(r_i) + (z_i - z_j) \frac{\partial f}{\partial z}(r_i). \tag{2.1}
\]

Even though the Greek letters as superscript takes the values 1,2,3, the expression \(r^2\) is never used in the thesis that represent the second spatial component of the vector.
In fact, any time a number is used as the superscript, it represents the exponent or power. For example, \((\mathbf{r} - \mathbf{r}')^2\) means \(\mathbf{r} - \mathbf{r}'\) squared.

Other notations used throughout the thesis are,

\((\cdot)_K\) is the SPH kernel approximation of a quantity,

\((\cdot)_S\) or \(\langle \cdot \rangle\) is the SPH particle approximation of a quantity,

\[
\frac{D}{Dt} = \frac{\partial}{\partial t} + (\mathbf{v} \cdot \nabla) \text{ is the material derivative,}
\]

\[
\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j, \mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j, f_{ij} = f_i - f_j, etc.,
\]

\[
W_{ij} = W(\mathbf{r}_{ij}, h) = W(\mathbf{r}_i - \mathbf{r}_j, h),
\]

\[
\nabla^\alpha \nabla^\beta f = \frac{\partial f}{\partial \mathbf{r}^\alpha} \frac{\partial f}{\partial \mathbf{r}^\beta},
\]

H.O.T. is short for higher order terms,

\(\mathbf{a} \otimes \mathbf{b} = a^\alpha b^\beta\) is the tensor/outer product of 2 vectors or first order tensor,

\(\mathbf{a} \cdot \mathbf{b} = a^\alpha b^\alpha\) is the inner product of 2 vectors or first order tensor,

\(\mathbf{A} : \mathbf{B} = A^{\alpha\beta} B^{\alpha\beta}\) is the double-dot product of 2 second order tensor,

\(\mathbf{A} \cdot \mathbf{b} = A^{\alpha\beta} b^\beta\) is the matrix-vector multiplication,

\(\mathbf{I}^{\alpha\beta}, I^{\alpha\beta\gamma}\) are the identity tensors,

and \(0^{\alpha\beta\gamma}\) is the third order zero tensor.

### 2.3 SPH derivatives approximation

#### 2.3.1 Kernel approximation

In a PDE system, the rate of change of physical quantities depend on the spatial derivatives of those physical quantities. For mesh-based numerical methods, such as the finite difference method, the derivatives are approximated using the information on neighboring grid points. In SPH, the kernel function helps to approximate the derivatives. First of all, for a quantity \(f\), the following identity always holds,

\[
f(\mathbf{r}) = \int_{\Omega} f(\mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') d\mathbf{r}', \quad \mathbf{r} \in \Omega \tag{2.2}
\]
where $\delta(r)$ is the Dirac delta function,

$$
\delta(r - r') = \begin{cases} 
1 & r = r' \\
0 & r \neq r',
\end{cases}
$$

(2.3)

where $dr'$ is the volume element and $\Omega$ is the spatial domain that contains $r$. Then the delta distribution is approximated by a kernel function,

$$
f_K(r) = \int_{\Omega} f(r') W(r - r', h) \, dr',
$$

(2.4)

where the function $W$ is the smoothing kernel, also known as kernel function or smoothing function. The variable $h$ is the smoothing length. As shown in Figure 2.1, through the kernel function, the entire fluid region of interest is covered. The fluid properties at any location can be interpolated from the value of those quantities of particles. The kernel function $W$ has three properties:

$$
\int_{\Omega} W(r - r', h) \, dr' = 1.
$$

(2.5)

This is the normalization condition and

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

(2.6)

In the limit as $h \to 0$, the kernel approximation is exact. In practice, one adds an additional requirement to the kernel function $W$ that

$$
W(r - r', h) = 0 \text{ when } |r - r'| > ch,
$$

(2.7)

where $c$ is a constant related to the kernel function. This property is called compact support. With this property, the integration is now over a local support domain instead of over the entire domain. The kernel approximation has 2nd order accuracy [41]. The detail of the error analysis will be shown in Section 2.3.5.
Figure 2.1: In SPH, a) the fluid is represented by particles with the kernel function. b) SPH kernel function with 2 key parameters: smoothing length $h$ and particle separation $p_{\text{sep}}$.

2.3.2 Kernel functions

There are many choices of kernel functions for SPH. The kernel function should be an even function with respect to $r - r'$ with the properties,

$$\int_{\Omega} W(r - r', h)dr' = 1,$$  \hspace{1cm} (2.8)

$$\lim_{h \to 0} W(r - r', h) = \delta(r - r'),$$  \hspace{1cm} (2.9)

$$W(r - r', h) = 0 \text{ when } |r - r'| > ch.$$  \hspace{1cm} (2.10)
In addition, the kernel function should be non-negative in the support domain. The reason is that negative values of the kernel function in a fluid simulation may result in nonphysical phenomena, such as negative density. Because of the symmetry, the kernel can be written in the form,

\[ W(r_{ij}, h) = \frac{1}{h^d} f \left( \frac{|r_{ij}|}{h} \right), \quad (2.11) \]

where \( d \) is the number of dimension. Gingold and Monaghan [23] use a Gaussian kernel in two dimension,

\[ f(s) = \frac{1}{h^2 \pi} e^{-s^2}, \quad (2.12) \]

where \( s = \frac{|r_{ij}|}{h} \). The Gaussian kernel satisfies condition (2.8) and (2.9); but it does not have compact support. However, by assuming the kernel function is Gaussian, it is easier to find the physical interpretation of a SPH equation. This is described as the first golden rule of SPH by Monaghan [38]. Kernel functions based on B-splines are used more commonly because they have compact support and are therefore computationally efficient. For example, a cubic spline in two dimension is,

\[
\begin{align*}
    f(s) &= \frac{5}{14 \pi} \begin{cases} 
    (2 - s)^3 - 4(1 - s)^3, & 0 \leq s < 1; \\
    (2 - s)^3, & 1 \leq s < 2; \\
    0, & 0 \leq s \geq 2.
    \end{cases} \quad (2.13)
\end{align*}
\]

The factor \( \frac{5}{14 \pi} \) is replaced by \( \frac{1}{6} \) in one dimension and \( \frac{1}{4 \pi} \) in three dimension. A quintic spline is another commonly used kernel by researchers [47, 19]

\[
\begin{align*}
    f(s) &= \frac{7}{478 \pi} \begin{cases} 
    (3 - s)^5 - 6(2 - s)^5 + 15(1 - s)^5, & 0 \leq s < 1; \\
    (3 - s)^5 - 6(2 - s)^5, & 1 \leq s < 2; \\
    (3 - s)^5, & 2 \leq s < 3; \\
    0, & s \geq 3.
    \end{cases} \quad (2.14)
\end{align*}
\]

Both of them are bell-shaped functions. The cubic spline is a 3rd order polynomial, and its second derivative is a piece-wise linear function (Figure 2.2c). Hence the third derivative of the cubic spline is discontinuous. Therefore, the second derivative of a
cubic spline is not a good choice for SPH derivative approximation.

Another class of radial function having compact support was derived by Wendland [58, 59]. For a Wendland kernel function, the variable $q$ is defined as $q \equiv s/2 = \frac{r_{ij}}{2h}$, and the function is zero if $q > 1$. The 5th order polynomial $C^2$ Wendland kernel (WC2 for short) is,

$$WC^2(s) = \frac{7}{\pi} \begin{cases} (1 - q)^4(4q + 1) & 0 \leq q < 1; \\ 0, & q \geq 1. \end{cases}$$

(2.15)

The WC4 kernel is an 8th order polynomial and belongs to $C^4$,

$$WC^4(s) = \frac{9}{\pi} \begin{cases} (1 - q)^6 \left(1 + 6q + \frac{35}{3}q^2\right), & 0 \leq q < 1; \\ 0, & q \geq 1. \end{cases}$$

(2.16)

And the WC6 is an 11th order polynomial,

$$WC^6(s) = \frac{78}{7\pi} \begin{cases} (1 - q)^8((1 + 8q + 25q^2 + 32q^3), & 0 \leq q < 1; \\ 0, & q \geq 1. \end{cases}$$

(2.17)

Recently, Dehnen and Aly [16] show that pairing instability can be solved by using Wendland kernels. Pairing instabilities happen in SPH when particles that are close pair and the effective number of particles are reduced inside the support region. Some of the Wendland kernels are sufficiently smooth, however, they require more computational effort while giving similar numerical performance to the quintic spline kernel for our numerical study. Thus, we use quintic spline kernels in our simulation.

Liu [34, 32] introduces a systematic way to build kernels that have a high order of completeness which means they can reproduce high-order polynomials. The idea is to set the higher even moment of the kernel function to be zero. The kernel functions constructed by this condition are not necessarily positive. For example, in order to get a 4th order kernel, Equation (2.33) needs to be satisfied so the kernel is negative in some region of its support domain. This may leads to unphysical phenomena in the simulation such as negative density or negative energy.
Figure 2.2: Various positive kernel functions used in SPH literatures. a) kernel functions; b) first derivative of kernel function; c) second derivative of kernel function.
Figure 2.3: Demonstration of the overlap $\beta$. Top: small overlap $\beta$. Bottom: large $\beta$, which results in more neighbors.

There are two key parameters to control the kernel functions: they are the smoothing length $h$ and the overlap $\beta$,

$$\beta = \frac{h}{p_{sep}}.$$  \hspace{1cm} (2.18)

The smoothing length $h$ describes the particle interaction radius, and the overlap describes the number of neighbor particles. The larger value of $\beta$ means the support domains of kernels have more overlap. The smoothing length $h$ and the overlap $\beta$ is related by the initial particle separation $p_{sep}$. The initial particle separation $p_{sep}$ is defined to be the initial separation distance between particles. For example, the particles can be placed on a lattice of square cells and $p_{sep}$ is the length of the sides of
those cells. Since the overlap is the ratio of the smoothing length and the particle separation, larger value of $\beta$ also implies that more neighbor particles are inside the support domain of a kernel (Figure 2.3). Overlap is an important concept in many meshfree methods, for example, the vortex method and the reproducing kernel particle method (RKPM) [34]. Some overlap for support domains of kernels is required to cover the computational domain, and to establish particle-particle interaction. If the overlap is too large, the increasing the number of neighbors requires more computational resources. Quinlan et al. [50] use analogy to mesh-based methods to interpret those two parameters. The smoothing length is analogous to the spatial discretization size in mesh-based methods. The overlap $\beta$ is analogous to the number of points in a stencil in a finite differences method. In traditional mesh-based methods, the computational stencil is a fixed characteristic of a method and the accuracy of the method is controlled by the spatial discretization. In SPH, convergence is not obtained by decreasing the smoothing length $h$ alone with a fixed overlap $\beta$, which is different from mesh-based methods. More details are discussed in Chapter 3.

As particles moves in the simulation, the positions of the particles can be disordered. The particle disorder is a nature concept but the theoretical definition and the quantitative measurement is difficult to identify. In SPH, at the beginning of a simulation, the particles are usually placed with a regular arrangement with a pattern, such as, a square lattice/grids or a polar coordinates lattice. The particles disorder describes the deviation of particle distribution from those regular arrangements. Antuono et al. [?] present a numerical algorithm that measures the disorder in particle distribution. The particle separation is no longer equal to the initial particle separation $p_{sep}$. For applications with incompressible flow, the spacing between particles is restricted by the incompressible condition, and large voids should not occur during the simulation. One approach to modeling fluids in SPH is based on the assumption that the fluid is slightly compressible. The pressure is determined by a equation of state to maintain low density variation. The particle separation during the simulation is restricted by
the pressure and it also maintains low variation even though the particle distribution is disordered. The smoothing length $h$ is fixed during the simulation.

2.3.3 First derivatives and second derivative

The SPH formulation of the gradient $\nabla f(\mathbf{r})$ is obtained by replacing $f(\mathbf{r})$ in (2.4) with $\nabla f(\mathbf{r})$,

$$(\nabla f)_K(\mathbf{r}) = \int_\Omega \nabla_{\mathbf{r}'} f(\mathbf{r}') W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}'$$

$$= \int_{\partial \Omega} f(\mathbf{r}') W(\mathbf{r} - \mathbf{r}', h)d\mathbf{s}' - \int_{\Omega} f(\mathbf{r}') \nabla_{\mathbf{r}'} W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}' \quad \text{(Divergence Theorem)}$$

$$= -\int_{\Omega} f(\mathbf{r}') \nabla_{\mathbf{r}'} W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}'$$

$$= \int_{\Omega} f(\mathbf{r}') \nabla_{\mathbf{r}} W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}', \quad (2.19)$$

where $\nabla_{\mathbf{r}}$ is the gradient with respect to $\mathbf{r}$ and $\nabla_{\mathbf{r}'}$ is the gradient with respect to $\mathbf{r}'$. The kernel function has compact support property (2.7) so that for problems with boundary at infinity or boundaries far enough, the surface term is zero. However, when boundaries are involved in the problem, the surface term does not necessarily have to be zero since the kernel function $W$ has been truncated by the boundary. This can cause problems in formulation and difficulties when dealing with boundary conditions. We will discuss this problem later in Chapter 4.

Similarly, the divergence of a vector function $\nabla \cdot \mathbf{f}(\mathbf{r})$ can be approximated by,

$$(\nabla \cdot \mathbf{f})_K(\mathbf{r}) = \int_{\Omega} \nabla \cdot \mathbf{f}(\mathbf{r}') W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}'$$

$$= \int_{\partial \Omega} \mathbf{f}(\mathbf{r}') W(\mathbf{r} - \mathbf{r}', h) \cdot \mathbf{n} d\mathbf{s}' - \int_{\Omega} \mathbf{f}(\mathbf{r}') \cdot \nabla_{\mathbf{r}'} W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}'$$

$$= \int_{\Omega} \mathbf{f}(\mathbf{r}') \cdot \nabla_{\mathbf{r}} W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}', \quad (2.20)$$

where $\mathbf{f}$ is a vector function and $\mathbf{n}$ is the outward normal of the surface $\partial \Omega$. Again, the surface term is zero assuming that the boundary is far enough away.

Using integration by parts, the differential operators are transferred and applied to the kernel function. Hence in SPH, the derivative of a scalar function is approximated
by the convolution of the function and the derivative of the kernel function. This is similar to the idea used with finite difference approximations. With finite differences, the function is first approximated by an interpolant, then the differential operator is directly applied to the interpolant. The kernel function establishes the connection between particles, and now without a mesh or a grid, the spatial derivative of a scalar function can be approximated by transferring the derivative to the kernel function.

As in the case of first derivative, the second derivatives of a scalar function can be obtained by taking the derivative of the kernel function twice. For example, the second derivative with respect to spatial variable \( x \), \( \frac{\partial^2 f}{\partial x^2} \), can be approximated by

\[
\left( \frac{\partial^2 f}{\partial x^2} \right)_K (r) = \int_{\Omega} \frac{\partial^2}{\partial x^2} f(r') W(r - r', h) \, dr' = \int_{\Omega} f(r') \frac{\partial^2}{\partial x^2} W(r - r', h) \, dr'.
\]  

(2.21)

However, this formulation is not commonly used for several reasons. First of all, it is very sensitive to particle disorder. Second, due to lack of differentiability of the kernel function, taking the second derivative of the kernel function may result in a step function or discontinuous function. For example, the second derivative of the cubic spline (2.13) with respect to \( s \) is,

\[
\frac{\partial^2 f(s)}{\partial s^2} = \frac{5}{14\pi} \begin{cases} 
18s - 12, & 0 \leq s < 1; \\
12 - 6s, & 1 \leq s < 2; \\
0, & 0 \leq s \geq 2.
\end{cases}
\]

(2.22)

This function is a piecewise linear function. Lack of smoothness of the second derivative of the kernel function affects the accuracy of the approximation of the second derivative of the function. For decades, pioneers in SPH research have studied the second derivative formulation and different expressions are used in the literature. A summary of their work will be provided in Section 2.5.4.

2.3.4 Particle approximation

In SPH, a fluid is represented by a finite set of particles that carry information of fluid properties. Therefore to evaluate integral (2.4) and those integrations in the
approximation of the derivatives, the integrals are approximated by summation over the mass element. This step is called particle approximation. The integral (2.4) can be rewritten as

$$f_K(r) = \int_{\Omega} f(r') W(r - r', h) \frac{\rho(r') dr'}{\rho(r')} ,$$  (2.23)

where $\rho(r') dr'$ is the mass element. Then,

$$f_S(r) = \sum_j \frac{m_j}{\rho_j} f_j W(r - r_j, h),$$  (2.24)

where $j$ is the particle index and the summation is over all particles. Here the particle at $r_j$ has mass $m_j$, density $\rho_j = \rho(r_j)$ and the value of the quantity $f$ at $r_j$ is denoted by $f_j$. In the above step, the continuous integral of kernel approximation is discretized into a summation over a set of particles. A function evaluated at position $r_i$, $f(r_i)$, can be expressed as,

$$f_S(r_i) = \sum_j \frac{m_j}{\rho_j} f_j W(r_i - r_j, h) = \sum_j \frac{m_j}{\rho_j} f_j W_{ij},$$  (2.25)

where $W_{ij} = W(r_i - r_j, h)$. The summation is over all particles in the compact support domain of the kernel function. Thus, Equation (2.25) expresses the value of the function at the position $r_i$ as the weighted average of its neighbor particles in the support domain of the kernel function.

