Truly incompressible approach for computing incompressible flow in SPH and comparisons with the traditional weakly compressible approach

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Contents

List of Figures ................................................. 9
List of Tables .................................................. 12
Abstract .......................................................... 13
Declaration ......................................................... 15
Copyright .......................................................... 17
Acknowledgements .............................................. 19

1 Introduction ................................................... 21
   1.1 Smoothed Particle Hydrodynamics (SPH) ................. 21
      1.1.1 SPH in Astrophysics ................................. 22
      1.1.2 SPH in Solid mechanics ......................... 24
      1.1.3 SPH in Fluid mechanics ......................... 24

2 An Overview of SPH and Incompressible Methodologies .... 31
   2.1 Fundamentals .............................................. 32
      2.1.1 Definition of a particle in SPH ................... 32
      2.1.2 SPH formulations .................................... 32
      2.1.3 The kernel function ................................ 35
      2.1.4 The choice of smoothing length $h$ ............... 37
   2.2 Weakly compressible SPH (WCSPH) ....................... 38
## CONTENTS

2.2.1 Weakly compressible algorithm ........................................... 38
2.2.2 Continuity equation ......................................................... 40
2.2.3 Momentum equation ....................................................... 40
2.2.4 State equation ............................................................. 41

2.3 Truly incompressible SPH (ISPH) ........................................... 42
2.3.1 Truly incompressible algorithm ......................................... 42
2.3.2 Prediction step ............................................................. 43
2.3.3 Pressure Poisson equation ............................................... 44
2.3.4 Correction step ............................................................. 45

2.4 Time integration .............................................................. 46
2.4.1 Time step ................................................................. 46
2.4.2 Temporal integration ...................................................... 48

2.5 Wall modelling and Boundary conditions ................................. 49
2.5.1 Dummy particles .......................................................... 49
2.5.2 Mirror particles ........................................................... 51
2.5.3 Repulsive forces .......................................................... 53

2.6 Velocity-pressure coupling technique .................................... 54
2.6.1 Projection method ......................................................... 54

2.7 Solution of a linear equation system ...................................... 57
2.7.1 Direct methods ............................................................ 57
2.7.2 Iterative methods ........................................................ 59
2.7.3 Convergence criteria ..................................................... 63

3 The ISPH SPARTACUS-2D code .............................................. 65
3.1 The original SPARTACUS-2D code ......................................... 65
3.1.1 Fundamental equations .................................................. 65
3.1.2 Kernels ................................................................. 67
3.1.3 Time step and temporal integration ................................ 68
3.1.4 Optimisation and algorithm structure ......................... 68

3.2 The ISPH SPARTACUS-2D code ............................................ 71
CONTENTS

3.2.1 Fundamental equations ........................................... 71
3.2.2 Wall modelling and boundary conditions ......................... 73
3.2.3 Time step and temporal integration ............................... 74
3.2.4 Iterative methods linear solvers ................................ 74
3.2.5 Code structure ......................................................... 75
3.2.6 Test of the Laplacian operator ................................... 75

4 2-D SPH Benchmark Test Cases ........................................ 81
4.1 Lid-driven cavity flow ................................................. 81
  4.1.1 Geometry of the system ........................................ 81
  4.1.2 System modelling .................................................. 82
  4.1.3 Simulation results ................................................ 84
  4.1.4 Partial conclusions .............................................. 92
4.2 Incompressible flow around a moving square in a rectangular box 95
  4.2.1 Geometry of the system ........................................ 95
  4.2.2 System modelling .................................................. 95
  4.2.3 Simulation results ................................................ 96
  4.2.4 Partial conclusions .............................................. 102

5 2-D Laminar Flow past a Bluff Body in a Channel .................. 111
5.1 Theoretical investigation ............................................ 111
5.2 Geometry of the system ............................................. 112
5.3 System modelling ..................................................... 112
  5.3.1 Fluid discretisation and wall modelling ........................ 112
  5.3.2 Simulation conditions ......................................... 113
5.4 Simulation results .................................................... 114
  5.4.1 A laminar flow past a bluff body at $Re_{A} = 20$ ........... 114
  5.4.2 A laminar flow past a bluff body at $Re_{A} = 100$ .......... 117
5.5 Partial conclusions ................................................... 122
List of Figures

1.1 Examples of SPH applications in astrophysics ........................................... 23
1.2 The collision of two rubber rings using SPH without artificial stress .......... 25
1.3 The collision of two rubber rings using SPH with artificial stress ................. 26
1.4 Comparisons of experimental and numerical results ......................................... 27
1.5 Wave over-topping on coral reefs with SPARTACUS-2D code ....................... 28
1.6 Comparisons of dam break between SPH and experiment ............................. 30

2.1 Neighbours of particle \( a \) with a compact support kernel .......................... 35
2.2 Instability condition .................................................................................. 37
2.3 Comparisons of exact and approximate projection operator ......................... 45
2.4 Truncation of the kernel support at the wall ............................................... 49
2.5 Sketch of dummy particles around a wall corner and curved wall ............... 50
2.6 The influence of different mass of circular cylinder ..................................... 52
2.7 Sketch of mirror particles depending on the type of wall boundaries .......... 53
2.8 Construction of artificial velocity for boundary particles ............................ 53

3.1 Determination of the closest neighbours relative to particle \( a \) ....................... 69
3.2 Adjacent cells relative to a periodic flow with respect to \( x \)-direction ............. 70
3.3 Simplified algorithm of SPARTACUS with the WCSPH approach ............... 70
3.4 Simplified algorithm of SPARTACUS with the ISPH approach .................... 76
3.5 Convergence test of the exact and approximate Laplacian operator .......... 78
3.6 Examination of the approximate and exact Laplacian operators .................. 79

4.1 Configuration of the 2-D lid-driven cavity flow ............................................ 82
4.2 ISPH convergence test in time for $Re = 400$ ........................................ 85
4.3 Comparisons of horizontal velocity field at $Re = 400$ ................................. 86
4.4 Comparisons of pressure at $Re = 400$ ............................................................. 87
4.5 Spatial resolution influence at $Re = 400$ ......................................................... 88
4.6 ISPH convergence test in time for $Re = 1,000$ ................................................ 89
4.7 Spatial resolution influence at $Re = 1,000$ ....................................................... 90
4.8 2-D ISPH lid-driven cavity flow error estimation ............................................. 91
4.9 2-D SPH lid-driven cavity flow pressure profiles ............................................. 91
4.10 2-D lid-driven cavity flow for uniform velocity vectors at $Re = 1,000$ ............... 94
4.11 Geometry of a moving square inside a rectangular box ................................... 95
4.12 One example of crashed simulation at $Re = 50$ ............................................. 97
4.13 WCSPH velocity magnitude at $Re = 100$ ...................................................... 98
4.14 Velocity magnitude at the physical time $t/T = 5.0$ for $Re = 100$ .................... 100
4.15 Velocity magnitude at the physical time $t/T = 8.0$ for $Re = 100$ .................... 101
4.16 Pressure at the physical time $t/T = 5.0$ for $Re = 100$ .................................... 102
4.17 Pressure at the physical time $t/T = 8.0$ for $Re = 100$ .................................... 103
4.18 Velocity magnitude at the physical time $t/T = 5.0$ for $Re = 50$ ....................... 104
4.19 Velocity magnitude at the physical time $t/T = 8.0$ for $Re = 50$ ....................... 105
4.20 Pressure at the physical time $t/T = 5.0$ for $Re = 50$ ........................................ 105
4.21 Pressure at the physical time $t/T = 8.0$ for $Re = 50$ ........................................ 106
4.22 Velocity magnitude at the physical time $t/T = 5.0$ for $Re = 150$ ...................... 106
4.23 Velocity magnitude at the physical time $t/T = 8.0$ for $Re = 150$ ...................... 107
4.24 Pressure at the physical time $t/T = 5.0$ for $Re = 150$ ...................................... 107
4.25 Pressure at the physical time $t/T = 8.0$ for $Re = 150$ ...................................... 108
4.26 Time histories of pressure drag coefficients .................................................... 109
5.1 Geometry of the 2-D bluff body in the case of square cylinder ......................... 113
5.2 Comparisons of horizontal velocity magnitude contours for $Re_d = 20$ ............. 115
5.3 Comparisons of horizontal velocity magnitude contours at $Re_d = 20$ ............... 116
5.4 ISPH horizontal velocity at the downstream of the channel at $Re_d = 20$ ........... 117
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.5</td>
<td>Comparisons of time-averaged $C_p$ for $Re_d = 20$</td>
<td>118</td>
</tr>
<tr>
<td>5.6</td>
<td>An example of time-averaged centreline $C_p$ from ISPH for $Re_d = 20$</td>
<td>119</td>
</tr>
<tr>
<td>5.7</td>
<td>Comparisons of time-averaged corrected centreline $C_p$ distributions</td>
<td>119</td>
</tr>
<tr>
<td>5.8</td>
<td>Comparisons of time-averaged $C_p$ on the square cylinder at $Re_d = 20$</td>
<td>119</td>
</tr>
<tr>
<td>5.9</td>
<td>Time-averaged velocity vectors behind of the square cylinder</td>
<td>120</td>
</tr>
<tr>
<td>5.10</td>
<td>Comparisons of horizontal velocity contours for $Re_d = 100$</td>
<td>122</td>
</tr>
<tr>
<td>5.11</td>
<td>ISPH horizontal velocity at the downstream of the channel at $Re_d = 100$</td>
<td>123</td>
</tr>
<tr>
<td>5.12</td>
<td>Comparisons of instantaneous pressure contours for $Re_d = 100$</td>
<td>123</td>
</tr>
<tr>
<td>6.1</td>
<td>Zoom of a free surface</td>
<td>129</td>
</tr>
<tr>
<td>6.2</td>
<td>Examples of surface particle tracking defect</td>
<td>130</td>
</tr>
<tr>
<td>6.3</td>
<td>Configuration of a dam breaking on dry bed</td>
<td>131</td>
</tr>
<tr>
<td>6.4</td>
<td>Pressure of dam breaking case for dry bed at $t = 0.186 \text{s}$</td>
<td>134</td>
</tr>
<tr>
<td>6.5</td>
<td>Pressure of dam breaking case for dry bed at $t = 0.278 \text{s}$</td>
<td>135</td>
</tr>
<tr>
<td>6.6</td>
<td>Pressure of dam breaking case for dry bed at $t = 0.650 \text{s}$</td>
<td>136</td>
</tr>
<tr>
<td>6.7</td>
<td>Pressure of dam breaking case for dry bed at $t = 1.860 \text{s}$</td>
<td>137</td>
</tr>
<tr>
<td>6.8</td>
<td>Pressure of ISPH dam breaking case with $k - L_m$ turbulence model</td>
<td>138</td>
</tr>
<tr>
<td>6.9</td>
<td>Configuration of a dam breaking on wet bed</td>
<td>139</td>
</tr>
<tr>
<td>6.10</td>
<td>Free surface evolution with the $L_m$ turbulence model</td>
<td>142</td>
</tr>
<tr>
<td>6.11</td>
<td>Free surface evolution with the $k - L_m$ turbulence model</td>
<td>143</td>
</tr>
<tr>
<td>6.12</td>
<td>Free surface evolution with the $k - \epsilon$ turbulence model</td>
<td>144</td>
</tr>
<tr>
<td>6.13</td>
<td>Measurement positions for 3-D dam-break experiment</td>
<td>146</td>
</tr>
<tr>
<td>6.14</td>
<td>General description of the system</td>
<td>147</td>
</tr>
<tr>
<td>6.15</td>
<td>General description of the system (box)</td>
<td>147</td>
</tr>
<tr>
<td>6.16</td>
<td>Snapshot of a 3-D dam-break at $t = 0.40 \text{s}$</td>
<td>150</td>
</tr>
<tr>
<td>6.17</td>
<td>Snapshot of a 3-D dam-break simulation at $t = 0.56 \text{s}$</td>
<td>151</td>
</tr>
<tr>
<td>6.18</td>
<td>Vertical water heights in the reservoir H4 and the tank H2</td>
<td>152</td>
</tr>
<tr>
<td>6.19</td>
<td>Pressure time histories at P1 and P3</td>
<td>153</td>
</tr>
<tr>
<td>6.20</td>
<td>Pressure time histories at P5 and P7</td>
<td>154</td>
</tr>
</tbody>
</table>
# List of Tables

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Minimum Residual (MR) algorithm</td>
<td>61</td>
</tr>
<tr>
<td>2.2</td>
<td>Unpreconditioned Bi-CGSTAB algorithm</td>
<td>62</td>
</tr>
<tr>
<td>3.1</td>
<td>Unpreconditioned Minimum Residual algorithm in the code</td>
<td>75</td>
</tr>
<tr>
<td>3.2</td>
<td>Unpreconditioned Bi-CGSTAB algorithm in the code</td>
<td>77</td>
</tr>
<tr>
<td>4.1</td>
<td>Fluid particle discretisation for the lid-driven cavity flow at $Re = 400$</td>
<td>82</td>
</tr>
<tr>
<td>4.2</td>
<td>Fluid particle discretisation for the lid-driven cavity flow at $Re = 1000$</td>
<td>83</td>
</tr>
<tr>
<td>4.3</td>
<td>Physical characteristics of the 2-D lid-driven cavity flow</td>
<td>83</td>
</tr>
<tr>
<td>4.4</td>
<td>The comparisons of the lid-driven cavity flow CPU time for $Re = 1000$</td>
<td>92</td>
</tr>
<tr>
<td>4.5</td>
<td>Fluid particle discretisation for a moving square inside a rectangular box</td>
<td>96</td>
</tr>
<tr>
<td>4.6</td>
<td>Effect of resolution vs $Re$</td>
<td>97</td>
</tr>
<tr>
<td>4.7</td>
<td>CPU time for WCSPH and ISPH with the resolution of $\delta r/L = 1/60$</td>
<td>108</td>
</tr>
<tr>
<td>5.1</td>
<td>Fluid, edge and dummy particle discretisation for the 2-D bluff body</td>
<td>113</td>
</tr>
<tr>
<td>5.2</td>
<td>Comparisons of the time-averaged drag and lift coefficients at $Re_d = 20$</td>
<td>117</td>
</tr>
<tr>
<td>5.3</td>
<td>Comparisons of the time-averaged drag and lift coefficients at $Re_d = 100$</td>
<td>121</td>
</tr>
<tr>
<td>5.4</td>
<td>CPU time for the bluff body flow at $Re_d = 100$</td>
<td>124</td>
</tr>
<tr>
<td>6.1</td>
<td>Set of coefficients for $k - L_m$ and $k - \epsilon$ model</td>
<td>128</td>
</tr>
<tr>
<td>6.2</td>
<td>Fluid particle discretisation of the dam break for dry bed</td>
<td>132</td>
</tr>
<tr>
<td>6.3</td>
<td>2-D dry-bed dam-break flow CPU time for WCSPH and ISPH</td>
<td>133</td>
</tr>
<tr>
<td>6.4</td>
<td>Fluid particle discretisation of the dam-break flow for wet bed</td>
<td>140</td>
</tr>
<tr>
<td>6.5</td>
<td>2-D wet-bed dam-break flow CPU time for WCSPH and ISPH</td>
<td>141</td>
</tr>
</tbody>
</table>
6.6 Fluid particle discretisation for the 3-D dam-break flow .................................... 148
6.7 3-D dam-break flow CPU time ................................................................................ 154
Abstract

In the Smoothed Particle Hydrodynamics (SPH) method for solving the Navier-Stokes equations the most widespread method to solve for pressure and mass conservation is the weakly compressible assumption (WCSPH). This includes hydraulics applications and leads to some drawbacks such as severe artificial pressure fluctuations and a limitation to very small time steps related to the WCSPH Mach number and explicit method.

The main goal of the PhD thesis is to develop an semi-implicit and truly Incompressible SPH (ISPH) algorithm in 2-D and 3-D and to compare this approach to the classical WCSPH method, showing how some of the problems encountered in WCSPH have been resolved by using ISPH to simulate hydraulic flows.

Mathematical models for each method are presented within the SPH formalism. Several standard boundary conditions with wall modellings are introduced. The true incompressibility is achieved by means of a velocity-pressure coupling technique: a projection method which is presented within an SPH formulation. Since the pressure is obtained by a linear solver, several linear solvers are also introduced.

The new algorithm with ISPH is examined through several applications and compared with WCSPH and also other numerical methods and/or experimental data. For 2-D laminar flow simulations, a lid-driven cavity flow and an incompressible flow around a moving square placed in a rectangular box are performed as a benchmarking test. A flow around a stationary bluff body is also studied. The results show that pressure fields extracted from WCSPH are very unreliable for all cases whereas ISPH predict pressures and forces in closer agreement with classical Finite Volume or Finite Difference CFD methods.

To demonstrate a free-surface flow case, 2-D and 3-D dam break cases are simulated. 2-D dam break cases, with dry or wet beds downstream, which demonstrate the ability of
ISPH to model highly nonlinear flows involving splash-up and impact effects. Turbulence models, mixing length $L_m$, $k - L_m$ and $k - \epsilon$, are also examined for the dam break problem and special attention is given to tracking the surface particles. A 3-D dam break with a box placed in the flow is also simulated without any turbulence modelling as a validation of the 3-D ISPH method. Both WCSPH and ISPH results are compared with Volume-Of-Fluid (VOF) and experimental data. The agreement is good although there are small discrepancies in the moving front speed due to not enough number of particles.

The WCSPH and ISPH results are verified with reference data from experiment and/or another numerical method. All the comparisons show superior results from ISPH than WCSPH and good agreement in general.
Declaration

No portion of the work referred to in the thesis has been submitted in support of an application for another degree or qualification of this or any other university or other institution of learning.
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Chapter 1

Introduction

The numerical study of fluid flows offers two distinctive approaches; one is Eulerian and the other is Lagrangian. The Eulerian approach examines the flow at a fixed spatial point as a function of time, whereas, the Lagrangian one follows the history of an individual fluid particle through space and time. Since the Eulerian technique has been studied for more than 50 years, most of commercial codes in Computational Fluid Dynamics (CFD) are based on this approach. For example, Fluent, Star-CD, CFX, Comet and Saturne are based on a finite volume method. Pronto and Telemac are based on a finite element method.

However, the Eulerian approach has difficulties to solve applications that involve large deformations and complex free-surface flows. For this, the Lagrangian approach (also sometimes referred to as a ‘particle method’) has been developed. In the Lagrangian approach, there are two ways to describe spatial fields depending on the existence of a mesh. For instance, ‘Marker-And-Cell’ (e.g. [24]), ‘Particle-In-Cell’ (e.g. [22] [23]) and ‘Lattice-Boltzmann’ (e.g. [60]) methods are mesh based. On the other hand, Vortex methods (e.g. [2]) and Smoothed Particle Hydrodynamics (SPH) do not need a grid and called are meshless technique. Numerical developments of the meshless Smoothed Particle Hydrodynamics are presented in detail in this work.

1.1 Smoothed Particle Hydrodynamics (SPH)

The fully Lagrangian Smoothed Particle Hydrodynamics (SPH) method was originally invented to deal with non axisymmetric problems in astrophysics (Lucy 1977 [40], Gingold &
Since then the use of SPH has expanded in many areas of solid and fluid dynamics (involving large deformations, impacts, free-surface and multiphase flows). For example, collision of rubber cylinders (Swegle et al., 1995 [58]) in solid mechanics, dam breaking and free-surface waves (Monaghan, 1994 [43]) and two-phase flows such as Rayleigh-Benard instability (Violeau, 1999 [65]) in fluid mechanics.

A major advantage of SPH over Eulerian methods is that the method does not need a grid to calculate spatial derivatives. Instead, they are found by summation of analytical differentiated interpolation formulae (Monaghan, 1992 [42]). The momentum and energy equations become sets of ordinary differential equations which are easy to understand in mechanical and thermodynamical terms. For example, the pressure gradient becomes a force between pairs of particles.

While Eulerian methods have difficulties to construct a mesh for the simulation domain when it has very complex interfaces, SPH is able to do it without any special front tracking treatment. Moreover, the convection term of Navier-Stokes equations can cause many problems in the Eulerian framework, which are only partially circumvented by introducing numerical diffusion when it is discretised. However, in SPH this term is implicitly considered. Some examples of SPH applications classified as astrophysics, solid and fluid mechanics are followed.

1.1.1 SPH in Astrophysics

SPH has been successfully applied in astrophysics such as stellar collisions (e.g. [1]), disks and rings (e.g. [25]), and formation of the moon and impact problems (e.g. [4] [6]), these applications using SPH are shown in Fig. 1.1. For instance, since the impact of a planet Mars-sized body with Earth cannot be reproduced experimentally, numerical simulations are indispensable. The simulation results are compared with small scale experimental data and then extrapolated to the larger scales. For example, the power of SPH has allowed Benz et al. [4] have studied the collision theory of the origin of the Moon.
1.1. Smoothed Particle Hydrodynamics (SPH) 23

(a) A deep collision between two equal-mass stars [1].

(b) A time sequence of moon-forming impact (beginning top left) [6].

(c) The gas disk in the axisymmetric collision at various times [32].

Figure 1.1: Examples of SPH applications in astrophysics.
1.1.2 SPH in Solid mechanics

When SPH is applied to solids the SPH particles mimic the behaviour of the atoms; if the solid is compressed, the atoms repel each other and if it is stretched, the atoms attract each other and oppose the stretch. However, when the material is stretched, the attraction cause the SPH particles to form clumps, which is commonly called the tensile instability. This instability in SPH is also known to occur in gas dynamics where the pressure is positive [52]. There have been number of attempts to remove this instability by dealing with the interpolation of kernels [52] or dissipative terms [50] or artificial stress [45] or combining normalised kernels (to reduce boundary errors) [29]. Gray et al. [18] added artificial stress to remove the tensile instability and presented in Figs. 1.2 and 1.3.

1.1.3 SPH in Fluid mechanics

As an illustration of industrial application, Ha and Cleary [21] carried out one of SPH validation tests on Gravity Die Casting (GDC) processes, which are capable of making complicated high integrity components, such as wheels, cylinder heads, engine blocks and brake callipers, at lower cost than most other casting methods. Figure 1.4 shows the SPH simulation result compared with experiment and another numerical tool, MAGMAsoft, which is a 3-D solidification and fluid flow package used in the die casting industry to model the molten metal flow and solidification in dies. MAGMAsoft employs the finite difference method to solve the heat and mass transfer on a rectangular grid [21]. The comparisons shows a good agreement among them and even better in SPH demonstrating the detailed features of the free surface shapes.

SPH is also known to be a good numerical method to simulate environmental flow, some examples of environmental flows applications by using SPH are demonstrated. Lee et al. [38] simulated 2-D wave over-topping on coral reefs with SPH based on 2-D experiments by Gourlay [17] and the results are presented in Fig. 1.5. Without any further treatment for the surface particles, the breaking events are well captured (Fig. 1.5 (a)). The main purpose of the experiment was to measure maximum wave set-up. SPH results are compared with the experimental result and another numerical method which is Boussinesq model, named...
Figure 1.2: The collision of two rubber rings using SPH without artificial stress [18].
Figure 1.3: The collision of two rubber rings using SPH with artificial stress \cite{18}.
1.1. Smoothed Particle Hydrodynamics (SPH)

MAGMAssoft experiment SPH

Figure 1.4: Comparisons of experimental and numerical results at selected times $t = 1.6s$, $2.0s$ and $3.4s$ during the die filling in gravity die casting [21].

BSQ in Fig. 1.5(b). Both numerical methods provide similar results to the experiment. The other example is 3-D SPH dam-break case, performed by Issa [26]. The results are compared with experimental results at the physical time indicated in Fig. 1.6 The agreements between numerical and experimental results are good.

Nevertheless, despite good agreements in general, some limitations are found in the SPH method such as very small time step, which lead to very expensive CPU cost, and pressure fluctuation. As explained later in this thesis, one of the most crucial problems of conventional SPH is the use of a weakly compressible formulation which leads to unphysical pressure
Chapter 1. Introduction

(a) Wave over-topping on coral reefs for wave period of $T = 1.48 \text{ s}$.

(b) Maximum wave set-up for various flow conditions.

Figure 1.5: Wave over-topping on coral reefs with SPARTACUS-2D code [38].
fields. To circumvent these problems, a different numerical scheme incorporating an incompressible solver has been adapted to the traditional SPH. The methodology of SPH with these two different numerical schemes are addressed in the following chapter.
Figure 1.6: Comparisons of dam break with SPARTACUS-3D code and experimental results at the indicated time [26].
Chapter 2

An Overview of SPH and Incompressible Methodologies

When modelling incompressible flows, traditional SPH solvers resort to a weakly compressible approach (hereafter referred to as WCSPH). The advantage is that it is easy to programme because the pressure is obtained from an algebraic explicit thermodynamic equation and diffusion terms are treated as explicit. However, some drawbacks appear. Firstly, WCSPH requires a very small time step associated with a numerical speed of sound. Secondly, small density errors always remain causing significant non-physical pressure fluctuations which can yield numerical instability. In a worst case scenario, it can lead to particle clumping (Issa, 2005).

