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**Theoretical development of the SPH method and application to transient
fluid structure interaction problems.**

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Abstract

The smoothed particle hydrodynamic method (SPH) is a meshless method that suffers from several shortcomings. These shortcomings are tensile instability and zero energy modes -which are characterised by unphysical particle clumping- lack of consistency and improper enforcement of essential boundary conditions. The capability of the method also lacks; with most applications limited to either fluid or very simple fluid-structure interactions.

This thesis addresses most of the issues that plague SPH as well as extending the capability to more complex fluid-structure interactions. Particle clumping has been reduced by the introduction and rigorous mathematical and code development of a mixed formulation procedure that while is prevalent in finite element, has never been applied to the SPH method. Unlike every other attempt in literature to solve the particle clumping problem, this approach addresses the cause as opposed to treat the symptoms, which gives it mathematical rigour and generality. Furthermore, a moving least squares procedure was applied to the code to smooth pressure by using a first order consistent scheme, this gave an unexpected side effect in the form of velocity differences between simulations that used the procedure and those that did not. This was investigated and conclusions drawn into the nature of why this difference occurred.

Extension of the capability of the method occurred by the addition of rotational boundary conditions and modification of the contact algorithm to account for a no-slip boundary condition to achieve successful simulation of complex fluid-structure interaction problems. These problems were three benchmark cases involving the interaction of an elastic body and free surface flow. Validation occurred throughout the development of the code and simulations. Code validation was by comparison to theory, while the results of the beam deflection were compared to LS-Dyna. The benchmark cases were compared to both experimental results and to another paper who modelled the problem using a partitioned finite volume solver. All coding and simulations in this work was done within in the inhouse Meshless continuum mechanics (MCM) code.

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Finally, thank you to my office mates. You have kept me sane and we will be friends for life.

Notation

$\mathbf{a}$ acceleration vector

$\mathbf{B}$ Strain displacement matrix

β Bulk modulus

$\mathbf{b}(\mathbf{x})$ linear basis

C_1 Constant for polynomial equation of state

$\mathbf{D}$ Rate of deformation tensor

$\mathbf{d}$ deviatoric

$\mathbf{e}$ error

f function

f^b body force vector

$\mathbf{F}$ Force

G Shear modulus

g_a gap function

g gravity

H_p Array of shape functions for pressure interpolation

$\mathbf{H}$ Array of shape functions for displacement interpolation

h SPH smoothing length

i particle of interest

j neighbour particle

$\mathbf{J}$ Jacobian matrix

K Bulk modulus

k incompressibility constant

m mass

$\mathbf{M}$ Mass matrix

N Number of particles

$NNBR$ Number of neighbour particles

N_P Number of particles
 $\hat{n}$ normal
 Q Contact stiffness parameter
 p Pressure
 P Power
 PS Pressure scale factor
 S deviatoric stress tensor
 t normal stress vector
 u displacement vector
 w SPH kernel
 X Lagrangian co-ordinate
 x co-ordinate
 x' Neighbour x co-ordinate
 y co-ordinate
 y' Neighbour y co-ordinate
 dV Volume integral
 $d\Gamma$ Surface integral
 dt timestep
 δ Virtual variation
 δ Dirac delta function
 Σ Sum notation
 Δ infinitesimal change
 ϵ Strain
 ρ density
 Γ Boundary
 σ Cauchy Stress tensor
 π Functional

Λ Lagrange multiplier

ϵ' deviatoric strain

Ω Volume Integral

∇ Gradient operator

ω trial function

Abbreviations

BC Boundary condition

CFD Computational Fluid Dynamics

EOS Equation of State

FE Finite Element

FSI Fluid Structure Interaction

IQN-ILS: Interface Quasi Newton Algorithm-Inverse Least Squares

MCM Meshless Continuum Mechanics

MEF Mixed Element Formulation

MLS Moving Least Squares

SPH Smoothed Particle Hydrodynamics

SVD Singular value decomposition

U-P Displacement-Pressure formulation

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1. Introduction

The ability to model Fluid Structure Interaction (FSI) scenarios are of increasing interest in many engineering and medical fields. This is in part due to industrial demand, but also advances in computer technology and research into numerical methods. The consequence of this is that more complex and wide ranging FSI problems can be modelled.

FSI modelling generally involves the simulation of fluid impact on structures; this impact creates deformation of the structure. A few examples of FSI are plane impact upon water (Hughes et al. 2013), wave impact on ships (Senjanovic & Fan 1995) and blood flow against an artery wall (Formaggia et al. 2006). This highlights the wide range of applications of FSI modelling. The ability to model large deformations and being able to successfully represent the interaction at the fluid/structure boundaries are among the challenges of FSI modelling. The main approach to model FSI is adopting a coupled FSI approach using a Computational Fluid Dynamics (CFD) solver to describe the fluid and a Finite Element (FE) solver to describe the structure. This same coupled approach is used when using Smoothed particle hydrodynamics (SPH) to model FSI problems (Hughes et al. 2013) (Hu et al. 2014). Generally fluid is simulated using an SPH solver and the structure FE (Fourey et al. 2010) (Yang 2012).

The capability of the SPH method has recently been extended to describe both the fluid and the structure in FSI interaction. This eliminated the need for coupling; however, this capability has only proved successful in simulating single phase flow impact on an elastic plate known as the elastic gate problem. When applied to a more complicated case in the form of the interaction between a skirt of a surface effect ship and water, results were incomplete indicating problems in extending the FSI capability reliably to a more complex case. Extension of the elastic gate problem to a sloshing tank scenario with a clamped beam immersed in the fluid has been proposed by Souto-Iglesias et al as a novel benchmark test of the SPH method. Experimental results are available for this benchmark test and the FSI problem considered in this review will be based upon this test.