The SPH first derivative (2.19) and (2.20) can also be expressed as,

$$(\nabla f)_S (r) = \sum_j \frac{m_j}{\rho_j} f_j \nabla_r W(r - r_j, h),$$  (2.26)

$$(\nabla \cdot f)_S (r) = \sum_j \frac{m_j}{\rho_j} f_j \cdot \nabla_r W(r - r_j, h),$$  (2.27)

and,

$$(\nabla f)_S (r_i) = \sum_j \frac{m_j}{\rho_j} f_j \nabla_i W_{ij},$$  (2.28)

$$(\nabla \cdot f)_S (r_i) = \sum_j \frac{m_j}{\rho_j} f_j \cdot \nabla_i W_{ij}. $$  (2.29)
Here $\nabla_i$ represents the gradient with respect to a particle at $r_i$.

In some SPH work, the kernel function $W$ is referred as an interpolation function and Equation (2.25) is considered an interpolation process [46, 11, 18, 15]. This interpretation is not true and misleading. The values given by (2.25) at sample particles are not the same as the function value given at those sample particles. In other words, $f_S(r_j) \neq f(r_j)$, where $j$ is the index of any particle. Hence, when the value of a quantity is used to solve a PDE system, the expression for the value needs to be chosen carefully, namely, $f_j$ or $f_S(r_j)$. For example,

$$\frac{D\rho_i}{Dt}, \quad \text{and} \quad \frac{D}{Dt} \sum_j \frac{m_j}{\rho_j} \rho_j W_{ij},$$

(2.30)

are different quantities. The first expression represents the rate of change of actual density at position $r_i$. The second expression represents the rate of change of the averaged density at position $r_i$. Monagan [40] uses the second expression (equation 4.22 in [40]) to show total mass conservation at each particle. However, the first expression is more commonly used in SPH equations [38, 41].

### 2.3.5 Error estimate

First let us look at the error introduced in the kernel approximation (2.4). Using the Taylor expansion of $f(r')$ at position $r$,

$$f_K(r) = \int_\Omega \left[ f(r) + (r - r')^\alpha \frac{\partial f(r)}{\partial r^\alpha} + (r - r')^\beta \frac{\partial f(r)}{\partial r^\beta} \right] W(r - r', h)dr' + O((r - r')^3).$$

(2.31)

Here the normalization condition (2.5) is used. And for the second term, if we require that the kernel function is an even function, then the integral,

$$\int_\Omega (r - r')^\alpha W(r - r', h)dr' = 0.$$

(2.32)
Therefore, the kernel approximation has second order accuracy \( O(h^2) \). If a higher order kernel function is designed such that the second moment of the kernel is zero,

\[
\int_\Omega (r - r')^\alpha (r - r')^\beta W(r - r', h) \, dr' = 0,
\]

then the kernel approximation has fourth order accuracy. The third moment of the kernel function is also zero because the kernel function is even.

The analysis of the error introduced by particle approximation \((2.25)\) is slightly different. Using the Taylor expansion,

\[
f_S(r_i) = \sum_j m_j \rho_j \left[ f(r_i) + (r_i - r_j)^\alpha \frac{\partial f(r_i)}{\partial r_i^\alpha} + O ((r_i - r_j)^2) \right] W_{ij}
\]

\[
= f(r_i) \sum_j m_j \rho_j W_{ij} + \frac{\partial f(r_i)}{\partial r_i^\alpha} \sum_j m_j \rho_j (r_i - r_j)^\alpha W_{ij} + O ((r - r')^2).
\]  

(2.34)

This shows that the particle approximation cannot reproduce a constant exactly unless the summation in the first term is one,

\[
\sum_j m_j \rho_j W_{ij} = 1.
\]  

(2.35)

In fact condition \((2.35)\) depends on the location of the particle \(i\). If the particle is close to the boundary, this condition is not true. If the particle is inside the domain of interest and the support domain of the particle doesn’t intersect with the boundary, then

\[
\sum_j m_j W_{ij} \approx 1, \quad \sum_j m_j (r_i - r_j)^\alpha W_{ij} \approx 0.
\]  

(2.36)

The particle approximation has second order accuracy under the condition \((2.36)\).

Similarly, for the kernel approximation of the first derivative \((2.19)\),

\[
(\nabla_r f)_K (r) = \int_\Omega \left[ f(r) + (r - r')^\alpha \frac{\partial f(r)}{\partial r^\alpha} + (r - r')^\beta \frac{\partial f(r)}{\partial r^\beta} \right] \nabla_r W(r - r', h) \, dr' + O ((r - r')^3).
\]

\[
= f(r) \int_\Omega \nabla_r W(r - r', h) \, dr' + \frac{\partial f(r)}{\partial r^\alpha} \int_\Omega (r - r')^\alpha \nabla_r W(r - r', h) \, dr' + O ((r - r')^2).
\]  

(2.37)
The integral of the first term is zero by the symmetry of the kernel function. The integral of the second term is equal to 1 if the kernel is normalized (performing integration by parts on (2.5) and use condition (2.7)). Hence the kernel approximation for the first derivative also has second order accuracy $O(h^2)$. And for the particle approximation (2.28),

$$
(\nabla f)_S (r_i) = \sum_j \frac{m_j}{\rho_j} \left[ f(r_i) + (r_i - r_j) \alpha \frac{\partial f(r_i)}{\partial r_i^\alpha} + O((r_i - r_j)^2) \right] \nabla_i W_{ij} \\
= f_i \sum_j \frac{m_j}{\rho_j} \nabla_i W_{ij} + \frac{\partial f(r_i)}{\partial r_i^\alpha} \sum_j \frac{m_j}{\rho_j} (r_i - r_j) \alpha \nabla_i W_{ij} + O((r_i - r_j)^2).
$$

(2.38)

Figure (2.4) shows that the summation in the first term is not zero if the particle is close to the boundary since the gradient of the kernel function $\nabla_i W_{ij}$ is truncated by the boundary. Thus the SPH particle approximation (2.28) of the first derivative is not a good approximation.

Figure 2.4: The summation $\sum_j \frac{m_j}{\rho_j} \nabla_i W_{ij}$ in (2.38) using the quintic kernel function (2.14) in one dimension is nonzero near the boundary $x = 0$ and $x = 1$, which results in deterioration in accuracy of the first derivative approximation.
2.3.6 Special techniques dealing with SPH derivatives

We showed in Equation (2.38) that the SPH approximation (2.28) for the first derivative is problematic. The formula cannot reproduce the derivative of a constant function. One simple modification introduced by Monaghan [41] is,

\[ \langle \nabla f(r_i) \rangle = \sum_j \frac{m_j}{\rho_j} (f_j - f_i) \nabla_i W_{ij}. \]  

(2.39)

The idea is to subtract the first term in (2.38) from the original particle approximation formula so that,

\[ \sum_j \frac{m_j}{\rho_j} (f_j - f_i) \nabla_i W_{ij} = \frac{\partial f(r_i)}{\partial r_i} - \sum_j \frac{m_j}{\rho_j} (\mathbf{r}_i - \mathbf{r}_j)^a \nabla_i W_{ij} + O ((\mathbf{r}_i - \mathbf{r}_j)^2). \]  

(2.40)

The accuracy of this modification still depends on the value of \( \sum_j \frac{m_j}{\rho_j} (\mathbf{r}_i - \mathbf{r}_j)^a \nabla_i W_{ij} \).

For divergence approximation of a vector function, a similar technique can be applied,

\[ \langle \nabla \cdot f(r_i) \rangle = \sum_j \frac{m_j}{\rho_j} (f_j - f_i) \cdot \nabla_i W_{ij}. \]  

(2.41)

Monaghan [41] and Prince [49] introduced the generalized formulae for first derivatives,

\[ \nabla f = \frac{1}{\Phi} [\nabla (f \Phi) - f \nabla \Phi], \]  

(2.42)

\[ \nabla f = \Phi \left[ \nabla \left( \frac{f}{\Phi} \right) + \frac{f}{\Phi^2} \nabla \Phi \right], \]  

(2.43)

\[ \nabla \cdot f = \frac{1}{\Phi} [\nabla \cdot (f \Phi) - f \cdot \nabla \Phi], \]  

(2.44)

and their corresponding SPH form,

\[ \langle \nabla f \rangle = \frac{1}{\Phi_i} \sum_j \frac{m_j}{\rho_j} \Phi_j (f_j - f_i) \nabla W_{ij}, \]  

(2.45)

\[ \nabla f = \Phi_i \sum_j \frac{m_j}{\rho_j} \left[ \frac{f_j}{\Phi_j} + \frac{f_i}{\Phi_i^2} \Phi_j \right] \nabla W_{ij}, \]  

(2.46)
\[ \langle \nabla \cdot \mathbf{f} \rangle = \frac{1}{\Phi_i} \sum_j \frac{m_j}{\rho_j} \Phi_j (f_j - f_i) \cdot \nabla W_{ij}. \quad (2.47) \]

Set \( \Phi = 1 \) in (2.45) and (2.47) we can get those new formulae (2.39) and (2.41). Now use (2.46) and set \( \Phi = \rho \) we can get the gradient for pressure,

\[
\langle \nabla P_i \rangle = \rho_i \left[ \sum_j \frac{m_j}{\rho_j} \frac{f_j}{\rho_j} \nabla W_{ij} + \frac{f_i}{\rho_i^2} \sum_j \frac{m_j}{\rho_j} \rho_j \nabla W_{ij} \right] \\
= \rho_i \sum_j m_j \left( \frac{f_i}{\rho_i^2} + \frac{f_j}{\rho_j^2} \right) \nabla W_{ij}. \quad (2.48)
\]

The reason that formula (2.46) is chosen instead of the formula (2.46) is that, the expression (2.48) conserves linear momentum. For example, consider the Euler equation of inviscid fluid, and the momentum equation is

\[ \frac{Dv}{Dt} = -\nabla P. \quad (2.49) \]

Applying the SPH scheme and consider the total linear momentum of the system,

\[
\frac{D}{Dt} \sum_j m_j v_j = \sum_j m_j \frac{D}{Dt} v_j = - \sum_j m_j \frac{\nabla P}{\rho} \\
= - \sum_i m_i \frac{\rho_i}{\rho} \sum_j m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla W_{ij} \\
= 0. \quad (2.50)
\]

The last double summation is zero since \( \nabla W_{ij} \) is antisymmetric. This shows the total linear momentum of the system is conserved exactly. Conservation can be a very important concept in designing numerical schemes. It assures that the numerical scheme describes the correct physics of the actual system and it also guarantees that there is no momentum produced by numerical error to be added to the numerical simulation.

Equation (2.39), (2.41) and (2.48) will be used to approximate first derivatives in an SPH formulation.
2.4 Lagrangian Fluid Dynamics

In fluid dynamics, a fluid element, sometimes also known as a fluid parcel or a fluid particle (which is a different concept from SPH fluid particles) means an infinitesimally small region of fluid usually used in mathematical formulation. A fluid element is associated with fluid properties, such as mass, density, and it is assumed to have a well defined position and velocity.

There are two different mathematical specifications of the flow field. In the Lagrangian specification of the flow field, the observer follows the fluid element through the flow. The fluid properties carried by the fluid element vary with time. The position, density, velocity and other fluid properties can be expressed as

\[ r(t), \rho(r(t), t), v(r(t), t) \ldots \] \hspace{1cm} (2.51)

In the Eulerian specification of the flow field, the observer stays on a fixed location in space and focuses on the fluid properties at this location with varying time. The density, velocity and other fluid properties are now functions of space coordinates and time together,

\[ \rho(r, t), v(r, t) \ldots, \] \hspace{1cm} (2.52)

where \( r \) here is a fixed point in space whereas in (2.51) \( r(t) \) is the position of the fluid element following the motion of the flow.

The Eulerian description and the Lagrangian description are related by the material derivative or the substantial derivative. Suppose for a quantity \( F(r, t) \) defined at a fixed position \( r \) and time \( t \), the time derivative of the quantity \( F \) is \( \frac{\partial F}{\partial t} \). This only measures the rate of change of the quantity \( F \) with time at a fixed location in space. The total rate of change of quantity \( F \) of a fluid element, following the flow field with the Eulerian description velocity \( v \), is called the material derivative of \( F \), denoted by \( \frac{DF}{Dt} \),

\[ \frac{DF}{Dt} = \frac{\partial F}{\partial t} + (v \cdot \nabla) F. \] \hspace{1cm} (2.53)
Numerical methods generally can also be classified into Eulerian numerical methods and Lagrangian numerical methods. Many hybrid methods have been developed over years, such as the semi-Lagrangian method and Arbitrary Lagrangian-Eulerian, but they will not be discussed in this thesis. In Eulerian methods, the variables in the underlying system depend on the time variable $t$ and the space variable $\mathbf{r}$ where $\mathbf{r}$ represents spatial position in a time-independent coordinate system, and the variables are usually solved on a mesh or a grid. Finite difference methods, finite element methods, finite volume methods and spectral methods are examples of Eulerian method. In Lagrangian methods, variables in the system are quantities carried by fluid elements that follow the flow field, or the characteristics of the system, mathematically speaking. Vortex method and smoothed particle hydrodynamics are examples of Lagrangian methods. The choice of method for a certain problem depends on the objective and characteristics of the problem.

2.5 SPH governing equations

2.5.1 Governing Equations of Fluid dynamics and Non-dimensionalization

Many phenomena in fluid dynamics and gas dynamics can be described by the Navier-Stokes equations and the Euler equations respectively. The Navier-Stokes equations consist of 3 equations. The momentum equation describes the convection and the diffusion of the fluid. The continuity equation describes the mass conservation. And the energy equation describes the conservation of the energy. Using the Lagrangian description and the material derivative discussed in last section,

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v}, \quad \text{(Mass conservation)} \quad (2.54)$$

$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla P + \nabla \cdot (\tau) + \rho \mathbf{F}, \quad \text{(Momentum conservation)} \quad (2.55)$$

$$\rho \frac{DE}{Dt} = -P \nabla \cdot \mathbf{v} + \nabla \cdot (k \nabla T) + \tau : \nabla \mathbf{v}, \quad \text{(Energy conservation)} \quad (2.56)$$
where $\tau$ is the second order stress tensor and $\mathbf{F}$ is the total body force applied in the system. The symbol $:=$ is the double contraction of two second order tensors. It is explained in Section 2.2. For isotropic Newtonian fluid, the stress tensor $\tau$ can be written as,

$$
\tau = \mu \left[ (\nabla \mathbf{v} + \nabla \mathbf{v}^T) - \frac{2}{3} \nabla \cdot \mathbf{v} \mathbf{I} \right].
$$

(2.57)

Here $\mu$ is the dynamic viscosity and $\mathbf{I}$ is the second order identity tensor.

Many problems of interest involve incompressible flow where the density within any fluid element (an infinitesimally small region of fluid) is constant. An equivalent way to describe the incompressibility in fluid dynamic is that the divergence of the velocity vector is zero,

$$
\nabla \cdot \mathbf{v} = 0.
$$

(2.58)

Using this condition and the stress expression for isotropic Newtonian fluid, the momentum equation within the incompressible Navier-Stokes equation is,

$$
\rho \frac{\text{D}\mathbf{v}}{\text{D}t} = -\nabla P + \nabla \cdot (\mu \nabla \mathbf{v}) + \rho \mathbf{F}.
$$

(2.59)

The continuity equation simply becomes Equation (2.58). Under the assumption of incompressibility, the energy equation usually reduces to,

$$
c_p \rho \frac{\text{D}T}{\text{D}t} = \nabla \cdot (k \nabla T),
$$

(2.60)

where $T$ is the temperature, $c_p$ is the specific heat at constant pressure, and $k$ is the coefficient of thermal conductivity.

Now if we focus only on Equations (2.58) and (2.59), we notice that there are three equations for the evolution of the velocity component in three dimension and one equation for the relation between these velocity components. But there is no separate equation for pressure which is an unknown variable to be solved. In general, an equation of state that describes the relation between state variables of the fluid needs to be introduced to the system. We will discuss the equation of state in Section 2.5.5.
Another approach is to use the incompressibility condition (2.58). Take the divergence of the momentum equation (2.59),

\[ \nabla^2 P = -\rho \nabla \cdot (\mathbf{v} \cdot \nabla \mathbf{v}) + \nabla \cdot \mathbf{F}. \]  

This equation is called pressure poisson equation, which replaces the incompressibility equation. It shows that the pressure now depends on the velocity field instead of the density and the temperature of the material.

It is useful to write the governing equations in non-dimensional form. Nondimensionalization (also known as scaling) reduces the number of free parameters in the problem to be studied and helps analyzing the behavior of the system regardless of the units used to measure the variables. To do this we need to select characteristic quantities to describe the system. Suppose we choose \( L \) to be the characteristic length, \( U_0 \) to be the characteristic velocity, \( P_0 \) to be the characteristic pressure, \( t_0 \) to be the characteristic time and \( \rho_0 \) to be the characteristic density. Following the definition of those characteristic quantities, we can define the non-dimensional variables,

\[ x' = \frac{x}{L}, \quad y' = \frac{y}{L}, \quad z' = \frac{z}{L}, \quad u' = \frac{u}{U_0}, \quad v' = \frac{v}{U_0}, \quad w' = \frac{w}{U_0}, \quad \rho' = \frac{\rho}{\rho_0}, \]

and further we choose \( t_0 = L/U_0 \) and define,

\[ t' = \frac{t}{L/U_0}, \quad P' = \frac{P - P_0}{\rho_0 U_0^2}. \]

Note that the definitions of the dimensionless variables are not unique, and they usually depend on the problem and have different expressions. The non-dimensional form of governing equations can be obtained using those definitions. For example the incompressible Navier-Stokes momentum equation with the absence of body force becomes,

\[
\begin{align*}
    \frac{\text{D} \mathbf{v}'}{\text{D}t} &= -\nabla P' + \frac{1}{Re} \nabla \cdot (\nabla \mathbf{v}'), \\
    \nabla \cdot \mathbf{v}' &= 0.
\end{align*}
\]  

(2.62)
Here the assumption is that the viscosity is a constant. \( Re \) is a dimensionless parameter called the Reynolds number. It is defined to be \( \frac{\rho_0 U_0 L}{\mu} \), which can be interpreted as the ratio of the convective force to the viscous force. If the Reynolds number is high, the convective force dominates and it usually results in turbulent flow. If the Reynolds number is low, the viscous force is dominating, and it results in laminar flow. In the latter case, since the viscous force is dominating, the proper choice of the characteristic time should be \( t_0 = \frac{L^2}{\nu} \), where \( \nu = \frac{\mu}{\rho} \) is the kinematic viscosity.