Circumventing those problems can be achieved by solving truly incompressible SPH (hereafter referred to as ISPH). Pressure and viscous forces are treated separately, the pressure being calculated by enforcing a divergence-free velocity field. The pressure is thus no longer a dependent variable but is computed from a pressure Poisson equation. The Courant condition is based on fluid velocities instead of the numerical speed of sound. Although larger time-steps can be used, the solution of the resulting elliptic pressure Poisson equation increases the total work per time-step (Cummins and Rudman). Hence, the CPU time for both WCSPH and ISPH method is compared in the present work to measure which method is less time consuming and how much benefit of it.

The main purpose of the PhD work here is to develop the incompressible algorithm in
an SPH code. Since incompressibility is a very generic but also difficult topic in CFD in general, not only SPH methods but also the other numerical tools for incompressible flows are discussed including, velocity-pressure coupling techniques and linear solvers.

2.1 Fundamentals

2.1.1 Definition of a particle in SPH

In physical space, fluid can be discretised by a finite number of macroscopic volumes of fluid. Each of these volumes $V$ is composed of several mesoscopic fluid elements. The mesoscopic elements are the particles defined in continuum mechanics formalism. In SPH, a particle $a$ represents a macroscopic volume of fluid. Each fluid particle, for example particle $a$, carries information of a mass $m_a$, a density $\rho_a$, a pressure $p_a$, a velocity $u_a$, position $r_a$ and other quantities depending on the nature of the flow and of the fluid. The mass is constant through the simulations, but, pressure, velocity, position and other physical quantities are updated every time step. Density is also updated every time step in weakly compressible approach (WCSPH) whereas constant density is set in truly incompressible approach (ISPH). Henceforth, the bold characters present vectors or tensors and plain ones are for scalar quantities.

2.1.2 SPH formulations

\`$\nabla$' and \`$\nabla'$ are respectively gradient and divergence operators. The overstrike bar indicates Reynolds averaging.

A basic principle in SPH is that a quantity $\alpha$ can be expressed in terms of a convolution product of $\alpha$ and the Dirac distribution $\delta$ over the whole domain, as:

$$\alpha(r) = \int_\Omega \alpha(r')\delta(r - r') \, dr'$$

(2.1)

where $\Omega$ is the volume of the fluid domain, and $dr'$ an elementary volume. The Dirac distribution can be approximated in discrete sense by a kernel function $w_h$ with smoothing length $h$, which allows any quantity to be expressed in terms of its values known at different particle locations (Lucy 1977 [40], Gingold and Monaghan 1977 [15], and Monaghan 1985 [41]).
2.1. Fundamentals

More precisely, any quantity $\alpha$ attached to a particle ‘$a$’ at a position $r_a$ is written as:

$$\alpha(r_a) \approx \sum_b \frac{m_b}{\rho_b} \alpha_b w_h(r_{ab})$$

(2.2)

where the subscript ‘$b$’ is used to describe any particle in the neighbourhood of particle ‘$a$’. The distance from ‘$a$’ to ‘$b$’ is $r_{ab} (= |r_{ab}|)$, $\alpha_b$ denotes the value of any quantity $\alpha$ at $r_b$ and the summation applies to all the particles including any particles denoted as boundary particles, with the volume $dr'$ in Eq. (2.1) replaced by the particle volume $\frac{m_b}{\rho_b}$ in Eq. (2.2).

According to Morris et al. (1997, [46]), a kernel function $w_h$ can be written in a general manner as:

$$w_h(r_{ab}) = \frac{1}{h^\sigma} f \left( \frac{r_{ab}}{h} \right)$$

(2.3)

where $\sigma$ is the dimension of the system and the smoothing length $h$ is proportional to the particle distance, which plays a role similar to the mesh size in Eulerian codes. The function $f \left( \frac{r_{ab}}{h} \right)$ is described in Section 2.1.3. As shown in Eq. (2.3), the kernel only varies with the distance $r_{ab}$ between particles, which ensures both linear and angular momenta conservation (Monaghan 1992 [42]). The kernel has to be at least $C^1$ for numerical consistency (Monaghan 1992 [42]).

The gradient of $\alpha$ is then expressed as a function of $\alpha$ and the kernel derivatives as:

$$\nabla \alpha(r_a) \approx \int_\Omega \nabla \alpha(r_a) w_h(r - r') dr' = \sum_b \frac{m_b}{\rho_b} \alpha_b \nabla_a w_h(r_{ab})$$

(2.4)

where the quantity $\nabla_a w_h(r_{ab})$ denotes the gradient of the kernel, which is taken as centred on the position of particle $a$.

Note that various ways exist to express gradients in continuous form, i.e.:

$$\nabla \alpha = \frac{1}{\rho} (\nabla (\rho \alpha) - \alpha \nabla \rho)$$

(2.5)

or

$$\nabla \alpha = \rho \left( \nabla \left( \frac{\alpha}{\rho} \right) + \frac{\alpha}{\rho^2} \nabla \rho \right)$$

(2.6)

which lead to different discrete SPH forms. For instance, combining Eqs. (2.4) and (2.5) gives the following SPH form:

$$\nabla \alpha(r_a) \approx \frac{1}{\rho_a} \sum_b m_b (\alpha_b - \alpha_a) \nabla_a w_h(r_{ab})$$

(2.7)
and with Eqs. (2.4) and (2.6):

$$\nabla \alpha(\mathbf{r}_a) \approx \rho_a \sum_b m_b \left( \frac{\alpha_a}{\rho_a^2} + \frac{\alpha_b}{\rho_b^2} \right) \nabla_a w_h(r_{ab})$$

(2.8)

Here, Eq. (2.7) is symmetric and (2.8) is antisymmetric when \(a\) and \(b\) are swapped. The second form ensures linear momentum conservation (Monaghan 1992 [42]) and is generally used for pressure gradient. Bonet [5] also suggested the following form:

$$\nabla \alpha(\mathbf{r}_a) \approx \sum_b \frac{m_b}{\rho_b} (\alpha_a + \alpha_b) \nabla_a w_h(r_{ab})$$

(2.9)

However, since \(\rho\) is constant for each particle \((\rho_a = \rho_b)\) for truly incompressible flow, Eqs. (2.7), (2.8) and (2.9) are identical to Eq. (2.4). As a proof, since \(\rho_a = \rho_b = \rho_0\), the right hand side of Eq. (2.8) can be split in two parts:

$$\rho_0 \sum_b m_b \frac{\alpha_a}{\rho_b^2} \nabla_a w_h(r_{ab}) + \rho_0 \sum_b m_b \frac{\alpha_b}{\rho_b^2} \nabla_a w_h(r_{ab})$$

(2.10)

Then it reduces to:

$$\alpha_a \sum_b \frac{m_b}{\rho_b} \nabla_a w_h(r_{ab}) + \sum_b \frac{m_b}{\rho_b} \alpha_b \nabla_a w_h(r_{ab})$$

(2.11)

If the kernel is built in such a way that for a constant field \(\alpha\), \(\nabla \alpha = 0\) holds, then one has:

$$\sum_b \frac{m_b}{\rho_b} \nabla_a w_h(r_{ab}) = 0$$

(2.12)

The first term of Eq. (2.11) then vanishes, which leads to the SPH formalism of Eq. (2.4). However, in the following, the kernel used here does not satisfy exactly the condition given by Eq. (2.12), thus Eq. (2.7), (2.8) or (2.9) is kept to estimate gradients. The conditions that hold for the gradient also holds for the divergence. Two examples of the divergence of a vector quantity \(\mathbf{V}\) can be written as:

$$\nabla \cdot \mathbf{V}_a \approx \frac{1}{\rho_a} \sum_b m_b (\mathbf{V}_b - \mathbf{V}_a) \cdot \nabla_a w_h(r_{ab})$$

(2.13)

$$\nabla \cdot \mathbf{V}_a \approx \rho_a \sum_b m_b \left( \frac{\mathbf{V}_a}{\rho_a^2} + \frac{\mathbf{V}_b}{\rho_b^2} \right) \cdot \nabla_a w_h(r_{ab})$$

(2.14)

As the gradient operator, the divergence can be written in a symmetric (Eq. (2.13)) and an antisymmetric (Eq. (2.14)) form. Note that other forms of gradient or divergence exist. Some of them are presented in Monaghan [42] also indicating their advantages and drawbacks.
2.1.3 The kernel function

By considering a domain of interest $\Omega$, the kernel function $w_h$ must satisfy the three following properties:

- The kernel summation over the whole domain $\Omega$ must be equal to unity:

$$\int_{\Omega} w_h(r - r')dr' = 1$$  \hspace{1cm} (2.15)

- When the smoothing length $h$ tends to zero, the kernel function must tend to Dirac distribution:

$$\lim_{h \to 0} w_h(r - r') = \delta(r - r')$$  \hspace{1cm} (2.16)

- The kernel must be at least once differentiable and its derivative must be continuous in order to avoid large fluctuations which would affect the solution [16].

![Figure 2.1: Neighbours of particle a with a compact support kernel.](image)

The kernel $w_h$ is, then, characterised by a compact support in order to spare computation time, that is $w_h(r_{ab})$ is zero if the distance $r_{ab}$ between two particles exceeds a limit value, which is the kernel support size $h_t$. Hence, the particles $b$ in the summation of equations above will be restricted to nearest neighbours of a particle $a$ (see Fig. 2.1). The support size $h_t$ is directly proportional to the smoothing length $h$:

$$h_t = \alpha h$$  \hspace{1cm} (2.17)
\( \alpha \) is a coefficient which depends on the order of kernel. The examples of 3\textsuperscript{rd}, 4\textsuperscript{th} and 5\textsuperscript{th} order of spline kernels for 2-D are as follows:

\[
f(q) = \frac{10}{7\pi} \begin{cases} 
1 - \frac{3}{2}q^2 + \frac{3}{4}q^3 & \text{if } 0 \leq q \leq 1 \\
\frac{1}{4} (2 - q)^3 & \text{if } 1 \leq q \leq 2 \\
0 & \text{if } q \geq 2 
\end{cases}
\]  
(2.18)

where \( q = r_{ab}/h \) and the kernel support size \( h_t \) for this case is equal to \( 2h \).

\[
f(q) = \frac{96}{1199\pi} \begin{cases} 
(\frac{3}{2} - q)^4 - 5 (\frac{3}{2} - q)^4 + 10 (\frac{1}{2} - q)^4 & \text{if } 0 \leq q \leq 0.5 \\
(\frac{3}{2} - q)^4 - 5 (\frac{3}{2} - q)^4 & \text{if } 0.5 \leq q \leq 1.5 \\
(\frac{3}{2} - q)^4 & \text{if } 1.5 \leq q \leq 2.5 \\
0 & \text{if } q \geq 2.5 
\end{cases}
\]  
(2.19)

where \( h_t = 2.5h \).

\[
f(q) = \frac{7}{478\pi} \begin{cases} 
(3 - q)^5 - 6 (2 - q)^5 + 15 (1 - q)^5 & \text{if } 0 \leq q \leq 1 \\
(3 - q)^5 - 6 (2 - q)^5 & \text{if } 1 \leq q \leq 2 \\
(3 - q)^5 & \text{if } 2 \leq q \leq 3 \\
0 & \text{if } q \geq 3 
\end{cases}
\]  
(2.20)

where \( h_t = 3h \). For 3-D case, the coefficient of the 3\textsuperscript{rd} order kernel is changed to \( \frac{1}{\pi} \).

Morris [46] mentioned that the 5\textsuperscript{th}-order of the kernel remained stable for simulations of very low Reynolds number, while the 3\textsuperscript{rd}-order one produced significant noise in pressure and velocity. The reason of this poor performance is that the stability properties of SPH equations are strongly depending on the 2\textsuperscript{nd} derivative of the kernel, which links to the tensile instability as mentioned in Section 1.1.2. Swegle et al. performed the SPH stability analysis [58] and mentioned that the system is conditionally stable if:

\[
w''T < 0
\]  
(2.21)

where \( w'' \) is the 2\textsuperscript{nd} derivative of the kernel and \( T \) the particle stress, where \( T < 0 \) corresponds to a compression state and \( T > 0 \) a tensile state. The stability of this system is achieved by limiting the time step. Figure 2.2 shows the stability regimes.
2.1. Fundamentals

Figure 2.2: Instability condition \( w': 1^{st} \) derivative of the kernel, \( w''': 2^{nd} \) derivative of the kernel, \( T: \) the particle stress, \( u: \) the initial inter-particle distance, \( h: \) the smoothing length) [58].

**Kernel correction**

As indicated in Section 2.1.2, the condition of Eq. (2.12) is not satisfied. This will be achieved by normalising the kernel. Several techniques to correct the kernels [5] [7] [20] are suggested and one simpler example taken from [5] is:

\[
\alpha(r_{ab}) \approx \frac{\sum_{b=1}^{N} \frac{m_b}{\rho_b} \alpha_b w(r_{ab})}{\sum_{b=1}^{N} \frac{m_b}{\rho_b} w(r_{ab})}
\]

(2.22)

According to Bonet [5], it provides a much improved interpolation, especially near the domain boundaries, even though it fails to satisfy a rotational invariance condition.

2.1.4 The choice of smoothing length \( h \)

The smoothing length \( h \) in SPH analogous to a cell size in an Eulerian code. As shown in Eq. 2.17 this parameter is directly linked to the kernel support and strongly influences the accuracy of results. Gingold and Monaghan [16] showed the existence of an optimal \( h \) depending on particle number. Higher number of particles and lower smoothing length \( h \) gives smaller error. This is consistent with what Speith [56] mentioned in his paper. He
proved that the accuracy of SPH results depends on the number of neighbours $N_i$:

$$N_i \propto \left( \frac{h}{\delta r} \right)^d N$$

(2.23)

where $N$ corresponds to the total number of particles and $d$ is the dimension of the problem and $\delta r$ the initial particle spacing. From this equation, a higher value of $h$ increases the number of particle neighbours by keeping $N$ as a constant. However, he concluded that the smoothing length $h$ determines the spatial resolution of the simulations, whereas the global accuracy depends on the mean interaction number $N_i$ [49]. The higher $N_i$ and the lower $h$ the better are the simulation results. Since this conclusion is self-contradictory, the compromise between $N_i$ and $h$ can be found by choosing the total particle number $N$.

### 2.2 Weakly compressible SPH (WCSPH)

By allowing 1% of density fluctuation, SPH has been applied to incompressible flow such as separated flows [27], free-surface flows [43] and low Reynolds number incompressible flows [46]. The advantages of using WCSPH are the following: it is robust and easy to program since it is a fully explicit method. The pressure is a thermodynamic variable obtained from an artificial state equation. However, one of the drawbacks of this method is the use of much smaller time steps compared to other numerical methods due to the numerical speed of sound. The application of this method is thus limited because of the expensive computation time. The following subsections are describing the fluid mechanics equations in SPH form briefly based on WCSPH approach.

#### 2.2.1 Weakly compressible algorithm

A classical method which solves weakly compressible equations in primitive variables (density $\rho$, velocity $\mathbf{u}$) is presented. The Lagrangian Reynolds-Averaged Navier-Stokes equations read:

$$\frac{1}{\rho} \frac{d\rho}{dt} + \nabla \cdot \mathbf{u} = 0$$

(2.24)

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\rho} \nabla p + \nabla \cdot (\nu_E \nabla \mathbf{u}) + \mathbf{F}^e$$

(2.25)
where \( \rho \) is the density, \( \overline{u} \) is the Reynolds averaged velocity vector, \( t \) the time, \( \overline{p} \) the Reynolds-averaged pressure, \( \nu_E = \nu + \nu_T \) the effective viscosity, \( \nu \) being the kinematic viscosity and \( \nu_T \) the turbulent viscosity, and \( F^e \) an external body force such as gravity. For turbulent flows, the turbulent viscosity \( \nu_{T,a} \) is estimated through turbulence closures such as mixing length \( (L_m) \), one equation \( (k-L_m) \) or two equations \( (k-\varepsilon) \) models. The detail of these turbulence closures as implemented in the SPARTACUS-2D code are presented in [62] and briefly introduced in Chapter 6.

The system composed of Eq. (2.24) and (2.25) is closed by a relation between \( \rho \) and \( \overline{p} \) taking the form of an appropriate equation of state for water:

\[
\overline{p} = \frac{\rho_0 c_0^2}{\gamma} \left( \left( \frac{\rho}{\rho_0} \right)^\gamma - 1 \right)
\]  

(2.26)

where \( \gamma = 7 \) is often chosen, \( \rho_0 \) is a reference density and \( c_0 \) is a numerical speed of sound which is normally taken ten times higher than the maximum fluid velocity in order to reduce the density fluctuation down to \( 1\% \) [43]. Due to the polytropic index \( \gamma \), small density fluctuations lead to large pressure fluctuations but the noise induced in the pressure field does not generally contaminate the flow evolution. This approach tends to keep the particle distances roughly constant by imposing a repelling force to a pair of particles when they come too close to each other.

The scheme is first order and fully explicit in time. The following equations give the sequence of the WCSPH algorithm. The velocity is calculated as:

\[
\overline{u}^{n+1} = \overline{u}^n + \left( -\frac{1}{\rho} \nabla \overline{p}^n + \nabla \cdot (\nu_E \nabla \overline{u}^n) + F^e \right) \Delta t
\]  

(2.27)

where superscripts \( n \) and \( n+1 \) indicate respectively previous and present time steps and \( \Delta t \) is the numerical time step.

Position and density are updated at the next time step by:

\[
r^{n+1} = r^n + \overline{u}^{n+1} \Delta t , \quad \rho^{n+1} = \rho^n - \rho^n \left( \nabla \cdot \overline{u}^{n+1} \right) \Delta t
\]  

(2.28)

Finally, the pressure at \( n+1 \) is obtained from Eq. (2.26) with the updated density.
2.2.2 Continuity equation

Density can be calculated directly from the SPH interpolation formulation Eq. (2.2):

$$\rho_a \approx \sum_b m_b w_h(r_{ab})$$  \hspace{1cm} (2.29)

or by solving the continuity equation Eq. (2.24) with one of the SPH divergence forms Eq. (2.13):

$$\frac{d\rho_a}{dt} \approx \sum_b m_b \overline{u}_{ab} \cdot \nabla w_h(r_{ab})$$  \hspace{1cm} (2.30)

where $\overline{u}_{ab} = \overline{u}_a - \overline{u}_b$. According to Monaghan [42] Eq. (2.30) has advantages over Eq. (2.29). Density with Eq. (2.29) drops significantly near the edge of the fluid, which is unphysical. However, density obtained from Eq. (2.30) will vary only when particles move relative to each other. There is also a computational advantage in using Eq. (2.30) since the rates of change of all physical variables can be computed in one subroutine.

2.2.3 Momentum equation

The pressure gradient term in Eq. (2.25) can be estimated with the SPH formulation of Eq. (2.8) or Eq. (2.9) as:

$$\frac{1}{\rho_a} \nabla \overline{p}_a \approx \sum_b m_b \left( \frac{\overline{p}_b}{\rho_b^2} + \frac{\overline{p}_a}{\rho_a^2} \right) \nabla w_h(r_{ab})$$  \hspace{1cm} (2.31)

or

$$\frac{1}{\rho_a} \nabla \overline{p}_a \approx \sum_b m_b \frac{\overline{p}_b + \overline{p}_a}{\rho_a \rho_b} \nabla w_h(r_{ab})$$  \hspace{1cm} (2.32)

The viscous term is not directly built as divergence of gradient, but as a combination of the finite difference approach and SPH formalism. According to Cleary and Monaghan [9], when this term was directly built, the result was too sensitive to particle disorder to be of practical use. A better approach was to explore integral approximation and the following form was suggested:

$$\nabla \cdot \left( \nu_E \nabla \overline{u}_a \right) \approx \sum_b m_b \frac{\nu_{E,a} + \nu_{E,b}}{\rho_a + \rho_b} \frac{\overline{u}_{ab} \cdot \overline{f}_{ab}}{r_{ab}^2 + \eta^2} \nabla w_h(r_{ab})$$  \hspace{1cm} (2.33)
Morris [46] also proposed a similar form as:

$$\nabla \cdot (\nu_E \nabla \underline{u})_a \approx \sum_b m_b \frac{\rho_a \nu_{E,a} + \rho_b \nu_{E,b}}{\rho_a \rho_b} \frac{\mathbf{r}_{ab} \cdot \nabla w_h(r_{ab})}{r_{ab}^2 + \eta^2} \underline{u}_{ab}$$

(2.34)

where \(\nu_{E,a} = \nu_a + \nu_{T,a}\), \(\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b\) and \(\eta^2 = 0.01h^2\) is a small parameter to avoid a zero denominator. For laminar flow, the eddy viscosity \(\nu_{T,a}\) will be dropped so that \(\nu_{E,a}\) is representing only kinematic viscosity \(\nu_a\), which is constant for all fluid particles. Monaghan’s viscous term for laminar flow is:

$$\nu \nabla^2 \mathbf{u}_a \approx \sum_b m_b \frac{8(\nu_a + \nu_b)}{\rho_a + \rho_b} \frac{\mathbf{u}_{ab} \cdot \mathbf{r}_{ab}}{r_{ab}^2 + \eta^2} \nabla w_h(r_{ab})$$

(2.35)

and Morris’s viscous term for laminar flow is:

$$\nu \nabla^2 \mathbf{u}_a \approx \sum_b m_b \frac{\mu_a + \mu_b}{\rho_a \rho_b} \frac{\mathbf{r}_{ab} \cdot \nabla w_h(r_{ab})}{r_{ab}^2 + \eta^2} \mathbf{u}_{ab}$$

(2.36)

with the dynamic viscosity \(\mu_a = \rho_a \nu_a\). Each particle carries its own molecular viscosity in order to allow modelling of multiphase flow. Morris et al. stated that both formulations conserves linear momentum exactly, while angular momentum is only approximately conserved by Eq. (2.36) and exactly by Eq. (2.35) [46]. However, Monaghan’s term is retained for the simulations presented in the following since the results from both methods show little difference [26].

There are several ways to express the momentum equation, e.g. by combining Eq. (2.31) and Eq. (2.34), it gives:

$$\frac{d\mathbf{u}_a}{dt} \approx - \sum_b m_b \left( \frac{\rho_b}{\rho_a} \frac{\mathbf{u}_b}{\rho_a} + \frac{\rho_b}{\rho_a} \frac{\mathbf{u}_a}{\rho_b} - 8 \frac{\nu_{E,a} + \nu_{E,b}}{\rho_a + \rho_b} \frac{\mathbf{r}_{ab} \cdot \mathbf{r}_{ab}}{r_{ab}^2 + \eta^2} \nabla w_h(r_{ab}) \right) + \mathbf{F}_a^e$$

(2.37)

or combining Eq. (2.31) and Eq. (2.34), it gives:

$$\frac{d\mathbf{u}_b}{dt} \approx - \sum_b m_b \left( \frac{\rho_b}{\rho_a} \frac{\mathbf{u}_b}{\rho_a} + \frac{\rho_b}{\rho_a} \frac{\mathbf{u}_a}{\rho_b} \right) \cdot \nabla w_h(r_{ab})$$

$$+ \sum_b m_b \frac{\rho_a \nu_{E,a} + \rho_b \nu_{E,b}}{\rho_a \rho_b} \frac{\mathbf{r}_{ab} \cdot \nabla w_h(r_{ab})}{r_{ab}^2 + \eta^2} \underline{u}_{ab} + \mathbf{F}_a^e$$

(2.38)

### 2.2.4 State equation

The pressure for each particle is obtained from a state equation, which was established by Batchelor [3] and Tait [59], then Monaghan [43] applied it by introducing a numerical speed
of sound in order to give a smaller speed of sound than the real one as:

\[
\overline{\rho_a} = \frac{\rho_0 c_0^2}{\gamma} \left[ \left( \frac{\rho_a}{\rho_0} \right)^\gamma - 1 \right]
\]  

(2.39)

As mentioned before, the choice of \( \gamma = 7 \) causes pressure to respond strongly to variations in density. For lower Reynolds numbers \( (Re \leq 1) \), more accurate pressure estimates are obtained if \( \gamma = 1 \) [46].

### 2.3 Truly incompressible SPH (ISPH)

While WCSPH is fully explicit in time, ISPH is semi-implicit: the pressure is solved by a fully implicit way, while the velocity is calculated explicitly.