SPH has four main shortcomings that can affect simulation performance and numerical convergence, ultimately leading to poor/inaccurate results and representation of behaviour. Tensile instability is one issue in which under tension particles un-physically clump together. This has the effect of the solution become unstable and ultimately useless. Another is zero energy modes where particle deformation occurs under zero strain energy, which is unphysical behaviour. Exact implementation of essential boundary conditions is not possible in the basic SPH method, due to the fact that the approximations in SPH do not have the property of strict interpolants; which means that the interpolated value of a variable at a particle does not equal the particle value of that variable (Vignjevic 2011). Finally, the basic SPH method is not even zero order consistent, and hence convergence of a numerical solution can be an issue. There is ongoing research to try to eliminate or reduce the impact of these problems to SPH simulations. The shortcomings described will have an impact on FSI simulation in SPH, so part of the research in the modelling of FSI using the SPH method will include work done in addressing some of the SPH shortcomings.

The aim of this thesis is broad in specification, but ultimately the work is about development of the capability of the method to make the method more mainstream and competitive in comparison to

other commercial modelling methods, while highlighting the development of meshless methods, which in theory should address any shortcomings in mesh based methods. Which is why a complex FSI test is an excellent illustration to show how the method has developed and what it is now capable of. To achieve this, the work in this thesis will address some of the shortcomings of the theory by applying a novel approach called mixed formulation to the SPH method. The work will also develop the capability of the theory to model a complex FSI test which will build on existing research. In order to achieve successful output, theory needs to be married with computational development; that is any theoretical development needs to be compatible with the in-house meshless continuum mechanics SPH code developed by Cranfield University. Therefore, the general structure of each chapter will initially discuss the theoretical development derived, then talk about the coding process and end with illustration of results and if necessary future developments.

1.1 Structure of the thesis

Chapter 2 is a literature overview on the SPH method. The overview will cover the research done in SPH in addressing consistency, particle clumping and extending the capability of the method to model FSI interactions without coupling. In addition, since this thesis is exploring a new mixed element formulation approach in addressing particle clumping that has never been researched in SPH, the literature overview will cover the research done in the FE method that has used this approach to address shortcomings in the FE method.

Chapter 3 builds upon chapter 2 by showing the mathematical development of the SPH method and research. The mathematics shown in this chapter shall form the basis of the novel mathematical development and the simulations in further chapters.

Chapter 4 begins the main part of the work undertaken in this thesis that will lead into the novel work of chapters 5,6 and 7. It begins by description and testing of a free surface problem that will illustrate pressure instability. From there, the work will use the moving least squares (MLS) approach discussed in chapter 3 to 'smooth' pressure by applying the MLS procedure to density. The mathematical derivation that was added to the code to achieve this density MLS update will be shown. Then using the same dambreak free surface problem, the MLS algorithms will be tested for 20,10 and every timestep MLS update. Results are shown and discussed

Chapter 5 extends on the work described in chapter 4 by investigation of an unintended velocity difference that occurs when using this procedure. The magnitude of the velocity difference between a no- pressure smoothed case and one that uses this is dependent on the number of timesteps that this procedure is used. The investigation details tests involving different particle densities, geometries and flow speeds. The frequency of application of the density update algorithm is considered and conclusions drawn from results.

Chapter 6 extended the capability of the SPH method to FSI problems by detailing simulations of complex FSI problems. The problems are described and a literature review of previous work done in SPH regarding fluid-structure interaction problems is shown. The underlying theory behind the benchmark problems such as sloshing, Eulerian-Lagrangian descriptions of motion is explained and complexities of modelling such scenarios highlighted. Modelling assumptions are described and code changes not described in chapters 2-4 are shown. The step by step process starting from simple

block impact testing to the final simulations of the benchmark problems is illustrated, with testing validation in the form of LS-Dyna comparison when modelling the beam and experimental comparison when modelling the water are shown. The end of the chapter will discuss the results and describe recommendations for future work.

Chapter 7 takes on the development of chapter 6 and details the results of the clamped elastic beam in the sloshing tank scenarios. Results are discussed and recommendations for future research and code development are highlighted. Results are presented for the free surface positions and beam deflections and compared to experiment and literature.

Chapter 8 moves on from the fluid-structure interaction case and concentrates on the particle clumping issue. Mixed formulation is introduced and it is explained why it is believed that this procedure can be used to cure SPH of particle clumping and conserve momentum. Different formulations are researched and derived in SPH form, before it is explained why displacement-pressure formulation is the formulation that this thesis will use to apply to SPH problems. From there, the displacement-pressure formulation is implemented; with different solution techniques to solve the fields that come because of the method are derived and investigated. Research into the nature of the fields is discussed and the chapter is concluded with the direction of the work that mixed formulation should take in the future.

Chapter 9 concludes the work in the thesis and presents recommendations for future work that will build upon the foundations and research laid out in this thesis.

Chapter 2 Literature review

The smoothed particle hydrodynamic (SPH) technique is a meshless method, developed independently by Lucy (Lucy 1977) and Gingold and Monaghan (Gingold & Monaghan 1977). In this work, development of the method arose due to difficulties in the finite difference method in dealing with distortions in spheric polytropes. For problems that did not exhibit spherical symmetry, to achieve adequate accuracy in the simulation, a number of particles required when compared to a non-distorted spherical symmetric case are of at least cubic times amount (Gingold & Monaghan 1982). For a numerical simulation - where the time of simulation is an important consideration - this situation was far from ideal.

To attempt to solve this problem, the fluid continuum was replaced by a Lagrangian description of the flow which represented the flow of discrete particles. An assumption was made that the fluid particles were of equal mass, so the number of particles per unit volume was proportional to the density. An additional assumption was made which was the particle positions are randomly distributed according to the density. This assumption made the link between the fluid flow problem and a probability distribution, as finding the density from a known sample of fluid particles was equivalent to finding the probability density from a sample of data. This would simplify the problem as now the fluid density was in the form of a probability distribution, it was in an integral form and the Monte-Carlo technique used to approximate an integral required far fewer data points than finite difference methods require. This in theory would solve the problem regarding simulation time as fewer points would need to be used to achieve the same accuracy.