### 2.5.2 Continuity equation

In SPH, the density can be calculated by applying Equation (2.24) to the density,

\[
\rho(\mathbf{r}) = \sum_j m_j W_{ij}.
\]

(2.63)

However, as Monaghan [39] points out, and also as discussed in Section 2.3.5, the summation suffers from the lack of fluid material outside the boundary, which leads to a deficiency of the quantity near the boundary. For particles near the boundary, the density drops to zero as the kernel function falls to zero at its support domain boundary. For a free surface problem, this may cause the density near the surface to be lower than expected.

Hence the original continuity equation is used with an equation of state [39],

\[
\begin{align*}
\frac{\text{D} \rho}{\text{D}t} + \rho \nabla \cdot \mathbf{v} &= 0, \\
P &= P(\rho).
\end{align*}
\]

(2.64)

The equation of state is chosen such that the density fluctuation is small. Therefore the flow is weakly compressible. Another disadvantage of the summation form of the density is that it has to be calculated before the calculation of other parameters. If the continuity equation is used, it is not necessary to calculate the density before other parameters are evaluated.
Using the special expression for approximation of divergence (2.41), the discretized continuity equation is given by

\[
\frac{D\rho_i}{Dt} = \sum_j m_j v_{ij} \cdot \nabla_i W_{ij},
\]

where \( v_{ij} = v_i - v_j \), \( r_{ij} = r_i - r_j \), and \( \nabla_i \) denotes that the gradient is taken respect
to position \( r_i \). This expression can also be interpreted in a microscopic way. The local change of density is directly related to the relative motion of the neighboring particles.

### 2.5.3 Momentum Equation

For incompressible flow, the momentum equation (2.59) is used to derive the corresponding SPH equation. As we mentioned in Section 2.3.6, the pressure term can be rewritten such that the linear momentum of the system is conserved exactly,

\[
\frac{\nabla P}{\rho} = \nabla \left( \frac{P}{\rho} \right) + \frac{P}{\rho^2} \nabla \rho. \quad \text{(Quotient Rule)} \tag{2.66}
\]

Hence the momentum equation for SPH is,

\[
\frac{Dv_i}{Dt} = - \sum_j m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla_i W_{ij} + \Pi_{ij}. \tag{2.67}
\]

We denote \( \Pi_{ij} \) as the viscous term which should be the SPH approximation for the term \( \frac{1}{\rho} \nabla \cdot (\mu \nabla v) \). This symmetric form of the pressure term also assures conservation of angular momentum of the system with the absence of the viscous term,

\[
\frac{D}{Dt} \sum_i r_i \times m_i v_i = - \sum_i m_i \sum_j m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) r_i \times \nabla_i W_{ij} = - \sum_i m_i \sum_j m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) r_i \times (r_i - r_j) \frac{\partial W_{ij}}{\partial r} \frac{1}{r_{ij}} (\text{where } r_{ij} = |r_{ij}|) = 0. \tag{2.68}
\]

The last term is zero because of the antisymmetry in the double sum (since \( r_i \times r_j = -(r_j \times r_i) \)).
2.5.4 Viscosity

A direct way to approximate the second derivative is to apply the particle approximation to the Equation (2.21). Hence with the assumption that the viscosity $\mu$ is a constant, the viscous term should be expressed as

$$\Pi_{ij} = \frac{\mu_i}{\rho_i} \sum_j \frac{m_j}{\rho_j} v_j \nabla^2 W_{ij}. \tag{2.69}$$

Here $\nabla^2 = \nabla \cdot \nabla = \Delta$ is the Laplacian. This approximation for the Laplacian has some advantages. First, it is lack of accuracy for low order kernel function. If the kernel function is not smooth enough (for example the cubic spline (2.13)), the second derivative or the Laplacian of the kernel function may be a step function or even discontinuous. Second, it is sensitive to the particle disorder. That means perturbations in particle distribution introduces large error in this approximation. Brookshaw [7] introduces a new expression for SPH second derivative approximation in one dimension for thermal conduction problems,

$$\langle \frac{\partial^2 T}{\partial t^2} \rangle_i = \frac{1}{2} \sum_j m_j \frac{T_i - T_j}{x_{ij}} \frac{\partial W_{ij}}{\partial x_i}, \tag{2.70}$$

where $T$ is the temperature and $x$ is the position of the particle. One problem in this formulation is that $x_{ij}$ could be very small. Thus, $\frac{x_{ij}}{x_{ij}^2 + \epsilon h^2}$ is used instead of $\frac{1}{x_{ij}}$. Following this idea, one commonly used scheme for viscosity is,

$$\Pi_{ij} = 2 \sum_j \frac{m_j}{\rho_i \rho_j} \frac{2 \mu_i \mu_j}{\mu_i + \mu_j} \frac{r_{ij} \cdot \nabla W_{ij}}{|r_{ij}|^2 + \eta^2 v_{ij}}, \tag{2.71}$$

where $\eta = 0.01h^2$ is a small parameter used to regularize the singularity. Equation (2.71) can be interpreted as a hybrid scheme that combines the finite differences first derivative and the SPH first derivative. In fact, let $\eta = 0$, then [52],

$$\lim_{r_j \to r_i} v_{ij} \frac{r_{ij}}{|r_{ij}|^2} = \lim_{r_i \to r_j} \frac{v_i - v_j}{|r_i - r_j|} \frac{r_{ij}}{|r_{ij}|} = D_d v \frac{r_{ij}}{|r_{ij}|}, \tag{2.72}$$

where

$$D_d v = \nabla v \cdot \frac{r_{ij}}{|r_{ij}|}, \tag{2.73}$$
is the directional derivative. The finite difference approximation is used to approximate the gradient of the velocity. In this way, the approximation suffers less from the particle disorder. This formulation conserves linear momentum exactly, but angular momentum is not conserved. We will refer to this formulation as Standard Diffusion Scheme. The term,
\begin{equation}
\frac{2\mu_i\mu_j}{\mu_i + \mu_j},
\end{equation}
calculates the effective viscosity if the viscosity term \( \mu \) is discontinuous. For example, for a two-phase flow problem, the viscosity may be discontinuous across the interface of the two materials. Equation (2.71) is investigated by Morris et al. [47] to model low Reynolds number incompressible flow through a periodic lattice of cylinders, with a slightly different form of viscosity \( \frac{\mu_i + \mu_j}{2} \). Hu and Adams [26] also use this form of viscosity to develop a multi-phase method for macroscopic and mesoscopic flows.

Cleary [12, 13] introduces a new formulation (2.5.4) which conserves both linear momentum and angular momentum.
\begin{equation}
\Pi_{ij} = \sum_j \xi \frac{m_j}{\rho_i\rho_j} \frac{2\mu_i\mu_j}{\mu_i + \mu_j} \frac{v_{ij} \cdot r_{ij}}{|r_{ij}|^2 + \eta^2} \nabla W_{ij}, \quad \eta = 0.01h^2.
\end{equation}

We will refer to this scheme as CSIRO diffusion scheme. Different values of \( \xi \) had been reported based on different numerical experiments and analysis. Cleary [12] calibrates the value of \( \xi = 4.9633 \) based on plane Couette flow computation using an equation of state for pressure. Cummins and Rudman suggestes that \( \xi = 4.1666 \). Monaghan [41] shows that the expression corresponds to both a shear viscosity and a bulk viscosity and that choosing \( \xi = 4 \) will match the shear viscosity to the real viscosity. Hu and Adams [25] give a theoretical proof that the value of \( \xi \) is 4.

In fact, using Taylor expansion, it can be shown [52] that in two dimensions,
\begin{align}
2 \sum_j \frac{m_j}{\rho_j} \frac{r_{ij} \cdot \nabla W_{ij}}{|r_{ij}|^2 + \eta^2} v_{ij} & \approx 2 \int_{\Omega} (\mathbf{v} - \mathbf{v}') \frac{\mathbf{r} - \mathbf{r}'}{|\mathbf{r} - \mathbf{r}'|^2} \nabla W(\mathbf{r} - \mathbf{r}', h) \, d\mathbf{r}' \\
& = \nabla \cdot (\nabla \mathbf{v}(\mathbf{r})) + \text{H.O.T.},
\end{align}

(2.76)
and,
\[
\sum_j \xi \frac{m_j}{\rho_j} \frac{v_{ij} \cdot r_{ij}}{|r_{ij}|^2 + \eta^2} \nabla W_{ij} \approx \xi \int_\Omega \frac{(v - v') \cdot (r - r')}{|r - r'|^2} \nabla W(r - r') \, dr' \\
= \frac{\xi}{4} \nabla \cdot \nabla v + \frac{\xi}{2} \nabla (\nabla \cdot v) + \text{H.O.T.} \tag{2.77}
\]

Artificial viscosity is another way to deal with the viscous diffusion. Monaghan [42] introduces artificial viscosity to simulate shock problems involving gas. It has the form,
\[
\Pi_{ij} = \begin{cases} \\ - \alpha \bar{c}_{ij} \frac{v_{ij} \cdot r_{ij}}{|r_{ij}|^2 + 0.01h^2} + \beta h^2 \left( \frac{v_{ij} \cdot r_{ij}}{|r_{ij}|^2 + 0.01h^2} \right)^2 \nabla W_{ij}, & \text{if } v_{ij} \cdot r_{ij} < 0; \\ 0, & \text{otherwise}, \end{cases} \tag{2.78}
\]

where, for example, \( \bar{c}_{ij} = (c_i + c_j)/2 \) and \( c \) is the sound of speed. This form of viscosity conserves linear momentum and angular momentum. Monaghan [41] shows that the shear viscosity coefficient \( \mu = \rho \alpha hc_8 \) for two dimension. Hence we define
\[
\mu_i = \frac{1}{8} \alpha_i \rho_i hc_i. \tag{2.79}
\]

Viscosity in the form (2.78) is same as the expression (2.5.4) with \( \xi = 4 \).

### 2.5.5 Equation of state

In many numerical methods, water is treated as incompressible since the speed of sound in water is much larger then the bulk flow speed (small Mach number). A further constraint on the velocity field should be taken into account to ensure that the divergence of velocity is zero. For SPH, incompressible fluid is treated as a weakly compressible fluid by introducing a suitable equation of state. Monaghan [39] suggests to use the equation of state for water introduced by Batchelor [4],
\[
P = \frac{\rho_0 c^2}{\gamma} \left( \left( \frac{\rho}{\rho_0} \right)^\gamma - 1 \right), \tag{2.80}
\]
where \( \gamma = 7 \) and \( \rho_0 \) is the reference density. The speed of sound \( c \) should be chosen to be large enough to mimic the behavior of the real flow, but it should not be so
large to limit the time step size. Monaghan [39] suggests that the speed of sound
\[ c = 10U_{\text{max}} \]
where \( U_{\text{max}} \) is the maximum speed of fluid. Thus the density fluctuation, which is proportional to the square of the Mach number \( M \) (\( M = U/c \), where \( U \) is the characteristic velocity), is about 1% of the fluid density. This expression gives large pressure due to small density fluctuation. Hence the density fluctuation is small even for high Reynolds number. Valizadeh and Monaghan [56] use this equation of state to simulate turbulent flow in a fixed and rotating box.

Another choice for the equation of state is,
\[ P = c^2 \rho, \quad (2.81) \]
where \( c \) is the speed of sound and again \( c = 10U_{\text{max}} \). Morris et al. [47] use this equation of state for low Reynolds number flow. They argue that Equation (2.80) would give a noisy result since it is too stiff for their simulation.

### 2.6 The time integration scheme

The SPH equations are integrated with a Runge-Kutta midpoint method. Runge-Kutta midpoint method is a second order method.

\[
\mathbf{r}^{1/2} = \mathbf{r}^0 + \frac{\Delta t}{2} \mathbf{v}^0, \quad (2.82)
\]

\[
\mathbf{v}^{1/2} = \mathbf{v}^0 + \frac{\Delta t}{2} \mathbf{a}(\mathbf{r}^0, \mathbf{v}^0), \quad (2.83)
\]

and then,

\[
\mathbf{r}^1 = \mathbf{r}^0 + \Delta t \mathbf{v}^{1/2}, \quad (2.84)
\]

\[
\mathbf{v}^1 = \mathbf{v}^0 + \Delta t \mathbf{a}(\mathbf{r}^{1/2}, \mathbf{v}^{1/2}), \quad (2.85)
\]

where \( f^0, f^{1/2} \) and \( f^1 \) denote the value of \( f \) at the beginning, halfway, and the end of the time step.
For the stability of a numerical method, the time step is controlled by a CFL condition,

\[ \Delta t \leq C_1 \frac{h}{c}, \quad (2.86) \]

where \( c \) is the speed of the sound. In SPH simulation, we set the value of the speed of the sound to be \( 10U_{\text{max}} \). \( C_1 \) is a constant that depends on the choice of kernel. For example, after trying various values for \( C_1 \), we choose \( C_1 = 0.4 \) for the quintic spline kernel. We also need to control time step by viscous diffusion,

\[ \Delta t \leq C_2 \frac{h^2}{\nu}. \quad (2.87) \]

The parameter \( \nu \) is the kinematic viscosity. Again, the constant \( C_2 \) depends on the choice of kernel. From simulation experiments, \( C_2 = 0.2 \) for the quintic spline kernel. If there is some extra body forces in the system, for example, the gravity, then an additional constraint for time step is needed,

\[ \Delta t \leq C_3 \min_a \left( \frac{h}{f_a} \right). \quad (2.88) \]

The minimum is taken over all fluid particles. \( C_3 \) can be determined by numerical experiments.

When the Reynolds number is small, the viscous diffusion is the dominated phenomenon. Hence (2.87) dominates the time constraint. On the other hand, when Reynolds number is large, the flow is dominated by advection. Therefore (2.86) dominates the time constraint. Therefore, the time step for SPH simulations should be,

\[ \Delta t = \min \left( 0.4 \frac{h}{c}, 0.2 \frac{h^2}{\nu}, C_3 \min_a \left( \frac{h}{f_a} \right) \right). \quad (2.89) \]
Chapter 3

CONVERGENCE OF SPH

3.1 Introduction

Convergence is a very important concept to numerical methods for partial differential equations. Convergence implies that solutions to the discretized equation approach those of the PDE, as discretization step sizes approach zero. If this does not occur, the associated numerical approximations are useless. The order of accuracy of a (convergent) method refers to how rapidly errors decrease in the limit as the step size tends to zero. However, it is not easy to study the convergence of SPH. There are some difficulties raised in the error analysis. First, the error in a summation approximation of an integral is not trivial to estimate, especially in higher dimensions. In higher dimensions, it is not clear how to divide the circular or the spherical compact support into small volumes associated with each particle. Second, particles get disordered as fluid moves. The error depends on the dynamics of the flow. Monaghan [41] notes that the error in kernel approximation is second order in smoothing length \( h \). This result does not account for the error in particle approximation. Cleary and Monaghan [11] suggests that if the particle separation \( p_{\text{sep}} \) decreases faster than the smoothing length \( h \), the overall error is \( O(h^2) \) even if particles are disordered. This implies that the overlap \( \beta \) is not a fixed number and as \( \beta \) increases the computational cost increases. Quinlan et. al. [50] performs rigorous error analysis and points out that the discretization error limits overall error as \( h \) decreases. The overall error they obtain for uniform particle spacing in one dimension is,

\[
\sum_j f_j W_{ij} p_{\text{sep}} - f_i' = f_i' \left( O \left( \beta^{-(\kappa + 2)} \right) \right) + f_i'' \left( O(h^2) + O \left( h^2 \beta^{-(\kappa + 2)} \right) \right), \tag{3.1}
\]
where $\beta = h/p_{\text{sep}}$ is the overlap and $\kappa$ is the boundary smoothness of the kernel function $W$. Boundary smoothness of a kernel function is defined as the largest integer $\kappa$ such that the $\kappa$th derivative and all lower derivatives are zero at the edges of the compact support [50]. The cubic spline kernel (2.13) has $\kappa = 2$. Theoretically, the Gaussian kernel has $\kappa \rightarrow \infty$. When the overlap $\beta$ is fixed, the number of particles in the summations which approximates kernel approximation integrals remains same even as smoothing length $h$ decrease. Hence the discretization error is a constant which dominates the smoothing error eventually.