#### 2.3.1 Truly incompressible algorithm

The truly incompressible approach dealing with pressure and velocity as primitive variables is presented in this section. The density is constant and Eq. (2.24) reduces to:

\[
\nabla \cdot \mathbf{u} = 0
\]  

(2.40)

The classical projection method ([8], [61]) is used to solve the velocity-pressure coupling problem. The discretised form of Eq. (2.25) is split into two parts; the first being the prediction step based on viscous and external forces:

\[
\mathbf{u}^{n+1} = \mathbf{u}^n + (\nu_F \nabla \mathbf{u}^n + \mathbf{F}^e) \Delta t
\]  

(2.41)

and the second the correction step based on pressure force:

\[
\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = -\frac{1}{\rho} \nabla \overline{p}^{n+1}
\]  

(2.42)

where \( \mathbf{u}^n \) is an auxiliary velocity. In the prediction step, Eq. (2.41) can be rewritten as:

\[
\mathbf{u}^+ = \mathbf{u}^n + (\nabla \cdot (\nu_F \nabla \mathbf{u}^n + \mathbf{F}^e) \Delta t
\]  

(2.43)

The auxiliary velocity field \( \mathbf{u}^+ \) is usually not divergence free but this is imposed upon \( \mathbf{u}^{n+1} \). Hence, the auxiliary velocity is projected on the divergence-free space by writing the divergence of Eq. (2.42) as:

\[
\nabla \cdot \left( \frac{\mathbf{u}^{n+1} - \mathbf{u}}{\Delta t} \right) = -\nabla \cdot \left( \frac{1}{\rho} \nabla \overline{p}^{n+1} \right)
\]  

(2.44)
With the condition of incompressibility on \( \bar{\mathbf{u}}^{n+1} \), this leads to the following pressure equation:

\[
\nabla \cdot \left( \rho \frac{1}{\rho} \nabla \bar{p}^{n+1} \right) = \frac{\nabla \cdot \bar{\mathbf{u}}}{\Delta t}
\]

(2.45)

Since a constant density is considered here, Eq. (2.45) can be rewritten as:

\[
\nabla^2 \bar{p}^{n+1} = \frac{\rho}{\Delta t} \nabla \cdot \bar{\mathbf{u}}
\]

(2.46)

where \( \nabla^2 \) is the Laplacian operator.

Once pressure is obtained from Eq. (2.46), the velocity is updated by the computed pressure gradient:

\[
\bar{\mathbf{u}}^{n+1} = \bar{\mathbf{u}} - \left( \rho \frac{1}{\rho} \nabla \bar{p}^{n+1} \right) \Delta t
\]

(2.47)

Finally, particles move only with this corrected velocity as:

\[
\mathbf{r}^{n+1} = \mathbf{r}^{n} + \bar{\mathbf{u}}^{n+1} \Delta t
\]

(2.48)

One should note that the updated velocity \( \bar{\mathbf{u}}^{n+1} \) is divergence free only to within the spatial truncation error due to the method of solving Eq. (2.46) (see Section 2.3.3). Hence errors are produced in particle positions; however, this error is still less than that of the WCSPH method (Cummins [12]). The details of velocity-pressure coupling algorithm are shown in Section 2.6.

### 2.3.2 Prediction step

The auxiliary velocity \( \bar{\mathbf{v}}_a \) can be predicted without pressure term in Eq. (2.37) or (2.38) as:

\[
\frac{d\bar{\mathbf{v}}_a}{dt} \approx \sum_b m_b \frac{\nu_{E,a} + \nu_{E,b} \bar{\mathbf{u}}_{ab} \cdot \mathbf{r}_{ab}}{\rho_a + \rho_b} \frac{\nabla \cdot \mathbf{r}_{ab} w_h (r_{ab})}{r_{ab}^2 + \eta^2} + \mathbf{F}^e_a
\]

(2.49)

or

\[
\frac{d\bar{\mathbf{v}}_a}{dt} \approx \sum_b m_b \frac{\rho_a \nu_{E,a} + \rho_b \nu_{E,b} \mathbf{r}_{ab} \cdot \nabla \cdot \mathbf{r}_{ab} w_h (r_{ab})}{\rho_a \rho_b} \frac{\nabla \cdot \mathbf{r}_{ab} w_h (r_{ab})}{r_{ab}^2 + \eta^2} + \mathbf{F}^e_a
\]

(2.50)

Then, its divergence will be obtained from:

\[
\nabla \cdot \bar{\mathbf{v}} \approx -\frac{1}{\rho_a} \sum_b m_b \mathbf{u}_{ab} \cdot \nabla \cdot \mathbf{r}_{ab} w_h (r_{ab})
\]

(2.51)

and used in the right hand side of Eq. (2.46).
2.3.3 Pressure Poisson equation

Cummins et al. [12] described two approaches to solve the pressure equation, the first by an exact discretisation of the Laplacian and the second by an approximation. They proposed the exact discretisation of the Laplacian with constant density as:

\[
\nabla \cdot (\nabla \tilde{p})_a \approx \sum_b \frac{m_b}{\rho_b} \left( \sum_c \frac{m_c}{\rho_c} \tilde{p}_c \nabla \tilde{b} w_h(r_{bc}) \right) \cdot \nabla \tilde{a} w_h(r_{ab}) \tag{2.52}
\]

Assuming that Eq. (2.12) is satisfied, the pressure gradient can be expressed with Eq. (2.4). It leads to the exact Laplacian form Eq. (2.52). Note that the double summation leads to a very large stencil (neighbours of the neighbour of a particle “a”). Cummins et al. tested this form on a simple 1-D hydrostatic equilibrium problem. They pointed out that the exact Laplacian operator produces a distinct pressure decoupling pattern similar to that observed in exact projection methods on co-located finite-difference grids [51] (see Fig. 2.3 (a)) and this co-location problem also hampers convergence when iterative techniques are used to perform the projection. Similar phenomena are also observed in our work and presented in Section 3.2.1.

Therefore, the alternative method was suggested which is an approximated operator similar to Eq. (2.34) as:

\[
\nabla \cdot \left( \frac{1}{\rho_a} \nabla \tilde{p} \right)_a \approx \sum_b \frac{m_b}{\rho_a \rho_a + \rho_b} \frac{\tilde{p}_a}{r_{ab}} \cdot \nabla \tilde{a} w_h(r_{ab}) \tag{2.53}
\]

The pressure gradient is here computed with a finite-difference approximation by using a Jacobian transform. This approximation is also examined and shown in Fig. 2.3 (b). In their work, the mirror particle technique is used at boundaries (see Section 2.5.2) and the velocity, pressure and position for those particles are shown in Fig. 2.7 (a) and (b).

Another example of the approximate Laplacian operator is the one used in our work, which is even closer to the diffusion term (i.e. analogous to Eq. (2.34), see [63] for coding details) and reads:

\[
\nabla \cdot \left( \frac{1}{\rho_a} \nabla \tilde{p} \right)_a \approx \frac{2}{\rho_a^2} \sum_b m_b \frac{\tilde{p}_{ab} \cdot \nabla \tilde{a} w_h(r_{ab})}{r_{ab}^2 + \eta^2} \tag{2.54}
\]
2.3. Truly incompressible SPH (ISPH)

(a) Exact projection operator. 

(b) Approximate projection operator.

Figure 2.3: Pressure vs $y$ and $t$. The results from the exact and approximate projection operator [12].

where $\vec{p}_{ab} = \vec{p}_a - \vec{p}_b$.

Shao (e.g. [55], [54]) also proposed the following form, similar to Eq. (2.33):

$$
\nabla \cdot \left( \frac{1}{\rho_a} \nabla \vec{p} \right)_a \approx \sum_b m_b \frac{8}{(\rho_a + \rho_b)^2} \frac{\vec{p}_{ab} \cdot \nabla_a \vec{w}_h(r_{ab})}{r_{ab}^2 + \eta^2} 
$$

These three operators have a compact stencil (single summation) but are not compatible with the $\Delta p = \nabla \cdot (\nabla p)$ relation in the discretised form.

2.3.4 Correction step

Once the pressure is obtained from Eq. (2.46), the auxiliary velocity $\vec{u}^*$ will be corrected by the gradient of pressure Eq. (2.31):

$$
\frac{d\vec{u}_a}{dt} \approx \frac{d\vec{u}^*_a}{dt} - \sum_b m_b \left( \frac{\vec{p}_b}{\rho_b^2} + \frac{\vec{p}_a}{\rho_a^2} \right) \nabla_a \vec{w}_h(r_{ab})
$$

or by the gradient of pressure Eq. (2.32):

$$
\frac{d\vec{u}_a}{dt} \approx \frac{d\vec{u}^*_a}{dt} - \sum_b m_b \frac{\vec{p}_b + \vec{p}_a}{\rho_a \rho_b} \nabla_a \vec{w}_h(r_{ab})
$$
The position of particles are changed with this corrected velocity only according to Eq. (2.28).

## 2.4 Time integration

### 2.4.1 Time step

The time step $\Delta t$ in our work takes into account three conditions, a CFL condition ($\Delta_{CFL}$), inertia forces ($\Delta t_{forces}$) and viscous ($\Delta t_{visc}$) forces. The time step is then chosen by the minimum of these three condition for both WCSPH and ISPH as:

$$\Delta t \leq \min(\Delta t_{CFL}, \Delta t_{forces}, \Delta t_{visc}) \quad (2.58)$$

While the conditions of the mass and viscous forces are identical for WCSPH and ISPH, the CFL condition is different between them.

**CFL condition**

The CFL condition imposes that the time step $\Delta_{CFL}$ is less or equal to the convection time on the smoothing length $h$, which is proportional to the initial particle spacing $\delta r$.

$$\Delta t_{CFL} \leq 0.4 \frac{h}{u_{ref}} \quad (2.59)$$

where the coefficient 0.4 was chosen through numerical tests [42]. The reference velocity $u_{ref}$ can be the numerical speed of sound $c_0$ for WCSPH and maximum fluid velocity $u_{max}$ for ISPH.

**Condition on the force per unit mass**

The time step based on force terms $\delta_{forces}$ can be chosen by the minimum of the magnitude of particle accelerations as:

$$\Delta t_{forces} \leq 0.25 \min_a \sqrt{\frac{h}{|f_a|}} \quad (2.60)$$

where $|f_a|$ is the magnitude of a particle acceleration [46].
2.4. Time integration

Condition on the viscous diffusion

The viscous diffusion condition is:

\[ \Delta t_{\text{visc}} \leq 0.125 \min_{a} \frac{h^2}{\nu_{E,a}} \]  \hspace{1cm} (2.61)

where the minimum of effective viscosity \( \nu_{E,a} \) among particles is taken into account. For laminar flow, the effective viscosity \( \nu_E \) will be replaced by the kinematic viscosity \( \nu \).

The examples of different coefficients in time step for a truly incompressible approach

Morris et al. [46] mentioned that the coefficients in Eq. (2.59) to Eq. (2.61) are influenced by the choice of kernel and the arrangement of particles. The following discussion introduces the different definition of time step used for a truly incompressible approach by changing these coefficients. According to Cummins and Rudman [12], the dominant time-step constraint is different depending on the resolutions (number of particles) in truly incompressible approach. Based on \( Re = 420 \), if the resolution is less than \( 50 \times 50 \), the time-step is governed by the CFL stability constraint with different coefficient used in Eq. (2.59) as:

\[ \Delta t_{\text{CFL}} \leq 0.25 \frac{h}{u_{\text{max}}} \]  \hspace{1cm} (2.62)

For higher resolutions, the viscous diffusion condition, \( \Delta t_{\text{visco}} \), is the dominant time-step constraint (see Eq. (2.61)). This is linked to the cell Peclet number \( Pe_{\text{cell}} \) in Eulerian methods. The cell Peclet number gives a relation between convection and diffusion coefficients as:

\[ Pe_{\text{cell}} = \frac{u \Delta x}{\nu} < 2 \]  \hspace{1cm} (2.63)

where \( \Delta x \) is the cell size and \( u \) the velocity, and it should be smaller than two [13].

This cell Peclet number can be related between the CFL condition and viscous diffusion condition in SPH as:

\[ Pe_{\text{cell, SPH}} = \frac{\Delta t_{\text{visco}} \left( \frac{h^3}{\nu} \right)}{\Delta t_{\text{CFL}} \left( \frac{h}{u_{\text{max}}} \right)} < 1 \]  \hspace{1cm} (2.64)

With the coefficients used by Cummins et al. in this case, it will be:

\[ \frac{\Delta t_{\text{visco}}}{\Delta t_{\text{CFL}}} = \frac{0.125 h^2}{0.25 \frac{h}{u_{\text{max}}}} < 1 \iff Pe_{\text{cell, SPH}} = \frac{u_{\text{max}} h}{\nu} < 2 \]  \hspace{1cm} (2.65)
By recalling that the role of the smoothing length $h$ is analogous to a cell size $\Delta x$ in an Eulerian scheme, the same criterion for the cell Peclet number can be found. According to Shao et al. [55] [53], initial particle spacing $\delta r$ is used for time step instead of the smoothing length $h$ as shown above. The CFL condition satisfies the following expression:

$$\Delta t_{CFL} \leq 0.1 \frac{\delta r}{u_{\text{max}}}$$

(2.66)

and the constraint of viscous diffusion is:

$$\Delta t_{\text{visco}} \leq 0.1 \frac{\delta r^2}{\nu}$$

(2.67)

2.4.2 Temporal integration

The Reynolds-averaged Navier-Stokes and the position equations can be integrated in time with fully explicit scheme for WCSPH and the predictor and corrector scheme for ISPH.

**WCSPH explicit scheme**

Integration with the explicit scheme for WCSPH gives:

$$\begin{align*}
\mathbf{u}^{n+1}_a &= \mathbf{u}^n_a + \Delta t M^n_a \\
\rho^{n+1}_a &= \rho^n_a + \Delta t N^n_a \\
r^{n+1}_a &= r^n_a + \Delta t (\mathbf{u}^{n+1}_a)
\end{align*}$$

(2.68)

where $M^n_a$ corresponds to the right hand side of Eq. (2.33) or Eq. (2.34) and $N^n_a$ for the right hand side of Eq. (2.30). Superscripts $n$ and $n + 1$ indicate respectively previous and present time steps.

**ISPH predictor-corrector scheme**

Integration with a predictor-corrector scheme in the context of the present work gives:

$$\begin{align*}
\mathbf{u}^n_a &= \mathbf{u}^n_a + \Delta t F^n_a \\
\mathbf{u}^{n+1}_a &= \mathbf{u}^n_a - \Delta t \left( \frac{1}{\rho} \nabla r^{n+1}_a \right) \\
r^{n+1}_a &= r^n_a + \Delta t (\mathbf{u}^{n+1}_a)
\end{align*}$$

(2.69)

where $F^n_a$ refers to the right hand side of Eq. (2.49) or Eq. (2.50).
2.5 Wall modelling and Boundary conditions

Unlike finite differences where skewed discretisations can be introduced near a wall to retain the same order (high order backward differencing), SPH has a large isotropic stencil which becomes truncated near a wall. With a crude discretisation we observe that particles can penetrate and even cross the walls. There are several ways to prevent this phenomenon, for example, by using some repulsive forces or dummy particles [55] or mirror particles [12], [43].

The number of neighbouring particles depends on the radius of the compact support $h_t$ of the kernel and have a strong influence on the accuracy of numerical prediction. When the particles are close to the wall, the number of neighbouring particles are getting smaller due to the truncation of the kernel (see Fig. 2.4).

![Figure 2.4: Truncation of the kernel support at the wall (E: Edge particles, F: Fluid particles).](image)

2.5.1 Dummy particles

Dummy particles are regularly distributed at the initial state and have zero velocity through the whole simulation, while several layers of dummy particles [55] are built as an extension of the edge particles surrounding the solid boundaries to ensure the same order of discretisation (in terms of kernel compact support) for particles located close to those boundaries, as for particles located in the core of the domain. This also makes the coding simpler (e.g. for parallelisation) as the same scheme is used for all particles with the only difference that wall particles anchor their initial position every time step. The number of dummy particle layers is decided from the radius of the compact support (i.e. such that the stencil is not truncated
This technique is chosen for ISPH and further developed to link the dummy particles to the edge particles in their normal direction. In the following simulations, three or four layers of dummy particles are built. These dummy particles and edge particles are once linked together, the dummy particles carry identical pressure as their normal direction edge particles. To illustrate the use of dummy particles, three types of wall configurations are shown: the first where the dummy particles are in the outer corner (see Fig. 2.5(a)), the second for the inner corner (see Fig. 2.5(b)) and the last for the curved wall (see Fig. 2.5(c)).

(a) Case of an outer corner (example of a cavity flow).

(b) Case of an inner corner (example of a square cylinder in a flow).

(c) Case of a curved wall (example of a circular cylinder in a flow).

Figure 2.5: Sketch of dummy particles around a wall corner and curved wall.

As shown in Fig. 2.5 this approach sometimes requires particular care depending on
2.5. Wall modelling and Boundary conditions

geometry. There is no special treatment when outer corners are considered in contrast to the treatment of inner corners where two pressure fields overlap with the presence of the two perpendicular walls. To circumvent this problem in this work, the diagonal particles carry the same pressure as the average of their four neighbouring particles. This treatment is done only for 2-D applications. In the case of circular cylinder (see Fig. 2.5(c)), the number of edge particles is decided from setting the length of the arc at the boundary very close to the initial particle distance $\delta r$, for example with 20 edge particles. In that case, the initial distribution of $\delta r$ is no longer constant; more dense particles (smaller $\delta r$, e.g. in Fig. 2.5(c)) for the concave and the less particles (larger $\delta r$) if the convex are considered. A bluff body case with circular cylinder case are performed with this consideration shown in Fig. 2.5(c) and presented in [37]. However, the dummy particles technique allows fluid particle penetration through the wall in certain cases. The bluff body case with a circular cylinder for example, the fluid particles were able to cross the cylinder. To circumvent this phenomenon, more numbers of edge and dummy particles are used for the cylinder and no fluid particles were crossed the boundary of the cylinder. However, denser edge and dummy particles repel the fluid particles with a stronger force (see Fig. 2.6).

2.5.2 Mirror particles

Unlike dummy particles, mirror particles are set in either a symmetric or antisymmetric way to fluid particle positions and have a non-zero velocity. In terms of velocity, if the mirror particles are set symmetrically, these particles carry identical velocity as the corresponding fluid velocity. With antisymmetric set, the mirror particles have the opposite velocity. Figure 2.7 shows that symmetric pressure and asymmetric velocity for the mirror particles, especially Fig. 2.7(a) and (b) represents the wall modelling and boundary condition applied by Cummins et al. [12] for the truly incompressible approach. Neumann boundary conditions for pressure $\frac{d\varphi}{dn} = 0$ at the wall are achieved by this way.

On corners or curved surfaces these particles no longer have homogeneous distribution of spacing (see Fig. 2.7(c)), which leads to large density variations. Two examples of boundary conditions are briefly introduced here to treat the curved wall. Firstly, Morris et al. [46] for the weakly compressible approach used the combination of dummy and mirror
Figure 2.6: The influence of different mass of circular cylinder. In each figure, \( k_{par} \) indicates the type of particles (blue: fluid particles, green: edge particles, red: dummy particles).

(a) The number of cylinder edge particles: 20  
(b) The number of cylinder edge particles: 30  
(c) The number of cylinder edge particles: 40

The other example is the Multiple Boundary Tangent (MBT) approach. This work is done for the truly incompressible SPH by Yildiz et al. but not applied in our work yet. This technique of building the mirror particles is different from the Morris et al.’s. The mirror particles technique; the actual SPH particles are built to represent the mirror particles and edge particles. As illustrated in Fig. 2.8 a tangential line relative to a fluid particle \( a \) can be drawn, then the normal distances \( d_a \) and \( d_B \) to the boundary are calculated for the fluid particle \( a \) and mirror particle \( B \). By assuming zero velocity on this tangential line itself, each mirror particle velocity \( v_B = -(d_B/d_a)v_a \) can be obtained from the velocity of fluid particle \( a \). This artificial velocity \( v_B \) is used to calculate viscous forces but this is not used for the position of the mirror particle.
2.5. Wall modelling and Boundary conditions

(a) Straight wall. (b) Right-angle corner wall. (c) Curved wall.

Figure 2.7: Sketch of mirror (ghost) particles depending on the type of wall boundaries.

Figure 2.8: Construction of artificial velocity for boundary particles to simulate a no-slip boundary conditions for a curved wall [46].

particles are not built as actual SPH particles. At each time, tangent lines are computed for all edge particles. The neighbouring particles of each edge particle in fluid domain are mirrored with respect to the tangent line of the corresponding edge particle. The detail can be found in [73].

2.5.3 Repulsive forces

With repulsive forces, only one layer of particles is placed on the wall, and as indicated by the name, they exert very large repulsive forces to prevent fluid particles from crossing the walls. The advantage of using the repulsive forces is that not only CPU time but also memory can be saved by not imposing the dummy or mirror particles. However, when a central repulsive force is used, particle disorganisation close to wall is found due to their discreteness. By reducing the distance between edge particles as four times less than the fluid
particle distance, the results are improved [44]. Instead of the central force, the idea of a
normal repulsive force was established by Monaghan [44]. This force is based on the normal
and tangential distances of the fluid particles to the edge particles. By comparing with the
central force, the normal repulsive force produces better results and does not require finer
discretisation for edge particles.

2.6 Velocity-pressure coupling technique

There are a number of coupling techniques between the velocity and pressure. Since the
projection method is used to solve the incompressibility for ISPH, this method is explained
with SPH formulation [64].

2.6.1 Projection method

The following is to highlight the velocity-pressure coupling algorithm in terms of the pro-
jected velocity field by considering a fluid domain $\Omega$, whose boundary is separated in two
parts $\partial \Omega_1$ and $\partial \Omega_2$. Two vector spaces $E$ and $F$ are defined by:

\[
E = \{ \mathbf{u} \in C^0(\Omega, \mathbb{R}^2), \mathbf{u} \cdot \mathbf{n} |_{\partial \Omega_1} = 0 \} \tag{2.70}
\]

\[
F = \{ \alpha \in C^0(\Omega, \mathbb{R}), \alpha |_{\partial \Omega_2} = 0 \} \tag{2.71}
\]

where $\mathbf{n}$ is the unit vector perpendicular to $\partial \Omega_1$. $E$ can be interpreted as the space of possible
velocity fields, while $F$ is the space of possible scalar fields (like pressure) defined on $\Omega$.
The separated boundaries $\partial \Omega_1$ and $\partial \Omega_2$ are respectively solid and liquid boundaries. The
boundary conditions specified in Eqs. (2.70) and (2.71) thus respectively correspond to a free-
slip condition for velocities on a solid wall and a zero-pressure condition for free surfaces.
Two products of vector and scalar on these space can be defined as:

\[
\langle \mathbf{u}, \mathbf{v} \rangle = \int_{\Omega} \mathbf{u} \cdot \mathbf{v} d\Omega \tag{2.72}
\]

\[
\langle \alpha, \beta \rangle = \int_{\Omega} \alpha \beta d\Omega \tag{2.73}
\]
2.6. Velocity-pressure coupling technique

The divergence (herein denoted by $D = \nabla \cdot$) and gradient ($G = \nabla$) operators are both linear functions, respectively from $E$ to $F$ and from $F$ to $E$. The following equality

$$
(\mathbf{u}, G\alpha) = \int_{\Omega} \mathbf{u} \cdot \nabla \alpha d\Omega
= \int_{\Omega} [\nabla \cdot (\alpha \mathbf{u}) - \alpha \nabla \cdot \mathbf{u}] d\Omega
= \int_{\partial\Omega} \alpha \mathbf{u} \cdot \mathbf{n} d\Gamma - \langle \alpha, D\mathbf{u} \rangle
$$

(2.74)

shows that $D$ and $-G$ are adjoint operators, thanks to the boundary conditions prescribed in Eqs. (2.70) and (2.71). Thus, $\text{Ker} \ D$ and $\text{Im} \ G$ are orthogonal spaces, which means that for each arbitrary velocity field $\mathbf{u}^\ast$ (“initial” estimation of the velocity field) there exists a unique vector field $\mathbf{u}$ in $\text{Ker} \ D$ and a unique scalar field $\alpha$ such that

$$
\mathbf{u}^\ast = \mathbf{u} + \nabla \alpha
$$

(2.75)

which is known as “Hodge’s decomposition”. Taking the divergence of Eq. (2.75) then yields:

$$
\nabla^2 \alpha = \nabla \cdot \mathbf{u}^\ast
$$

(2.76)

Hence $\mathbf{u}$ is the projection of $\mathbf{u}^\ast$ on the subspace of the divergence-free velocity fields, and this is achieved by correcting $\mathbf{u}^\ast$, through Eq. (2.75), $\alpha$ being estimated by solving Eq. (2.76). Comparing Eq. (2.76) with (2.46) shows that the role of $\alpha$ is here played by the pressure (with proportionality factor). One should emphasise the fact that Pythagoras’ theorem then states that the function

$$
f(\nabla) = \int_{\Omega} (\mathbf{u}^2 - \nabla^2) d\Omega
$$

(2.77)

defined for all velocity fields $\nabla$ in $\text{Ker} \ D$ is minimum for $\nabla = \mathbf{u}$, meaning that the projected field is the incompressible velocity field closest to the initial estimation $\mathbf{u}^\ast$ in the sense of kinetic energy. With the notations of Section 2.3, similar considerations can be applied to the SPH numerical method.