Despite the good results highlighted by (Gingold & Monaghan 1977) (Lucy 1977), the method did not conserve linear and angular momentum as highlighted in Monaghan's historical review of the SPH method (Monaghan 2005). However, this was corrected. (Gingold & Monaghan 1982).

A pure stability analysis was done in (J. Swegle, D. Hicks, S. Attaway 1995), where it was shown that SPH was unstable in tension (further work also showed instability in compression as well, but as this was only within the region of less than $2/3$ of the smoothing length, this was undetected in simulations). Visually this was shown by unphysical particle clumping. This particle clumping is also a consequence of another shortcoming of the SPH method called zero energy modes. This led to research focussed on the development of ways to improve stability.

Given that a key requirement for a stable scheme is that of completeness as defined by the Lax-Wendroff theorem (Piskunov & Freytag 2005) and that Belytschko (Belytschko et al. 1998), highlighted issues with completeness and consistency in the SPH method, research focussed on improving SPH completeness and consistency (Liu et al. 1995) (Belytschko et al. 1998) (Dilts 1999). (Liu et al. 1995) (Belytschko et al. 1996) and (Dilts 1999) used the MLS approach to ensure first order completeness. This approach will form part of the method to smooth pressure in further chapters. Randles and Libersky (Randles & Libersky 1996) and Vignjevic and Campbell (Vignjevic et al. 2000) developed a normalised first order consistent version of the SPH method with improved accuracy.

However, in the review of SPH conducted by Vignjevic (Vignjevic 2011), he noted that research had confirmed what Swegle (J. Swegle, D. Hicks, S. Attaway 1995) had shown in his paper. Namely that

instability doesn't result from the numerical time integration algorithm, but rather from an effective stress resulting from a nonphysical negative modulus being produced by the interaction between the constitutive relation and the kernel interpolation. In other words, the kernel interpolation used in spatial discretisation changes the nature of original partial differential equations. These changes in the effective stress amplify, rather than reduce, perturbations in the strain (Vignjevic 2011). A comprehensive review of SPH completeness and consistency is shown in (Belytschko et al. 1998) (Liu & Liu 2010).

One approach to tackle the root cause of the instability was called non-collocational SPH in which stress is calculated at points other than at SPH particle positions, hence the term non-collocational as stress was calculated at different points to other quantities. This was suggested as a way to address tensile instability (DYKA et al. 1997), however due to the fact that stress is calculated from strain which is the rate of change of displacement, this could have also addressed the zero energy issue. This was due to the fact that the whole mechanism comes from the fact that field variables and their derivatives are calculated at the same points as explained by (Vignjevic et al. 2000). With this technique, it wouldn't be the case and Dyka (Dyka & Ingel 1995) showed that method can also address Tensile instability. (DYKA et al. 1997) explained how this would solve the tensile instability problem by stating that if $w''\sigma > 0$ wasn't satisfied – which it is in conventional SPH – then the instability wouldn't occur as the Von Neumann analysis done by Swegle et al (J. Swegle, D. Hicks, S. Attaway 1995) showed tensile instability to occur when the equation was satisfied. By computing stresses at different points, the i particle is included in the stress calculations and so the equation is not satisfied. This was tested with different variants of the SPH equations; however, this was shown to remove the instability only for a momentum equation that does not conserve momentum, in addition, the computational cost is high. Another approach to solve tensile instability involved addressing the Kernel itself. This approach called adaptive kernel estimation (Sigalotti & López 2008) in which the kernel is varied so that only minimum smoothing is required. This allows redevelopment of a more stable set of SPH equations that do not suffer from tensile instability. However, testing was limited to a fluid with a Van Der Waals equation of state.

Vignjevic (Vignjevic et al. 2000) explained that there were 2 main approaches to address the particle clumping issue. The first approach has been discussed, the second was to find a way to suppress the oscillation as opposed to developing a method that doesn't suffer from the oscillation in the first place. The most recent work in this field was described in (Ganzenmuller 2015), where the author developed an approach that suppresses the growth of the zero-energy modes and hence the rank deficiency in the solution does not occur. This approach is analogous to the hourglass control algorithm in SPH where a correction force is added to suppress the growth. The author concluded that the positive results imply there is a lot of promise in this area of research as it increases the range of deformations that can be simulated in an accurate manner. Mehra (Mehra et al. 2012) tested two numerical approaches designed to deal with tensile instability - Monaghan artificial stresses (Monaghan 2000) and the Godunov - type SPH for high impact problems.

Furthermore, Belytschko and Xiao (Belytschko & Xiao 2002) studied the stability of particle methods based on the Shepard function with corrected derivatives. They considered both Eulerian and Lagrangian kernels with nodal integration, as in standard SPH. They realised that the tensile instability originates as a distortion of the material instability induced by Eulerian kernels and that a Lagrangian kernel with the addition of stress points effectively eliminates it.

Vignjevic et al (Rade Vignjevic et al. 2006) actually solved the tensile instability problem by introducing a Total Lagrange Formulism in SPH. In this approach, the Lagrangian kernel is a function of initial position and initial smoothing length which is different from the usual Eulerian Kernel which is a function of current position and smoothing length and allows a varying neighbourhood. As a function of initial position, it meant that the number of neighbours is fixed as the initial position does not change. This has been shown to cure the tensile instability problem but at the cost of not being able to extreme material deformations (Rade Vignjevic et al. 2006). However, it does lack versatility as primarily SPH models are run using a Eulerian kernel rather than Lagrangian due to the fact SPH mainly models fluids.

All in all, it can be seen from the literature overview that there the research to address the particle clumping issue has gone in many different directions.