### 3.1.1 Numerical test: Double Periodic problem

To examine the convergence of SPH, we consider a 2D flow problem in a rectangle region, $[0,L] \times [-L,L]$ with periodic boundary conditions on each side of the boundaries of the region. Initially, the velocity of the fluid in the subregion $[0,L] \times [0,L]$ is set to 1 and the velocity of the fluid in the subregion $[0,L] \times [-L,0]$ is set to 0. Because of the periodic boundary conditions on each side of the domain, this problem is equivalent to an unbounded problem. Hence the accuracy of the simulation is not affected by any approximation of solid boundary conditions. The exact solution of this problem can be found,

$$v_x(y,t) = \frac{1}{2} - \sum_{k=1}^{\infty} \frac{2}{(2k-1)\pi} \sin \left( \frac{(2k-1)\pi y}{L} \right) \exp \left( -\frac{1}{Re} \left( \frac{(2k-1)\pi}{L} \right)^2 t \right).$$  

(3.2)

The flow is unidirectional and the pressure is close to zero. The dominating force is the viscous force. Thus we tried different viscous schemes to test the convergence of SPH. We set $L = 1$ in the simulation, and the overlap $\beta$ is set to 1.2. The SPH solution was compared with the exact solution to determine the error. The error was computed at all particles over the computational domain, and results are presented in the form of $L_2$ norm error. Results are presented in Figure 3.1 as a function of smoothing length $h$. For all viscous diffusion schemes, the error is limited at low $h$ by discretization error. Therefore, none of the viscous schemes is satisfying. Many SPH works [11, 41] have focused on the conservation properties of these SPH schemes. However, if the result of
3.2 Gradient correction

The common SPH first derivative for a scalar function $f$ is,

$$\langle \nabla f \rangle_i = \sum_j \frac{m_j}{\rho_j} (f_j - f_i) \nabla W_{ij}. \quad (3.3)$$

Using Taylor’s expansion, we have,

$$\langle \nabla f \rangle_i = \sum_j \frac{m_j}{\rho_j} (f_j - f_i) \nabla W_{ij}$$

$$= \sum_j \frac{m_j}{\rho_j} \left( -r_{ij}^\alpha \nabla^\alpha f_i \big|_i + \frac{1}{2} r_{ij}^\alpha r_{ij}^\beta \nabla^\alpha \nabla^\beta f_i \big|_i - \frac{1}{6} r_{ij}^\alpha r_{ij}^\beta r_{ij}^\lambda \nabla^\alpha \nabla^\beta \nabla^\lambda f_i \big|_i + \text{H.O.T.} \right) \nabla W_{ij}. \quad (3.4)$$

Figure 3.1: The L2 norm relative error of the calculated velocity for Double periodic flow against the smoothing length $h$ with different viscous diffusion schemes.
Therefore, the error for this scheme is,

\[
\langle \nabla f \rangle_i - \nabla f_i = \sum_j \frac{m_j}{\rho_j} \left( f_j - f_i \right) \nabla W_{ij} = \nabla^\alpha f_i - \sum_j \frac{m_j}{\rho_j} r^\alpha_{ij} \nabla^\delta W_{ij} - \left( \sum_j \frac{m_j}{\rho_j} r^\alpha_{ij} r^\beta_{ij} \nabla^\delta W_{ij} \right)
\]

\[
+ \nabla^\alpha \nabla^\beta \nabla^\lambda f_i \left( - \frac{1}{6} \sum_j \frac{m_j}{\rho_j} r^\alpha_{ij} r^\beta_{ij} r^\lambda_{ij} \nabla^\delta W_{ij} \right) + \text{H.O.T.}
\]  

(3.5)

The first term is nonzero. Figure 3.2 shows the term \( - \sum_j \frac{m_j}{\rho_j} r^\alpha_{ij} \nabla^\delta W_{ij} \) for different kernels in one dimension.

Hence, Bonet and Lok [?] introduced the modified first derivative,

\[
\langle \nabla f \rangle_i |F_1\rangle = \sum_j \frac{m_j}{\rho_j} \left( f_j - f_i \right) B_i \cdot \nabla W_{ij} = \sum_j \frac{m_j}{\rho_j} \left( f_j - f_i \right) B_{i}^{\alpha\beta} \nabla^\delta W_{ij},
\]  

(3.6)

where,

\[
B_i = \left[ - \sum_j \frac{m_j}{\rho_j} r^\alpha_{ij} \nabla^\delta W_{ij} \right]^{-1}.
\]  

(3.7)

The error of the new scheme can be obtained,

\[
\langle \nabla f \rangle_i |F_1\rangle = \nabla^\alpha f_i + \nabla^\alpha \nabla^\beta f_i \left( \frac{1}{2} \sum_j \frac{m_j}{\rho_j} r^\alpha_{ij} r^\beta_{ij} B_{i}^{\alpha\beta} \nabla^\delta W_{ij} \right)
\]

\[
- \nabla^\alpha \nabla^\beta \nabla^\lambda f_i \left( \frac{1}{6} \sum_j \frac{m_j}{\rho_j} r^\alpha_{ij} r^\beta_{ij} r^\lambda_{ij} B_{i}^{\alpha\beta} \nabla^\delta W_{ij} \right) + \text{H.O.T.}
\]

(3.8)
This method is first-order consistent which means the scheme can exactly calculate the gradient of a linear function.

3.3 Fatehi’s Laplacian approximation

The standard scheme for viscous diffusion of a scalar function $f$, assuming constant viscosity $\mu$, is,

$$\left\langle \frac{1}{\rho} \nabla \cdot (\mu \nabla f) \right\rangle_i = \frac{\mu_i}{\rho_i} 2 \sum_j \frac{m_j}{\rho_j} (f_i - f_j) \frac{r_{ij} \cdot \nabla W_{ij}}{|r_{ij}|^2 + \eta^2}. \quad (3.9)$$

Here $\eta = 0.1h$ is a small parameter that prevents singularity. Hence, the standard scheme for the Laplacian of a scalar function $f$, is

$$\left\langle \nabla \cdot \nabla f \right\rangle_i = 2 \sum_j \frac{m_j}{\rho_j} (f_i - f_j) \frac{r_{ij} \cdot \nabla W_{ij}}{|r_{ij}|^2 + \eta^2} = 2 \sum_j \frac{m_j}{\rho_j} (f_i - f_j) \frac{e_{ij} \cdot \nabla W_{ij}}{|r_{ij}| e_{ij} \cdot \nabla W_{ij}}. \quad (3.10)$$

We drop the $\eta$ term for now to simplify the analysis and the vector $e_{ij}$ is defined by

$$e_{ij} = \frac{r_{ij}}{|r_{ij}|}. \quad (3.11)$$

Since,

$$\nabla^\delta W = \nabla^\delta W(|r - r'|) = \frac{\partial W(r)}{\partial r} \nabla^\delta |r - r'| = \frac{\partial W(r)}{\partial r} \frac{(r - r')^\delta}{|r - r'|}, \quad r = |r - r'|,$$

and

$$e_{ij} \cdot e_{ij} = 1.$$
Therefore we can rewrite (3.11),

\[
\langle \nabla \cdot \nabla f \rangle |_i = \nabla^\alpha f |_i \left( 2 \sum_j \frac{m_j}{r_{ij}^3} \nabla^\alpha W_{ij} \right) + \nabla^\alpha \nabla^\beta f |_i \left( - \sum_j \frac{m_j}{r_{ij}^3} r_{ij}^\beta \nabla^\alpha W_{ij} \right) \\
+ \nabla^\alpha \nabla^\beta \nabla^\lambda f |_i \left( \frac{1}{3} \sum_j \frac{m_j}{r_{ij}^3} r_{ij}^\beta r_{ij}^\lambda \nabla^\alpha W_{ij} \right) + \text{H.O.T.} \quad (3.12)
\]

So the error of this scheme is,

\[
\langle \nabla \cdot \nabla f \rangle |_i - \nabla \cdot \nabla f |_i = \nabla^\alpha f |_i \left( 2 \sum_j \frac{m_j}{r_{ij}^3} \nabla^\alpha W_{ij} \right) + \nabla^\alpha \nabla^\beta f |_i \left( B_{i}^{-1} - I \right) \\
+ \nabla^\alpha \nabla^\beta \nabla^\lambda f |_i \left( \frac{1}{3} \sum_j \frac{m_j}{r_{ij}^3} r_{ij}^\beta r_{ij}^\lambda \nabla^\alpha W_{ij} \right) + \text{H.O.T.} \quad (3.13)
\]

The first term is zero for interior uniformly arranged particles, and it is nonzero for non-uniform arrangement and for particles near the boundary. The second term is also nonzero and \( O(\beta^{-\kappa+1}) \) for uniformly spaced particles.

The leading term of the error needs to be eliminated in the scheme. The difficulty is that it contains the first derivative of \( f \) evaluated at \( r_i \). One option is to use the numerical approximation of \( \nabla f \) and a good choice is the scheme mentioned in Section 3.2. Hence, substitute (3.8) into (3.11),

\[
2 \sum_j \frac{m_j}{r_{ij}^3} \frac{f_i - f_j}{|r_{ij}|} e_{ij} \cdot \nabla W_{ij} \\
= 2 \sum_j \frac{m_j}{r_{ij}^3} \left\{ e_{ij} \left[ \langle \nabla^\xi f \rangle |_i F_1 - \nabla^\alpha \nabla^\beta f |_i \left( \frac{1}{2} \sum_j \frac{m_j}{r_{ij}^3} r_{ij}^\alpha r_{ij}^\beta B_i^\delta \nabla^\delta W_{ij} \right) \right] \\
+ \nabla^\alpha \nabla^\beta \nabla^\lambda f |_i \left( \frac{1}{6} \sum_j \frac{m_j}{r_{ij}^3} r_{ij}^\alpha r_{ij}^\beta r_{ij}^\lambda B_i^\delta \nabla^\delta W_{ij} \right) + \text{H.O.T.} \right\} e_{ij} \nabla^\theta W_{ij} \\
+ \nabla^\alpha \nabla^\beta f |_i \left( - \sum_j \frac{m_j}{r_{ij}^3} e_{ij}^\alpha r_{ij}^\beta e_{ij}^\theta \nabla^\theta W_{ij} \right) \\
+ \nabla^\alpha \nabla^\beta \nabla^\lambda f |_i \left( \frac{1}{3} \sum_j \frac{m_j}{r_{ij}^3} e_{ij}^\alpha r_{ij}^\beta r_{ij}^\lambda e_{ij}^\theta \nabla^\theta W_{ij} \right) + \text{H.O.T.} , \quad (3.14)
\]
\[ 2 \sum_j \frac{m_j}{\rho_j} \left( \frac{f_i - f_j}{|r_{ij}|} - e_{ij}^a \langle \nabla^a f \rangle_i |F_1 \rangle \right) e_{ij} \cdot \nabla W_{ij} \]

\[ = - \nabla^a \nabla^b f_i \sum_j \frac{m_j}{\rho_j} \left\{ e_{ij}^\epsilon \left( \sum_j \frac{m_j}{\rho_j} r_{ij}^\alpha r_{ij}^\beta B_i^\epsilon \nabla^\delta W_{ij} \right) + e_{ij}^\alpha r_{ij}^\beta \right\} e_{ij}^\epsilon \nabla^\delta W_{ij} \]

\[ + \nabla^a \nabla^b \nabla^\lambda f_i \sum_j \frac{m_j}{\rho_j} \left\{ e_{ij}^\epsilon \left( \sum_j \frac{m_j}{\rho_j} r_{ij}^\alpha r_{ij}^\beta r_{ij}^\lambda B_i^\epsilon \nabla^\delta W_{ij} \right) + e_{ij}^\alpha r_{ij}^\beta r_{ij}^\lambda \right\} e_{ij}^\epsilon \nabla^\delta W_{ij} \]

\[ + \text{H.O.T.}. \]

(3.15)

Since we are attempting to approximate the Laplacian of the function \( f \) using particles randomly placed in the space, the first term in (3.15) involves mixed derivatives which are not desired. Fatehi [21] suggests to rewrite the dot product \( e_{ij} \cdot \nabla W_{ij} \) to an outer/dyadic product \( e_{ij} \otimes \nabla W_{ij} \) to raise the degree of freedom, in order to correct the leading error term in (3.15). All the algebraic calculations in error analysis are done the same except that we change the dot product to the outer product,

\[ 2 \sum_j \frac{m_j}{\rho_j} \left( \frac{f_i - f_j}{|r_{ij}|} - e_{ij}^a \langle \nabla^a f \rangle_i |F_1 \rangle \right) e_{ij} \otimes \nabla W_{ij} \]

\[ = - \nabla^a \nabla^b f_i \sum_j \frac{m_j}{\rho_j} \left\{ e_{ij}^\epsilon \left( \sum_j \frac{m_j}{\rho_j} r_{ij}^\alpha r_{ij}^\beta B_i^\epsilon \nabla^\delta W_{ij} \right) + e_{ij}^\alpha r_{ij}^\beta \right\} e_{ij}^\epsilon \nabla^\delta W_{ij} \]

\[ + \nabla^a \nabla^b \nabla^\lambda f_i \sum_j \frac{m_j}{\rho_j} \left\{ e_{ij}^\epsilon \left( \sum_j \frac{m_j}{\rho_j} r_{ij}^\alpha r_{ij}^\beta r_{ij}^\lambda B_i^\epsilon \nabla^\delta W_{ij} \right) + e_{ij}^\alpha r_{ij}^\beta r_{ij}^\lambda \right\} e_{ij}^\epsilon \nabla^\delta W_{ij} \]

\[ + \text{H.O.T.}. \]

(3.16)

Now a new renormalization second order tensor \( \hat{\mathbf{B}}_i \) is introduced such that,

\[ \sum_j \frac{m_j}{\rho_j} \left[ e_{ij}^\epsilon \left( \sum_j \frac{m_j}{\rho_j} r_{ij}^\alpha r_{ij}^\beta B_i^\epsilon \nabla^\delta W_{ij} \right) + e_{ij}^\alpha r_{ij}^\beta \right] e_{ij}^\epsilon \nabla^\delta W_{ij} : \hat{\mathbf{B}}_i = -\mathbf{I} \]

(3.17)

where \( ^4\mathbf{A} \) is a fourth order tensor, and \( \hat{\mathbf{B}}_i \) is symmetric. This leads to a \( 3 \times 3 \) system of equations for two dimensional problems, \( 6 \times 6 \) system of equations for three dimensional problems. The new scheme for Laplacian is,

\[ \langle \nabla \cdot \nabla f \rangle_i |S_1 = \hat{\mathbf{B}}_i : 2 \sum_j \frac{m_j}{\rho_j} \left( \frac{f_i - f_j}{|r_{ij}|} - e_{ij}^a \langle \nabla^a f \rangle_i |F_1 \rangle \right) e_{ij} \otimes \nabla W_{ij} \].

(3.18)
Now the leading term of the error is,

\[ \langle \nabla \cdot \nabla f \rangle_i |_{S_1} - \langle \nabla \cdot \nabla f \rangle_i = \nabla^\alpha \nabla^\beta \nabla^\lambda f_i \{ \frac{1}{3} \sum_j \frac{m_j}{\rho_j} \left[ e^i_{ij} \left( \sum_j \frac{m_j}{\rho_j} r_{ij}^\alpha r_{ij}^\beta r_{ij}^\lambda \mathbf{B}_i^\xi \nabla^\delta W_{ij} \right) + e^i_{ij} r_{ij}^\alpha r_{ij}^\beta \right] e^\theta_{ij} \nabla^\epsilon W_{ij} : \hat{\mathbf{B}}_i \} \]

+ H.O.T.

Fatehi[21] claims that the order of the leading term in its truncation error is

\[ |\nabla^3 f_i| \times O \left( \tilde{d}^{\kappa+1} \right) \]

for non-uniform particle spacing where \( \tilde{d} \) is the deviation distance. Since the deviation distance is assumed smaller than \( p_{sep} \), this method has first order accuracy.