In the SPH formalism, considerations regarding incompressibility can be written in a way similar to the developments made at the end of Section 2.3.1. One defines a finite set of
particles \( A \) (playing the role of \( \Omega \) in a discrete Lagrangian formalism). Then one defines two vector spaces \( E_{SPH} \) and \( F_{SPH} \) by:

\[
E_{SPH} = \{ \vec{u}_A \in C^0(\mathbb{R}^2) \} \tag{2.78}
\]

\[
F_{SPH} = \{ \alpha_A \in C^0(\mathbb{R}) \} \tag{2.79}
\]

where the subscript \( A \) means that the considered fields are defined on the set \( A \) (\( \vec{u}_A \) is the collection of all the particle velocities \( \vec{u}_a \)). Then, two discrete scalar products are defined by:

\[
\langle \vec{u}_A, \vec{v}_A \rangle = \sum_{a \in A} \frac{m_a}{\rho_a} \vec{u}_a \cdot \vec{v}_a \tag{2.80}
\]

\[
\langle \alpha_A, \beta_A \rangle = \sum_{a \in A} \frac{m_a}{\rho_a} \alpha_a \beta_a \tag{2.81}
\]

Considering the SPH divergence and gradient discrete operators given by Eqs. (2.13) and (2.8), respectively denoted by \( D_{SPH} \) and \( G_{SPH} \), leads to:

\[
(\vec{u}, (G_{SPH} \alpha)_A) + \langle (D_{SPH} \vec{u})_A, \alpha_A \rangle = \sum_{a \in A} \frac{m_a}{\rho_a} \vec{u}_a \cdot (G_{SPH} \alpha)_a + \sum_{a \in A} \frac{m_a}{\rho_a} (D_{SPH} \vec{u}_a)_a \alpha_a
\]

\[
= \sum_{a,b \in A} m_a m_b \left[ \frac{\alpha_a}{\rho_a^2} \vec{u}_a + \frac{\alpha_b}{\rho_b^2} \vec{u}_b \right] \cdot \nabla_a w_h(r_{ab})
\]

\[
= \sum_{a,b \in A} m_a m_b \left( \frac{\alpha_b}{\rho_b^2} \vec{u}_a + \frac{\alpha_a}{\rho_a^2} \vec{u}_b \right) \cdot \nabla_a w_h(r_{ab}) \tag{2.82}
\]

The latter expression vanishes by re-arranging the discrete labels \( a \) and \( b \), provided the kernel is a function of the particle distance only, which ensures \( \nabla_b w_h(r_{ba}) = -\nabla_a w_h(r_{ab}) \). Thus \( D_{SPH} \) and \(-G_{SPH}\) are skew adjoint operators, meaning that Hodge’s decomposition still stands in our discrete formalism. As a consequence, any discrete estimated velocity field \( \vec{u}^*_A \) can be projected on the SPH-divergence-free space by correcting it through a discrete pressure field satisfying a Poisson equation analogous to Eq. (2.76) or (2.46):

\[
(D_{SPH} G_{SPH} \vec{p})_A = \frac{\rho_A}{\Delta t} (D_{SPH} \vec{u}^*_A) \tag{2.83}
\]

with Neumann boundary condition \( \frac{\vec{p}}{\vec{n}} = 0 \), where \( n \) is the normal unit vector of the boundary. When this equation is solved, one should use the exact SPH operators defined by Eqs. (2.13)
and (2.8). However, this would involve too many computational resources through the double summation required to write the left hand side of Eq. (2.83) and also leads to a checkerboard effect on the solution. Thus, it is usually preferred to use an approximate form of the combined operator $D_{SPH}G_{SPH}$, namely the SPH form of the Laplace operator (Eq. (2.34)) [10].

2.7 Solution of a linear equation system

In CFD, the linear equation system is written as:

$$AF = B$$

(2.84)

where $A$ is a matrix of known coefficients, $B$ is a vector of given coefficients and $F$ a vector of unknowns such as density, velocity or temperatures for each particles. This system is usually solved by the iterative method which requires storage of the order $n$ instead of $n^2$ as required in direct methods. Some examples of direct and iterative methods are introduced here.

2.7.1 Direct methods

Gauss Elimination

Gauss elimination is the basic method for solving linear systems of algebraic equations. This is based on the systematic reduction of large systems of equations to smaller ones.

$$A = \begin{pmatrix}
  a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\
  a_{21} & a_{22} & a_{23} & \cdots & a_{2n} \\
  \vdots & \vdots & \vdots & \ddots & \vdots \\
  a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn}
\end{pmatrix}$$

(2.85)

The reduction of the system is done by eliminating certain elements of the matrix replacing it with zero. For example, the first column of the matrix, $a_{21}, a_{31}, \ldots, a_{n1}$, are eliminated from the $2^{nd}$ row by:

$$a_{i1} = a_{i1} - \frac{a_{i1}}{a_{11}}$$

(2.86)
Then, all of the elements below $a_{11}$ are eliminated. When this process is complete for the $1^{st}$ column, the same procedure is carried out for the $2^{nd}$ column below the $2^{nd}$ row until the column $n - 1$. After this process is complete, the original matrix has been replaced by an upper triangular one:

$$U = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ 0 & a_{22} & a_{23} & \cdots & a_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_{nn} \end{pmatrix} \quad (2.87)$$

This is called forward elimination and the elements of the right hand side of the equation, $b_i$, are also modified during the procedure. The last equation (last row) in Eq. (2.87) contains only one variable $f_n$ then:

$$f_n = \frac{b_n}{a_{nn}} \quad (2.88)$$

The next to the last equation contains only $f_{n-1}$ and $f_n$, and $f_{n-1}$ can be solved since $f_n$ is known. Then, the $i^{th}$ equation yields $f_i$:

$$f_i = \frac{b_i - \sum_{k=i+1}^{n} a_{ik} f_k}{a_{ii}} \quad (2.89)$$

**LU Decomposition**

Any matrix $A$ can be factored into the product of lower ($L$) and upper ($U$) triangular matrices as:

$$A = LU \quad (2.90)$$

Then, Eq. (2.84) can be rewritten as:

$$AF = LUF = B \quad (2.91)$$

The existence of this factorisation allows the solution of the system Eq. (2.84) in two stages as $UF = P$ and $LP = B$. Once $LP = B$ is solved for $P$, $UF = P$ can be calculated for $F$ as shown previously.

The advantage of $LU$ decomposition over Gauss elimination is that the factorisation can be
performed without knowing the vector $B$. As a result, if many systems involving the same
matrix are to be solved, considerable savings can be obtained by performing the factorisation
first; the system can then be solved as required \[13\]. Variations on $LU$ factorisation are the
basis of some of the better iterative methods of solving systems of linear equations.

### 2.7.2 Iterative methods

There are numerous iterative methods to solve the pressure Poisson equation \(2.45\) such as
GMRES, Pre-conditioned Conjugate Gradient, Bi-CGSTAB. Only two of them are presented
here; one is the minimum residual method (MR) and the other is Bi-CGSTAB.

**Minimum residual (MR) method**

The minimum residual method is a very basic and simple among iterative methods. The
following information concerning the MR is taken from the MSc lecture notes of UMIST
\[34\].

The matrix $A$ can be decomposed as $L + D + U$, where lower matrix $L$, diagonal one $D$ and
upper one $U$. For example, the $j$th equation based on matrix $A$ is:

$$a_{j1}f_1 + a_{j2}f_2 + \cdots + a_{jj}f_j + \cdots + a_{jn}f_n = b_j \tag{2.92}$$

This can be rewritten by using the $L$, $D$ and $U$ decomposition as:

$$l_{j1}f_1 + l_{j2}f_2 + \cdots + d_{jj}f_j + \cdots + u_{jn}f_n = b_j \tag{2.93}$$

Then, the sequence of approximation is $F^{(0)}, F^{(1)}, ..., F^{(r)}$. At the iteration $F^{(r)}$, $F^{(r-1)}$ is
known. The Gauss Seidel Method simply uses the last known values when solving the $j$th
equation for $f_j$. In short, $F^{(r)}$ can be expressed with $L$, $D$, $U$ notation as:

$$F^{(r)} = (L + D)^{-1} \left[ B - UF^{(r-1)} \right] \tag{2.94}$$

By defining the residual vector $R$ as:

$$R^{r-1} = B - AF^{r-1} \tag{2.95}$$
The residual tends toward zero as the sequence of $F^{(r)}$ converges to the solution $F^{sol}$ since $AF^{sol} = B$. By rewriting Eq. (2.95) with $L$, $D$ and $U$ decomposition as:

$$R^{(r-1)} = B - (L + D + U)F^{(r-1)} = B - UF^{(r-1)} - (L + D)F^{(r-1)} \quad (2.96)$$

Adapting the Gauss Seidel method for the sequence of $F^{(r)}$, then combining Eqs. (2.96) and (2.94), gives:

$$F^{(r)} = (L + D)^{-1} \left[ R^{(r-1)} + (L + D)F^{(r-1)} \right] \quad (2.97)$$

This will be:

$$F^{r} = F^{(r-1)} + (L + D)^{-1}R^{(r-1)} \quad (2.98)$$

By introducing the over (or under)-relaxation parameter $\omega$, the convergence can be accelerated:

$$F^{(r)} = F^{(r-1)} + \omega (L + D)^{-1}R^{(r-1)} \quad (2.99)$$

This will be over-relaxation if $\omega > 1$ and this is called SOR (Successive Over Relaxation) method and under-relaxation is when $\omega < 1$.

Although the pre-conditioning method has not been used in the context of present work yet, for general explanation, pre-conditioning $P = L + D$ is introduced, then Eq. (2.99) can be rewritten as:

$$F^{(r)} = F^{(r-1)} + \omega P^{-1}R^{(r-1)} \quad (2.100)$$

Then, the next residual is:

$$R^{(r)} = B - AF^{(r)} \quad (2.101)$$

Putting Eq. (2.100) into Eq. (2.101),

$$R^{(r)} = B - A \left( F^{(r-1)} + \omega P^{-1}R^{(r-1)} \right) \quad (2.102)$$

The right hand side of Eq. (2.102) can be rewritten as (see Eq. (2.95)):

$$R^{(r-1)} = A\omega P^{-1}R^{(r-1)} \quad (2.103)$$
Then, the norm of Eq. (2.102) is:

\[ |R^{(r)}|^2 = (R^{(r-1)})^2 - 2\omega (R^{(r-1)}, AP^{-1}R^{(r-1)}) + \omega^2 (P^{-1}R^{(r-1)})^2 \]  

(2.104)

where the scalar product of vectors is written \((U, V) = \sum_{i=1}^{n} u_iv_i\). The residual is minimum when the differentiation of Eq. (2.104) in \(\omega\) is zero:

\[ \frac{d |R^{(r)}|^2}{d\omega} = -2 (R^{(r-1)}, AP^{-1}R^{(r-1)}) + 2\omega (P^{-1}R^{(r-1)})^2 = 0 \]  

(2.105)

Finally, \(\omega\) is defined as:

\[ \omega = \frac{(R^{(r-1)}, AP^{-1}R^{(r-1)})}{(AP^{-1}R^{(r-1)}, AP^{-1}R^{(r-1)})} \]  

(2.106)

This is minimum residual method pre-conditioned by \(P^{-1}\). The algorithm of the minimum residual method is Table 2.1.

| \(R^{(r-1)} = B - AF^{(r-1)}\) |  |
| \(z^{r} = P^{-1}R^{(r-1)}\) |  |
| \(\omega^{r} = \frac{(R^{(r-1)}, Az^{r})}{(Az^{r}, Az^{r})}\) |  |
| \(F^{(r)} = F^{(r-1)} + \omega^{(r)}z^{(r)}\) |  |

Table 2.1: Minimum Residual (MR) algorithm.

The approximation of the solution is seen as a \(z\) search directions along the optimum \(\omega\) is looking for:

\[ F^{(r)} = F^{0} + \omega^{(1)}z^{(1)} + \omega^{(2)}z^{(2)} + \cdots + \omega^{(r)}z^{(r)} \]  

(2.107)

This single direction of searches make the convergence slower. This algorithm with SPH formulations is interpreted in Section 3.2.4.

**Unpreconditioned Bi-CGSTAB**

Despite the relative simplicity of the minimum residual method, a more effective method is required to have more than one direction of search for solution. For this, unpreconditioned Bi-CGSTAB, which has two different directions of searching solution, is applied. Bi-CGSTAB
is one of variants of conjugate gradient methods, precisely Bi-CG. The advantage of Bi-CGSTAB over conjugate gradient method is that it can be applied to not only symmetric problems but also asymmetric ones [13][68]. The residual vector $r^i$ is orthogonal with respect to another row of vectors $r_0^0, r_1^0, \cdots, r_{i-1}^0$, and, vice versa, $\hat{r}^j$ is orthogonal with respect to $r_0^0, r_1^0, \cdots, r_{i-1}^0$. The detail of Bi-CGSTAB can be found in Vorst [68] and its algorithm is shown in Table 2.2. In order to restrict on memory traffic, both updates to the current solution

| $f^0$ is an initial guess; $r^0 = b - Af^0$; |
| $\hat{r}^0$ is an arbitrary vector, such that $(\hat{r}^0, r^0) \neq 0$, e.g., $\hat{r}^0 = r^0$; |
| $\gamma^0 = \alpha = \omega^0 = 1$; |
| $\zeta^0 = \eta^0 = 0$; |
| for $i = 1, 2, 3, \cdots$, |
| $\gamma^i = (\hat{r}^0, r^{i-1})$; $\beta = (\gamma^i / \gamma^{i-1})(\alpha / \omega^{i-1})$; |
| $\eta^i = r^{i-1} + \beta(\eta^{i-1} - \omega^{i-1}\zeta^{i-1})$; |
| $\zeta^i = A\eta^i$; |
| $\alpha = \gamma^i / (\hat{r}^0, \zeta^i)$; |
| $s = r^{i-1} - \alpha\zeta^i$; |
| $t = As$; |
| $\omega^i = (t, s)/(t, t)$; |
| $f^i = f^{i-1} + \alpha\eta^i + \omega^i s$; |
| if $f^i$ is accurate enough then quit; |
| $r^i = s - \omega^i t$ |

end

Table 2.2: Unpreconditioned Bi-CGSTAB algorithm [68].

$f$ in one single step, while the updates to the residual $r$ had to be done separately ($s = r^{i-1} - \alpha\zeta^i$ and $r^i = s - w^i t$). The iteration might terminate as soon as $\|s\|$ is small enough, but in that case, before stopping the algorithm, the current solution has to be updated appropriately as $f^i = f^{i-1} + \alpha\eta^i$ in order to compatible with the current residual $s$ (and the computation of $t, w^i$, as well as the second update $w^i s$ should be skipped). The implementation of this
2.7. Solution of a linear equation system

procedure in ISPH is indicated in Section 3.2.4.

2.7.3 Convergence criteria

When the iterative solvers are used, it is important to know when the iterations should be stopped. Iteration can be stopped when the residual norm has been reduced to some fraction of its original size, usually by three or four orders of magnitude. Within this level, the error is likely to have fallen by 0.1% of the solution [13]. According to [13] the residual and the error usually do not fall in the same way at the beginning of iteration process; if the matrix is poorly conditioned, the error may be large even when the residual is small. However, note that the ISPH numerical solution still provides good results even with the large residual norm, its tolerance is prescribed for every application.

Many iterative solvers require calculation of the residual. Hence, it is better if the residual is normalised by its initial level value at every time step since it does not require additional computation. For each particle \( a \), the residual \( (R)_a \) is defined as \( (R)_a = (B)_a - (Lp)_a \), where \( (B)_a = (\rho \nabla \cdot \bar{u}^*/\Delta t)_a \) and \( (Lp)_a = (\nabla^2 \bar{p})_a \). The convergence is obtained when:

\[
\frac{\|R\|_2}{\|R_0\|_2} < \theta
\]

(2.108)

where \( R_0 \) is the initial residual, \( \theta \) the convergence criterion and \( \| \cdot \|_2 \) the \( l_2 \)-norm calculated as:

\[
\|R\|_2 = \sqrt{\frac{1}{N} \sum_{a=1}^{N} R_a^2}
\]

(2.109)

where \( N \) is the number of particles. A convergence criterion \( \theta \) can be adjusted from case to case. In the context of the present work the criterion is thus indicated in the section of simulation condition for each application.

The next chapter presents the exact algorithmic details of the incompressible solver incorporated into the SPARTACUS SPH code.
Chapter 3

The ISPH SPARTACUS-2D code

The development of the truly incompressible SPH (ISPH) has been achieved through development of a pre-existing industrial code, SPARTACUS-2D and 3D, which is initially developed with the WCSPH approach at the “Laboratoire National d’Hydraulique et d’Environnement” of EDF (Electricité de France) since 1998 by Violeau and by Issa at Manchester (see [26]). The SPARTACUS code is modified for the ISPH approach. Before explaining the ISPH SPARTACUS code, the original code is briefly introduced.

3.1 The original SPARTACUS-2D code

A standard solution in SPARTACUS-2D code is based on the weakly compressible approach and briefly summarised in this section.

3.1.1 Fundamental equations

The continuity equation

The continuity equation (2.30) in the code is expressed as:

$$\frac{d \rho_a}{dt} \approx \sum_b m_b \mathbf{u}_{ab} \cdot \nabla w_h (r_{ab})$$

where \( \mathbf{u}_{ab} = \mathbf{u}_a - \mathbf{u}_b \).
Chapter 3. The ISPH SPARTACUS-2D code

The momentum equation

There are several ways to express the momentum equation. In the code, two pressure gradient forms and two viscous forms have been implemented. By combining the pressure gradient form of either Eq. (2.31) or Eq. (2.32) with Monaghan’s viscous term of Eq. (2.33), gives:

\[
\frac{d\mathbf{p}_a}{dt} \approx - \sum_b m_b \left( \frac{\overline{p}_b}{\rho_b^2} + \frac{\overline{p}_a}{\rho_a^2} - 8 \frac{\nu_{E,a} + \nu_{E,b} \mathbf{u}_{ab} \cdot \mathbf{r}_{ab}}{\rho_a + \rho_b \frac{r_{ab}^2}{\eta^2}} \right) \nabla_a w_h(r_{ab}) + \mathbf{F}_a^e
\] (3.2)

or

\[
\frac{d\mathbf{p}_a}{dt} \approx - \sum_b m_b \left( \frac{\overline{p}_b}{\rho_b} + \frac{\overline{p}_a}{\rho_a} - 8 \frac{\nu_{E,a} + \nu_{E,b} \mathbf{u}_{ab} \cdot \mathbf{r}_{ab}}{\rho_a + \rho_b \frac{r_{ab}^2}{\eta^2}} \right) \nabla_a w_h(r_{ab}) + \mathbf{F}_a^e
\] (3.3)

The same pressure gradient forms with Morris’s viscous term Eq. (2.34), it gives:

\[
\frac{d\mathbf{p}_a}{dt} \approx - \sum_b m_b \left( \frac{\overline{p}_b}{\rho_b^2} + \frac{\overline{p}_a}{\rho_a^2} \right) \nabla_a w_h(r_{ab}) + \sum_b m_b \frac{\rho_a \nu_{E,a} + \rho_b \nu_{E,b} \mathbf{r}_{ab} \cdot \nabla_a w_h(r_{ab})}{\rho_a \rho_b} \frac{r_{ab}^2}{r_{ab}^2 + \eta^2} \mathbf{u}_{ab} + \mathbf{F}_a^e
\] (3.4)

or

\[
\frac{d\mathbf{p}_a}{dt} \approx - \sum_b m_b \left( \frac{\overline{p}_b}{\rho_b} + \frac{\overline{p}_a}{\rho_a} \right) \nabla_a w_h(r_{ab}) + \sum_b m_b \frac{\rho_a \nu_{E,a} + \rho_b \nu_{E,b} \mathbf{r}_{ab} \cdot \nabla_a w_h(r_{ab})}{\rho_a \rho_b} \frac{r_{ab}^2}{r_{ab}^2 + \eta^2} \mathbf{u}_{ab} + \mathbf{F}_a^e
\] (3.5)

where \( \mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b \) and \( \mathbf{F}_a^e \) is the external force for a particle \( a \).

External forces

When gravity effects are considered, the external forces \( \mathbf{F}_a^e \) in Eqs. (3.2) to (3.5) are replaced with gravity \( \mathbf{g} \). The other example of the external forces is a propelling force. There are two main ways to set a fluid in motion in the code: firstly, a constant force \( F \), which is considered as an external volumetric force, can be applied to all fluid particles. Secondly, the correct mass flow rate at an “inlet” boundary can be imposed at each time step by updating the forcing term \( F \) [26].
3.1. The original SPARTACUS-2D code

The state equation

The state equation is implemented as:

\[ \bar{p}_a = \frac{\rho_0 c_0^2}{\gamma} \left[ \left( \frac{\rho_a}{\rho_0} \right)^\gamma - 1 \right] \]  \hspace{1cm} (3.6)

where \( \gamma = 7 \) is chosen in the code, \( \rho_0 \) is the reference density and \( c_0 \) the numerical speed of sound, which should be at least ten times superior to the maximum fluid velocity.

Particle position

The particles move with the simple relation as:

\[ \frac{d\mathbf{r}_a}{dt} = \mathbf{u}_a \]  \hspace{1cm} (3.7)

No XSPH correction \[42\] is applied.

3.1.2 Kernels

Based on the 3rd, 4th and 5th order spline kernels described in Section 2.1.3 the first derivative of them were respectively implemented as Eqs. (3.8), (3.9) and (3.10):

\[ w'_h(q) = \frac{10}{7\pi h^2} \begin{cases} 
-3q + \frac{9}{4}q^2 & \text{if } 0 \leq q \leq 1 \\
-\frac{3}{4}(2-q)^2 & \text{if } 1 \leq q \leq 2 \\
0 & \text{if } q \geq 2 
\end{cases} \]  \hspace{1cm} (3.8)

\[ w'_h(q) = \frac{96}{1199\pi h^2} \begin{cases} 
-4\left(\frac{5}{2} - q\right)^3 + 20\left(\frac{3}{2} - q\right)^3 - 40\left(\frac{1}{2} - q\right)^3 & \text{if } 0 \leq q \leq 0.5 \\
-4\left(\frac{5}{2} - q\right)^3 + 20\left(\frac{3}{2} - q\right)^3 & \text{if } 0.5 \leq q \leq 1.5 \\
-4\left(\frac{5}{2} - q\right)^3 & \text{if } 1.5 \leq q \leq 2.5 \\
0 & \text{if } q \geq 2.5 
\end{cases} \]  \hspace{1cm} (3.9)

\[ w'_h(q) = \frac{7}{478\pi h^2} \begin{cases} 
-5(3 - q)^4 + 30(2 - q)^4 - 75(1 - q)^4 & \text{if } 0 \leq q \leq 1 \\
-5(3 - q)^4 + 30(2 - q)^4 & \text{if } 1 \leq q \leq 2 \\
-5(3 - q)^4 & \text{if } q \geq 3 \\
0 & \text{if } q \geq 3 
\end{cases} \]  \hspace{1cm} (3.10)

where \( q \) denotes the ratio \( r_{ab}/h \). However, most of the time the 4th-order kernel is applied in this work.
3.1.3 Time step and temporal integration

Time step

The time step is chosen by the minimum among the three conditions as (see Section 2.4):

\[
\Delta t \leq \min \left( 0.4 \frac{h}{c_0}, 0.25 \min_a \frac{h}{|f_a|}, 0.125 \min_a \frac{h^2}{\nu_{E,a}} \right)
\]  

where \( h \) is smoothing length, \( c_0 \) the numerical speed of sound, \( f_a \) the force per unit mass. Each term respectively represents the condition of CFL, mass forces and viscous term.

Temporal integration

The Reynolds-averaged Navier-Stokes and the position equations can be integrated in time with fully explicit scheme as:

\[
\begin{align*}
\mathbf{u}_a^{n+1} &= \mathbf{u}_a^n + \Delta t M_n^a \\
\rho_a^{n+1} &= \rho_a^n + \Delta t N_n^a \\
r_a^{n+1} &= r_a^n + \Delta t (\mathbf{u}_a^{n+1})
\end{align*}
\]  

where \( M_n^a \) corresponds to the right hand side of Eq. (2.33) or Eq. (2.34) and \( N_n^a \) for the right hand side of Eq. (2.30). Superscripts \( n \) and \( n + 1 \) indicate respectively previous and present time steps.

3.1.4 Optimisation and algorithm structure

Link list

Since SPH formulations are based on the summations of each particle pair, the CPU time would scale as \( N^2 \) where \( N \) denotes the total particle number. However, each particle \( a \) is only linked to its closest neighbours \( b \) due to the compact support in the kernel function. It is thus essential to construct an optimal link list for searching the neighbouring particles at each time step and its algorithm is as follows:

1. A coarse grid, composed of cells measuring \( h_t \) (see Fig. 3.1), is first applied to the whole domain.
3.1. The original SPARTACUS-2D code

Figure 3.1: Determination of the closest neighbours relative to particle $a$ ([26], $h_t$: compact support size).

2. The corresponding cell of each particle $a$ is determined.

3. For each particle $a$, particles $b$ located in cell $a$ and in the eight adjacent cells are considered. Only those for which $r_{ab} < h_t$ are considered as $a$-neighbours.