Another issue of accurate modelling in SPH is the calculation of density. A simple way of calculating density is known as summation density, which is simply the sum of a particles neighbour masses in its support domain weighted by the kernel function. This was appealing due to its simplicity but is poor near boundaries due to the truncation of the kernel function, leading to a calculation of a smaller density than expected because of a lack of neighbours. However, this particle density deficiency does give approximately correct behaviour at free surfaces (Vignjevic & Campbell 2009). This is due to the fact that because of the deficiency, it will give 0 pressure at the free surface boundary, which is the correct behaviour as a free surface has 0 pressure (normal stress) at the water/gas boundary. However, Hoover (Hoover 1998) showed that the basic SPH method leads to fictitious surface tension effects. In addition, for near or incompressible SPH and for situations with breaking waves the correct behaviour is not captured, so research into this field is ongoing. For example, Becker and Tescher (Becker & Teschner 2007) developed a surface tension model based on cohesion forces that can deal with large curvature in the free surface, while Fang (Fang et al. 2009). focused on developing a more consistent SPH framework by using an energy based framework to ensure linear consistency of angular momentum.

Research in consistency was expanded to more specific cases. For example (Colagrossi & Landrini 2003) state that neglecting of air dynamics and hence free surface effects lead to the incorrect representation of pressure maxima, minima and oscillations. They used a Moving Least Squares (MLS) approach like Dilts, but applied to the density field only. This was shown to smooth pressure oscillations and provided a less noisy pressure flow for free surface and multiphase flows.

SPH research mainly focussed on modelling of fluids, not structures or FSI which is the focus of this thesis. Lobovsky (Lobovsky & Kren 2007) began extending the method to FSI interactions without the need of a coupled code with promising results for the future of complex FSI interactions modelled in SPH. The capability of the SPH method has recently been extended to describe both the fluid and the structure in FSI interaction (Antoci et al. 2007). This eliminated the need for coupling; however, this capability has only proved successful in simulating single phase flow impact on an elastic plate known as the elastic gate problem. When applied to a more complicated case in the form of the interaction between a skirt of a surface effect ship and water, results were incomplete indicating problems in extending the FSI capability reliably to a more complex case (Paredes & Imas 2011). Extension of the elastic gate problem to a sloshing tank scenario with a clamped beam immersed in the fluid has been proposed by Souto-Iglesias et al ((Vera et al. 2010) as a novel benchmark test of

the SPH method. This same test has also been considered as a way to test the particle finite element method which aims to use the advantages of both particle and mesh based methods (Idelsohn et al. 2008).

One of the difficulties of representing FSI interaction is that of contact and boundaries. The contact boundary condition has been largely ignored in the conventional Smooth Particle Method (SPH), with contact between two bodies simply handled by the conservation equations (R. Vignjevic et al. 2006).

Monaghan (Monaghan 1989) was the first to address this by preventing inter-penetration, which was a consequence of contact between materials treated simply as neighbour interpolation and hence mixing could occur. However, this did not prevent the other two issues that occur by treating contact in this manner, which is generation of non-physical tensile forces, resisting separation of two bodies. And the generation of shear stresses preventing friction-less or low friction sliding (R. Vignjevic et al. 2006). Belytschko began the process of a more robust treatment of contact by developing a 'pinball' contact algorithm designed to enforce impenetrability between elements (Belytschko et al. 1990). (Campbell et al. 2000) built upon this idea by introducing a particle to particle contact approach to contact.

Using the particle to particle contact approach, a robust contact algorithm based on Monaghan's repulsive force (Monaghan 2000) was derived (R. Vignjevic et al. 2006) (De Vuyst 2003; Vignjevic 2011). This is done by imposing a contact potential which approximated the interaction between a pair of particles, the force between particles is then calculated by the gradient of the potential. While the contact algorithm solved the issues mentioned by (R. Vignjevic et al. 2006), the derivation only focussed on the repulsive aspect of contact.

The key point made in (Layton 1999) is that possibilities of allowing attraction has not been investigated, furthermore the force does not include non-slip conditions given by $\mathbf{u} \cdot \hat{\mathbf{t}} \approx 0$ on Γ . To address the no-slip condition (Layton 1999) showed that there are 3 natural ways to do this, they are:

- 1) Lagrange multiplier implementation with equation as a constraint
- 2) Penalty term imposing equation approximately
- 3) Replacing no slip with friction slip with a friction factor which increases as the separation approaches 0.

In the SPH method (Müller et al. 2004) developed a contact algorithm, which generated an attractive force as well as the repulsive part based on the Leonard Jones force. While this is useful in the sense that it simulates adhesion for fluids and deformable solids, there are no significant results. This approach used by (Akinci et al. 2012) was developed by using a two-way coupling approach that simulated adhesion for fluids and rigid bodies (Akinci et al. 2012), which does not present the same challenge due to the fact they do not deform. In this instance, it is far simpler to simulate adhesion by use of ghost or boundary particles that have no ghost or particle pairs. By utilising equal and opposite forces concepts, these particles will stick. However, for a deformable body that will move and interact with different particles during time evolution of the simulation, this approach is insufficient. Research done by Akinci (Akinci 2014) does show promise in extending the work to simulating adhesion with deformable bodies. This involves the coupling of an SPH solver to the

structure composed of a triangular mesh and the generation of boundary particles for the mesh using the technique proposed by (Akinci et al. 2012). This does, however, lead to under sampling of the boundary particles and regardless is not suitable for our purposes since (Akinci 2014) states that this technique can only work if the deformations can be mapped to a triangle mesh, which given the fact the FSI interaction modelled in this body of work are all comprised of SPH particles, it makes this work insufficient for our purposes. What it does highlight, however, is the challenge of the simulation of adhesion is not just solved by the correct representation of the Leonard Jones force, but care and attention need to be given to the particle interactions at the interface. This issue is particularly highlighted in the review of work done to enforce no-slip boundary conditions in SPH conducted by (Souto Iglesias et al. 2010), where after reviewing the main techniques used in SPH to represent boundary particles such as ghost particles (Colagrossi & Landrini 2003) -where particles are replaced by ghost particles that mirror their opposite numbers behaviour-, imaginary particles (Takeda et al. 1994) and fixed zero velocity particles. The conclusion was that convergence to the exact solution seems feasible for all models and that future studies should be conducted for practical SPH simulations with a limited number of neighbours and disordered particles. Considering that all the research so far in SPH focuses on fixed boundaries, this indicates the depth of research still needed to develop accurate contact for highly deformable structures. The work done modelling FSI interaction with a deformable beam in this thesis is based on the contact algorithm developed by (De Vuyst 2003) as this is part of the MCM code. Chapter 3 will outline the nature of the algorithm more, while the work in this thesis will highlight the limitations of this contact algorithm.