### 3.4 New derivative operators

Here is a list of common SPH derivative formulae,

\[ \langle \nabla f \rangle = \sum_j \frac{m_j}{\rho_j} (f_j - f_i) \nabla W_{ij}, \quad \text{(3.19)} \]

\[ \langle \nabla f \rangle |_{F_1} = \sum_j \frac{m_j}{\rho_j} (f_j - f_i) \mathbf{B}_i \cdot \nabla W_{ij} = \sum_j \frac{m_j}{\rho_j} (f_j - f_i) \mathbf{B}_i^{\alpha \beta} \nabla^\beta W_{ij}, \quad \text{(3.20)} \]

\[ \langle \nabla \cdot \nabla f \rangle_i = 2 \sum_j \frac{m_j}{\rho_j} \left( \frac{f_i - f_j}{|r_{ij}|} \right) e_{ij} \cdot \nabla W_{ij}, \quad \text{(3.21)} \]

\[ \langle \nabla \cdot \nabla f \rangle_i |_{S_1} = 2 \sum_j \frac{m_j}{\rho_j} \left( \frac{f_i - f_j}{|r_{ij}|} - e_{ij}^\alpha \langle \nabla^\alpha f \rangle_i |_{F_1} \right) e_{ij}^\theta \hat{\mathbf{B}}_i^{\delta \beta} \nabla^\delta W_{ij}. \quad \text{(3.22)} \]

Compared to Equation (3.19), a gradient correction is done in Equation (3.20) by introducing the corrected kernel gradient,

\[ \nabla W_{ij} = \mathbf{B}_i^{\alpha \beta} \nabla^\beta W_{ij}, \quad \text{(3.23)} \]

Similarly, Equation (3.22) also used another corrected kernel gradient,

\[ \nabla W_{ij} = \hat{\mathbf{B}}_i^{\delta \beta} \nabla^\delta W_{ij}, \quad \text{(3.24)} \]

The idea is to introduce \( \mathbf{B} \) and \( \hat{\mathbf{B}} \) to raise the degree of freedom so that the consistency of the approximation can be improved. Following this idea, we can create a different kernel to satisfy more conditions.
3.4.1 Gradient correction

Now we define a new kernel gradient $\nabla W$

$$\nabla W_{ij} \equiv B^\alpha_{\beta\gamma\delta\epsilon} (s_1)_{ij}^\beta (s_2)_{ij}^\gamma (s_3)_{ij}^\delta \nabla^\epsilon W_{ij}. \quad (3.25)$$

The 5th order tensor $\overline{B}$ has thirty-two unknowns in two dimension, where

$$(s_1)_{ij} = (s_2)_{ij} \equiv r_{ij} + r^2_{ij}, \quad (s_3)_{ij} \equiv e_{ij} + e^4_{ij}. \quad (3.26)$$

Using Taylor’s expansion of $f_j$ at position $i$ for Equation (3.19), with new gradient kernel $\overline{\nabla W}$, we get,

$$\langle \nabla f \rangle = \sum_j \frac{m_j}{\rho_j} (f_j - f_i) \overline{\nabla W}$$

$$= \sum_j \frac{m_j}{\rho_j} \left[ -r^\eta_{ij} \nabla^\eta f_i + \frac{1}{2} r^\eta_{ij} r^\theta_{ij} \nabla^\eta \nabla^\theta f_i + \frac{1}{6} r^\eta_{ij} r^\theta_{ij} r^\lambda_{ij} \nabla^\eta \nabla^\theta \nabla^\lambda f_i + \text{H.O.T.} \right] \overline{\nabla W}$$

$$= \nabla^\eta f_i \left( - \sum_j \frac{m_j}{\rho_j} r^\eta_{ij} \nabla^\eta W_{ij} \right) + \nabla^\eta \nabla^\theta f_i \left( \frac{1}{2} \sum_j \frac{m_j}{\rho_j} r^\eta_{ij} r^\theta_{ij} \nabla^\eta W_{ij} \right)$$

$$+ \nabla^\eta \nabla^\theta \nabla^\lambda f_i \left( \frac{1}{2} \sum_j \frac{m_j}{\rho_j} r^\eta_{ij} r^\theta_{ij} r^\lambda_{ij} \nabla^\eta W_{ij} \right) + \text{H.O.T.} \quad (3.27)$$

Hence, to get a more accurate approximation of $\nabla f$, we first require that

$$- \sum_j \frac{m_j}{\rho_j} r^\alpha_{ij} \nabla^\alpha W_{ij} = -\overline{B}_{ij}^{\alpha\beta\gamma\delta\epsilon} \left[ \sum_j \frac{m_j}{\rho_j} r^\eta_{ij} \nabla^\eta (s_1)_{ij}^\beta (s_2)_{ij}^\gamma (s_3)_{ij}^\delta \nabla^\epsilon W_{ij} \right] = I^\alpha. \quad (3.28)$$

There are four equations in two dimension since the index $\alpha = 1, 2$ and $\eta = 1, 2$ representing $x$ and $y$ component of the vector. Then we set the next 2 error terms in (3.27) to zero,

$$\frac{1}{2} \sum_j \frac{m_j}{\rho_j} r^\eta_{ij} r^\theta_{ij} \nabla^\eta W_{ij} = \overline{B}_{ij}^{\alpha\beta\gamma\delta\epsilon} \left[ \frac{1}{2} \sum_j \frac{m_j}{\rho_j} r^\eta_{ij} \nabla^\eta (s_1)_{ij}^\beta (s_2)_{ij}^\gamma (s_3)_{ij}^\delta \nabla^\epsilon W_{ij} \right] = 0^{\alpha\theta}. \quad (3.29)$$

$$\frac{1}{6} \sum_j \frac{m_j}{\rho_j} r^\eta_{ij} r^\theta_{ij} r^\lambda_{ij} \nabla^\eta W_{ij} = \overline{B}_{ij}^{\alpha\beta\gamma\delta\epsilon} \left[ \frac{1}{2} \sum_j \frac{m_j}{\rho_j} r^\eta_{ij} r^\theta_{ij} r^\lambda_{ij} \nabla^\eta (s_1)_{ij}^\beta (s_2)_{ij}^\gamma (s_3)_{ij}^\delta \nabla^\epsilon W_{ij} \right] = 0^{\alpha\theta\lambda}. \quad (3.30)$$
With the varying indices, there should be eight equations in Equation (3.29) and sixteen equations in Equation (3.30) in two dimension. However, since $\eta$, $\theta$ and $\lambda$ are the indices of the same term $r_{ij}$, there are duplicate equations. In fact, there are six equations instead of eight in Equation (3.29) and eight equations instead of sixteen in Equation (3.30). On the other hand, since $(s_1)_{ij}$ and $(s_2)_{ij}$ are same, the elements of tensor $\overline{B}$ have repetition. Hence, there are in total twenty four unknown elements in $\overline{B}$. Put Equation (3.28), Equation (3.29) and Equation (3.30) together,

$$
\left[ \begin{array}{c} 
\sum_j \frac{m_j}{\rho_j} r_{ij}^\eta (s_1)_{ij}^{\beta} (s_2)_{ij}^\gamma (s_3)_{ij}^\delta \nabla^\epsilon W_{ij} \\
\sum_j \frac{m_j}{\rho_j} r_{ij}^\eta r_{ij}^\epsilon (s_1)_{ij}^{\beta} (s_2)_{ij}^\gamma (s_3)_{ij}^\delta \nabla^\epsilon W_{ij} \\
\sum_j \frac{m_j}{\rho_j} r_{ij}^\eta r_{ij}^\theta r_{ij}^\lambda (s_1)_{ij}^{\beta} (s_2)_{ij}^\gamma (s_3)_{ij}^\delta \nabla^\epsilon W_{ij} 
\end{array} \right] \overline{B}_{\alpha\beta\gamma\delta\epsilon} = \\
\left[ \begin{array}{c} -I^{\eta\alpha} \\
0_{\eta\rho\alpha} \\
0_{\eta\theta\theta\lambda}
\end{array} \right].
$$

There are eighteen equations in this system and twenty four unknowns. This is an under-determined system. We can simply set six elements of $\overline{B}$ equal to zero and solve the system.

Therefore, the new scheme takes the following form,

$$
\langle \nabla f \rangle_i |_{\text{new}} \equiv \sum_j \frac{m_j}{\rho_j} (f_j - f_i) \overline{B}_{i}^{\alpha\beta\gamma\delta\epsilon} (s_1)_{ij}^{\beta} (s_2)_{ij}^\gamma (s_3)_{ij}^\delta \nabla^\epsilon W_{ij}.
$$

(3.32)

Similar to (3.8), the truncation error of the new scheme becomes,

$$
\langle \nabla f \rangle_i |_{\text{new}} = \nabla^\alpha f |_i \\
+ \nabla^\eta \nabla^\theta \nabla^\lambda \nabla^\epsilon f |_i \left( \frac{1}{24} \sum_j \frac{m_j}{\rho_j} r_{ij}^\eta r_{ij}^\theta r_{ij}^\lambda \overline{B}_{i}^{\beta\gamma\delta\epsilon} (s_1)_{ij}^{\beta} (s_2)_{ij}^\gamma (s_3)_{ij}^\delta \nabla^\epsilon W_{ij} \right) \\
+ \text{H.O.T.}
$$

(3.33)

All the terms including $\nabla^\eta f |_i$ and $\nabla^\eta \nabla^\theta f |_i$ vanish. The normalization tensor $\overline{B}$ makes the consistency of the scheme two orders of magnitude higher than the scheme (3.6).

The convergence of this scheme depends on the choices of $s_1$, $s_2$ and $s_3$. We will show in Section 3.4.3 that our choice (3.26) of those vectors gives this scheme higher order of convergence.
3.4.2 Laplacian correction

For the correction of Laplacian approximation, we replace the term \( e^\theta_{ij} B^\delta_i \nabla^\delta W_{ij} \) in Equation (3.22) with,

\[
Y_{ij} \equiv \tilde{B}_i^\alpha \gamma^\delta (s_4)_{ij}^\alpha (s_5)_{ij}^\beta (s_6)_{ij}^\gamma \nabla^\delta W_{ij},
\]  

(3.34)

with

\[
(s_4)_{ij} \equiv e_{ij} + e^2_{ij}, \quad (s_5)_{ij} \equiv e^3_{ij}, \quad (s_6)_{ij} \equiv e_{ij} + e^4_{ij}.
\]  

(3.35)

The error analysis is similar to Equation (3.16) in Section 3.3. In Equation (3.16) the corrected gradient operator is used to approximate the gradient of the function \( \nabla f \).

Hence, substitute this new gradient kernel (3.25) from previous section and \( Y_{ij} \) into the error analysis Equation (3.16), we get,

\[
2 \sum_j \frac{m_j}{\rho_j} \left( \frac{f_i - f_j}{|r_{ij}|} - e^\phi_{ij} \frac{\nabla^\phi f_i}{|\nabla^\phi f_i|_{\text{new}}} \right) Y_{ij}
\]

\[
= - \nabla^\nu \nabla^\theta f_i \| \sum_j \frac{m_j}{\rho_j} \left\{ e^\phi_{ij} \left( \sum_j \frac{m_j}{\rho_j} r^\eta_{ij} r^\theta_{ij} \nabla^\phi W_{ij} \right) + e^\eta_{ij} r^\theta_{ij} \right\} Y_{ij}
\]

\[
+ \nabla^\nu \nabla^\theta \nabla^\lambda f_i \| \frac{1}{3} \sum_j \frac{m_j}{\rho_j} \left\{ e^\phi_{ij} \left( \sum_j \frac{m_j}{\rho_j} r^\eta_{ij} r^\theta_{ij} r^\lambda_{ij} \nabla^\phi W_{ij} \right) + e^\eta_{ij} r^\theta_{ij} r^\lambda_{ij} \right\} Y_{ij}
\]

\[
+ \nabla^\nu \nabla^\theta \nabla^\xi f_i \| \frac{1}{12} \sum_j \frac{m_j}{\rho_j} \left\{ e^\phi_{ij} \left( \sum_j \frac{m_j}{\rho_j} r^\eta_{ij} r^\theta_{ij} r^\lambda_{ij} r^\xi_{ij} \nabla^\phi W_{ij} \right) + e^\eta_{ij} r^\theta_{ij} r^\lambda_{ij} r^\xi_{ij} \right\} Y_{ij}
\]

\[
+ \text{H.O.T.}
\]

(3.36)

Therefore, we have the system,

\[
\begin{bmatrix}
\sum_j \frac{m_j}{\rho_j} \left\{ e^\phi_{ij} \left( \sum_j \frac{m_j}{\rho_j} r^\eta_{ij} r^\theta_{ij} \nabla^\phi W_{ij} \right) + e^\eta_{ij} r^\theta_{ij} \right\} (s_4)_{ij}^\alpha (s_5)_{ij}^\beta (s_6)_{ij}^\gamma \nabla^\delta W_{ij}
\end{bmatrix}
\equiv \alpha^\beta^\gamma^\delta
\begin{bmatrix}
\tilde{B}_i^n \\
\tilde{B}_i^\phi \\
\tilde{B}_i^\theta \\
\tilde{B}_i^\lambda \\
\tilde{B}_i^\xi
\end{bmatrix}
\]

\[
\tilde{B} = \begin{bmatrix}
-\tilde{I}^\phi \\
0^\theta^\phi \\
0^\theta^\lambda \\
0^\theta^\xi
\end{bmatrix}.
\]

(3.37)

In this system, the terms

\[
\sum_j \frac{m_j}{\rho_j} r^\eta_{ij} r^\theta_{ij} \nabla^\phi W_{ij} = 0,
\]

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\[
\sum_j \frac{m_j}{\rho_j} \rho_j r_{ij}^\eta r_{ij}^\theta \sum_k \eta_{ij} r_{ij}^\eta \sum_k \eta_{ij} r_{ij}^\theta W_{ij} = 0,
\]

since this is part of the system when we try to solve \( \overline{B} \) (Equation (3.29) and Equation (3.30)). Hence,

\[
\begin{bmatrix}
\sum_j m_j \rho_j \{ \eta_{ij} r_{ij}^\eta (s_4)_{ij} (s_5)_{ij} (s_6)_{ij} \} \nabla^\delta W_{ij} \\
\sum_j m_j \rho_j \{ \eta_{ij} r_{ij}^\theta (s_4)_{ij} (s_5)_{ij} (s_6)_{ij} \} \nabla^\delta W_{ij} \\
\sum_j m_j \rho_j \{ \eta_{ij} r_{ij}^\phi (s_4)_{ij} (s_5)_{ij} (s_6)_{ij} \} \nabla^\delta W_{ij}
\end{bmatrix}
\hat{B} =
\begin{bmatrix}
-\mathbf{I}^\phi \\
0^\phi\theta \\
0^\phi\theta\lambda \\
\end{bmatrix}.
\]

(3.38)

Since \( e_{ij} = r_{ij}/|r_{ij}| \), we have \( e_{ij}^1 r_{ij}^2 = e_{ij}^2 r_{ij}^1 \), where the superscripts indicates the first and second components of those vectors. Therefore there are duplicated equations in the system (3.38). The elements of \( \hat{B} \) have no repetition since we choose \( s_4, s_5 \) and \( s_6 \) differently. Thus, the system (3.38) represent twelve equations with sixteen unknowns in two dimension. Again, this system is underdetermined. We set four of the unknowns to zero, and solve the linear system.

Hence our new scheme for Laplacian approximation is,

\[
\langle \nabla \cdot \nabla f \rangle_i \mid_{\text{new}} = 2 \sum_j \frac{m_j}{\rho_j} \left( \frac{f_i - f_j}{|r_{ij}|} - e_{ij}^\alpha \langle \nabla^\alpha f \rangle_i \mid_{\text{new}} \right) \hat{B}_i \left( s_4 \right)_{ij} \left( s_5 \right)_{ij} \left( s_6 \right)_{ij} \nabla^\delta W_{ij}.
\]

(3.39)

The truncation error of our new Laplacian approximation is,

\[
\langle \nabla \cdot \nabla f \rangle_i \mid_{\text{new}} = \nabla \cdot \nabla f_i + \nabla^\eta \nabla^\theta \nabla^\lambda \nabla^\xi \nabla^\nu f_i \times
\left\{ \frac{1}{60} \sum_j m_j \rho_j \left[ e_{ij}^\phi \left( \sum_j m_j \rho_j r_{ij}^\eta r_{ij}^\theta r_{ij}^\phi \nabla^\phi W_{ij} \right) + e_{ij}^\eta r_{ij}^\theta \nabla^\xi r_{ij}^\phi \nabla^\xi Y_{ij} \right] \right\}
\]

+ H.O.T.

(3.40)

Now the leading term of the truncation error includes all the fifth derivatives of \( f \). This scheme has fourth order consistency and can evaluate the Laplacian of a fourth order polynomial exactly. The convergence of this scheme again depends on the choices of the vector \( s_4, s_5 \) and \( s_6 \). The scheme using our choice of those vectors (3.35) is accurate to the fourth order of the smoothing length \( h \).
3.4.3 Test new derivative operators with functions

The new operators in previous two sections are defined by Equation (3.32) and Equation (3.39),

\[
\langle \nabla f \rangle_i^\text{new} \equiv \sum_j \frac{m_j}{\rho_j} (f_j - f_i) \bar{B}_i^{\alpha\beta\gamma\delta} (s_1)_{ij} (s_2)_{ij} (s_3)_{ij} \nabla^\epsilon W_{ij}.
\]

and

\[
\langle \nabla \cdot \nabla f \rangle_i^\text{new} = 2 \sum_j \frac{m_j}{\rho_j} \left( \frac{f_i - f_j}{|r_{ij}|} - e_{ij}^\alpha \langle \nabla f \rangle_{ij}^F \right) \hat{\bar{B}}_i^{\alpha\beta\gamma\delta} (s_4)_{ij} (s_5)_{ij} (s_6)_{ij} \nabla^\delta W_{ij},
\]

where \( \bar{B} \) and \( \hat{\bar{B}} \) is solved by linear system (3.31) and (3.38), respectively. The divergence operator is defined by,

\[
\langle \nabla f \rangle_i^\text{new} \equiv \sum_j \frac{m_j}{\rho_j} (f_j - f_i) \cdot \bar{B}_i^{\alpha\beta\gamma\delta} (s_1)_{ij} (s_2)_{ij} (s_3)_{ij} \nabla^\epsilon W_{ij}.
\] (3.41)

where \( \bar{B} \) is also solved from linear system (3.31).

We first test the consistency of the numerical operators. Belytschko et al. [11] define the order of consistency for mesh free method as the maximum order of polynomial that can be reproduced exactly by numerical scheme. For example, a numerical scheme that has “zero order consistency” means the numerical scheme can reproduce a constant exactly. The order of consistency affects the accuracy of the scheme. Fatehi [21] has found that their gradient approximation has first order consistency, which means the gradient of a linear function using their gradient approximation is exact. Their Laplacian operator has second-order consistency. Based on our error analysis, the new gradient approximation has third-order consistency and the new Laplacian approximation has fourth-order consistency.

First, consider the polynomial \( f(x, y) = x^2 y \) in the region \([-1, 1] \times [-1, 1]\). The particles are placed on a Cartesian grid with \( \Delta x = \Delta y = p_{\text{sep}} \) and the smoothing length is chosen to be \( h = 1.3 p_{\text{sep}} \). Boundary particles are placed on the boundary to mimic a proper boundary condition. For a function test rather than a dynamic flow test, a boundary condition is not needed. However, since the support domains of some particles are
truncated by the boundaries, boundary particles are added to show the presence of
the boundary and, more importantly, to improve the accuracy of the scheme. The
kernel function we are using is the quintic spline function (2.14) for all the numerical
experiments. The top figure in Figure 3.3 shows the results of the $L_2$-norm error versus
the particle separation with a fixed overlap ratio $\beta = h/p_{sep} = 1.3$. The new gradient
approximation gives the error $10^{-14}$, about the machine error, which proves that new
gradient scheme has third order consistency. Meanwhile, Fatehi’s gradient scheme (3.6)
does not reproduce the gradient of the third order polynomial. The bottom figure in
Figure 3.3 shows that result of approximation of the Laplacian of a forth order poly-
nomial $f(x, y) = x^2y^2$ in $[-1, 1] \times [-1, 1]$. The new Laplacian scheme gives error about
$10^{-7}$. This is not machine error (about $10^{-16}$). We think this is due to the roundoff
error when solving the linear system (3.38) that has large condition number. Hence
our new scheme reproduces the Laplacian of a cubic polynomial.