This algorithm makes the CPU time proportional to $N$. When constructing the link list, the pair of particles which interact is only counted once due to the symmetric or antisymmetric contributions in the SPH formulations (see details in [26]). This makes not only the CPU time smaller but also the memory by a factor of 2.

Periodic conditions

In the code, periodic conditions (e.g. with respect to $x$ in Fig. 3.2) are achieved by considering that particles located at one end boundary are linked to particles at the other end boundary. The cells adjacent to the $a$-particle one are therefore completed by those located in the vicinity of the opposite boundary by considering that particle $b$ of Fig. 3.2 is located at $x_b = (x_{max} - x_{min})$ and vice versa.

Code structure

The simplified algorithm of the original SPARTACUS code is shown in Fig. 3.3.
Define the geometry

Set the simulation domain boundaries, physical and numerical parameters in a parameter file

Define the initial conditions

Search for the neighbouring particles

Compute the kernel derivative for each particle pair

Calculate the acceleration and velocity of the particles

Determine the time step

Update the position of particles

Update the density of particles

Update the pressure of particles

Figure 3.2: Adjacent cells relative to a periodic flow with respect to $x$-direction [26].

Figure 3.3: Simplified algorithm of SPARTACUS with the WCSPH approach.
3.2 The ISPH SPARTACUS-2D code

The new development of the SPARTACUS-2D code for the truly incompressible approach is described in this section and shortly highlighted as follows:

- One single step algorithm in the original code breaks down to two steps (prediction and correction steps) algorithm.

- Laplacian operator for pressure Poisson equation is developed.

- Two iterative methods (minimum residual method and Bi-CGSTAB) without pre-conditioning are implemented in the code.

- Dummy particles have a link with edge particles in their normal direction.

- Surface particle tracking method is also developed (see Section 6.2) for free-surface flow.

3.2.1 Fundamental equations

The continuity equation

Since density is constant for ISPH, the continuity equation is written only with the divergence of velocity and its SPH formulation is:

\[
\nabla \cdot \vec{u}_a \approx -\rho_a \sum_b m_b \vec{u}_{ab} \cdot \nabla w_h(r_{ab})
\]

(3.13)

where \( \vec{u}_{ab} = \vec{u}_a - \vec{u}_b \). This term is mainly used to obtain the right hand side of the pressure Poisson equation, which is the divergence of the temporal velocity \( \vec{u}_a^e \) (see Eq. (3.16)).

The momentum equation in the prediction step

As explained in the previous chapter, the momentum equation is split into two parts; one is the prediction step and the other is the correction step. In the prediction step, the momentum equations are based on the viscous term and external forces. Two forms of viscous term by
Monaghan and Morris are available in the SPARTACUS code, respectively:

\[
\frac{d\vec{u}_a}{dt} \approx \sum_b 8m_b \frac{\nu_{E,a} + \nu_{E,b}}{\rho_a + \rho_b} \frac{\vec{u}_{ab} \cdot \vec{r}_{ab}}{r_{ab}^2 + \eta^2} \nabla_a w_h(r_{ab}) + F_a^e
\]  

or

\[
\frac{d\vec{u}_a}{dt} \approx \sum_b m_b \frac{\rho_a \nu_{E,a} + \rho_b \nu_{E,b}}{\rho_a \rho_b} \frac{\vec{r}_{ab} \cdot \nabla_a w_h(r_{ab})}{r_{ab}^2 + \eta^2} \vec{u}_{ab} + F_a^e
\]  

where \( F_a^e \) corresponds to external forces applied on a particle \( a \).

### The pressure Poisson equation

Instead of the state equation in the original SPARTACUS code, pressure here is obtained from the pressure Poisson equation:

\[
\nabla^2 p_{n+1} = \frac{\rho}{\Delta t} \nabla \cdot \vec{u}^n
\]

where \( \nabla^2 \) is the Laplacian operator. The expression of \( \nabla \cdot \vec{u}^n \) is obtained from the procedure in Eq. (3.13). As it is known that the exact Laplacian shows the pressure decoupling effect (see Section 2.3.3), the approximated Laplacian operator is chosen and the form is as:

\[
\nabla^2 p_a \approx \frac{2}{\rho_a} \sum_b m_b \frac{\vec{p}_{ab} \cdot \nabla_a w_h(r_{ab})}{r_{ab}^2 + \eta^2}
\]

where \( \vec{p}_{ab} = \vec{p}_a - \vec{p}_b \). As mentioned in Section 2.7.2, two types of linear system solver are implemented without pre-conditioning; one is the Minimum Residual (MR) method and the other is the Bi-CGSTAB method [68]. The system is solved for fluid and edge particles only with indirect contributions of dummy particles. In other words, dummy particles are contributing to the right hand side of the pressure solution. The coding detail of the system is indicated in Section 3.2.4.

In addition, the exact Laplacian operator is also performed, which is slightly different from the one Cummins et al. proposed in Eq. (2.52) by considering the gradient of a constant is zero (see Eq. (2.12)). As mentioned in Section 2.1.2, the gradient of constant in SPH formulation does not satisfy zero near the boundaries due to the truncation of the kernel.
3.2. The ISPH SPARTACUS-2D code

compact support. Hence the exact Laplacian in the code is built from Eq. (2.32) and Eq. (3.13) as:

\[ G_a = (G_{SPH}p)_a = \frac{1}{\rho_a} \nabla p_a \approx \sum_b m_b \left( \frac{p_b}{\rho_a} + \frac{p_a}{\rho_b} \right) \nabla w_h(r_{ab}) \]  
(3.18)

then, divergence of this is:

\[ (D_{SPH}G_{SPH}p)_a = \nabla \cdot G_a \approx -\frac{1}{\rho_a} \sum_b m_b G_{ab} \cdot \nabla w_h(r_{ab}) \]  
(3.19)

where \( G_{ab} = G_a - G_b \). This is justified by the skew adjointness of both operators through Eq. (2.82).

The momentum equation in correction step

After the pressure is known, the predicted momentum equation is corrected as either:

\[ \frac{d\mathbf{u}_a^{n+1}}{dt} \approx \frac{d\mathbf{u}_a^n}{dt} - \sum_b m_b \left( \frac{p_a^{n+1}}{\rho_a} + \frac{p_b^{n+1}}{\rho_b} \right) \nabla w_h(r_{ab}) \]  
(3.20)

or

\[ \frac{d\mathbf{u}_a^{n+1}}{dt} \approx \frac{d\mathbf{u}_a^n}{dt} - \sum_b m_b \left( \frac{p_a^{n+1}}{\rho_a^2} + \frac{p_b^{n+1}}{\rho_b^2} \right) \nabla w_h(r_{ab}) \]  
(3.21)

The positions of particles

Some authors include the temporal positions \( r_a^* \) by the predicted velocity at the prediction step (e.g. [12]) though, the particles move only with the corrected velocity as Eq. (3.7) in our code.

3.2.2 Wall modelling and boundary conditions

The truly incompressible approach is developed with the dummy particles technique due to its simplicity. The wall is supported by one layer of edge particles and several layers of dummy particles. The number of dummy particles layer can be decided from the radius of compact support \( h_t \) [55]. When the pressure is obtained from the pressure Poisson equation for fluid and edge particles, dummy particles carry an identical pressure to edge particles normal to the wall. For this procedure, all the dummy particles have to be linked with the edge particles.
in their normal direction. In the case of free-surface flow, surface particles should be searched in order to apply zero pressure free-surface boundary condition, hence, a new algorithm to track the surface particles is implemented and explained in Chapter 6.

3.2.3 Time step and temporal integration

The only difference between WCSPH and ISPH in time step is the CFL condition by replacing the numerical speed of sound $c_0$ by maximum fluid velocity $u_{max}$ in Eq. (3.11) as:

$$\Delta t \leq \min \left( 0.4 \frac{h}{u_{max}}, 0.25 \min_a \left( \frac{h}{E_a} \right), 0.125 \min_a \left( \frac{h^2}{\nu_{E,a}} \right) \right)$$  (3.22)

The Reynolds-averaged Navier-Stokes and the position equations can be integrated in time with the predictor and corrector scheme as:

$$\begin{align*}
\mathbf{u}_a^{n+1} &= \mathbf{u}_a^n + \Delta t F_a^n \\
\mathbf{r}_a^{n+1} &= \mathbf{r}_a^n + \Delta t \left( \frac{1}{\rho} \nabla p_a^{n+1} \right) \\
\end{align*}$$  (3.23)

where $F_a^n$ correspond to the right hand side of Eq. (3.14) or (3.15).

3.2.4 Iterative methods linear solvers

By interpreting the system $AF = B$ for the pressure Poisson equation (see Section 3.2.1), the unpreconditioned Minimum Residual (MR) and Bi-CGSTAB method is rewritten in SPH formulation by replacing $A$ for the Laplacian operator $L$, $F$ for the pressure and $B$ for the right hand side of Eq. (3.16). The algorithms are rewritten corresponding to ISPH procedure.

Unpreconditioned Minimum Residual (MR) method

For each particle $a$, the right hand side of Eq. (3.16) is:

$$b_a = \frac{\rho_a}{\Delta t} \nabla \cdot \mathbf{u}_a$$  (3.24)

where $\mathbf{u}_a$ is expressed with SPH formulation in Eq. (3.13). According to Eq. (3.17),

$$L \mathbf{p}_a \approx \frac{2}{\rho_a} \sum_b m_b \frac{\mathbf{p}_{ab} \mathbf{r}_{ab} \cdot \nabla w_h(r_{ab})}{r_{ab}^2 + \eta^2}$$  (3.25)
3.2. The ISPH SPARTACUS-2D code

As defined in Table 2.1, \( z \) is pre-conditioned residual. However, since pre-conditioning has not been applied in this work yet, this plays the role of the residual itself. By substituting \( Lz_a \) for \( L\eta_a \), it gives:

\[
Lz_a \approx \frac{2}{\rho_a} \sum_b m_b \frac{z_{ab} r_{ab} \cdot \nabla_a \omega_b(r_{ab})}{r_{ab}^2 + \eta^2}
\]  

(3.26)

\[
\begin{align*}
  r^{r-1}_a &= b_a - L\eta^{r-1}_a \\
  z^r_a &= r^{r-1}_a \\
  \omega^r &= \frac{(r^{r-1}_a, Lz^r_a)}{(Lz^r_a, Lz^r_a)} \\
  p^r_a &= p^{r-1}_a + \omega^r z^r_a
\end{align*}
\]

Table 3.1: Unpreconditioned Minimum Residual algorithm in the code. Note that \((U, V) = \sum_{i=1}^{N} u_i v_i \) where \( N \) is the number of particles.

Unpreconditioned Bi-CGSTAB

As the same manner as shown previously, the identical expression is applied for \( L\eta_a \) and \( Ls_a \) in the algorithm (see Table 3.2), by replacing \( p_a \) with \( \eta_a \) and \( s_a \).

3.2.5 Code structure

The structure of the code is briefly introduced. Several algorithms for the ISPH approach have been examined (e.g. [35]) and one shown in Fig. 3.4. All the applications presented in this thesis are based on this algorithm.

3.2.6 Test of the Laplacian operator

The purpose of this test is to examine the Laplacian operators themselves. By replacing the pressure \( \mathbf{p} \) with a function \( f \) and setting the density and mass to unity in Eq. (3.17), 1-D problem is considered in an infinite channel as:

\[
\frac{\partial^2 f(z)}{\partial z^2} = -1
\]  

(3.27)
Chapter 3. The ISPH SPARTACUS-2D code

Figure 3.4: Simplified algorithm of SPARTACUS with the ISPH approach.
3.2. The ISPH SPARTACUS-2D code

\[ p_0^a \text{ is an initial guess; } r_0^a = b_a - L p_0^a; \]
\[ r_0^a \text{ is an arbitrary vector, such that } (r_0^a, r_0^a) \neq 0, \text{ e.g., } r_0^a = r_0^a; \]
\[ \gamma^0 = \alpha = \omega^0 = 1; \]
\[ \zeta_0^a = \eta_0^a = 0; \]

for \( i = 1, 2, 3, \ldots, \)
\[ \gamma^i = (r_0^a, r_0^{i-1}); \]
\[ \beta = (\gamma^i / \gamma^{i-1}) (\alpha / \omega^{i-1}); \]
\[ \eta_i^a = r_i^{i-1} + \beta (\eta_i^{i-1} - \omega^{i-1} \zeta_i^{i-1}); \]
\[ \zeta_i^a = L \eta_i^a; \]
\[ \alpha = \gamma_i / (r_0^a, \zeta_i^a); \]
\[ s_a = r_i^{i-1} - \alpha \zeta_i^a; \]
\[ t_a = L s_a; \]
\[ \omega^i = (t_a, s_a) / (t_a, t_a); \]
\[ p_i^a = p_i^{i-1} + \alpha \eta_i^a + \omega^i s_a; \]
if \( p_i^a \) is accurate enough then quit;
\[ r_i^a = s_a - \omega^i t_a \]

end

Table 3.2: Unpreconditioned Bi-CGSTAB algorithm in the code. Note that \((U, V) = \sum_{i=1}^{N} u_i v_i\) where \(N\) is the number of particles.

Its solution with zero boundary condition for \( f(z) \) is:
\[ f(z) = \frac{1}{2} z (H - z) \quad (3.28) \]

where \(H\) is the channel height.

For the numerical simulation, the channel size is defined as the ratio of the length to the width as 2 and it represents an infinite channel by using a periodic condition. In total, 1,189 particles are used (779 fluid particles, 82 edge particles and 328 dummy particles) having the particle distance \( \delta r / H = 0.05 \), where the channel width \( H = 1 \) m. In terms of SPH parameters, 3\(^{rd}\)-order kernel and the ratio of smoothing length \( h / \delta r = 1.3 \) are used with this number of particles. This test is carried out only for one time step and the convergence of the iterative method for the approximated and exact Laplacian operators is also compared.
The criterion $\theta$ to stop the iterative method is set at $10^{-4}$ (see Eq. (2.108)) for the approximate Laplacian operator and takes only 8 iterations. As shown in Fig. 3.5, the exact Laplacian does not converge at the same criterion as the approximated Laplacian, the criterion is thus changed to $\theta = 0.2$ and takes 98 iterations. While the result from the approximate Laplacian operator is perfectly matched with the analytical solution given by Eq. (3.28), the exact Laplacian shows overestimation along the channel depth with decoupling effect near the boundary (see Fig. 3.6). These decoupling and the convergence problems in the exact Laplacian operator are also mentioned by Cummins et al. [12].

Note that the approximate Laplacian operator shows a good performance here, but this is a very specific case. All the error sources are eliminated such as boundary conditions and numerical problems. These are discussed in the following chapters.

(a) Scale depending on the approximate one. (b) Scale depending on the exact one.

Figure 3.5: Convergence test of the exact and approximate Laplacian operator in the SPARTACUS-2D code.
3.2. The ISPH SPARTACUS-2D code

Figure 3.6: Examination of the approximate and exact Laplacian operators by solving 1-D problem Eq. (3.27) in the SPARTACUS-2D code (left: 2-D view, right: the comparisons with analytical solution).
Chapter 4

2-D SPH Benchmark Test Cases

Two test cases, lid-driven cavity flow and incompressible flow around a moving square inside a rectangular box, are taken from the SPHERIC list of verification test cases. SPHERIC (SPH European Research Interest Community) is an ERCOFTAC special interest group. The purpose of these tests is to validate truly incompressible (ISPH) algorithms of the SPARTACUS-2D code. Weakly compressible SPH (WCSPH) is also run to compare these two different approaches and show their benefits and drawbacks.

4.1 Lid-driven cavity flow

The lid-driven cavity flow has been widely used as a benchmark test case for various numerical methods in the last decades and is thus suitable for testing the WCSPH and ISPH algorithms. Two different Reynolds numbers, based on the lid velocity and the size of the cavity, namely 400 and 1,000, are studied and results are compared to Ghia et al. data [14] and to a finite volume based software (STAR-CD) data. The last set of results is referred to as “FV”.

4.1.1 Geometry of the system

This geometry corresponds to the one listed in the SPHERIC website [70] and shown in Fig. 4.1, the size $L$ is set at 1 m in both horizontal and vertical direction.
Figure 4.1: Configuration of the 2-D lid-driven cavity flow \((L = 1 \, m, U_{Lid} = 1 \, m/s)\).

### 4.1.2 System modelling

#### Fluid discretisation and wall modelling

The lid wall and solid walls consist of one layer of edge particles and four layers of dummy particles. Three different resolutions of initial fluid particle discretisations are presented for both WCSPH and ISPH at \(Re = 400\) as shown in Table 4.1.

<table>
<thead>
<tr>
<th>Fluid particles</th>
<th>1,521</th>
<th>4,761</th>
<th>9,801</th>
</tr>
</thead>
<tbody>
<tr>
<td>Edge particles</td>
<td>170</td>
<td>290</td>
<td>408</td>
</tr>
<tr>
<td>Dummy particles</td>
<td>720</td>
<td>1,200</td>
<td>1,672</td>
</tr>
<tr>
<td>Total particle number</td>
<td>2,411</td>
<td>6,251</td>
<td>11,881</td>
</tr>
</tbody>
</table>

Table 4.1: Fluid, edge and dummy particle discretisation for the 2-D lid-driven cavity flow at \(Re = 400\).

At \(Re = 1,000\), four different initial fluid particle distributions are presented for both WCSPH and ISPH, starting from the coarsest one with \(\delta r = 1/20 \, m\). The other distributions are respectively based on \(\delta r = 1/40 \, m\), \(\delta r = 1/80 \, m\), and finally \(\delta r = 1/160 \, m\). Going from one distribution to a finer one means that the number of fluid and boundary particles is
4.1. Lid-driven cavity flow

Fluid particles quadrupled.

<table>
<thead>
<tr>
<th></th>
<th>Fluid particles</th>
<th>361</th>
<th>1,521</th>
<th>6,241</th>
<th>25,281</th>
</tr>
</thead>
<tbody>
<tr>
<td>Edge particles</td>
<td>90</td>
<td>170</td>
<td>330</td>
<td>650</td>
<td></td>
</tr>
<tr>
<td>Dummy particles</td>
<td>400</td>
<td>720</td>
<td>1,360</td>
<td>2,640</td>
<td></td>
</tr>
<tr>
<td>Total particle number</td>
<td>851</td>
<td>2,411</td>
<td>11,881</td>
<td>28,571</td>
<td></td>
</tr>
<tr>
<td>Initial particle spacing: ( \delta r ) (m)</td>
<td>1/20</td>
<td>1/40</td>
<td>1/80</td>
<td>1/160</td>
<td></td>
</tr>
</tbody>
</table>

Table 4.2: Fluid, edge and dummy particle discretisation for the 2-D lid-driven cavity flow at \( Re = 1,000 \) for WCSPH and ISPH.

FV simulations are performed on a grid identical to that of Ghia et al. [14] who used 128 cells in horizontal and vertical directions (\( \delta r = 1/128 \) m).

**Simulation conditions**

The Reynolds number \( Re \) is defined as:

\[
Re = \frac{L \cdot U_{Lid}}{\nu}
\]

where \( U_{Lid} \) is the lid velocity and \( \nu \) the viscosity. The test case depends only on the Reynolds number, and in practice we chose to vary the viscosity, *i.e.* the cavity size \( L \), the constant lid velocity \( U_{Lid} \) and the density \( \rho \) are set to unity, as 1 m, 1 m/s and 1 kg/m\(^3\) respectively, such that \( \nu = \frac{1}{Re} \) as described in Table 4.3.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th>400</th>
<th>1,000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reynolds number: ( Re )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Viscosity: ( \nu ) (m(^2)s(^{-1}))</td>
<td>0.0025</td>
<td>0.001</td>
<td></td>
</tr>
</tbody>
</table>

Table 4.3: Physical characteristics of the 2-D lid-driven cavity flow.

In terms of SPH parameters, a \( 4^{th} \)-order kernel with a smoothing length ratio \( h/\delta r \) of 1.3 is used in both WCSPH and ISPH. Two sets of the numerical speed of sound in WCSPH is shown; one is ten times higher than lid velocity \( c_0 = 10U_{Lid} \) according to the usual practice...
in the SPH community and the other is much higher $c_0 = 100 U_{Lid}$ according to Issa et al. recommendations. In ISPH, the convergence is reached at the tolerance of $\theta = 0.01$ (see Eq. (2.108)) for both Reynolds numbers.

In FV, the spatial discretisation is second-order accurate, the velocity coupling is achieved by the SIMPLE algorithm, and the steady state is reached for a non-dimensional tolerance of $10^{-4}$ (see Eq. (2.108)) for both $Re = 400$ and 1,000.

4.1.3 Simulation results

All the results are presented with dimensionless quantities; the length is normalised by the cavity size $L$, the velocity components by the lid velocity $U_{Lid}$, the pressure by $\frac{1}{2} \rho U_{Lid}^2$ and the time by $T = \frac{L}{U_{Lid}}$, which is 1 s here.

The cavity flow at $Re = 400$

The convergence test in time is made with ISPH and presented in Fig. 4.2 based on the initial particle distance $\delta r/L = 1/100$. The horizontal and vertical velocity component profiles at the centre of the cavity are drawn at the physical time $t/T$ of 5.2, 15.6, 26.0, 52.0 and 260.0. From the physical time of $t/T = 15.6$, the ISPH results are getting close to Ghia et al.’s steady-state data [14] and it is even closer at $t/T = 260.0$. However, the differences of the profiles between at $t/T = 52.0$ and $t/T = 260.0$ are indistinguishable compared to the CPU time. All the following tests on the cavity flow are compared at $t/T = 52.0$. Now, the comparisons of horizontal velocity field between WCSPH and ISPH are shown in Fig. 4.3 including two different values of the numerical speed of sound in WCSPH based on the initial particle distance $\delta r/L = 1/100$. A void appears at the centre of the cavity with the normal definition of the numerical speed of sound $c_0 = 10 U_{Lid}$ (see Fig. 4.3 (a)). Such voids had also appeared in the recirculation behind backward-facing step [27], in the recirculation past a square cylinder presented in Chapter 5 or in a back-step flow or just behind the front corners of a moving square box in Section 4.2, inducing us to use a Mach number of 0.01 in most applications rather than $Ma = 0.1$ as mentioned in [27]. Although the void disappeared with higher numerical speeds of sound, the fluctuation of pressure in WCSPH is then extremely
4.1. Lid-driven cavity flow

Figure 4.2: ISPH convergence test in time for $Re = 400$ on 2-D lid-driven cavity flow at the centre of the domain at the given physical time $t/T$ with the initial particle spacing $\delta r/L = 0.01$.

large (see Fig. 4.4) and the positions of particles near the boundary in WCSPH are not as ordered as in ISPH (see Fig. 4.3 (a) and (b) for WCSPH and (c) for ISPH). The agreement between the ISPH and FV for both pressure and velocity fields is good, far superior than WCSPH.

Next, the influence of spatial resolution is examined and the results are plotted in Fig. 4.5 along with FV result, which correspond to Ghia et al.’s data. Horizontal and vertical velocity component profiles from WCSPH for $\delta r/L = 1/40$ look unrealistic. Higher resolutions produce more realistic results but are still far from FV data (see Fig. 4.5 (a) and (c)). On the other hand, ISPH gives a much improved estimation of both horizontal and vertical velocity components, even with the lowest resolution $\delta r/L = 1/40$ (see Fig. 4.5 (b) and (d)).

The cavity flow at $Re = 1,000$

The Reynolds number is increased to 1,000 and the convergence test in time is also made in ISPH with $\delta r/L = 1/100$ at the identical physical time as $Re = 400$ (see Fig. 4.6). While the ISPH results at $Re = 400$ are getting close to Ghia et al. data from the physical time of
Figure 4.3: Comparisons of horizontal velocity field from WCSPH, ISPH and converged FV for the 2-D lid-driven cavity flow at $Re = 400$. The initial particle spacing $\delta r/L = 0.01$ and the physical time is at $t/T = 52.0$ for both SPH methods.

At $t/T = 15.6$, the ISPH results at $Re = 1,000$ are from $t/T = 26.0$. As for the results from $t/T = 52.0$ and $t/T = 260.0$ are identical, the following results are compared at $t/T = 52.0$.