In addressing particle clumping, this thesis will be applying a novel approach which has not been used in SPH before. This approach is called mixed element formulation and has been researched extensively in FE. Mixed methods are initially used in a finite element for analysis of incompressible materials and volumetric locking in equilibrium problems (Bathe 1996). This involved using a two-field displacement-pressure formulation, however, research has expanded beyond this. (Wang & Bathe 1997) extended the displacement pressure formulation to fluids and in the same paper extended the two-field displacement-pressure formulation to a three-field formulation that included as an independent variable a parameter α that was a vorticity co-efficient designed to suppress spurious rotational nodes. For dynamic problems, there exists a principle of virtual power and this is used to develop a three-field velocity, rate of deformation and stress mixed formulation. The two field displacement pressure (u-p) formulation has been extended to plasticity problems (Commend et al. 2004), a three field u-p-0 where 0 represents discontinuous volume parameter (Taylor 2000), crack propagation (Borja 2008) and contact. Further novel applications of this approach that have been published are the development of a three-field u-p- α approach to derive new equations that describe the motion of sloshing in a tank (Felippa & Ohayon 1990) and the use of a two field displacement-stress approach for simulation of photonic band cells (Srivastava & Nemat-Nasser 2014). The method has been shown to have to satisfy the Brezzi condition (Bathe 1996) and research has focused on finding the elements and solution spaces that satisfy this (VOHRALÍK & WOHLMUTH 2013). Overall, like the research in SPH on particle clumping, there is a diverse spectrum of research in the use of this technique to address FE shortcomings and application to various real-world problem modelling.

3 Mathematical development

This section shall detail the non-novel mathematics of SPH and mixed formulation. The mathematics in this chapter will show the development of the consistency of SPH, the contact algorithm developed by (De Vuyst 2003), SPH equations in the Total-Lagrange formulation and Mixed element formulation. The mathematics in this chapter will form the basis of the novel mathematical development of the mixed element formulation in chapter 8, the density update MLS algorithm chapter 4 and the changes to the contact algorithm chapter 6.

3.1 SPH Development and Consistency

SPH is a meshless numerical scheme. This means that there is no connectivity between nodes (or particles as they are called in SPH). In addition, each particle carries physical properties such as mass, velocity, stress and so on.

The basic step of the method for domain discretization, field function approximation and the numerical solution can be summarised as follows (Liu & Liu 2003). The continuum is decomposed into a set of arbitrarily distributed particles with no connectivity (meshless); 2. The integral representation method is used to approximate a field function 3. Particle approximation is introduced for converting integral representation into a finite summation by replacing the integral by a sum.

A field function is a function that satisfies the axioms of a field (Earl 2012).

A field consists of a set F and two binary operations “+” (addition) and “.” (multiplication), defined on R , for which the following conditions are satisfied: 1. $(F, +, \cdot)$ is a ring.

2. Multiplicative commutative: For any $M, N \in F$, $M \cdot N = N \cdot M$.

3. Multiplicative identity: There exists $1 \in F$ such that $N \cdot 1 = 1 \cdot N = N$ for all $A \in F$.

4. Multiplicative inverse: If $M \in F$ and $M \neq 0$, there exists $N \in F$ such that $M \cdot N = N \cdot M = 1$.

The integral representation is based on the following convolution integral (Liu & Liu 2010).

$$f(x) = \int f(x') \bar{\delta}(x - x') dx' \quad (1)$$

Where:

$\bar{\delta}(x - x')$ is the Dirac delta and has the properties:

$$\bar{\delta}(x - x') = 1 \text{ at } x = x', 0 \text{ elsewhere} \quad (2)$$

As long as the Dirac Delta is used, the integral representation shown in (1) is exact (Nastasescu & Gavrilă 2011). However, the Dirac Delta lacks continuity and differentiability, which makes it unsuitable to use in interpolation as further field approximations such as finding the stress of a particle is a function of the interpolation derivative. While continuity is a strong requirement of stability of a numerical scheme.

To retain the desirable properties of the Dirac Delta, the technique of the SPH method is to choose a smooth kernel as an interpolation function that mimics these properties (Li & Liu 2007) and has continuity and differentiability. This function is represented as W and is a function of position and width of kernel h .

This gives the integral representation as:

$$f(x) = \int f(x')W(x - x', h)dx' \quad (3)$$

Which as it is now an approximation, (3) now takes the form.

$$\langle f(x) \rangle = \int f(x')W(x - x', h)dx' \quad (4)$$

Where h is now the influence area of the kernel. As the kernel is not the Dirac delta, then the kernel serves only as an approximation. The kernel is chosen to be an even function. An even function has the property $f(x) = f(-x)$ and is symmetric about the y axis. This ensures that the Kernel is symmetric and has the consequence that particles from the same distance but different positions should have equal effect on a given particle.

Various research has gone into different types of Kernels such as Gaussian distribution or cubic splines, but they all must satisfy the following requirements (Nastasescu & Gavrila 2011).

Normalisation condition:

$$\int W(x - x', h)dx' = 1 \quad (5)$$

This ensures that the integral over the support domain of smoothing function is equal to 1, which is a necessary condition for a statistical distribution as it ensures that all outcomes are possible.