We then investigate the convergence of the new scheme for other analytic functions. We
choose the function $f(x, y) = \sin(2\pi(x + y))$ inside $[-1, 1] \times [-1, 1]$. Periodic boundary
conditions are applied on each side of the boundary. The top figure in Figure 3.4 shows
the $L_2$-norm error of the SPH gradient approximation versus particle separation $p_{sep}$.
Fatehi’s gradient scheme gives a convergence rate about 1.5, while the new gradient
scheme shows a convergence rate of 3. Both of the methods shows a constant conver-
gence rate with fixed overlapping ratio $\beta = h/p_{sep} = 1.3$. The bottom of Figure 3.4
shows the result for SPH Laplacian approximation. Again, Fatehi’s Laplacian has a
convergence rate about 1.5, while the new scheme gives a convergence rate of 4.

We then test the new scheme on a perturbed grid. A randomness parameter $\varepsilon$ is
added through,

$$ r_{perturb} = r_{reg} + \varepsilon \times \text{RNG} \times p_{sep}, $$

(3.42)

where RNG is the random number generator, and in the experiment we generate the
random number from a uniform distribution between -1 and 1. With $\varepsilon = 0.05$, Figure
3.5 shows a similar result compared to the regular particle arrangement.
The convergence of the method is obtained by decreasing the particle separation $p_{\text{sep}}$ with a fixed overlap $\beta = h/p_{\text{sep}}$. The error is not limited by the discretization error even with a fixed number of neighbor particles. In the work of Quinlan et al. [50], it shows that standard SPH schemes are near second-order convergence if $\beta \propto h^{-1}$. It implies that more and more particles are needed in each one of the support domain. For example, if the smoothing length $h$ is halved, in order to achieve second-order convergence, the overlap $\beta$ needs to be doubled. Hence the number of neighbor particles needs to be doubled and $p_{\text{sep}}$ is reduced to $p_{\text{sep}}/4$. Our new scheme solves the dilemma of balancing between the accuracy and the computational effort. Compared to Fatehi’s method, the new method improves both the consistency results and the convergence. The accuracy of the new gradient scheme is one order of magnitude higher than the gradient approximation (3.6) and the accuracy of the new Laplacian approximation is two orders of magnitude higher than Fatehi’s scheme (3.18).
Figure 3.3: Consistency result with new operator versus Fatehi’s operator. Top figure shows that the gradient of the function $x^2y$ is reproduced exactly with new operator. The bottom figure shows that the Laplacian of the function $x^2y^2$ is reproduced exactly with the new operator.
Figure 3.4: $L_2$-norm error of SPH derivative schemes versus particle separation $p_{\text{sep}}$ for fixed overlap ratio $\beta = h/p_{\text{sep}} = 1.3$ on a regular Cartesian lattice.
Figure 3.5: $L_2$-norm error of SPH derivative schemes versus particle separation $p_{sep}$ for fixed overlap ratio $\beta = h/p_{sep} = 1.3$ on an irregular Cartesian lattice, with randomness $\varepsilon = 0.05$. 
For particle methods like SPH, complex boundaries can be easily represented by particles, but implementing correct boundary conditions has been a challenging topic for SPH. As we mentioned, the integral form or the summation form of SPH has suffered from boundary deficiency, as the integral or the summation is truncated by the boundary. Physical quantities calculated from the SPH equations drop near the boundary as the kernel function drops to zero. Even though for some applications velocity drops to zero near the boundary, however, quantities like density do not. On the other hand, for incompressible flow, physical boundary conditions need to be properly addressed, such as a no-slip condition and a no-penetration condition. For example, the simple Couette flow describes the flow between two parallel plates generated purely by momentum, where one of the plates moves relative to the other. The momentum is transferred from the boundary into the fluid. However, in the context of SPH, the particles only interact with particles inside the fluid. Special treatment needs to be done to mimic the proper physical boundary condition.

There are some recent improvements in treating boundary conditions. Libersky and Petschek [30] introduce ghost particles to mimic a “reflective” or “transmissive” boundary condition. Takeda et. al [55] use imaginary particles that fill the space outside the boundary to specify the no-slip boundary condition. Monaghan [39] introduces boundary particles that locate on the solid boundary and exert repulsive forces to the fluid particles near the boundary, which can prevent fluid particles from penetrating the solid boundary.
4.1 Ghost particle

Ghost particles are virtual particles created outside the fluid domain. For any fluid particle within $\alpha h$ (radius of the support domain) away from the boundary, the corresponding ghost particle is generated by reflecting the fluid particle across the boundary. The ghost particle is assigned the density, the mass and the pressure same as the fluid particle. The velocity of the ghost particle is of opposite sign, producing a repulsive force in normal direction at the boundary and a shear stress in tangential direction to achieve the no-slip condition. In other words, the velocity of the fluid particle is extrapolated across the boundary to give the ghost particle an artificial velocity, assuming zero velocity on the boundary. If the boundary moves, the velocity of ghost particle can be calculated similarly, using the velocity of fluid particle relative to the boundary,

$$v_{\text{ghost}} = 2v_{\text{wall}} - v_{\text{fluid}}.$$  \hspace{1cm} (4.1)

![Figure 4.1: Ghost particles are placed beyond the boundary to obtain the no-slip condition and the no-penetration condition](image)

The velocity field at the boundary can be estimated by SPH summation formula
\[ v(r_w) = \sum_j \frac{m_j}{\rho_j} v_j W(r - r_j) \]
\[ = \sum_{j \in \text{Fluid}} \frac{m_j}{\rho_j} v_j W(r - r_j) + \sum_{k \in \text{Ghost}} \frac{m_k}{\rho_k} v_k W(r - r_k) \]
\[ = \sum_{j \in \text{Fluid}} \frac{m_j}{\rho_j} v_j W(r - r_j) + \sum_{k \in \text{Ghost}} \frac{m_k}{\rho_k} (2v_{\text{wall}} - v_{\text{fluid}}) W(r - r_k) \]
\[ = \sum_{j \in \text{Fluid}} \frac{m_j}{\rho_j} v_j W(r - r_j) + \sum_{j \in \text{Fluid}} \frac{m_j}{\rho_j} (2v_{\text{wall}} - v_j) W(r - r_j) \]
\[ = 2v_{\text{wall}} \sum_{j \in \text{Fluid}} \frac{m_j}{\rho_j} W(r - r_j). \] (4.2)

Here the summation in the last equation is a discretized approximation of the integral \[ \int W(r - r') dr'. \] The region of the integration is the portion of the compact support of the particle at the wall that lies within the fluid domain. If the boundary is a line/plane, then the integration region is a half circle/sphere. Therefore the summation is approximately \( \frac{1}{2} \) since the kernel is normalized to 1. Thus \( v(r_w) \approx v_{\text{wall}}. \)

This estimation still works for a curved boundary. For a curved boundary, additional resolution is needed to resolve the physics near corners or turns. The smoothing length needs to be small enough to capture the dynamics of the fluid in those regions. Hence, with a much smaller smoothing length, the portion of the curved boundary inside the compact support of the kernel is approximately a straight line/flat plane. Thus the value of the summation is again approximately \( \frac{1}{2}. \)

The ghost particles are generated at each time step. They are used in the momentum equation to evaluate the acceleration of fluid particles, but their positions do not evolve in time. The ghost particles are also used in the continuity equation. Therefore they contribute to the density calculation, and correct the density deficiency problem near the boundary.

The ghost particle method is widely used in SPH for many applications. Libersky and Petschek [30] first introduces ghost particles to simulate solid wall boundary conditions with the sign of normal velocity of the ghost particle reversed. Colagrossi [14] implements the ghost particle method for the free slip boundary condition to study
interfacial flow with different fluids separated by sharp interfaces. The normal com-
ponent of the velocity is defined same as (4.1) to generate the repulsive force, but the
tangential component is defined by,

\[ v_{t,\text{ghost}} = v_{t,\text{wall}}. \] (4.3)

This condition essentially implements the Neumann condition \( \frac{\partial v_t}{\partial n} = 0 \) which implies
that the shear stress on the boundary is zero. Therefore the fluid achieves free-slip at
the boundary. Morris [47] introduces fixed virtual particles outside the boundary to
achieve the no-slip boundary condition. Instead of being generated at each time step,
the virtual particles are placed on a Cartesian grid and fixed during simulation. They
can be interpreted as extrapolation points outside the computational domain. For each
fluid particle, the velocities of virtual particles that lay inside its compact support are
calculated at each step. The signs of both normal and tangential components of the
velocity are reversed. The magnitude of the velocity relates to the ratio of the distance
\( d_{\text{fluid}} \) between the fluid particle and the tangent plane and the distance \( d_{\text{fluid}} \) from the
virtual particle to the tangent plane.

\[ v_{\text{fluid}} - v_{\text{virtual}} = \beta v_{\text{fluid}}, \] (4.4)

where

\[ \beta = \max \left\{ \beta_{\text{max}}, 1 + \frac{d_{\text{virtual}}}{d_{\text{fluid}}} \right\}. \] (4.5)

The drawback of the ghost particle method is that, it is complicated to implement when
the computational domain has complex boundaries. For example, if the boundary has
acute angle, it is likely that the ghost particle is placed in the fluid region (Figure 4.3).

Szewc et. al. [54, 53] discusses the situation where three ghost particles are
needed for the fluid particle near a corner with a right angle. If a no-slip condition is
required on both walls of the corner, there is no way to assure the proper velocity in
the vicinity of the corner. The reason is that there is a singular point if the velocities
Figure 4.2: Fixed virtual particles introduced by Morris [47] are placed outside the boundary for the no-slip boundary condition.

Figure 4.3: Demonstration of the drawback of the ghost particle method. The ghost particle $a'$ for fluid particle $a$ is placed inside the fluid region.

of those two walls are different. The authors suggest adding a free parameter in the calculation of the velocity of the ghost particle so the velocity developed in the corner is continuous and satisfies one of the boundary conditions on those walls. They also state that the free-slip boundary condition is preferred to get rid of the discontinuity of the velocity.
4.2 Boundary force

The boundary force method is another commonly used boundary treatment. Monaghan [39] first introduces the boundary force method to SPH when simulating free surface flow. In this method, particles called boundary particles are generated along the boundary to represent the rigid body. To include interactions between fluid and the rigid body, boundary particles exert a repulsive force to prevent fluid particles from penetrating the boundary. The Lennard-Jones type force in molecular dynamics is chosen to be the form of the repulsive force,

\[
f(r) = \begin{cases} 
\frac{D}{r} \left( \left( \frac{r_0}{r} \right)^{12} - \left( \frac{r_0}{r} \right)^6 \right), & 0 < r < r_0; \\
0, & r > r_0.
\end{cases}
\]  

(4.6)

Here \( r \) is the distance between a fluid particle and a boundary. The force is set to zero when \( r > r_0 \) so that it is a purely repulsive force and there is no attraction. The coefficient \( D \) is chosen by considering the physics of the problem. For example, for problems involve gravity and the fluid with the depth \( H \), \( D = 5gH \). And for weakly incompressible problems without gravity, \( D \) is estimated so that the particle with the maximum velocity cannot penetrate the boundary. In [45], to simulate the impact between fluid and a rigid body, \( D = U_{\text{max}}^2 \), where \( U_{\text{max}} \) is the estimated max speed of the fluid relative to the boundary.

Besides the repulsive force in normal direction to prevent penetrating, a no-slip condition in the tangential direction needs to be correctly implemented. In the boundary force method, this is done by including boundary particles in the viscous force calculation. The velocity of the boundary particle is assigned with the velocity of the boundary. Hence at each step, boundary particles generate momentum through the interaction with fluid particles and transfer the momentum into fluid.

This form of boundary force can be easily implemented. However, if a fluid particle travels along the boundary with a constant distance, the normal force exerted on the
Figure 4.4: Lennard-Jones force and boundary force are plotted against the distance to the boundary. Red solid line represents Lennard-Jones force in Molecular Dynamics where both repulsion and attraction are included. The blue dotted line represents the boundary force.

Figure 4.5: Illustration of the boundary force method.
particle is not uniform, and the tangential force is nonzero. The reason is that the dir-
rection of the repulsive force is aligned with the line segment connecting the boundary
particle and the fluid particle. Therefore if a fluid particle is between two boundary
particles, the tangential component of the boundary force is nonzero. This method is
improved by Monaghan and Kos [45] by defining the boundary force/mass in the form
of,
\[ f_{ak}(x, y) = \frac{U_{\text{max}}^2}{y} \frac{2m_k}{m_a + m_k} \Gamma(y) \chi(x) \mathbf{n}_k. \]  
(4.7)
Here \( f_{ak} \) is the force exerted to the fluid particle \( a \) due to the boundary particle \( k \). The
variables \( x \geq 0 \) and \( y \geq 0 \) are the local tangential and vertical coordinates measured
from the boundary particle \( k \). The function \( \chi(x) \) is defined by,
\[ \chi(x) = \begin{cases} 
1 - \frac{x}{p_{\text{sep}}} , & 0 \leq x < p_{\text{sep}}; \\
0 , & \text{otherwise}, 
\end{cases} \]  
(4.8)
where \( p_{\text{sep}} \) is the separation distance between fluid particles. It is also the separation
distance between boundary particles. Let us assume the fluid particle is \( x_1 \) right from
the left boundary particle \( k_1 \) and \( x_2 \) left from the right boundary particle \( k_2 \). We know
that \( x_1 + x_2 = p_{\text{sep}} \). If we further assume the mass of those two boundary particles are
equal, denoted by \( m_b \), then the boundary force exerted on this fluid particle is,
\[ f = f_{ak_1}(x_1, y) + f_{ak_2}(x_2, y) \]
\[ = \frac{U_{\text{max}}^2}{y} \frac{2m_b}{m_a + m_b} \Gamma(y) \left( \chi(x_1) + \chi(x_2) \right) \]
\[ = \frac{U_{\text{max}}^2}{y} \frac{2m_b}{m_a + m_b} \Gamma(y) \left( 1 - \frac{x_1}{p_{\text{sep}}} + 1 - \frac{x_2}{p_{\text{sep}}} \right) \]
\[ = \frac{U_{\text{max}}^2}{y} \frac{2m_b}{m_a + m_b} \Gamma(y). \]  
(4.9)
Now the boundary force depends only on \( y \), which means the tangential component of
the boundary force is zero. Since the boundary force is a function of the normal distance
to the boundary \( y \), the fluid particles with the same distance from the boundary have
the same boundary force exerted on them. The function \( \Gamma(y) \) has the form of the
gradient of the kernel function $W$, and is defined in terms of the variable $s = \frac{y}{h}$. For example, for the cubic spline kernel (2.13), the function $\Gamma(y)$ is,

$$
\Gamma(y) = \begin{cases} 
\frac{2}{3}, & 0 < s < 2/3; \\
\frac{5}{14\pi} \left[3(2 - s)^2 - 12(1 - s)^2\right], & 2/3 < s < 1; \\
\frac{5}{14\pi} \left[3(2 - s)^2\right], & 1 < s < 2; \\
0, & \text{otherwise.}
\end{cases}
$$ (4.10)

We replace the value of the gradient of the kernel inside $0 < s < 2/3$ with its maximum value. The factor $U_{max}^2$ is again the estimate force/mass to stop the particle at an estimated speed $U_{max}$. The factor $1/y$ is used to prevent particles with faster speed. The form of the force is similar to the gradient of the kernel function since the repulsive boundary force is against the force generated by the gradient of the pressure. The SPH form of the pressure gradient involves the gradient of the kernel function. For this choice of boundary force, $f_{ak} = -f_{ka}$ where $f_{ka}$ is the force on boundary particle $k$ due to the fluid particle $a$. Thus, the linear momentum and the angular momentum of the entire system are conserved, in the absence of external forces.

Monaghan [43] introduces another updated boundary force scheme. He argues that for boundary with complex geometries, or even a simple concave boundary, the normal vectors at the position of different boundary particles can cross. Hence the direction of the normal is not clear and the direction of the repulsive force is ambiguous. Monaghan then proposes a new boundary force scheme. The force per mass on a SPH fluid particle $a$ due to a boundary particle $k$ has the form,

$$
f_{ak} = \frac{K}{\beta} \frac{2m_k}{m_a + m_k} \frac{r_{ak}}{|r_{ak}|^2} W(r_{ak}, h).
$$ (4.11)

Here $K$ is a parameter that measures the magnitude of the force to stop fluid particles from penetrating the boundary. The constant $\beta$ makes sure the total force acting on the fluid particle remains unchanged if the spacing of the boundary particle changes. For example, if the spacing of the boundary particles is halved, then the number of
boundary particles in the compact support of a fluid particle is doubled. This means that the total force exerted on the fluid particles are doubled. To make the total force invariant with the boundary particle spacing change, the magnitude of force from each boundary particle needs to be halved, and hence $\beta$ should be doubled.