Four different spatial discretisation are now examined with an initial particle distance $\delta r/L$ between the closest neighbouring particles of $1/20$, $1/40$ $1/80$ and $1/160$. Horizontal
4.1. Lid-driven cavity flow

Figure 4.4: Comparisons of pressure from WCSPH, ISPH and converged FV for the 2-D lid-driven cavity flow at \( Re = 400 \). The initial particle spacing \( \delta r/L = 0.01 \) and the physical time is at \( t/T = 52.0 \) for both SPH methods.

and vertical velocity components depending on the initial particle distributions are plotted in Fig. 4.7 against Ghia et al. and FV data (\( \delta r/L = 1/128 \)). Again, WCSPH shows significant influence of the resolution or initial particle distribution, with results for the coarser cases \( \delta r/L = 1/20 \) and \( 1/40 \) being very far from the FV profiles (see Fig. 4.7 (a) and (c)). With WCSPH, the central solid body rotation effect seems to be captured reasonably but the wall
boundary layers are significantly thicker and this leads to severely underestimated velocity profile extremes. It is as if the viscosity was being strongly increased for coarser resolutions. This may be attributed to the random motion of particles (“wobble” due to large pressure fluctuations) which enhances momentum diffusion in a Brownian-like fashion. The results indicate that this “wobble” is much smaller with ISPH than WCSPH. ISPH shows a much smoother pattern (see Fig. 4.5 (b) and (d)) with regular but perhaps slow asymptotic con-
4.1. Lid-driven cavity flow

Figure 4.6: ISPH convergence test in time for $Re = 1,000$ on 2-D lid-driven cavity flow at the centre of the domain at the given physical time $t/T$ with the initial particle spacing $\delta r/L = 0.01$.

Convergence towards the accurate results of Ghia et al. [14]. This improved behaviour must be attributed to the correct pressure field from the ISPH.

The error analysis is performed for the error on the minimum and maximum of the vertical and horizontal velocity components rather than the classical $l_2$-norm. The absolute value of those quantities are plotted against particle spacing $\delta r/L$ in Fig. 4.8. The ISPH spatial order of accuracy is approximately unity. While the symmetrical formulation of SPH may lead one to expect second-order accuracy, this is clearly not the case for several reasons. This flow is dominated by viscous forces and boundary conditions. The latter can seriously decrease the order and the discretisation of the Laplacian operator, whether by Eq. (2.33) or (2.34), is rather crude. Further effects that reduce the order are for instance the irregular distribution of the particles (as opposed to the initial square lattice distribution) and the ratio of smoothing length to particle spacing, see Quinlan et al. [49] for instance.

Comparisons of pressure profiles are also plotted; the horizontal variation of pressure for both SPH methods with FV are shown in Fig. 4.9(a) and the bottom left - top right diagonal variation of pressure for ISPH with FV in Fig. 4.9(b). The pressure field is smooth for ISPH
in contrast to the WCSPH pressure field, which is very noisy. Moreover ISPH isobars show
a trend very close to FV. The most important factor is the pressure gradient than the pressure
value itself. The shifting between pressure from ISPH and FV plotted in Fig. 4.9 (a) is hence
no relevant.

Velocity vectors are now compared at the corners of the cavity. WCSPH and ISPH sim-
ulations both capture the secondary flows observed at this Reynolds number in the left and
4.1. Lid-driven cavity flow

Figure 4.8: 2-D ISPH lid-driven cavity flow error estimation with spatial resolution influences for $Re = 1,000$.

Figure 4.9: 2-D SPH lid-driven cavity flow pressure profiles at $t/T = 52.0$ against to converged FV for $Re = 1,000$.

right bottom corners of the cavity. An enlargement of the right bottom corner vortex from WCSPH, ISPH and FV is drawn in Fig. 4.10 (b) (d) (f), where unit vectors are used to show direction. The centre of the right secondary vortex is well predicted by all methods: WCSPH
(0.85; 0.10), ISPH (0.87; 0.11) and FV (0.86; 0.11). However, the velocity in the first layer of fluid particles is not very smooth when predicted by WCSPH. An enlargement of the left top corner is also presented in Fig. 4.10 (a) (c) (e) from each method. Once again, the WCSPH wall treatment is not smooth. Overall, ISPH shows more coherent velocity fields while WCSPH exhibits small scale instabilities mentioned earlier.

The simulations were carried out on a Intel (R) PENTIUM D CPU 3.2GHz with 2.0 G RAM with 32 bits. The time step and CPU time for the case of \( \text{Re} = 1,000 \) are indicated in Table 4.4.

<table>
<thead>
<tr>
<th></th>
<th>WCSPH ((c_0 = 100 U_{\text{Lid}}))</th>
<th>ISPH</th>
<th>FV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time step: ( \delta t/T )</td>
<td>3.25 (10^{-5})</td>
<td>3.25 (10^{-3})</td>
<td>steady</td>
</tr>
<tr>
<td>CPU time ((h))</td>
<td>179.0</td>
<td>19.5</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Table 4.4: The comparisons of the 2-D lid-driven cavity flow CPU time for \( \text{Re} = 1,000 \) with \( \delta r/L = 1/160 \) for all methods, up to the physical time \( t/T = 52.0 \) for the SPH cases. Note that the linear solver in ISPH is without pre-conditioning.

The longer CPU time in WCSPH can be explained by the fact that high numerical speed of sound was required to prevent the appearance of a void in the cavity centre thus imposing the use of a very small time step. It must be noted that some fluid particles exited from the cavity in ISPH and WCSPH with the normal definition of the numerical speed of sound. For example ISPH with \( \delta r/L = 1/160 \), the fluid particles lost were about 2.0% from the top two corners, where velocity discontinuities occur due to the moving lid on the top and stationary walls on both sides. With the finer spatial resolutions, there were less proportionally exiting particles. In the case of WCSPH with \( c_0 = 10 U_{\text{Lid}} \), about 0.3% of fluid particles were going out along the lid and top corners. However, this did not occur in WCSPH with the higher numerical speed of sound.

### 4.1.4 Partial conclusions

Two different Reynolds number \( \text{Re} = 400 \) and \( \text{Re} = 1,000 \) were performed on 2-D lid-driven cavity flow for WCSPH and ISPH. The lower Reynolds number simulations converged
faster than the higher Reynolds number ones. As well-known for SPH, the pressure in WC-SPH is very noisy but the velocities are predicted with acceptable results. Smoother pressure and velocity fields and shorter CPU time are found in ISPH. Due to the velocity discontinuity at the wall, some particles exited in both ISPH and WCSPH with normal definition of speed of sound method but this did not occur in WCSPH with higher speed of sound.
Figure 4.10: 2-D lid-driven cavity flow for uniform velocity vectors at the top left and bottom right corners at $Re = 1,000$ from WCSPH, ISPH and FV. The initial particle distance for both SPH methods is $\delta r/L = 1/160$ and $\delta r/L = 1/128$ for FV.
4.2 Incompressible flow around a moving square in a rectangular box

This work deals with comparisons between ISPH and a Finite Difference solver (henceforth FD) to compute an incompressible flow around a moving square set in a rectangular box and also presented in Lee et al. [39]. All comparisons are made in terms of velocity magnitude and pressure at $Re = 50$, $100$ and $150$. WCSPH is also compared at only $Re = 100$.

4.2.1 Geometry of the system

The geometry is defined according to the SPHERIC benchmark [69] and shown in Fig. 4.11. The square in the geometry is at $t = 0.0$ s and moves along the horizontal direction with a prescribed motion, starting from rest and accelerating to a final steady maximum velocity.

![Fig. 4.11: Geometry of 2-D incompressible flow around a moving square inside a rectangular box (unit: m).](image)

4.2.2 System modelling

Fluid discretisation and wall modelling

Four different initial fluid particle discretisations are presented in Table 4.5. All the results shown in this section are based on $\delta r = 1/60$ m, which is the same as the grid size used in
FD. The square moving box and rectangular solid walls consist of a layer of edge particles and four layers of dummy particles.

<table>
<thead>
<tr>
<th>Fluid particles</th>
<th>19,260</th>
<th>43,590</th>
<th>77,720</th>
<th>175,380</th>
</tr>
</thead>
<tbody>
<tr>
<td>Edge particles</td>
<td>680</td>
<td>1,020</td>
<td>1,360</td>
<td>2,040</td>
</tr>
<tr>
<td>Dummy particles</td>
<td>2,720</td>
<td>4,080</td>
<td>5,440</td>
<td>8,160</td>
</tr>
<tr>
<td>Total particle number</td>
<td>22,660</td>
<td>48,690</td>
<td>84,520</td>
<td>185,580</td>
</tr>
<tr>
<td>Initial particle spacing: $\delta r (m)$</td>
<td>1/20</td>
<td>1/30</td>
<td>1/40</td>
<td>1/60</td>
</tr>
</tbody>
</table>

Table 4.5: Fluid, edge and dummy particle discretisation for the 2-D incompressible flow around a moving square set inside a rectangular box for WCSPH and ISPH.

Simulation conditions

The square moving box size $L$, the maximum velocity of the box $U_{\text{max}}$ and the density $\rho$ are set to unity, as 1 $m$, 1 $m/s$ and 1 $kg/m^3$ respectively, such that $\nu = \frac{1}{Re}$. Three different Reynolds numbers ($Re = 50, 100, 150$) are examined with ISPH and compared with the result from FD and WCSPH only at $Re = 100$. The movement of the box is identical with FD. In terms of SPH parameters, a $4^{th}$-order kernel with a smoothing length ratio $h/\delta r$ of 1.3 is used in both WCSPH and ISPH. Two different numerical speed of sound are presented; one is the normal definition of $c_0 = 10U_{\text{max}}$ and the other is higher at $c_0 = 100U_{\text{max}}$. In ISPH, the convergence is reached at the tolerance of $\theta = 0.1$ instead of $\theta = 0.01$ for the linear solver (see Eq. (2.108)) possibly due to compressible effects in accelerating flow. The results with the tolerance of $\theta = 0.01$ in ISPH and the numerical speed of sound $c_0 = 30U_{\text{max}}$ in WCSPH were presented in Lee et al. [39].

4.2.3 Simulation results

Again, all the results are presented with dimensionless quantities; the length is normalised by the moving square size $L$, the velocity magnitude by the maximum velocity of the box $U_{\text{max}}$, the pressure by $\rho U_{\text{max}}^2$ and the time by $T = \frac{L}{U_{\text{max}}}$, which is 1 $s$. $ModV$ and $Press$ in each
4.2. Incompressible flow around a moving square in a rectangular box

Figure indicate that \( \text{ModV} = \sqrt{\frac{u^2 + u^2}{U_{\text{max}}}} \) and \( \text{Press} = \frac{p(x, z) - p(0, 0)}{\rho U_{\text{max}}^2} \), where \( p(0, 0) \) is the pressure of left bottom corner of the rectangular box.

Before presenting the results for each Reynolds number, the relations between time step, spatial resolutions and Reynolds number are performed. Table 4.6 shows the procedure of the simulation depending on spatial resolutions and Reynolds number at the time step used in FD, which is \( \delta t / T = 9.009 \times 10^{-3} \); ‘yes’ indicates that the simulation runs until the end of the simulations, ‘no’ for the crashed simulations. This can be explained with Fourier

<table>
<thead>
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<th></th>
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<th>50</th>
<th>100</th>
<th>150</th>
</tr>
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<td>yes</td>
<td>yes</td>
<td></td>
</tr>
<tr>
<td>( \delta r / L = 1/40 )</td>
<td>no</td>
<td>yes</td>
<td>yes</td>
<td></td>
</tr>
<tr>
<td>( \delta r / L = 1/60 )</td>
<td>no</td>
<td>no</td>
<td>no</td>
<td></td>
</tr>
</tbody>
</table>

Table 4.6: Effect of resolution vs \( Re \) at the time step \( \delta t / T = 9.009 \times 10^{-3} \) used in FD.

![Velocity and Pressure](image)

(a) At the physical time \( t / \delta t = 14 \)

(b) At the physical time \( t / \delta t = 15 \)

Figure 4.12: One example of crashed simulation at \( Re = 50 \) with the time step \( \delta t = 9.009 \times 10^{-3} \) s. The initial particle distance \( \delta r / L = 1/60 \).

number \( \frac{v \Delta t}{\delta r^2} \). For explicit method in Eulerian schemes, this method will be stable if Fourier
number is less than 0.5. In SPH, this criteria is reduced to 0.125 (see Section 2.4), and the
smoothing length $h$ is used instead of $\delta r$ since the smoothing length is similar to the mesh
size in Eulerian methods. Then, the time step used in FD is larger than this condition and it
causes the simulations to crash by erroneously locating the fluid particles as shown in Fig.
4.12. Here, two different snap shots can be seen, just before crashing, for both velocity and
pressure.

**Comparisons among WCSPH, ISPH and FD at $Re = 100$**

First of all, WCSPH results with the numerical speed of sound $c_0 = 10U_{max}$ are shown in
Fig. 4.13 in terms of the velocity magnitude at $t/T = 5.0$ and $8.0$. The voids appear in the
wake and just behind the front corners of the moving box as occurred at the centre of the
cavity in 2-D lid-driven cavity flow. As already shown earlier in this chapter, increasing the
numerical speed of sound reduces the size of the voids. By increasing the numerical speed

![WCSPH Velocity Magnitude](image1)

(a) At the physical time $t/T = 5.0$

![WCSPH Velocity Magnitude](image2)

(b) At the physical time $t/T = 8.0$

Figure 4.13: WCSPH velocity magnitude at $Re = 100$ with the numerical speed of sound
$c_0 = 10U_{max}$. The initial particle distance $\delta r/L = 1/60$. 
of sound as \( c_0 = 100U_{\text{max}} \) in WCSPH, the voids are very tiny and repeated appearance and disappearance while the moving square is approaching near to the opposite end. A very tiny void at \( t/T = 8.0 \) appears around the front top and bottom corners (not possible to show this using contouring software). The ISPH results are compared with WCSPH and FD at \( t/T = 5.0 \) and 8.0.

In terms of velocity magnitude, all three patterns look similar but the maximum backflow behind the cylinder is one level lower in WCSPH (see Figs. 4.14 and 4.15) and the sharp angle of the isolines in front at the symmetry line in both WCSPH and ISPH is in contrast with the rounded FD solution (see Fig. 4.14).

In terms of pressure contours, WCSPH shows extreme levels of fluctuations which cannot be interpreted as a physical pressure field, mainly in the wake of the square box. ISPH pressure pattern compares realistically with FD, even if the peak in front and depletion at the rear appear slightly different (see Figs. 4.16 and 4.17).

This case with ISPH is simulated also for the lower spatial resolutions indicated in Table 4.5. All the results from lower resolutions are similar to the ones presented here except the case with \( \delta r/L = 1/20 \); the sharp angle of the isolines in front is not shown and even better agreement in pressure at the upstream is found.

**Comparisons between ISPH and FD at \( Re = 50 \)**

Comparisons between ISPH and FD are now presented at \( Re = 50 \) at \( t/T = 5.0 \) and 8.0 (see from Fig. 4.18 to Fig. 4.21).

The same general agreement as obtained previously is observed with the velocity magnitude for the wake and acceleration around the corners, especially at \( t/T = 8.0 \) (see Fig. 4.19). However the sharp angle of the isolines in front at the symmetry line is seen to be exacerbated at this Reynolds number (see Fig. 4.18).

In terms of pressure, the stagnation point pressure build-up at this Reynolds number propagates far upstream compared to the FD solution (see Fig. 4.20).
Figure 4.14: Velocity magnitude at the physical time $t/T = 5.0$ for $Re = 100$. The spatial discretisation $\delta r/L = 1/60$ for both SPH methods and FD.

**Comparisons between ISPH and FD at $Re = 150$**

Again, the results from ISPH and FD are compared at $Re = 150$ at $t/T = 5.0$ and 8.0 (see from Fig. 4.22 to Fig. 4.25). The same fair agreement and similar behaviour as shown with $Re = 50$ and 100 are repeated for the wake and acceleration around the corners. The ISPH pressure prediction gives slightly better results than for the lower Reynolds number cases.
4.2. Incompressible flow around a moving square in a rectangular box

Figure 4.15: Velocity magnitude at the physical time $t/T = 8.0$ for $Re = 100$. The spatial discretisation $\delta r/L = 1/60$ for both SPH methods and FD.

Comparisons of pressure drag coefficients

Time histories of pressure drag coefficients for each Reynolds number are presented in Fig. 4.26 by comparing the ISPH results against FD ones. Slight overestimation of the drag coefficient is shown for $Re = 50$ while the ISPH predictions for $Re = 100$ and 150 are scattered around the FD solution.

The simulations were carried out on a Intel (R) PENTIUM D CPU 3.2GHz with 2.0 G
Figure 4.16: Pressure at the physical time $t/T = 5.0$ for $Re = 100$. The spatial discretisation $\delta r/L = 1/60$ for both SPH methods and FD.

RAM with 32 bits. The time step and CPU time for each Reynolds number are indicated in Table 4.7.

### 4.2.4 Partial conclusions

Comparisons of ISPH and FD in the case of a moving square box set in a rectangular box are performed at $Re = 50$, 100 and 150. Generally speaking, the results from ISPH are
4.2. Incompressible flow around a moving square in a rectangular box

Figure 4.17: Pressure at the physical time \( t/T = 8.0 \) for \( Re = 100 \). The spatial discretisation \( \delta r/L = 1/60 \) for both SPH methods and FD.

Close to FD’s. ISPH shows a major improvement compared to WCSPH in computing flows involving bluff bodies, as no voids and no strong pressure fluctuations appear with ISPH. The void in WCSPH might be cured by increasing the numerical speed of sound, but the pressure fluctuation still remains. ISPH pressure pattern is much smoother, looks fairly similar to FD’s and is physically more realistic. The scattered pressure drag coefficients from ISPH need to be investigated further with different spatial resolutions or discretisation of the viscous forces. This chapter has shown that the ISPH solver performs well for difficult test cases. In the next
Chapter 4. 2-D SPH Benchmark Test Cases

Figure 4.18: Velocity magnitude at the physical time $t/T = 5.0$ for $Re = 50$. The spatial discretisation $\delta r/L = 1/60$ for both ISPH and FD.

Chapter, the ISPH solver will be applied to flow past a stationary square cylinder.
4.2. Incompressible flow around a moving square in a rectangular box

Figure 4.19: Velocity magnitude at the physical time $t/T = 8.0$ for $Re = 50$. The spatial discretisation $\delta r/L = 1/60$ for both ISPH and FD.

Figure 4.20: Pressure at the physical time $t/T = 5.0$ for $Re = 50$. The spatial discretisation $\delta r/L = 1/60$ for both ISPH and FD.
Figure 4.21: Pressure at the physical time $t/T = 8.0$ for $Re = 50$. The spatial discretisation $\delta r/L = 1/60$ for both ISPH and FD.

Figure 4.22: Velocity magnitude at the physical time $t/T = 5.0$ for $Re = 150$. The spatial discretisation $\delta r/L = 1/60$ for both ISPH and FD.
4.2. Incompressible flow around a moving square in a rectangular box

Figure 4.23: Velocity magnitude at the physical time $t/T = 8.0$ for $Re = 150$. The spatial discretisation $\delta r/L = 1/60$ for both ISPH and FD.

Figure 4.24: Pressure at the physical time $t/T = 5.0$ for $Re = 150$. The spatial discretisation $\delta r/L = 1/60$ for both ISPH and FD.
Figure 4.25: Pressure at the physical time $t/T = 8.0$ for $Re = 150$. The spatial discretisation $\delta r/L = 1/60$ for both ISPH and FD.

Table 4.7: CPU time and adjusted time steps for WCSPH and ISPH with the resolution of $\delta r/L = 1/60$ ($\delta t_F = 9.009 \times 10^{-3}$ s): the time step used in FD). Note that the linear solver in ISPH is without pre-conditioning.
4.2. Incompressible flow around a moving square in a rectangular box

Figure 4.26: Time histories of pressure drag coefficients ($C_{Dp}$). The spatial discretisation $\delta r/L = 1/60$ for ISPH (blue) and FD (red).
Chapter 5

2-D Laminar Flow past a Bluff Body in a Channel

Separated flows often take place in engineering problems as seen, for example, in flows over steps and fences, and around bluff bodies (Nakagawa et al. [47]). This is therefore a fundamental flow phenomenon. As a starting point, a laminar flow in a closed channel without a bluff body was simulated and reported in [35]. By locating a cylinder in a channel, laminar simulations around a bluff body are attempted at various different Reynolds numbers \( Re_d = 2, 20, 50 \) and 100, based on the mean bulk velocity at the inlet \( U_0 \) and the width of the cylinder \( d \). However, the present work comparing WCSPH, ISPH and FV (STAR-CD) is made only at \( Re_d = 20 \) and 100 with a square cylinder since some other parts of these results are already presented in [36]. The simulations on a circular cylinder are also carried out, however, these are not presented here but can be found in Lee et al. [37].

5.1 Theoretical investigation

In a laminar channel flow, by assuming the fluid velocity is not changed in time the momentum equation can be written as:

\[
0 = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \frac{\partial^2 u}{\partial z^2} + F^e
\]

(5.1)
where $F^e$ denotes an external force per unit mass to drive the fluid where it is required. Since the horizontal variation remains constant, Eq. (5.1) can be rewritten as:

$$\nu \frac{\partial^2 u}{\partial z^2} = -F^e \tag{5.2}$$

By integrating this with the zero velocity boundary condition, the horizontal velocity $u(z)$ will be obtained as:

$$u(z) = \frac{F^e}{2\nu} z(H - z) \tag{5.3}$$

where $H$ is a channel depth. Then, the mean bulk velocity $U$ is derived from:

$$U = \frac{1}{H} \int_0^H u(z)dz = \frac{H^2}{12\nu} F^e \tag{5.4}$$

The horizontal velocity $u(z)$ with the mean bulk velocity $U$ is:

$$u(z) = \frac{6U}{H^2} z(H - z) \tag{5.5}$$

### 5.2 Geometry of the system

The geometry of the configuration is based on Kim et al. [30] and shown in Fig. 5.1. The cylinder of dimension $d$ is located centrally in-between two flat plates placed a distance of $5d$ apart; the upstream end of the domain is $3d$ from the cylinder and the length to the downstream end $L_d = 28d$ for $Re_d = 20$ and $L_d = 98d$ for $Re_d = 100$, to ensure that the flow re-develops downstream of the cylinder.

### 5.3 System modelling

#### 5.3.1 Fluid discretisation and wall modelling

The fluid discretisations are described in Table 5.1 by having a uniform initial particle spacing of $1/10$ m or $1/20$ m. Again, one layer of edge particles and four layers of dummy particles are used for wall and square cylinder boundaries.

For FV (STAR-CD) simulations, a uniform mesh with spacing equal to the SPH particle spacing $\delta r = 0.05$ m is used for both Reynolds number. The mesh has 63,600 cells for $Re_d = 20$ and 203,600 cells for $Re_d = 100$. 
5.3. System modelling

![Geometry of the 2-D bluff body in the case of square cylinder (d = 1 m).](image)

Figure 5.1: Geometry of the 2-D bluff body in the case of square cylinder (d = 1 m).

<table>
<thead>
<tr>
<th></th>
<th>$L_d = 28 d$</th>
<th>$L_d = 98 d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluid particles</td>
<td>15,608</td>
<td>63,018</td>
</tr>
<tr>
<td>Edge particles</td>
<td>682</td>
<td>1,362</td>
</tr>
<tr>
<td>Dummy particles</td>
<td>2,648</td>
<td>5,368</td>
</tr>
<tr>
<td>Total particle number</td>
<td>18,938</td>
<td>69,748</td>
</tr>
<tr>
<td>Initial particle spacing: $\delta r$ (m)</td>
<td>0.1</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Table 5.1: Fluid, edge and dummy particle discretisation for the 2-D bluff body (d: the width of the square cylinder (= 1 m), $L_d$: the length from the cylinder to the downstream end).

5.3.2 Simulation conditions

This is a purely numerical test case so the square cylinder size d, the mean bulk velocity at the inlet $U_0$ and the density $\rho$ are set to unity as 1 m, 1 m/s and 1 kg/m$^3$ respectively, such that $\nu = \frac{1}{Re_d}$.

Periodic inflow-outflow boundary conditions are imposed, the flow being driven by a force relative to the prescribed mean bulk velocity at the inlet, which allows constant flow rate at each time step.

In terms of SPH parameters, a $4^{th}$-order kernel and smoothing length ratio $h/\delta r$ of 1.3 are used both for WCSPH and ISPH. For the CFL condition (see Eq. (3.22)), the numerical speed of sound $c_0 = 100$ m/s for WCSPH and maximum fluid velocity $u_{max} = 2$ m/s for ISPH are set. Running WCSPH with the usual numerical speed of sound value leads to the
appearance of a void downstream of the cylinder, this phenomenon having also been observed for the lid-driven cavity case (see Section 4.1) and the moving box (Section 4.2). In ISPH, the convergence is reached at the tolerance of $\theta = 0.01$ for $Re_d = 20$ and $0.2$ for $Re_d = 100$ to obtain pressure (see Eq. (2.108)).

For FV (STAR-CD) simulations, the first case at $Re_d = 20$ is run in steady motion. The second case at $Re_d = 100$ is treated as a transient flow, with a PISO algorithm to solve the velocity-coupling and an Euler implicit time-stepping scheme. This combination (PISO and Euler) has been proved to be second order accurate in time (Perić [48]). For both Reynolds numbers, a central difference scheme is used for convection and the time step is $0.025$ s.

5.4 Simulation results

All the results are presented as dimensionless quantities; the length is normalised by the width of the cylinder $d$, the velocity components by the mean bulk velocity at the inlet $U_0$, the pressure by $\frac{1}{2} \rho U_0^2$ and the time by $T = \frac{d}{U_0}$, which is 1 s.