Compact support:

$$W(x - x', h)dx' = 0 \text{ for } |x - x'| > kh \quad (6)$$

Positive smoothing function for any point at x' within the support domain:

$$W(x - x', h)dx' > 0 \quad (7)$$

The smoothing function value must satisfy the Dirac delta function condition as the smoothing length approaches to zero:

$$\lim_{h \rightarrow 0} W(x - x', h) = \bar{\delta}(x - x') \quad (8)$$

The smoothing function value must be monotonically decreasing with the increase of the distance away from the particle.

Equation (8) begins the journey into SPH being a consistent scheme as it tells us that as the Kernel function smoothing length approaches 0, the function gets closer and closer to representing the Dirac Delta. This is a requirement for a **consistent** function. Belytechko (Belytschko et al. 1998) defines from finite element literature that consistency is the ability of an approximation to exactly represent a differential equation as the number of points goes to infinity and the distance between them go to 0. This is an example of 0 order consistency as the Dirac delta is a constant rather than a p order differential equation.

To highlight this visually, taking the Kernel as a Gaussian (which satisfies (5)-(8)), it can be seen that if you squash the Gaussian, its width will approach 0 and its height infinity and will get closer and closer to approximating the Dirac Delta.

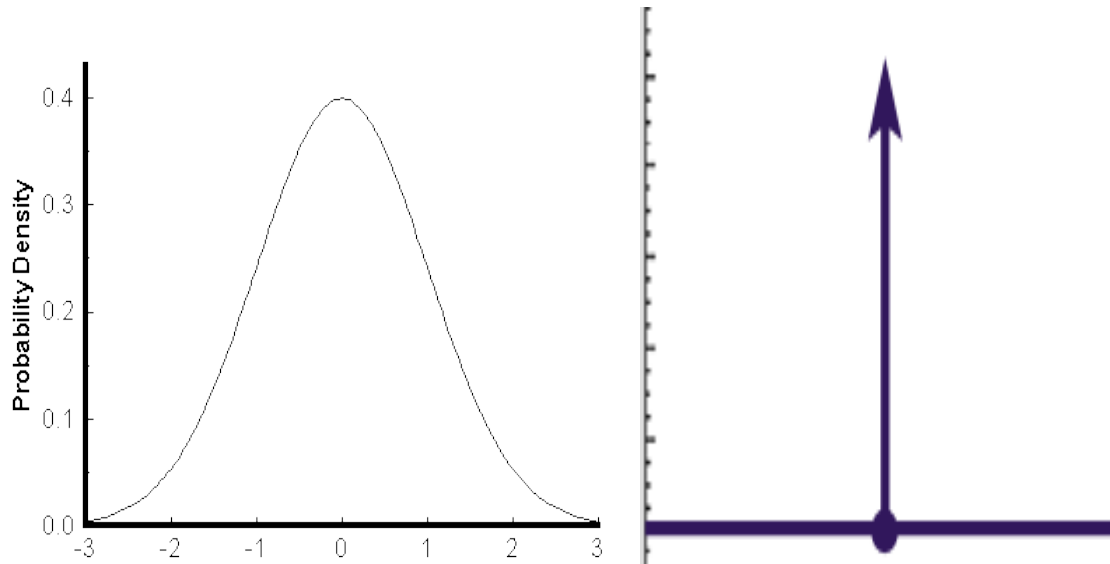


Figure 1: Comparison between the Gaussian bell function and the Dirac Delta

The next stage in the SPH derivation is the particle approximation phase. Equation (4) integral is replaced by a summation, which gives

$$f(x_i) = \sum_{j=1}^N f(x_j)W(x - x_j, h)\Delta V_j \quad (9)$$

Here the integral has been replaced by a summation procedure with the total volume integral dV now replaced by a sum of volumes up to the number N . This is also an example of a consistent technique as the more the integral is divided into sums, the closer it will represent the exact integral, with the limit being that an infinite number of divisions in the integral with 0 width will exactly represent the integral.

While in an intuitive sense it has been shown the scheme to be consistent, this work will now outline it in a more mathematical way using the proof outlined in (Liu & Liu 2003)

Starting from equation (4), suppose we wish to write $f'(x)$ in terms of $f(x)$, to do this, a Taylor series expansion is applied. The purpose of a Taylor series is to approximate a function with a polynomial by adding up n powers of its series and see if it converges.

If $f(x')$ is expanded as a Taylor series around x up to second order, we get the Taylor series of $f(x')$ as:

$$f(x') = f(x) + f'(x)(x' - x) + \frac{1}{2}f''(x)(x' - x)^2 \quad (10)$$

Which can be rewritten according to (Liu & Liu 2003) as:

$$\sum_{k=0}^n \frac{-1^k h^k f^k(x)}{k!} \left(\frac{x - x'}{h} \right)^k + r_n \left(\frac{x - x'}{h} \right) \quad (11)$$

With $r_n \left(\frac{x - x'}{h} \right)$ the residual in the Taylor series.

Substituting (11) into (4) we get:

$$\langle f(x) \rangle = \int \sum_{k=0}^n \frac{-1^k h^k f^k(x)}{k!} \left(\frac{x - x'}{h} \right)^k W(x - x', h) dx' + r_n \left(\frac{x - x'}{h} \right) \quad (12)$$

Which can be rewritten as:

$$\langle f(x) \rangle = \sum_{k=0}^n \frac{-1^k h^k f^k(x)}{k!} \int \left(\frac{x-x'}{h} \right)^k W(x-x', h) dx' + r_n \left(\frac{x-x'}{h} \right) \quad (13)$$

Rearranging to equate $f(x)$ to $f^k(x)$ we get:

$$f(x) = \sum_{k=0}^n A_k f^k(x) + r_n \left(\frac{x-x'}{h} \right) \quad (14)$$

Where:

$$A_k = \frac{-1^k h^k}{k!} \int \frac{(x-x')}{h} W(x-x', h) dx' \quad (15)$$

For $f(x)$ to be approximated to n th order, left hand side coefficients must equal right hand side coefficients and since the left hand side coefficients is just $f(x)$ then for this to be satisfied $f(x) = f^0(x)$. This will only occur if $A_0=1$ and $A_1=A_2=A_n=0$

Hence:

$$A_0 = \int W(x-x', h) dx' = 1 \quad (16)$$

$$A_1 = -h \int \left(\frac{x-x'}{h} \right) W(x-x', h) dx' = 0 \quad (17)$$

Equation (16) is the normalisation property showed in equation (5). While equation (17) gives us the symmetry property. This ensures that SPH approximation of a function is consistent to 1st order is consistent (Cossins 2010). A similar procedure exists for $f'(x)$ except with the addition of another criterion:

$$W(x-x', h)|_{\Gamma} = 0 \quad (18)$$

This equation simply means that the Kernel will vanish on the surface of the support domain. This gives us our compact support condition, which states that beyond the support domain, the kernel will be 0 and hence there will be no neighbour influence on the interpolation. This is necessary from a computational point of view as if the domain included all particles, this would increase the computational time of the simulation significantly.