Monaghan [43] states that the essential idea of the new boundary force scheme is to design a smooth boundary particle force so that the total force on a fluid particle obtained by summing over boundary particle forces is independent of the discrete nature of the boundary to a high degree of accuracy. Consider a straight line boundary lying on the $x$-axis and a fluid particle located at $(x_a, y_a)$. The vertical distance between the particle and the boundary is $y_a$. Now the tangential and the normal component of the boundary force per mass are given by,

$$f_x = \sum_{j=-\infty}^{\infty} \frac{x_a - x_j}{r_{aj}} \Phi(r_{aj}), \quad (4.12)$$

and

$$f_y = \sum_{j=-\infty}^{\infty} \frac{y_a}{r_{aj}} \Phi(r_{aj}), \quad (4.13)$$

where $r_{aj}$ is the distance between the fluid particle and the boundary particle $j$. The force is along the radial direction and the magnitude of the force is given by the function $\Phi$. We further assume boundary particles are equally spaced with spacing $\Delta$ so that $x_j = j \Delta$. Now using Poisson summation formula, those summations can be approximated by integrals,

$$f_x \approx \int_{-\infty}^{\infty} \frac{x_a - q}{r} W(r) \, dq, \quad (4.14)$$

where $r = \sqrt{(x_a - q)^2 + y_a^2}$. If we change the variable $q' = x_a - q$, it is clear that the integrand is an odd function of $q'$ so the integral is zero. Hence the tangential component of the force is approximately zero because the error in the Poisson summation integration approximation is negligible. The normal component of the force is, using the new variable $q'$,

$$f_y \approx y_a \int_{-\infty}^{\infty} \frac{W(r')}{r'} \, dq'. \quad (4.15)$$
The normal force depends only on the normal distance between the fluid particle and the boundary, and it is independent of $x_a$.

Back to Equation (4.11), the function $W$ has the form of a SPH kernel function. In Section 2.3.1 and 2.3.2, we mentioned that the kernel function is normalized to 1. However, for the kernel function used in the boundary force, it is used to represent the magnitude of the radial force, and different constraints are required. Monaghan [43] points out that the normalization factor is chosen to keep the fluid particle $p_{sep}$ distance away from the boundary, where $p_{sep}$ is the fluid particle separation.

Using boundary particles, the boundary force method can be easily implemented for problems with complex boundary geometry. However, the magnitude of the force is determined by the parameter $K$ which describes the force/mass required to stop a fluid particle with estimated maximum speed penetrating the boundary. The definition of $K$ is not clear and the value of $K$ is problem dependent. For example, for any problem with both the presence of gravity and the motion of fluid, it is not sure whether the parameter $K$ should be $gH$ or $U_{max}^2$ or the sum of those two expressions. On the other hand, without any virtual particles outside of the boundary, the accuracy of SPH will suffer from the deficiency of the SPH summation. This method may have a non-uniform convergence.

4.3 New scheme for solid boundary condition

The solid wall boundary conditions we focus on are the no-slip condition and the no-penetration condition. In conventional mesh-based numerical methods, the penetration is not a concern since the flow field is usually described in Eulerian reference frame. The no-slip boundary condition describes that the fluid velocity at the solid wall boundary is zero relative to the velocity of the boundary. Because the velocity is prescribed at a given location, no-slip condition is an example of Dirichlet boundary condition. In finite difference methods or finite element methods, the no-slip boundary condition is achieved by simply assigning the boundary velocity to the points on the
boundary. In SPH, Dirichlet boundary condition is not implemented using only bound-
dary particles with the proper boundary velocity since standard SPH approximations
suffer from the boundary deficiency. Even if particles are placed on the boundary, there
is still a portion of the support domain truncated by the boundary. The gradient and
the Laplacian of the variables are poorly approximated near the boundary. The ghost
particle method captures the no-slip and the no-penetration boundary conditions by
using ghost particles filling the space beyond the boundary, which fixed the boundary
deficiency problem. The boundary force method introduces repulsive forces attempt-
ting to correct the pressure gradient near the boundary in the momentum equation of
Navier-Stokes equations, but never try to recover the viscous diffusion term accurately.

The new SPH approximations described in previous chapter not only give high or-
der of consistency and convergency but improve the accuracy of the method near the
boundary. Figure 4.6a shows the relative spatial error of different SPH gradient ap-
proximations of the function $f(x, y) = \sin(2\pi x)$ using 1600 particles in two dimensions.
The relative spatial error of approximation (2.26) is very large in the entire domain.
Equation (2.39) gives same results for interior particles as Equation (3.6) but it is
much worse near the boundary. Our new scheme (3.32) is much better than the correc-
tion (3.6) in approximating the gradient for both interior particles and particles near
the boundary. Figure 4.6b demonstrates a similar result for different SPH Laplacian
approximations. The new Laplacian approximation (3.39) is better than any other
Techniques.

The superb performance of the new schemes near the boundary give us the option
to use only boundary particles to impose the no-slip condition. Just like implementing
Dirichlet boundary condition in finite differences methods, the boundary particles are
assigned with the velocity of the boundary. The momentum can be transferred from
the boundary particles to the fluid particles through the new Laplacian approximation
(3.39) more accurately. On the other hand, since the gradient of the pressure can be
evaluated more precisely at the boundary using the new gradient operator (3.32), there
Figure 4.6: Relative spatial error of different SPH approximations using 1600 particles in 2D. The top figure shows the SPH gradient approximations of the function $f(x, y) = \sin(2\pi x)$. The bottom figure shows the SPH Laplacian approximations of the same function.
is no need for a repulsive boundary force, unlike the boundary force method proposed by Monaghan [43]. The boundary particles are considered as a layer of fluid particles that stick to the solid boundary. Therefore, the density and the pressure of the boundary particles are prescribed initially just as any other fluid particles and the values are fixed during the simulation. The no-penetration boundary condition can be well handled by the new boundary technique. Let us consider that a fluid particle moves towards the boundary. As the fluid particle approaches the boundary, the local density increases and the local pressure also increases according to equation of state (2.80) or (2.81). Hence the fluid particle is pushed away by boundary particles due to the pressure gradient. The no-penetration boundary condition is satisfied automatically. The position of the boundary particles do not evolve with time. However, boundary particles should be placed more carefully to prevent fluid particles penetrating from the position between two adjacent boundary particles. At each time step, for each fluid particle within one particle separation $p_{sep}$ from the boundary, a corresponding boundary particle is generated at the position where the fluid particle is closest to the boundary.

The new boundary technique reduces the computational cost from layers of ghost particles/virtual particles. The new SPH scheme allows a simpler representation of boundaries than existing schemes like boundary force and ghost particles. Furthermore, the new SPH scheme with the new boundary method capture the no-slip and no-penetration conditions with better accuracy than existing techniques.
Chapter 5
NUMERICAL RESULTS

Three benchmark problems have been examined for the purpose of verification of the new algorithms. In the first test, the doubly periodic flow with periodic boundary conditions posed on each side of the domain is revisited. This is a good measure of how the new SPH schemes work without solid boundary conditions. In the second problem, plane Couette flow is simulated in SPH with different boundary conditions and the results are compared to the analytical solution. In the third test problem, circular Couette flow is studied where the flow between two concentric circles is generated due to the rotation of the outer circle with a constant angular speed. This test demonstrates the ability of the new boundary technique handling curved boundaries.

For the rest of the chapter, there are mainly three different SPH formulations for Navier-Stokes equations:

1. The Standard SPH formulation with Standard Diffusion Scheme or CSIRO Diffusion Scheme,

\[
\begin{align*}
\frac{d\rho_i}{dt} &= \sum_j m_j v_{ij} \cdot \nabla_i W_{ij}, \\
\frac{dv_i}{dt} &= -\sum_j m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla_i W_{ij} + \Pi_{ij}, \\
\frac{dr_i}{dt} &= v_i, \\
P &= \rho_0 c_s^2 \left[ \left( \frac{\rho}{\rho_0} \right)^\gamma - 1 \right],
\end{align*}
\]

with

\[
\Pi_{ij} = 2 \sum_j \frac{m_j}{\rho_i \rho_j} \frac{2\mu_i \mu_j}{\mu_i + \mu_j} \frac{r_{ij} \cdot \nabla W_{ij}}{|r_{ij}|^2 + \eta^2} v_{ij}, \quad \text{(Standard Diffusion)}
\]

\[
\Pi_{ij} = \sum_j \xi \frac{m_j}{\rho_i \rho_j} \frac{2\mu_i \mu_j}{\mu_i + \mu_j} \frac{v_{ij} \cdot r_{ij}}{|r_{ij}|^2 + \eta^2} \nabla W_{ij}, \quad \eta = 0.01h^2, \xi = 4. \quad \text{(CSIRO Diffusion)}
\]
2. The Fatehi’s SPH formulation,

\[
\begin{align*}
\frac{d\rho_i}{dt} &= \sum_j m_j v_{ij} \cdot (B_i \cdot \nabla \rho_i), \\
\frac{dv_i}{dt} &= -\frac{1}{\rho_i} \sum_j m_j (P_j - P_i) B_i \cdot \nabla W_{ij} + \sum_j m_j \left( \frac{v_i - v_j}{|r_{ij}|} - e_{ij}^\alpha \langle \nabla^\alpha v \rangle_{i|F_1} \right) e_{ij} \otimes \nabla W_{ij}, \\
\frac{dr_i}{dt} &= v_i, \\
P &= \frac{\rho_0 c^2}{\gamma} \left( \left( \frac{\rho}{\rho_0} \right)^\gamma - 1 \right),
\end{align*}
\]

where $B_i$ and $\hat{B}_i$ is calculated from Equation (3.7) and (3.17), respectively. The gradient approximation $\langle \nabla^\alpha v \rangle_{i|F_1}$ is defined by Equation (3.6).

3. The new SPH formulation,

\[
\begin{align*}
\frac{d\rho_i}{dt} &= \sum_j m_j v_{ij} \cdot \nabla W_{ij}, \\
\frac{dv_i}{dt} &= -\frac{1}{\rho_i} \sum_j m_j (P_j - P_i) \nabla W_{ij} + 2 \sum_j m_j \left( \frac{v_i - v_j}{|r_{ij}|} - e_{ij}^\alpha \langle \nabla^\alpha v \rangle_{i|\text{new}} \right) Y_{ij}, \\
\frac{dr_i}{dt} &= v_i, \\
P &= \frac{\rho_0 c^2}{\gamma} \left( \left( \frac{\rho}{\rho_0} \right)^\gamma - 1 \right),
\end{align*}
\]

where $\nabla W_{ij}$ and $Y_{ij}$ are defined by Equation (3.25) and (3.34), respectively. The gradient approximation $\langle \nabla^\alpha v \rangle_{i|\text{new}}$ is defined by Equation (3.32).

5.1 Doubly periodic problem

The doubly periodic problem is described in Section 3.1.1. The periodic boundary condition in SPH is implemented for both the particle movement and the particle interaction (Figure 5.1). In the particle movement, a fluid particle that moves out of the computational domain through a boundary is immediately inserted back through the opposite boundary. In the particle interaction, a fluid particle within the distance of the radius of the compact support from a boundary interacts with particles near the opposite boundary. This is implemented by copying all particles within the distance of the radius of the compact support from a boundary and placing them by the opposite boundary. In the simulation, for the analytical solution (3.2), we add as many terms
as possible of the summation until the absolute value of the next term to be added is less than the machine precision.

Figure 5.1: Implementation of periodic boundary conditions in SPH.

Figure 5.2: Doubly periodic flow.
Figure 5.3: Particles are placed initially on a 20×20 Cartesian grid with periodic boundary condition for doubly periodic problem.

We first study the velocity profiles at various time instant compared with the analytical solution. The particles are initially placed on a 20×20 Cartesian grid in the domain [0, 1] × [−0.5, 0.5] shown in Figure 5.3. Virtual particles for periodic boundary conditions are generated outside the boundary. The initial velocity for all the particles that have a positive y-coordinate is (1, 0) and for all the particles that have a negative y-coordinate, the initial velocity is set to be (0, 0). A very small time step $dt = 0.005 \Re h^2$ is found to be necessary in order to avoid numerical instability of the new scheme. The Reynolds number used in the simulation is 0.01. The speed of sound is 10 times the maximum speed $U_{\text{max}} = 1$ and the dynamic viscosity $\mu = 1$. The smoothing length $h$ used is 1.3 times more than the initial particle separation $p_{\text{sep}}$. For the quintic kernel with the radius of the support domain $3h$, there are 45
neighbor particles initially in the kernel support domain. In Figure 5.4, we show the results of the new formulation for the transient solution at a sequence of times until the velocity profile reaches its steady-state regime where $v_x = 0.5$. Here $v_x$ denotes the $x$ component of the velocity $v$. This flow is unidirectional, thus the particles on the same

![Figure 5.4: The development of the velocity profile of doubly periodic flow at time $t = 0.001, 0.01, 0.03, 0.05,$ and 0.1 with $Re = 0.01$.](image)

streamline move with the same velocity. Each data point in the figure corresponds to a column of such particles. Compared with the exact solution given by (3.2), the maximum relative error in the velocity is about 0.01% at time $t = 0.1$. Furthermore, the maximum and the minimum of the density at time $t = 0.1$ are $\rho_{\text{max}} = \rho_0 + 9 \times 10^{-6}\rho_0$ and $\rho_{\text{min}} = \rho_0 - 10^{-5}\rho_0$, which indicates the incompressibility is well maintained for the simulation using the new formulation.

Figure 5.5 shows the particle distribution during a simulation of the doubly periodic
problem with Reynolds number Re = 10. Figure 5.5a shows the initial particle distribution and particle distribution at $t = 0.5$. The particles move horizontally according to the velocity profile. The particle distribution at $t = 1$ is shown in Figure 5.5b. The particles marked by star move out of the right boundary and reenter from the left boundary due to the periodic boundary condition. The particles are now disordered, but in a 'orderly' way.

A convergence study is conducted for different SPH formulations. The spatial convergence rate is evaluated based on $L_2$ norm relative error,

$$E_{L_2} = \sqrt{\frac{\sum (\mathbf{v}_{\text{sph}} - \mathbf{v}_{\text{exact}})^2}{\sum \mathbf{v}_{\text{exact}}^2}},$$  

(5.1)

where $\mathbf{v}_{\text{sph}}$ is the velocity simulated by SPH and $\mathbf{v}_{\text{exact}}$ is the velocity calculated from the analytical solution. The summation is over all fluid particles but not boundary particles or any virtual particles. Figure 3.1 already shows the $L_2$ norm error for the Standard SPH formulation against the smoothing length $h$ with a fixed overlap $\beta = 1.3$. The overall error has the convergence rate close to 2 for both Standard Diffusion scheme (SD) and CSIRO scheme when the smoothing length is large. As $h$ decreasing, the overall error is dominated by the discretization error and the Standard SPH formulation does not converge any more. Figure 5.6 presents the $L_2$ norm relative error of the calculated velocity for doubly periodic flow against the smoothing length $h$ with Fatehi’s formulation and the new formulation. Compared to the results of the standard formulation, both Fatehi’s formulation and the new formulation obtain relative errors 2 to 3 orders of magnitude less than those of the standard formulation. More importantly, both formulations have a constant convergence rate independent of the smoothing length $h$. Fatehi’s formulation is accurate to second order in the smoothing length $h$, while the new formulation has third-order accuracy. The result implies that the new formulation handles purely viscous diffusion very well without solid wall boundary conditions. Note that since both Fatehi’s formulation and the new formulation are not in a symmetric form, both linear and angular momenta of
Figure 5.5: Particle distribution during the simulation of the doubly periodic problem with Re = 10. The top figure shows the initial particle distribution (circle) and the particle distribution at $t = 0.5$ (triangle). The bottom figure shows the particle distribution at $t = 1$. The particles marked by star enter from the left boundary due to the periodic boundary condition.
Figure 5.6: The L2 norm relative error of the calculated velocity for doubly periodic flow against the smoothing length $h$ with Fatehi’s formulation and the new formulation.
the system are not conserved. However, with the truly convergent techniques, the conservation error for the new formulation will converge to zero rapidly.

5.2 Couette flow

The Couette flow is a fluid flow between two infinite plates located at \( y = -L/2 \) and \( y = L/2 \) (Figure 5.7). The fluid is at rest initially and at the beginning of the simulation the upper plate moves at a constant speed \( U \) horizontally. The velocity has a linear profile when the flow reaches the steady state,

\[
\mathbf{v}_x(y) = \frac{U}{L} \left( y + \frac{L}{2} \right).
\]  (5.2)

The solution of the transient problem can be expressed as a series solution,

\[
\mathbf{v}_x(y, t) = \frac{U}{L} \left( y + \frac{L}{2} \right) + \sum_{n=1}^{\infty} \frac{2U}{n\pi} (-1)^n \sin \left( \frac{n\pi}{L} \left( y + \frac{L}{2} \right) \right) \exp \left( -\frac{1}{Re} \frac{n^2\pi^2}{L^2} t \right). \quad (5.3)
\]

Figure 5.7: Plane Couette flow.

The flow is simulated in a rectangular domain \([0, 1] \times [-0.5, 0.5]\) with \(15 \times 15\) particles placed initially on a Cartesian grid. The upper plate moves with a constant speed \( U = 1 \). The periodic boundary condition is applied in \( x \) direction. The ghost particle
method is implemented for the no-slip conditions on the top boundary and the bottom boundary for Standard SPH formulation and Fatehi’s formulation, and the new boundary technique is applied at the upper and lower plates for the new scheme. The Reynolds number in this test is set to be Re = 0.1. Other configurations are identical to previous test. In the simulation, for the analytical solution (5.3), we add as many terms as possible of the summation until the absolute value of the next term to be added is less than the machine precision.

![Figure 5.8: The development of the velocity profile of the plane Couette flow at time $t = 0.005, 0.03, 0.08,$ and $0.2$ with Re = 0.1.](image)

Figure 5.8 demonstrates the development of the velocity profile of the plane Couette flow at various time instants using the new formulation. The velocity of SPH simulation is compared with the analytical solution at the dimensionless time $t = 0.005, 0.03, 0.08,$ and $0.2$. The new formulation predicts the analytical solution very well with only 225 particles. The maximum density at time $t = 0.2$ is $\rho_{max} = \rho_0 + 9.5 \times 10^{-7}\rho_0$ and the
minimum density is \( \rho_{\text{min}} = \rho_0 - 4 \times 10^{-7} \rho_0 \).