5.4.1 A laminar flow past a bluff body at $Re_d = 20$

Since the flow is symmetrical about the longitudinal axis in this case, the fluid domain is divided at $Z/d = 0$; the upper part is the SPH results and the lower is the FV results in the figures of the comparisons of horizontal velocity magnitude contour. Both SPH results are compared at the physical time $t/T = 322.0$ against the converged FV; the comparisons WC-SPH against FV is in Fig. 5.2 (a) and ISPH against FV is in Fig. 5.2 (b) for different spatial resolution between SPH ($\delta r/d = 0.1$) and FV ($\delta r/d = 0.05$). Identical spatial resolution ($\delta r/d = 0.05$) for both SPH methods and FV is presented in Fig. 5.3.

The trend observed for the cavity flow is repeated here, i.e. ISPH shows a smoother velocity field than WCSPH which was obvious with the coarse spatial resolution. The finer spatial resolution gives smoother horizontal velocity for both SPH methods and even better agreement of ISPH with FV while WCSPH is less good (see Fig. 5.3). The flow near to the downstream is also illustrated and compared with the analytical solution given by Eq. (5.5) at the outlet to prove that the flow outlet does not have the influence of the bluff body located
5.4. Simulation results

(a) WCSPH at $t/T = 322.0$ (up, $\delta r/d = 1/10$) vs converged FV (down, $\delta r/d = 1/20$)

(b) ISPH at $t/T = 322.0$ (up, $\delta r/d = 1/10$) vs converged FV(down, $\delta r/d = 1/20$)

Figure 5.2: Comparisons of horizontal velocity magnitude contours for $Re_d = 20$. A zoom from $X/d = -4$ to $X/d = 10$ is presented.

near upstream (see Fig. 5.4).

Both SPH results are time-averaged for post-processing reasons and the time-averaged pressure and velocity vectors are also presented against FV results. The time-averaged pressure contour from $X/d = -4$ to $X/d = 6$ is shown in Fig. 5.5. The time-averaged pressure from WCSPH now has a physical flow pattern and comparable with ISPH and FV while the instantaneous pressure field shows high fluctuations.

The central pressure profile in the channel along the axial direction is also plotted in Fig. 5.7. Since the flow is driven by the constant mass flow rate at the inlet with periodic boundary condition, the pressure obtained from SPH is periodic. As a result, it does not show the pressure drop (see Fig. 5.6). This periodic pressure thus needs to be corrected to
Chapter 5. 2-D Laminar Flow past a Bluff Body in a Channel

Figure 5.3: Comparisons of horizontal velocity magnitude contours with \( \delta r/d = 1/20 \) for all methods at \( Re_d = 20 \). A zoom from \( X/d = -4 \) to \( X/d = 10 \) is presented.

obtain the real pressure by subtracting the body force, which can be assumed from Eq. (5.4).

The pressure drop for WCSPH, ISPH and FV is plotted in Fig. 5.7 and a good agreement is observed.

The time-averaged pressure drag coefficients are now calculated for the WCSPH and ISPH method and steady state pressure drag coefficient for FV. Each drag coefficient is indicated in Table 5.2. Although a good agreement on the pressure pattern is found for both WCSPH and ISPH method, the pressure drag coefficient shows discrepancies. Hence, the pressure on the cylinder is shown in Fig. 5.8. WCSPH shows a large fluctuation on the cylinder leading to the high pressure-drag coefficient. For ISPH, the pressure near corners (left side of top and bottom) seemed to be smoothed compared to FV ones. As shown in Section
5.4. Simulation results

(a) 2-D view from $X/d = 18$ to $X/d = 28$  
(b) Velocity profile at the outlet with analytical solution Eq. (5.5).

Figure 5.4: ISPH horizontal velocity at the downstream of the channel at $t/T = 322.0$ with $\delta r/d = 1/20$ for $Re_d = 20$.

<table>
<thead>
<tr>
<th>Methods</th>
<th>WCSPH</th>
<th>ISPH</th>
<th>FV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drag coefficient: $C_{D,p}$</td>
<td>14.56</td>
<td>3.48</td>
<td>4.31</td>
</tr>
<tr>
<td>Ratio of SPH to FV</td>
<td>3.38</td>
<td>0.81</td>
<td>–</td>
</tr>
</tbody>
</table>

Table 5.2: Comparisons of the time-averaged drag and lift coefficients at $Re_d = 20$ with $\delta r/d = 0.05$ for SPH and FV.

Pressures at the corner for dummy particles are averaged, and so might be the reason for the lower estimation of the pressure drag coefficient. This has clearly demonstrated that drag coefficients based on the WCSPH are unreliable.

Lastly, time-averaged velocity vectors are plotted in Fig. 5.9 to compare the recirculation length among WCSPH, ISPH and FV with the influence of the spatial resolution. The recirculation in WCSPH are poorly predicted for both spatial resolution, an asymmetrical behaviour behind of the cylinder is even produced by finer one. On the other hand, ISPH shows a good agreement with FV and is improved with finer spatial resolution.

5.4.2 A laminar flow past a bluff body at $Re_d = 100$

The horizontal velocity magnitude contours of $Re_d = 100$ are plotted in Fig. 5.10 by comparing WCSPH, ISPH and FV at the physical time $t/T = 520.0$. The WCSPH result appears
Figure 5.5: Comparisons of time-averaged pressure coefficient \( (C_p) \) distributions for \( Re_d = 20 \) with the spatial resolution \( \delta r/d = 1/20 \) for all methods. A zoom from \( X/d = -4 \) to \( X/d = 6 \) is presented.
5.4. Simulation results

Figure 5.6: An example of time-averaged centreline pressure coefficient ($C_p$) from ISPH for $Re_d = 20$. Note that the pressure at the inlet and outlet is identical due to the periodic boundary condition.

Figure 5.7: Comparisons of time-averaged corrected centreline pressure coefficient ($C_p$) distributions from WCSPH (black), ISPH (blue) and FV (red) methods for $Re_d = 20$.

Figure 5.8: Comparisons of time-averaged pressure coefficient on the square cylinder edge for $Re_d = 20$ with the spatial resolution $\delta r/d = 1/20$ for all methods.
Figure 5.9: Time-averaged WCSPH and ISPH velocity vectors behind of the square cylinder against converged FV for $Re_d = 20$. Velocity vectors are uniformly distributed.
to be very noisy and the shedding itself is not realistic. A void downstream of the cylinder is again present. Whereas ISPH and FV simulations look to be in phase and show the same shedding past the cylinder.

The frequency of the vortex shedding is compared for ISPH and FV. The Strouhal number $f d / U_0$, where $f$ is frequency, is calculated. ISPH gives a period $1/f$ of 2.05 and FV of 2.0 which leads to $St = 0.49$ for ISPH and $St = 0.50$ for FV. The flow near to the downstream is also illustrated and compared with the analytical solution given by Eq. (5.5) at the outlet to prove that the flow outlet does not have an influence of the bluff body located near upstream (see Fig. 5.11).

The pressure contours at $t/T = 520.0$ are also depicted in Fig. 5.12 from $X/d = -4$ to $X/d = 14$ only for ISPH against FV. Low pressure regions are located at the centre of each vortex that has been shed. The ISPH scheme correctly predicts this validating the method. There is a small asymmetry either side of the cylinder.

The time-averaged pressure drag and lift coefficients are calculated for ISPH and FV and shown in Table 5.3. The lift coefficient of 0.03 in ISPH might be a consequence of asymmetry at the upstream. It might be due to periodic boundary condition and the domain might be not long enough for the wake to become fully symmetrical again.

<table>
<thead>
<tr>
<th>Methods</th>
<th>$C_D$</th>
<th>$C_L$</th>
</tr>
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<tbody>
<tr>
<td>ISPH</td>
<td>2.46</td>
<td>0.03</td>
</tr>
<tr>
<td>FV</td>
<td>3.10</td>
<td>0.00</td>
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Table 5.3: Comparisons of the time-averaged pressure drag and lift coefficients at $Re_d = 100$ with $\delta r/d = 0.1$ for ISPH and $\delta r/d = 0.05$ for FV ($C_D$: drag coefficient, $C_L$: lift coefficient).

The CPU time for all methods is given in Table 5.4 with same spatial discretisation $\delta r/d = 1/10$ for SPH and FV. The small CPU time for ISPH is due to the small number of iterations needed for convergence of the pressure Poisson equation in this case. This demonstrates the robustness and advantage of the ISPH scheme.
Figure 5.10: Comparisons of instantaneous horizontal velocity magnitude contours for $Re_d = 100$ at the physical time $t/T = 520.0$ for all methods. A zoom from $X/d = -4$ to $X/d = 12$ is presented.

5.5 Partial conclusions

A laminar flow around a bluff body in a closed channel were examined for various flow conditions, $Re_d = 2, 20, 50$ and 100, with ISPH approach. The vortex shedding in ISPH ap-
5.5. Partial conclusions

(a) 2-D view from $X/d = 88$ to $X/d = 98$

(b) Velocity profile at the outlet with analytical solution Eq. (5.5).

Figure 5.11: ISPH horizontal velocity at the downstream of the channel at $t/T = 520.0$ with $\delta r/d = 1/10$ for $Re_d = 100$.

(a) ISPH ($\delta r/d = 1/10$)

(b) FV ($\delta r/d = 1/20$)

Figure 5.12: Comparisons of instantaneous pressure contours for $Re_d = 100$ at the physical time $t/T = 520.0$ for all methods. A zoom from $X/d = -4$ to $X/d = 16$ is presented.

appeared at $Re_d = 50$. However, only two cases at $Re_d = 20$ and 100 with a square cylinder are presented in this work by comparing the results among WCSPH, ISPH and FV. Velocity, pressure and pressure drag and lift coefficients are evaluated. Strouhal number is also estimated
<table>
<thead>
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<th>Methods</th>
<th>WCSPH</th>
<th>ISPH</th>
<th>FV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time step: $\delta t/T$</td>
<td>$5.2 \times 10^{-3}$</td>
<td>$2.6 \times 10^{-1}$</td>
<td>$5 \times 10^{-1}$</td>
</tr>
<tr>
<td>CPU time (h)</td>
<td>305.5</td>
<td>13.0</td>
<td>42.9</td>
</tr>
</tbody>
</table>

Table 5.4: CPU time for the bluff body flow at $Re_d = 100$ with $\delta r/d = 0.1$ at the same physical time $t/T = 520.0$.

for $Re_d = 100$ for ISPH and FV. In general, the ISPH results for both $Re_d = 20$ and 100 showed a good agreement to the FV. WCSPH was less good and even worse at $Re_d = 100$. A time-average of pressure for WCSPH showed similar patterns as ISPH and FV. However, the pressure drag coefficient in WCSPH was relatively high, which is a consequence of the high fluctuation of the pressure on the cylinder facing to upstream. Moreover, the recirculation zone was also not accurately predicted by WCSPH. When using the periodic inflow-outflow boundary conditions, the channel length must be long enough to re-develop the laminar flow at the outlet. It requires very expensive CPU time. Alternatively, a non-periodic inlet-outlet boundary condition should be developed.
Chapter 6

2-D and 3-D Dam-break Flows

Dam-break flows are a serious practical problem in civil engineering and have long been the subject of analytical and experimental study [57]. In terms of numerical study, it highlights free surface and impact against wall boundary conditions. As it is highly aerated flow with entrapped air pockets with the exception of Volume-of-Fluid (VOF), it is a very difficult problem for numerical schemes. At the same time, the geometry is very simple and the flow is driven by only gravity. Thus, it can reduce some problems caused by geometry itself. Several test cases of dam break are presented in this chapter by comparing ISPH with WC-SPH and/or experimental results and/or the other numerical results such as Volume-of-Fluid (VOF) methods.

Two sets of 2-D simulations are presented, the first deals with a dry bed and the second is with a wet bed. The wet bed one is based on an experimental configuration (Jánosi et al. [28]). In SPARTACUS-2D, three different turbulence approaches, mixing length ($L_m$) model, $k - L_m$ model and $k - \epsilon$ model, have been implemented by Violeau and Issa [66], these models are hence examined for 2-D dam-break applications. The results with $k - \epsilon$ turbulence model on these both cases are presented in Lee et al. [36].

The SPARTACUS-3D dam-break case is run without any turbulence approach; WCSPH is run with a parallel SPARTACUS-3D code with 16 processors by Issa at EDF and ISPH is run with a serial SPARTACUS-3D code. These are compared with VOF numerical results and experimental ones from [31].
6.1 Turbulence models in SPARTACUS-2D

The turbulence models are implemented in SPARTACUS code by Violeau and Issa [66] such as mixing length $L_m$, $k - L_m$ and $k - \epsilon$ models, are explained briefly here.

6.1.1 Mixing length model $L_m$

The mixing length $L_m$ is defined as an initial particle distance:

$$L_{m,a} = \delta r$$  \hspace{1cm} (6.1)

Then, the eddy viscosity $\nu_{T,a}$ is expressed with mixing length $L_m$ as:

$$\nu_{T,a} = L_{m,a}^2 \sqrt{2\sigma_{ij,a}\sigma_{ij,a}} = L_{m,a}^2 S_a$$ \hspace{1cm} (6.2)

where $\sigma_{ij}$ is the rate of strain, $S^2 = 2\sigma_{ij}\sigma_{ij}$. The rate of strain is defined with the velocity gradient as follows:

$$\sigma_{ij,a} = \frac{1}{2} \left[ \frac{\partial u_i}{\partial x_j} \bigg|_a + \frac{\partial u_j}{\partial x_i} \bigg|_a \right]$$ \hspace{1cm} (6.3)

The velocity gradient for a particle $a$ can be estimated by:

$$\left. \frac{\partial u_i}{\partial x_j} \right|_a = -\frac{1}{\rho_a} \sum_b m_b u_{i,ab} \otimes (\nabla_a w_h(r_{ab}))_j$$ \hspace{1cm} (6.4)

Alternatively, Violeau [66] suggested a formulation to estimate $S_a$ directly as:

$$S_a^2 = -\frac{1}{2} \sum_b \frac{\rho_a + \rho_b}{\rho_a \rho_b} \frac{\overline{u}_{ab}^2}{r_{ab}^2} + \frac{r_{ab}^2}{\eta^2} \nabla_a w_h(r_{ab})$$ \hspace{1cm} (6.5)

where $\overline{u}_{ab} = |\overline{u}_{ab}|$.

6.1.2 $k - L_m$ model

The eddy viscosity is defined as:

$$\nu_{T,a} = C_{\mu} \frac{k_a^2}{\epsilon_a}$$ \hspace{1cm} (6.6)
where the turbulent kinetic energy $k$ can be obtained from solving a transport equation for $k$ as:

$$
\frac{dk_a}{dt} = \sum_b m_b \frac{\mu_{k,a} + \mu_{k,b}}{\rho_a \rho_b} k_{ab} \frac{r_{ab}}{r_{ab}^2 + \eta^2} \mathbf{r}_{ab} \cdot \nabla_a w_h(r_{ab}) + P_a - \epsilon_a
$$

(6.7)

where $\mu_{k,a} = \mu_a + \frac{\nu r_{a,a}}{\sigma_{k}}$, $k_{ab} = k_a - k_b$, production term $P$ and dissipation term $\epsilon$. The production term $P$ can be defined in two ways; one is the classical model and the other is by Guimet & Laurence [19] in order to avoid over-estimation of $k$. The classical one is:

$$
P_a = \nu_{T,a} S_a = C_\mu \frac{k_a^2}{\epsilon_a} S_a
$$

(6.8)

The modified one by Guimet & Laurence is:

$$
P_a = \min \left( \sqrt{C_\mu}, C_\mu \frac{k_a}{\epsilon_a} S_a \right) k_a S_a
$$

(6.9)

The simulations of the turbulent flow here are based on Violeau’s strain model and Guimet & Laurence’s production model. Then, the dissipation, $\epsilon$, is estimated from $k$ and $L_m$:

$$
\epsilon_a = C_\mu^2 \frac{k_a^3}{L_{m,a}}
$$

(6.10)

This method is thus called the $k - L_m$ model.

### 6.1.3 $k - \epsilon$ model

In a similar manner as $k$, a transport equation for $\epsilon$ can be modelled as follows:

$$
\frac{d\epsilon_a}{dt} = \sum_b m_b \frac{\mu_{\epsilon,a} + \mu_{\epsilon,b}}{\rho_a \rho_b} \frac{\epsilon_{ab}}{r_{ab}^2 + \eta^2} \mathbf{r}_{ab} \cdot \nabla_a w_h(r_{ab}) + \frac{\epsilon_a}{k_a} \left( C_\epsilon \frac{P_a}{k_a} - \frac{\epsilon_a}{k_a} \right)
$$

(6.11)

where $\mu_{\epsilon,a} = \mu_a + \frac{\nu r_{a,a}}{\sigma_{\epsilon}}$ and $\epsilon_{ab} = \epsilon_a - \epsilon_b$. The Dirichlet wall boundary conditions are applied for $k$ and $\epsilon$ as follows:

$$
k = \frac{u_{*,a}^2}{\sqrt{C_\mu}} \quad \text{and} \quad \epsilon = \frac{u_{*,a}^3}{\kappa \delta}
$$

(6.12)

where $u_*$ is friction velocity, von Karman’s constant $\kappa = 0.41$ and $\delta$ is a small distance from the wall, which is smaller than particle size but larger than bed roughness thickness. In
addition, one more condition is considered for $\epsilon$ at the wall. Define the boundary condition for diffusion term of $\epsilon$ at the wall as:

$$
(diff \, \epsilon)_a = \frac{u^4}{\sigma_\epsilon \delta^2}
$$

By replacing the diffusion term in Eq. (6.11) with this at the wall, the $\epsilon$ at the wall will be compared with the value from Eq. (6.12). The maximum value between them will be chosen for $\epsilon$ at the wall. The coefficients used in $k - L_m$ and $k - \epsilon$ model are presented in Table 6.1, suggested by Launder and Spalding [33].

<table>
<thead>
<tr>
<th>$C_\mu$</th>
<th>$\sigma_k$</th>
<th>$\sigma_\epsilon$</th>
<th>$C_{e1}$</th>
<th>$C_{e2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.09</td>
<td>1.0</td>
<td>1.3</td>
<td>1.44</td>
<td>1.92</td>
</tr>
</tbody>
</table>

Table 6.1: Set of coefficients for $k - L_m$ and $k - \epsilon$ model.

### 6.1.4 Wall function

Since turbulence models are used, the particles at the wall (edge particles) no longer have zero velocity but the positions of these particles do not change. This is referred to here as “wall function”.

$$
\bar{u} = u_* \left( \frac{1}{\kappa} ln \frac{\delta}{\xi} + D \right)
$$

(6.14)

where $u_*$ is the friction velocity and $\xi$ is bed roughness thickness and $D = 8.5$ [26].

### 6.2 Surface particle tracking

No dummy particles are used to set the zero pressure free surface boundary conditions. For that reason, the number of neighbouring particles are insufficient since the support of the kernel is truncated shown in Fig. 6.1. This feature is used to define the free surface and to impose zero pressure on the surface particles for ISPH. There are several ways of searching the surface particles based on this. For example, Shao [53] defined the density according to equation [2.29] and used this equation to track the surface particles. Since density is constant in
6.3 2-D dam-break simulations on dry-bed

Figure 6.1: Zoom of a free surface. Description of the kernel compact support for a surface particle.

In our work, divergence of a particle position is used to track the surface particles. Divergence of a particle position in SPH reads:

\[
\nabla \cdot \mathbf{r} = \sum_b \frac{m_b}{\rho_b} r_{ab} \cdot \nabla_a w_h(r_{ab})
\]  

(6.15)

This is equal to 2 for 2-D simulations and 3 for 3-D in the core of the domain and far below for surface particles. An optimum criterion of 1.5 is used to determine which particles belong to the surface in 2-D and 2.4 for in 3-D. This criterion can be adjusted depending on the applications and the compact support size \(h_t\). The identified surface particles from Eq. (6.15) are shown in Fig. 6.2 at different times. Most surface particles are identified correctly but not all of them. This defect is acceptable as the undetected surface particles still have a pressure very close to zero. However, this could be further improved. This surface particle tracking technique can be also used in WCSPH with \(k - L_m\) and \(k - \epsilon\) turbulence models to apply zero conditions on these particles for \(k\), \(\epsilon\), \(\nu_T\) and \(P\). This is applied only for 2-D SPH dam-break benchmark test case, which is the simulation over the wet bed.

6.3 2-D dam-break simulations on dry-bed

The main purpose of this case is to compare the pressure distributions and surface shape between WCSPH and ISPH by applying three different turbulent approaches for both methods. The result with \(k - \epsilon\) are also presented in [36].
Figure 6.2: Examples of surface particle tracking defect (dam breaking case, top left: $t = 0.186 \text{ s}$, top right: $t = 0.278 \text{ s}$, bottom left: $t = 0.650 \text{ s}$, bottom right: $t = 1.860 \text{ s}$).
6.3.1 Geometry of the system

The geometry of a 2-D dam break is shown in Fig. 6.3 with the dimensions of $H_w$, $L_w$, $H_f$ and $L_f$ defined as the wall height and width, and the water height and width, respectively. The height of both side walls is set four times higher than the initial water height.

![Figure 6.3: Configuration of a dam breaking on dry bed (unit: m).](image)

6.3.2 System modelling

**Fluid discretisation and wall modelling**

The fluid discretisations are described in Table 6.2. The initial particle spacing $\delta r$ is set as $1/80H_f$. One layer of edge particles and four layers of dummy particles are used for wall particles.

**Simulation conditions**

All the dam-break simulations are performed with water and its real properties are taken for density and kinematic viscosity as $\rho = 1000 \text{ kg/m}^3$ and $\nu = 10^{-6}\text{m}^2/\text{s}$. In terms of SPH parameters, a 4th-order kernel and smoothing length ratio $h/\delta r$ of 1.3 are used. Not to violate the CFL condition in Eq. (3.22), the numerical speed of sound $c_0$ for WCSPH is set...
Table 6.2: Fluid, edge and dummy particle discretisation of the 2-D dam break for dry bed.

<table>
<thead>
<tr>
<th>Particles</th>
<th>Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluid particles</td>
<td>$40 \times 80$</td>
</tr>
<tr>
<td>Edge particles</td>
<td>802</td>
</tr>
<tr>
<td>Dummy particles</td>
<td>3,248</td>
</tr>
<tr>
<td><strong>Total particle number</strong></td>
<td>7,250</td>
</tr>
<tr>
<td>Initial particle distance: $\delta r , (m)$</td>
<td>$2.5 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

at 28.0 m/s and approximation of the maximum fluid velocity for ISPH is at 2.8 m/s from the theory of characteristic curves [57]:

$$u_{max} \leq 2 \sqrt{gH_f} \quad (6.16)$$

where $g$ is gravity and $H_f$ initial water depth. The criterion for surface particle tracking (see Section 6.2) is set at 1.5. Once the surface particles are identified, zero pressure is given to those particles for ISPH. In ISPH, the convergence is reached at the tolerance of $\theta = 0.1$ to obtain pressure (see Eq. (2.108)). Initially, hydrostatic pressure is set for all fluid particles as:

$$p_a = \rho_a g (H_f - z_a) \quad (6.17)$$

### 6.3.3 Simulation results

Dam-breaking flow for WCSPH and ISPH are plotted at the given times by comparing different turbulent approaches from Fig. 6.4 to 6.7. All the results in this section are enlarged in the vertical direction from $z = -0.01 \, m$ to $z = 0.3 \, m$.

In terms of surface shape, WCSPH and ISPH show very similar behaviour with all different turbulent approaches until the reflection of the wave on the opposite wall, then there are some small differences with more splash in ISPH (Fig. 6.6) with $k - \epsilon$ turbulence model, then a slightly different reflected wave speed (Fig. 6.7).

Regarding the pressure fields, again ISPH significantly reduces the pressure noise in comparison with WCSPH. One fact is that ISPH with the $k - L_m$ model showed perturbations
on pressure (see Figs. 6.4 and 6.7). When the criterion of 0.1 (see Eq. (2.108)) was set, it had 3 to 10 number of iterations each time step. Hence, an identical simulation with $k - L_m$ model was run again by restricting the number iteration for the linear solver as only two (see Section 3.2.1). Then, the result showed smoothed pressure pattern in Fig. 6.8. Note that the bluff body simulation at $Re_d = 100$ also required a small number of iterations, otherwise, the simulation was crashed. It seems that the linear solver needs to have smaller criterion (or smaller number of iterations) for unsteady flow. The exact reason has not been studied yet.

In the WCSPH results, some particles were stuck to the left-hand side of the wall while no particles were found in the same place with ISPH. However, a loss of particles through the boundary were found with ISPH. This might be due to pressure boundary conditions with surface particle tracking and/or no free divergence of the velocity, which can accumulate the error in particle position. As the pressure on the wall estimates are lower than the fluid particles’ pressure, the fluid particles are able to penetrate through the wall with the force of gravity. About 1.9% of fluid particles, equivalent to 60 out of 3,200 fluid particles, were lost in mixing length $L_m$ model and 4.3% in $k - L_m$ model and 5.0% in $k - \epsilon$ model.