While consistency has been discussed, another requirement is that of completeness. If an approximation that can represent exactly a polynomial to order k , the approximation will be **complete** to order k (Belytschko et al. 1998).

Clearly, the integral representation of SPH is at least 0 order complete, as it has been shown that $f(x) = f^0(x) = c$ if and only if the integral of the kernel is equal to one. For first order completeness, it must be shown that:

$$f(x) = c_0 + c_1 x \quad (19)$$

Which can only occur if (17) is satisfied, hence the Kernel properties lead to completeness of the scheme.

The particle approximation phase of SPH is not as simple. Numerous books and papers (Gingold & Monaghan 1982; Liu & Liu 2003; Vignjevic & Campbell 2009) illustrate the failings of the particle approximation to satisfy even zero order completeness. This is evident in cases with irregular spaced particles and truncated boundaries. To correct this, Shepard functions restore zero order consistency to particle approximation.

Particle approximation of SPH is given by:

$$u^h(x) = \sum_i^n W_{ij} u(x) \quad (20)$$

Where u is a field variable (e.g. density, velocity). This is analogous to equation (1) with the function of x now represented as a variable (nodal value) and the integral now replaced by a summation.

Shepard functions restore 0 order consistency simply by dividing (20) by the sum of kernels, as they cancel out it just leaves us with:

$$W_{shep}(x) = \frac{W_i(x)}{\sum_j W_j(x)} \rightarrow u^h(x) = W_{shep}(x) c \rightarrow \frac{\sum_i W_i(x)}{\sum_j W_j(x)} c \rightarrow c \quad (21)$$

Linear completeness can be shown by using a moving least squares function. The principle behind the least squares technique is that in an overdetermined system, that is a system with more equations than unknowns, an attempt is made to fit the data through the best straight line between the points. Because of the nature of the system, at each point there will be an error between the position of the point and where the line of best fit is drawn. Furthermore, there will be more than one best line of fit. For example, one line may have a line of best fit nearer to point one than point three, another may be the opposite. Because there is no exact solution to an overdetermined system in this form, the question remains what is the best solution?

The application of the least squares technique is to make the sum of the errors of the squares as small as possible. Mathematically this is defined as:

$$e_1^2 + e_2^2 \dots e_m^2 = \min \|f - Au\|^2 \quad (22)$$

Where A is the overdetermined matrix, u is the vector of unknown coefficients and f is the solution vector. Equation (22) is called the least squares approach. Weighted least squares are similar except a weighting factor is introduced. This weighting factor considers the distance between the approximation and the position of the data points and is hence a function of Euclidian distance. Moving least squares is the same principle as weighted least squares except that you begin with an arbitrary fixed point and that fixed point is moved to the problem domain. The key difference is that in the least and weighted least squares, the data points are fixed but in moving least squares, a point is moved and hence weighted least squares fit is computed for each individual point.

Mathematically, MLS works as follows. Given a set of scattered N points at position x_i in the realm of real numbers with $i \in [1 \dots N]$ that carry scalar values f_i , the least squares technique is concerned with finding the best fit function that minimises the error as described in equation (22). Hence it can be written this as:

$$f(x) = b(x)^T \cdot c(x) \quad (23)$$

With equation (22) being rewritten as:

$$J = \sum_i^n |b(x)^T \cdot c(x) - f_i|^2 \quad (24)$$

Where **b** is a polynomial basis vector and **c** the vector of unknown coefficients of the basis functions that will be minimised. For example a linear basis in 3d is given by **b(x)** = [1,x,y,z], while a quadratic basis in 2d would be given as **b(x)** = [1,x,y,z, x², x²y,xy²y²]. Consider that as the whole idea of the least squares and hence moving least squares approximation is to minimise the distance between the scattered points and the approximating function, it is essentially a minimisation problem. As it is a minimisation problem, to find the minimum can be done by setting the partial derivatives of all **c_i** to 0.

Hence by use of chain rule we get:

$$\frac{\partial J_i}{\partial c_i} = 2 \sum_i^n |b(x_i)^T b(x_i) c_i - b(x_i) f_i| = 0 \quad (25)$$

Divide by 2 and rearranging gives:

$$\sum_i^n b(x_i)^T b(x_i) c_i = \sum_i^n b(x_i) f_i \quad (26)$$

Rearranging for c gives:

$$c = \sum_i^n [b(x_i)^T b(x_i)]^{-1} \sum_i^n b(x_i) f_i \quad (27)$$

If $A = \sum_i [b(x_i)^T b(x_i)]^{-1}$ is non-singular, then substitution into $f(x)$ gives us our values for c which give the best fit function $f(x)$.

This illustrates how the least square procedure works, for the weighted least squares procedure we minimise:

$$J = \sum_i^n \bar{w}(\bar{x} - x_i) |b(x)^T \cdot c(x) - f_i|^2 \quad (28)$$

The function $\bar{w}$ is a weighting function that weights the error between $\bar{x}$ and positions of data points x_i . $\bar{x}$ in this case is a fixed point and now J will be minimised with respect to a fixed point. Another key difference is that the minimisation is within a local domain R ($\bar{x} - x < R$) with anything outside of this being 0. This gives a local least squares approximation. Hence equation is written as:

$$f(x)_{\bar{x}} = b(x)^T \cdot c(\bar{x}) \quad (29)$$

As the unknown coefficients are local solutions with respect to the point of interest, rather than global solutions as in the least squares technique.