Figure 5.9: The L2 norm relative error of the calculated velocity for plane Couette flow against the smoothing length \( h \) with different SPH formulations.

The convergence results for different SPH formulations are shown in Figure 5.9. With the fixed overlap \( \beta = 1.3 \), the error of standard formulation with CSIRO diffusion scheme does not decrease with a constant slope. Similar to doubly periodic flow case, the error is dominated by a constant \( \beta^{-(\kappa+1)} \) (Equation (3.1)). The standard formulation with Standard Diffusion scheme behaves like second-order method with a constant convergence rate. On the other hand, Fatehi’s formulation has a constant convergence rate about 2 with the ghost particles implemented for the no-slip boundary condition. The convergence rate of the new formulation with the new boundary particle treatment is about 3. This again validates that the new SPH formulation converges with a constant rate requiring only a fixed number of neighbor particles inside the compact support of the kernel.
5.3 Circular Couette flow

The two-dimensional circular couette flow is a fluid flow between two concentric circle located at \( r = r_1 \) and \( r = r_2 \) \( (r_1 < r_2) \). The fluid is viscous, incompressible, and initially stationary. Two circle boundaries start to rotate with different angular velocities \( \Omega_1 \) and \( \Omega_2 \), and eventually the fluid reaches a steady state. With no-slip condition at the two boundaries, the steady state solution is,

\[
v_\theta(r) = \frac{1}{r} \left( \frac{\Omega_1 - \Omega_2}{r_1^{-2} - r_2^{-2}} \right) + r \left( \frac{\Omega_1 r_1^2 - \Omega_2 r_2^2}{r_1^2 - r_2^2} \right). \tag{5.4}\]

The series solution for the time dependent problem can be found using polar coordinates since the flow is only in the \( \theta \) direction (see Appendix A). In our experiment, the location of the circle is \( r_1 = 1 \), and \( r_2 = 2 \). At the beginning of the simulation, the outer circle starts rotating with angular velocity \( \Omega_2 = 1 \) and \( \Omega_1 = 0 \). The computational domain we choose is a section of annulus with \( \theta = \frac{\pi}{6} \). The value of \( \theta \) is chosen to be \( \pi/6 \) so that the number of particles in radial direction and the number of particles on the most outer ring are approximately same. The periodic boundary conditions are applied to the inlet and outlet boundaries and the implementation is similar as shown in Figure 5.1. The periodic boundary conditions are implemented by rotating

Figure 5.10: Circular Couette flow.
the particles with the distance of the radius of the kernel support domain with $\theta = \frac{\pi}{6}$ (Figure 5.11). The ghost particle method is applied to the outer and inner rings for the standard formulation and Fatehi’s formulation while the new boundary particles treatment is implemented for the new formulation. The particles are initially places on 10 concentric rings separated by $p_{\text{sep}}$ with radii between $r_1$ and $r_2$. On each concentric ring, the particles are distributed uniformly and the arc length between two adjacent particles is approximately $p_{\text{sep}}$. Therefore the number of particles on each ring is not identical.

The velocity profiles of SPH simulation at different time is shown in Figure 5.12 compared with theoretical solution.

Figure 5.13 shows the convergence study on circular Couette flow for 4 different techniques. The standard formulations with both Standard Diffusion and CSIRO Diffusion do not converge with a constant slope. The rate of convergence of Fatehi’s formulation is 2, whereas the new formulation also presents a convergence rate of 2 but the error

![Figure 5.11: The initial particle distribution of circular Couette flow simulation. Periodic boundary conditions is applied to inlet and outlet boundaries. Boundary particles are placed on the outer and the inner rings for the simulation of the new SPH formulation.](image-url)
Figure 5.12: The development of the velocity profile of the circular Couette flow at dimensionless time $t = 0.01, 0.04, 0.1$ and $0.2$ with $Re = 0.01$.

Figure 5.13: The $L_2$ norm relative error of the calculated velocity for circular Couette flow against the smoothing length $h$ with different SPH formulations.
is one order of magnitude smaller than with Fatehi’s formulation.

To investigate the loss of accuracy compared to the plane Couette test, a function test is performed without fluid dynamics. The gradient and the laplacian of the function \( \sin(x + y) \) is approximated by the new schemes (3.32) and (3.39) in the sector same as the computation domain for the circular Couette test with boundary particles placed on the domain boundary. The initial particle distribution is same as the one described in the fluid test section (Figure 5.11).

Figure 5.14 shows the convergence results of the approximations. The convergence rate for the new SPH gradient approximation is two and the accuracy is lost. This shows that the loss of accuracy is not caused by dynamics of the fluid. We further investigate the spatial error distribution in the sector region. Figure 5.15 shows the contour plot of the spatial error of the new SPH approximations of the gradient and the laplacian of the function \( \sin(x + y) \) in the sector region \( 1 \leq r \leq 2, \ 0 \leq \theta \leq \frac{\pi}{6} \). The spatial error distribution does not show any patterns of note and there are particles (red dots) where the error has extreme values (spikes) compared to surrounding particles. The large error spikes on particular particles may caused by the large condition number of the linear systems 3.31 and 3.38. All these phenomena are due to particle disorder. For a circular geometry, it is not possible to arrange particles with a perfectly uniform separation. The disorder of particles causes the loss of accuracy as shown in Section 3.4.3. Hence, we think the particle disorder is the reason that the convergence rate for the circular Couette flow is one order less than the rate for the plane Couette flow.
Figure 5.14: $L_2$-norm error of SPH derivative schemes versus initial particle separation $p_{sep}$ for the function $\sin(x + y)$ on a sector domain. The top figure shows the convergence result for the new SPH gradient approximation. The bottom figure shows the convergence result for the new SPH laplacian approximation.
Figure 5.15: The contour plots of the spatial error of the new SPH derivative approximations for the function $\sin(x + y)$ in the sector region $1 \leq r \leq 2$, $0 \leq \theta \leq \frac{\pi}{6}$. The top figure: the new SPH gradient approximation. The bottom figure: the new SPH laplacian gradient approximation. The red dot (located at (0.1,1.0) on the top figure, (0.5,1.0) on the bottom figure) corresponds to the particle that have huge error compared to the error of neighboring particles.
6.1 Conclusion

SPH is an efficient computational algorithm because of the mesh-free nature of the method. The fundamental concepts and the essential formulations of SPH are reviewed. This thesis focuses on the convergence and the boundary techniques for the SPH method for simulating slightly compressible fluid flows.

The convergence of SPH is affected by the smoothing length and the overlap. Using a two-dimensional doubly periodic flow test, we confirmed that the convergence cannot be obtained for traditional SPH formulation with a fixed overlap value. The smoothing error dominates when the smoothing length is large and the SPH method demonstrates a second-order accuracy. However, the overall error is dominated by a constant discretization error with small smoothing length and the SPH method does not converge. Theoretically the convergence can be gained as the smoothing length tends to zero and the overlap tends to infinity simultaneously however in practice the computational cost is very expensive. Two existing techniques are shown with kernel corrections. The gradient approximation is corrected so that it has first-order consistency. The corrected laplacian approximation has second-order consistency. The error decrease monotonically as smoothing length is reduced even if the overlap is a constant. Following those ideas, we developed new algorithms that has higher-order accuracy and consistency. The new gradient approximation is consist enough to exactly represent the first derivative of a cubic function and the new laplacian approximation can exactly predict the second derivative of a fourth-order polynomial. Examining the new
techniques with two-dimensional analytic function on a regular Cartesian grid showed that the new gradient approximation has third-order accuracy and the new laplacian approximation has fourth-order accuracy. The same test is also performed on an irregular Cartesian grid with the particles perturbed by 5% $p_{\text{sep}}$ and the result showed that the new techniques have better accuracy in comparison with the best scheme available. The new schemes do not conserve linear and angular momenta but the conservation error will converge fast so that the conservation error is low enough to be accepted.

The boundaries of the computational domain is easy to represent in SPH but correctly and efficiently implementing the boundary conditions is difficult. Two commonly used boundary treatments are reviewed including the concepts and the formulations. The ghost particle method is similar to the ghost points in finite difference methods. Ghost particles are generated outside the boundary by mirroring fluid particles close to the boundary with the same pressure, density and mass as fluid particles. The normal component of the velocity has opposite sign and the tangential component of the velocity has the opposite sign or same sign as those of fluid particles. The ghost particle method work great for boundaries with straight lines. The disadvantage of the ghost particle method is the difficult configuration of ghost particles for boundaries with complex geometry. The boundary force method is another technique to treat solid wall boundary conditions. Particles are placed on the boundary that exert repulsive forces to prevent fluid particles from penetrating. However, the magnitude of the force is not determined rigorously. A new boundary treatment is developed that adopts the idea of boundary particles from the boundary force method but without imposing repulsive forces. The boundary particles act like boundary points in finite difference methods and Dirichlet boundary conditions can be easily implemented on those boundary particles.

The new algorithms with the new boundary treatment are first tested with the doubly periodic flow. The results show that the method has third-order convergence
rate without the restraint of solid wall boundary conditions whereas the standard SPH formulation does not converge with a constant slope and Fatehi’s formulation has second-order convergence. Our new algorithm is indeed a high-order method that converges with a fixed number of neighboring particles. In the plane Couette flow test, the new formulation works very well with the new boundary technique where boundary particles are used to impose the no-slip boundary condition. The convergence study is similar to the one with doubly periodic flow. The new schemes are then tested for circular Couette flow where the computational domain is a section of annulus. Compared with the available schemes, the error of the new formulation is at least one order of magnitude less and the new scheme behaves second-order accurate.

6.2 Future work

In order to improve the overall performance of our new algorithms for different applications, more rigorous analysis should be performed in the future.

- The time step used in our numerical simulation is very small, more suitable time stepping schemes should be implemented for SPH, such as implicit time stepping techniques.

- The computational cost for calculating the correction tensors at each time step for each particle is large. It is important to explore an algorithm to accelerate the calculation without damaging the convergence property of the current method.

- In order to remedy the drawbacks associated with particle disorder, remeshing techniques can be implemented to reinitialize the particle location.
BIBLIOGRAPHY


Appendix

ANALYTICAL SOLUTION OF THE CIRCULAR COUETTE FLOW

The circular Couette flow is the fluid flow generated between two rotating concentric cylinders. The solution of the flow is obtained in cylindrical coordinates, $v = v(r, \theta, z)$ and the components of the velocity vector are $v_r$, $v_\theta$ and $v_z$. Several assumptions are made to simplify the full Navier-Stokes equations in cylindrical coordinates,

- There is no flow in $z$ direction and in $r$ direction, $v_z = v_r = 0$
- The velocity $v_\theta$ depends only on $r$ and $\theta$, $v_\theta = v_\theta(r, \theta)$.
- There is no pressure gradient in $z$ direction and in $\theta$ direction, $p = p(r)$

The continuity equation $\nabla \cdot v = 0$ becomes

\[ \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} = 0. \]  (A.1)

This equation implies that $v_\theta$ depends only on $r$, $v_\theta = v_\theta(r)$. Therefore, the Navier-Stokes equations with boundary conditions are simplified to,

\[ \frac{\partial v_\theta}{\partial t} = \frac{1}{\text{Re}} \left[ \frac{\partial^2 v_\theta}{\partial r^2} + \frac{1}{r} \frac{\partial v_\theta}{\partial r} - \frac{v_\theta}{r^2} \right] \quad r_1 < r < r_2, \quad t > 0, \]
\[ v_\theta(t, r_1) = \Omega_1 r_1 \quad t > 0, \]
\[ v_\theta(t, r_2) = \Omega_2 r_2 \quad t > 0, \]
\[ v_\theta(0, r) = 0 \quad r_1 < r < r_2. \]  (A.2)

The steady state solution $v_\theta^S$ of the equation is,

\[ v_\theta^S(r) = \frac{1}{r} \left( \frac{\Omega_1 - \Omega_2}{r_1^2 - r_2^2} \right) + r \left( \frac{\Omega_1 r_1^2 - \Omega_2 r_2^2}{r_1^2 - r_2^2} \right). \]  (A.3)
The time-dependent solution of this equation can be expressed in a series using separation of variables,

\[ v_\theta = v_\theta^S + \sum_{n=1}^{\infty} A_n \exp \left( -\frac{1}{\text{Re} \lambda_n} t \right) \left[ J_1(\sqrt{\lambda_n} r) - \frac{J_1(\sqrt{\lambda_n} r_1)}{Y_1(\sqrt{\lambda_n} r_1)} Y_1(\sqrt{\lambda_n} r) \right], \quad (A.4) \]

where the function \( J_1 \) is the first order Bessel function of the first kind and the function \( Y_1 \) is the first order Bessel function of the second kind. The so-called eigenvalue \( \lambda_n \) is the solution to the equation,

\[ J_1(\sqrt{\lambda_n} r_1) Y_1(\sqrt{\lambda_n} r_2) - J_1(\sqrt{\lambda_n} r_2) Y_1(\sqrt{\lambda_n} r_1) = 0. \quad (A.5) \]

There are infinite number of real solutions to this equation and they can be ordered,

\[ 0 < \lambda_1 < \lambda_2 < \lambda_3 < \cdots < \lambda_n < \cdots \to \infty. \]

The solutions of this equation can be calculated numerically using root finding algorithms. We now define the variable \( k_n \equiv \sqrt{\lambda_n} \) to simplify expressions. The coefficient \( A_n \) in the equation (A.4) is,

\[ A_n = \frac{\int_{r_1}^{r_2} (-v_\theta^S) r \left[ J_1(k_n r) - \frac{J_1(k_n r_1)}{Y_1(k_n r_1)} Y_1(k_n r) \right] dr \int_{r_1}^{r_2} r \left[ J_1(k_n r) - \frac{J_1(k_n r_1)}{Y_1(k_n r_1)} Y_1(k_n r) \right]^2 dr }{\text{top} \ space \ text{bottom}}. \quad (A.6) \]

These integral can be evaluated numerically or analytically. Using the help of Maple, we get,

\[ \text{top} = -\frac{1}{\lambda_n} \left[ C_2 J_0(r_1 k_n)k_n - 2 C_1 r_1 J_1(r_1 k_n) + C_1 r_1^2 J_0(r_1 k_n)k_n \right. \]
\[ + 2 \alpha C_1 r_1 Y_1(r_1 k_n) - \alpha C_1 r_2^2 Y_0(r_1 k_n)k_n - C_2 \alpha Y_0(r_1 k_n)k_n \]
\[ - C_2 J_0(r_2 k_n)k_n + 2 C_1 r_2 J_1(r_2 k_n) - C_1 r_2^2 J_0(r_2 k_n)k_n \]
\[ - 2 \alpha C_1 r_2 Y_1(r_2 k_n) + \alpha C_1 r_2^2 Y_0(r_2 k_n)k_n + C_2 \alpha Y_0(r_2 k_n)k_n \left. \right], \quad (A.7) \]
and,

$$\text{bottom} = -\frac{1}{2k_n} r_1^2 \left[ (J_1 (r_1 k_n))^2 k_n - 2 r_1 J_0 (r_1 k_n) J_1 (r_1 k_n) \right. \\
+ r_1^2 (J_0 (r_1 k_n))^2 k_n - 2 \alpha r_1^2 J_1 (r_1 k_n) Y_1 (r_1 k_n) k_n \\
+ 2 r_1 \alpha Y_0 (r_1 k_n) J_1 (r_1 k_n) - 2 \alpha r_1^2 Y_0 (r_1 k_n) J_0 (r_1 k_n) k_n \\
+ 2 r_1 \alpha J_0 (r_1 k_n) Y_1 (r_1 k_n) + \alpha^2 r_1^2 (Y_1 (r_1 k_n))^2 k_n \\
- 2 r_1 \alpha^2 Y_0 (r_1 k_n) Y_1 (r_1 k_n) + \alpha^2 r_1^2 (Y_0 (r_1 k_n))^2 k_n \\
- r_2^2 (J_1 (r_2 k_n))^2 k_n + 2 r_2 J_0 (r_2 k_n) J_1 (r_2 k_n) \\
- r_2^2 (J_0 (r_2 k_n))^2 k_n + 2 \alpha r_2^2 J_1 (r_2 k_n) Y_1 (r_2 k_n) k_n \\
- 2 r_2 \alpha Y_0 (r_2 k_n) J_1 (r_2 k_n) + 2 \alpha r_2^2 Y_0 (r_2 k_n) J_0 (r_2 k_n) k_n \\
- 2 r_2 \alpha J_0 (r_2 k_n) Y_1 (r_2 k_n) - \alpha^2 r_2^2 (Y_1 (r_2 k_n))^2 k_n \\
+ 2 r_2 \alpha^2 Y_0 (r_2 k_n) Y_1 (r_2 k_n) - \alpha^2 r_2^2 (Y_0 (r_2 k_n))^2 k_n \right] , \tag{A.8}$$

where,

$$C_1 = \frac{\Omega_1 r_1^2 - \Omega_2 r_2^2}{r_1^2 - r_2^2} , \tag{A.9}$$

$$C_2 = \frac{\Omega_1 - \Omega_2}{r_1^2 - r_2^2} , \tag{A.10}$$

$$\alpha = \frac{J_1 (k_n r_1)}{Y_1 (k_n r_1)} . \tag{A.11}$$

and the function $J_0$ is the zero order Bessel function of the first kind and the function $Y_0$ is the zero order Bessel function of the second kind.