The CPU time between WCSPH and ISPH are indicated in Table 6.3.

<table>
<thead>
<tr>
<th></th>
<th>WCSPH</th>
<th>ISPH</th>
</tr>
</thead>
<tbody>
<tr>
<td>time step (s)</td>
<td>$4.64 \times 10^{-5}$</td>
<td>$4.64 \times 10^{-4}$</td>
</tr>
<tr>
<td>CPU time (h)</td>
<td>1.10</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Table 6.3: 2-D dam-break flow CPU time for the physical time of $t = 1.86 \text{ s}$ for WCSPH and ISPH.

### 6.3.4 Partial conclusions

Pressure and surface shape of WCSPH and ISPH methods are compared with different turbulence approaches. In general, ISPH showed again the smoother pressure and $k - \epsilon$ turbulence model showed more splash when the flow was reflected by the opposite wall. ISPH with $k - L_m$ required even lower iteration numbers for stopping the linear solver in this case by showing unrealistic pressure pattern such as high pressure near surface. It is observed that
some particles penetrate through the wall in ISPH about 2.0 % to 5.0 % depending on the turbulence model.
6.3. 2-D dam-break simulations on dry-bed

Figure 6.5: Pressure of dam breaking case for dry bed at \( t = 0.278 \text{ s} \).
Figure 6.6: Pressure of dam breaking case for dry bed at $t = 0.650$ s.
6.3. 2-D dam-break simulations on dry-bed

Figure 6.7: Pressure of dam breaking case for dry bed at $t = 1.860 \, s$. 

**WCSPH**

**ISPH**

**Mixing length $L_m$ model**

**$k - L_m$ model**

**$k - \epsilon$ model**
Figure 6.8: Corrected the pressure perturbation of ISPH dam breaking case with $k - L_m$ turbulence model.
6.4 2-D SPH dam-break benchmark test case

The aim of this simulation is to compare the surface shape against experimental results \cite{28} and \cite{57} on wet bed. This is also one of SPHERIC benchmark test cases \cite{71}.

6.4.1 Geometry of the system

In the experiment reported by Jánosi \textit{et al.} \cite{28}, various water depths $d$ were examined by keeping the water depth in reservoir $d_0 = 0.15$ m and the gate velocity of $1.5$ m/s. However, in the numerical simulation only one case where the water depth $d = 0.018$ m was chosen and compared.

![Configuration of a dam breaking on wet bed (unit: m).](image)

6.4.2 System modelling

Fluid discretisation and wall modelling

The fluid discretisations are described in Table \ref{table:fluid_discretisation} for both WCSPH and ISPH. One layer of edge particles and four layers of dummy particles are located for wall particles.

Simulation conditions

In terms of SPH parameters, a 4th-order kernel and smoothing length ratio $h/\delta r$ of 1.5 are used. Unlike the previous case, pressure is initially set at zero for all fluid particles. For the CFL condition (see Eq. \ref{eq:cfl_condition}), the numerical speed of sound $c_0$ for WCSPH is set at $12.50$ m/s and maximum fluid velocity for ISPH is at $1.25$ m/s ($> \sqrt{gd_0}$). Increasing this
<table>
<thead>
<tr>
<th>Particle Type</th>
<th>Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluid particles</td>
<td>17,805</td>
</tr>
<tr>
<td>Edge particles</td>
<td>792</td>
</tr>
<tr>
<td>Dummy particles</td>
<td>3,208</td>
</tr>
<tr>
<td>Total particle number</td>
<td>21,805</td>
</tr>
<tr>
<td>Initial particle spacing: $\delta r (m)$</td>
<td>0.002</td>
</tr>
</tbody>
</table>

Table 6.4: Fluid, edge and dummy particle discretisation of the 2-D dam-break flow for wet bed.

velocity had negligible influence in the result (although a smaller time step was needed) in ISPH while WCSPH shows better agreement in early stage with mixing length turbulence model, the consistent WCSPH results are shown in [67].

The gate is moved instantly with the velocity of 1.5 $m/s$. The criterion for surface particle tracking (see Section 6.2) is set at 1.5 to set the zero pressure boundary condition on the surface particles for ISPH. Beside, zero eddy viscosity $\nu_T$, turbulent kinetic energy $k$, dissipation $\epsilon$ and production $P$ are applied for the surface particles in both WCSPH and ISPH. In ISPH, the convergence is reached at the tolerance of $\theta = 0.1$ (see Eq. (2.108)).

Results are recorded every 0.062 $s$ equivalent to the experimental physical time indicated in [28]. Nevertheless, there is a small gap in time (0.043 $s$) between the experiments and numerical results. For instance, the experimental result at 0.219 $s$ is actually compared with the numerical result at 0.176 $s$ [67].

### 6.4.3 Simulation results

The results shown in Figs. from 6.10 to 6.12 are mainly to compare the surface shape at the different stages. Each figure also represents the influence of different turbulence approaches. The digitised experimental data of Jánosi et al. [28] is provided from SPHERIC [71] and compared with SPH results.

The initial stages of surface shapes in WCSPH and ISPH are different from experiment [28] although the initial mushroom shapes were observed and predicted in [57]. With almost instantaneous dam removal, these shapes are also shown in the present figures for earlier
times. In [28] the plate is said to be removed with a speed of 1.5 \( m/s \) which would take a time 0.1 \( s \). Due to inertia effects the time will inevitably be longer and this could explain the difference between the experimental results in [28] and [57].

In general, WCSPH and ISPH show similar patterns of surface shape, however there are more splashes and voids in ISPH except with the mixing length \( L_m \) turbulence model. The voids in ISPH (the last three figures from the bottom in Figs. 6.11 and 6.12) are also observed in the experiment. Both methods produce quite realistic representation of the various phenomena: the detaching and breaking front wave which then rebounds as a second breaking wave and enclosing a large void especially with \( k - L_m \) and \( k - \epsilon \) model.

This example does not allow one to conclude as to whether one or the other solver is superior, but shows that both are equally robust for representation of violent surface motion.

The CPU time between WCSPH and ISPH are indicated in Table 6.5. Again, 0.3\% of fluid particles were lost in ISPH.

<table>
<thead>
<tr>
<th></th>
<th>WCSPH</th>
<th>ISPH</th>
</tr>
</thead>
<tbody>
<tr>
<td>time step: ( \delta t ) (s)</td>
<td>9.6 ( 10^{-5} )</td>
<td>9.6 ( 10^{-4} )</td>
</tr>
<tr>
<td>CPU time (h)</td>
<td>1.0</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Table 6.5: 2-D dam-break flow CPU time for the physical time of \( t = 0.48 \) \( s \) for WCSPH and ISPH.

### 6.4.4 Partial conclusions

Mainly the surface shape of the dam-break flow on the wet bed with the gate movement is simulated with WCSPH and ISPH to compared with the experiment results. Three different turbulent approaches are also examined and \( k - L_m \) and \( k - \epsilon \) predictions in ISPH look quite similar each other with some splashes while the single \( L_m \) model yield worse prediction in this work. We note that some particles are penetrating through the wall in ISPH about 0.3\% while this does not happen in WCSPH. The movement of the gate has an influence on the initial stage of the surface shape.
Figure 6.10: Free surface evolution from WCSPH and ISPH with the mixing length $L_m$ turbulence model. Comparisons of the surface shape with experimental data from Jánosi et al. [28] (empty square) and Stansby et al. [57] (black delta). Note equivalent times for [57] are in bracket. The comparisons are made where $0.38 \, m \leq x \leq 1.04 \, m$ and $0.0 \, m \leq z \leq 0.13 \, m$. 

$\begin{align*}
t &= 0.156 \, s \\
(0.206 \, s) \quad t &= 0.219 \, s \\
(0.28 \, s) \quad t &= 0.281 \, s \\
t &= 0.343 \, s \\
t &= 0.406 \, s \\
t &= 0.468 \, s \\
t &= 0.531 \, s
\end{align*}$
6.4. 2-D SPH dam-break benchmark test case

Figure 6.11: Free surface evolution for WCSPH (left) and ISPH (right) with the $k - L_m$ turbulence model. Comparisons of the surface shape with experimental data from Jánosi et al. [28] (empty square) and Stansby et al. [57] (black delta). Note equivalent times for [57] are in bracket. The comparisons are made where $0.38 \, m \leq x \leq 1.04 \, m$ and $0.0 \, m \leq z \leq 0.13 \, m$. 
Figure 6.12: Free surface evolution for WCSPH (left) and ISPH (right) with the $k - \epsilon$ turbulence model. Comparisons of the surface shape with experimental data from Jánosi et al. [28] (empty square) and Stansby et al. [57] (black delta). Note equivalent times for [57] are in bracket. The comparisons are made where $0.38 \ m \leq x \leq 1.04 \ m$ and $0.0 \ m \leq z \leq 0.13 \ m$. 
6.5 3-D SPH dam-break benchmark test case

This 3-D dam-break experimental work has been carried out at the Maritime Research Institute Netherlands (MARIN). This case is also one of the validation cases listed in SPHERIC web-site [72]. Kleefsman et al. made a comparison between a numerical method VOF and an experiment with this case and presented in [31]. 3-D ISPH are run and compared with Kleefsman et al.’s results and 3-D WCSPH done by Issa at EDF.

6.5.1 The SPARTACUS-3D code

The SPARTACUS-2D ISPH code is extended to 3-D. This is quite straight forward by adding span-wise direction component in 2-D SPH equations. The 3-D SPH equations are thus not presented here except the kernel derivative. As in SPARTACUS-2D, the first derivative of the 3rd, 4th and 5th order spline kernels are considered as follows:

\[ w_h'(q) = \frac{1}{\pi h^3} \begin{cases} 
-3q + \frac{9}{4}q^2 & \text{if } 0 \leq q \leq 1 \\
-\frac{3}{4}(2-q)^2 & \text{if } 1 \leq q \leq 2 \\
0 & \text{if } q \geq 2 
\end{cases} \]  \tag{6.18}

\[ w_h'(q) = \frac{96}{1199\pi h^3} \begin{cases} 
-4\left(\frac{5}{2} - q\right)^3 + 20\left(\frac{3}{2} - q\right)^3 - 40\left(\frac{1}{2} - q\right)^3 & \text{if } 0 \leq q \leq 0.5 \\
-4\left(\frac{5}{2} - q\right)^3 & \text{if } 0.5 \leq q \leq 1.5 \\
-4\left(\frac{3}{2} - q\right)^3 & \text{if } 1.5 \leq q \leq 2.5 \\
0 & \text{if } q \geq 2.5 
\end{cases} \]  \tag{6.19}

\[ w_h'(q) = \frac{7}{478\pi h^3} \begin{cases} 
-5(3-q)^4 + 30(2-q)^4 - 75(1-q)^4 & \text{if } 0 \leq q \leq 1 \\
-5(3-q)^4 + 30(2-q)^4 & \text{if } 1 \leq q \leq 2 \\
-5(3-q)^4 & \text{if } q \geq 3 \\
0 & \text{if } q \geq 3 
\end{cases} \]  \tag{6.20}

with \( q \) denoting the ratio \( r_{ab}/h \).
6.5.2 Geometry of the system

In the experiment, a large tank of $3.22 \times 1 \times 1 \ m$ is used with an open roof. Water depth is $0.55 \ m$ and enclosed by a door on the right part of the tank. The water is released when the door is pulled up almost instantly. From the right end of the tank to the door will be called as reservoir. Figure 6.13 shows the geometry and the measurement positions; the locations of H1, H2, H3 and H4 are to examine the water heights and from P1 to P8 are for the pressure sensor on the box. The detail dimensions of the system and the exact measurement positions are described in Figs. 6.14 and 6.15.

![Figure 6.13: Measurement positions for water heights (H1 to H4) and pressures (P1 to P8) in the dam-break experiment [31] (unit: m). The right figure is an enlargement on the obstacle.](image)

6.5.3 System modelling

Fluid discretisation and wall modelling

The fluid discretisations are described in Table 6.6 for WCSPH and ISPH. The initial particle distance is decided by locating 30 fluid particles along the water height. One layer of edge particles and three layers of dummy particles are located for wall particles. The smaller number of particles in ISPH is due to the side walls of $x-z$ plane being replaced by periodicity in span-wise direction. However, WCSPH runs without periodicity by building the tank as indicated in the experiment.
6.5. 3-D SPH dam-break benchmark test case

Figure 6.14: General description of the system: top (top figure) and side (bottom figure) views (unit: m).

Figure 6.15: General description of the system: top (top figure) and side (bottom figure) views (unit: m).
Table 6.6: Fluid, edge and dummy particle discretisation for the 3-D dam-break flow for WCSPH and ISPH.

<table>
<thead>
<tr>
<th></th>
<th>WCSPH</th>
<th>ISPH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluid particles</td>
<td>$67 \times 54 \times 30$</td>
<td></td>
</tr>
<tr>
<td>Edge particles</td>
<td>38,142</td>
<td>16,079</td>
</tr>
<tr>
<td>Dummy particles</td>
<td>113,592</td>
<td>49,101</td>
</tr>
<tr>
<td>Total particle number</td>
<td>260,274</td>
<td>173,720</td>
</tr>
<tr>
<td>Initial particle spacing: $\delta r$ (m)</td>
<td>55/3000</td>
<td></td>
</tr>
</tbody>
</table>

Simulation conditions

The water in the reservoir is at rest initially. When the simulation is started, the water starts to flow into the empty part of the tank due to gravity.

As mentioned above, ISPH runs this case with $y$-direction periodicity. Initially, hydrostatic pressure (see Eq. (6.17)) is given to all fluid particles. During the simulation, zero pressure is given to the surface particles every time step. The criterion to define the surface particles (see Section 6.2) on this case is 2.4. In terms of SPH parameters in ISPH, a 3rd-order kernel and smoothing length ratio $h/\delta r$ of 1.0 are used. The time step in ISPH is 0.001, same as the one used in VOF. Several cases show that the less iteration number (smaller tolerance) also provide reasonable results, even better (see Sections 4.2, 5.3.2 and 6.3). Hence, only two iterations are considered for the pressure Poisson equation.

3-D parallel WCSPH are carried out with 16 processors, each processor has 3.2GHz of CPU and 4G RAM. For WCSPH, a 4th-order kernel with smoothing length ratio $h/\delta r$ of 1.5 and the numerical speed of sound $c_0 = 60$ m/s are used. No turbulence model is used on this simulation for both WCSPH and ISPH, instead, constant viscosity $10^{-6}$ m$^2$s$^{-1}$ is applied.

For VOF, a fine grid of $236 \times 76 \times 68$ grid cells has been used with some stretching towards the bottom of the tank with non-constant viscosity.
6.5.4 Simulation results

The presented results are based on the comparisons between VOF and the experiment made by Kleefsman et al. in [31].

First of all, the snapshots at the physical time of \( t = 0.4 \) s and 0.56 s are shown in Figs. 6.16 and 6.17 for VOF, experiment, WCSPH and ISPH. Note that WCSPH results are at the slightly different physical time as \( t = 0.41 \) s and \( t = 0.60 \) s. In each figure, the small pictures on the top right is the water in reservoir. The water in reservoir from WCSPH and ISPH are presented in terms of pressure. Consistent results for pressure as shown in previous cases are shown, fluctuated pressure for WCSPH and smoother one for ISPH. Kleefsman et al. mentioned that the free surface in VOF has some ripples by using the reconstruction aligned with the coordinate axes in their work [31], however, WCSPH and ISPH do not have those ripples and their presentation are with the horizontal water velocity. Again, a smoother velocity pattern is found in ISPH than in WCSPH. Both SPH results show the water speed is slower than the VOF, the experimental result is difficult to judge from this photo, and ISPH shows splashed water than VOF and WCSPH when the water hits the box in front. This splash-up in ISPH is better predicted than the other methods.

The time histories of water height at the locations of H4 and H2 are depicted in Fig. 6.18. The global behaviour in WCSPH and ISPH is pretty much similar but slightly shifted about 0.2 s after 2.5 s in the reservoir (profile at H4) and 4.5 s in the tank (profile at H2). Kleefsman et al. also pointed out that the water speed was slow with the coarse grid by testing a grid refinement study. The spikes in ISPH at H2 is due to the splashed particles after the water hit the box.

The pressure at the point of P1 and P3 at the front of the box and P5 and P7 at the top of the box are shown in Figs. 6.19 and 6.20. WCSPH results are presented only at P1 and P3 and showed strong fluctuations, whereas ISPH is smoother and showed similar behaviour with the experiment except the underestimation when the water hits the box (P1 and P3). At the second impact about 4.7 s, it is also visible in ISPH but, as mentioned earlier, the predicted flow is slower. The pressure on the top of the box (P5 and P7) shows fairly good agreement and the fluctuations in the early stages might be due to the wall treatment with dummy particles.
With VOF, several spikes appear at the same physical time in the pressure profile at all positions. According to Kleefsman et al., these spikes occur because some water enters an empty cell that is completely surrounded by cells with fluid. When the water enters the empty cell, there is no empty cell left in the neighbourhood, so this cell changes to a fluid cell in one time step without being a surface cell in-between. This discontinuous change in label and the corresponding restoration of $\nabla \cdot \mathbf{u} = 0$, results in a pressure peak over the whole
Figure 6.17: Snapshot of a 3-D dam-break simulation with a box in the flow compared with VOF simulations and experiment at $t = 0.56$ s VOF simulations and experiment results are taken from [31]. The small picture in each figure is water in reservoir.

pressure field.

The CPU time between WCSPH and ISPH are also indicated in Table 6.7. One of the reasons of the shorter CPU time in ISPH is that the difference of total particle numbers between WCSPH and ISPH. By using the $y$-periodicity in ISPH, 86,544 particles are less used. Moreover, about 2.6% of the fluid particles were lost during the simulation.
6.5.5 Partial conclusions

Comparisons in terms of water height and pressure on the box at each location have been performed for WCSPH, ISPH, VOF and the experiment on 3-D dam-break simulation. In general, the time history of water heights at each location showed a good agreement except for the slower water speed. It might be required to have a finer spatial resolution or a turbulence model. Again, Pressure with WCSPH shows unphysical behaviour while ISPH shows a good agreement except some underestimation when the flow hit the box. One should note that
Figure 6.19: Pressure time histories at P1 and P3. VOF simulations and experiment results are taken from [31].

some particles are penetrating through the wall in ISPH representing about 2.6% of the fluid particles.
Figure 6.20: Pressure time histories at P5 and P7. VOF simulations and experiment results are taken from [31].

<table>
<thead>
<tr>
<th>Methods</th>
<th>WCSPH</th>
<th>ISPH</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of processor</td>
<td>16</td>
<td>1</td>
</tr>
<tr>
<td>Time step: $\delta t$ (s)</td>
<td>$1.833 \times 10^{-4}$</td>
<td>$1.0 \times 10^{-3}$</td>
</tr>
<tr>
<td>Physical time: $t$ (s)</td>
<td>5.5 s</td>
<td>6.0 s</td>
</tr>
<tr>
<td>CPU time (h)</td>
<td>32.0 / processor</td>
<td>48.5</td>
</tr>
</tbody>
</table>

Table 6.7: 3-D dam-break flow CPU time.
Chapter 7

Conclusions and Future Work

7.1 Conclusions

This thesis has presented a truly Incompressible SPH (ISPH) scheme for both 2-D and 3-D flows. The main features of this new ISPH algorithm are: firstly, a constant density is used in our work, hence the right hand side of the pressure Poisson equation is obtained from the divergence of temporal velocity. Secondly, no temporal particles positions are introduced in the prediction step. Thirdly, slight different formulation of approximate Laplacian operator is developed. Then, a linear solver is implemented in SPH formulation rather than using a linear solver package. Finally, no matrix for the pressure Poisson equation is built. Instead, the pressure Poisson equation itself is solved for each particle iteratively by the implemented linear solver. Moreover, in the author’s knowledge, this is first time a 3-D application has been simulated with the truly incompressible SPH and validated with other numerical and experimental work.

The development of a truly incompressible approach for SPH has been presented and validated through various applications for 2-D and 3-D including benchmark test cases. In terms of 2-D applications, both laminar and turbulent flows are examined by comparing WCSPH and ISPH results with the results from other numerical methods, such as finite difference or finite volume, and/or experiments. For 2-D laminar flow simulations, the lid-driven cavity flow and the moving square set in a rectangular box are performed as a benchmark test case. The flow around a bluff body located between two flat plates is also run to examine the ability
of the code to capture the vortex shedding.

In general, WCSPH must have much higher numerical speed of sound to avoid the void, for example, at the centre of the cavity, around the moving body and wake, and just behind of the bluff body in each case. This higher numerical speed of sound leads to much smaller time step and very expensive CPU time. Moreover, the spatial discretisation has a strong influence on the accuracy of the results.

The ISPH results show generally good agreement with the other methods even with coarser spatial discretisation. Moreover contrary to WCSPH no spurious voids ever appeared.

For the lid-driven cavity flow case, an error analysis was carried out using various spatial resolutions. Although the error shows a first-order scheme convergence rate, on the coarser resolutions ISPH approaches a flow field that is much closer to the exact solution than the WCSPH results which are very noisy and seem to correspond to a much more viscous flow regime. At higher Reynolds number and with a finer discretisation, the WCSPH results are improved and are closer to ISPH one. However, short range and very intense pressure fluctuations produced by WCSPH in the instantaneous fields are so large that they mask the mean pressure variation. This is also generally true for unsteady pressure distributions in the moving square set, bluff body and dam break problems.

For the 2-D dam break case on dry and wet bed, three different turbulence models, mixing length $L_m$, $k - L_m$ and $k - \varepsilon$ model, are examined with these cases. The simulations over a dry bed are compared only between WCSPH and ISPH for these turbulence models. Mainly pressure and surface shape are compared between them and again far smoother pressure fields in ISPH are observed than WCSPH. The benchmark dam-break case over wet bed also compares the surface shape only; WCSPH and ISPH results are compared with two experimental data [28], [57] and shows close agreement.

A 3-D dam-break benchmark test case is run with constant viscosity, which means no turbulence models are used, and compared with Volume-of-Fluid (VOF) and experimental results. Unlike 2-D dam-break case, an obstacle in the form of a square box is located in the downstream region. The comparisons are made in terms of the time history of water heights and pressure on the obstacle at the indicated locations. Although 3-D SPH results show slower water speed than the VOF and experiment, water heights from both SPH results
7.2. Recommendations and Future work

are close to the experiment. In terms of pressure, the WCSPH results predicted strong fluctuations again, which proves that the typical WCSPH is not able to predict the pressure on the solid body accurately, while ISPH gives reasonable pressure time history except some underestimation and small scale of fluctuations. Also, ISPH produces splash-up which is closer to the experiment than the one simulated by the WCSPH and VOF.

Overall, ISPH yields much more reliable results than WCSPH; velocity and pressure fields in particular are smoother in every case. The CPU time required by ISPH is shorter, by about a factor of 2 to 8 depending on the cases. The CPU time in WCSPH is dominated by the choice of the numerical speed of sound while it is the linear solver in ISPH. Certain cases, for instance the bluff body case for higher Reynolds number, the smaller CPU time is in consequence of the larger tolerance for the linear solver. Moreover, there is a loss of fluid particles in cavity flow and dam-break simulations, which also affect the CPU time.

7.2 Recommendations and Future work

Although ISPH method provides promising results so far, this method still requires further investigation. Firstly, the error in ISPH is dominated by the approximate Laplacian operator and boundary conditions. Due to the approximate Laplacian operator to solve the pressure Poisson equation, this method still does not satisfy the free divergence of velocity field, which leads to the error in particle position. The divergence free velocity will be achieved by a compatible Laplacian operator, however, this operator in SPH shows the same pressure decoupling effect as found in an Eulerian method with co-located pressure and velocity. To satisfy the divergence free velocity field without the decoupling, the combination of compatible and approximate operators could be considered.

Even though several layers of dummy particles were used in ISPH, impermeability is not satisfied for certain cases. Although it might be linked with the error of particle positions, the wall modelling and boundary condition must be improved. Since the property of wall particles is the same as fluid particles, not real solid wall property, different density of edge and dummy particles could be applied. Also, the coupling of SPH and Eulerian method on the wall boundary could be considered by building mesh near the boundary and boundary
itself. Due to the movement of particles, it is not easy to have Neumann pressure boundary condition at the wall and in fact, this Neumann boundary condition is not satisfied with the approximate Laplacian operator.

Since the behaviour of the iterative method for the linear solver is not consistent for every case; some cases converged better with a smaller number of iterations and we need to define a better convergence criteria for some cases. The linear solver needs to be made more robust by implementing pre-conditioning.

Not only for ISPH but also for WCSPH in the case of channel flow, it is necessary to have non-periodic inlet and outlet boundary condition. Due to the kernel truncation at boundaries, normalisation technique on the kernel can be taken into account.

The major concern in ISPH should be the Laplacian operator and pre-conditioning for linear solver with boundary conditions. Then, turbulence models can be applied for 3-D ISPH.
Bibliography