A weighting function that has a limited domain and decreases as distance between the points increases satisfies the SPH kernel and so the SPH kernel can be used in the weighted least squares technique. Replacing $\bar{w}$ by SPH kernel w , we get:

Hence:

$$c(\bar{x}) = \sum_i [w(x - x_i) b(x_i)^T b(x_i)]^{-1} \sum_i w(x - x_i) b(x_i) f_i \quad (30)$$

If $A = \sum_i [b(x_i)^T b(x_i)]^{-1}$ is non-singular, then substitution into $f(x)$ gives us our values for c which give the best fit function $f(x)$. This approach exhibits a lot of characteristics of the SPH method as the same weighting function can be used and the weighting of influence particles over a domain or neighbourhood is the crux of the SPH method.

Moving least squares takes the concept of weighting least squares but instead of the point being fixed, the point moves across the entire domain. Given that SPH particles are moving, the technique is now suitable for SPH implementation.

3.2 MLS and consistency:

Starting from equation (23) and using equation (20) we get:

$$u_h(x) = \sum_i^n b(x)^T \cdot c(x) \quad (31)$$

With J being:

$$J = \sum_i^n w(\bar{x} - x_i) |b(x)^T \cdot c(x) - u_i|^2 \quad (32)$$

Hence:

$$c(\bar{x}) = \sum_i^n [w(x - x_i) b(x_i)^T b(x_i)]^{-1} \sum_i^n w(x - x_i) b(x_i) u_i \quad (33)$$

Setting:

$$A = \sum_i^n [w(x - x_i) b(x_i)^T b(x_i)]^{-1} \quad (34)$$

We get:

$$B = \sum_i^n w(x - x_i) b(x_i) \quad (35)$$

$$\mathbf{c}(\bar{\mathbf{x}}) = \mathbf{A}^{-1} \mathbf{B} \mathbf{u} \quad (36)$$

Recall that:

$$u_h(x) = \sum_i^m b(x)^T \cdot c(x) \quad (37)$$

Hence $u_h(x)$ can be written as:

$$u_h(x) = \sum_i^m b(x)^T \cdot \mathbf{A}(x)^{-1} \mathbf{B}(x) u_i \quad (38)$$

Comparison to equation (20) gives:

$$W_{ij} = b(x)^T \mathbf{A}(x)^{-1} \mathbf{B}(x) \quad (39)$$

This is the moving least squares kernel. Recall that $b(x)$ was the basis function. Therefore, if the basis function was constant (0 order as no polynomial terms) we would get:

$$\frac{W_i(x)}{\sum_j W_j(x)} \quad (40)$$

Which is our Sheppard function kernel, defined as 0 order complete as we could exactly represent the polynomial to 0 order.

Using a linear basis, we can prove the moving least squares technique gives us first order completeness.

If u_i equal α_i a constant, then the derivative of a constant will be 0 and hence be a minimum. Therefore, if J vanishes we get:

$$u_h(x) = \sum_i^m b(x)^T \cdot \alpha_i = u(x) \quad (41)$$

Therefore, any function in the basis is reproduced exactly. This is not just exclusive to constant and linear bases.

Chapter 4 will use this MLS approach to the updating of density fields.

3.3 Contact modelling in MCM

This section shall detail more the development of the frictionless contact algorithm described in the literature review. This will form the backbone of the FSI contact modelling in chapters 6 and 7 as simulation of contact between the material boundaries will use this algorithm.

A particle j is usually considered a neighbour of particle i , if it is within a distance of $2h$ of i . The parameter h varies in size but my simulations take h as 1.3 times the particle spacing. This same principle is used in registering contact between particles; hence if a boundary is within $2h$ of a particle, contact occurs. This is given as:

$$ga = \|x^i - x^j\| - (h^i + h^j) \quad (42)$$

Where x^i and x^j are position vectors of particles i and j respectively, h the smoothing length of particles i and j and ga the gap function. if $ga < 0$ contact occurs as from equation (42) it can be seen that this will only occur if and only if $\|x^i - x^j\|$ - the distance between particles i and j - is less than $2h$.

Equation (42) shows the criteria for contact between particles to occur. The contact potential and subsequently force is derived from the strong form momentum equation and contact conditions. The proof is shown in (De Vuyst 2003) and will be highlighted here in order to provide illustration.

Contact is derived by first considering the strong form momentum equation with constraints. This is given by:

$$\nabla \sigma + \rho f^b = \rho a \quad (43)$$

With boundary conditions

$$\sigma \cdot \hat{n} = t \text{ on } \Gamma_t \quad (44)$$

$$u = \bar{u} \text{ on } \Gamma_t \quad (45)$$

To derive the SPH form of the weak form momentum equation, it suffices to multiply equation (43) by a trial function w and integrate over the domain. After simplifying certain terms by employing Greens theorem and applying boundary conditions, SPH interpolations are then substituted in which yields a SPH version of the FE weak form.

However, this does not take into account contact conditions which are given by (R. Vignjevic et al. 2006)

$$t_a = -t_b, \Gamma_c = \Gamma_a \cap \Gamma_b \quad (46)$$

$$t_n > 0, g_a \leq 0, t_n \cdot g_a = 0 \quad (47)$$

Multiplying equation (43) by a trial function ω and integrating over the domain gives:

$$\int_{\Omega} \omega \nabla \cdot \sigma dV = \int_{\Omega} \omega \rho (a - f^b) dV - \int_{\Gamma} \omega t d\Gamma \quad (48)$$

The trial function is arbitrary and it is this arbitrariness that is crucial as otherwise a weak form of the partial differential equations that govern the system would not be equivalent to the strong form. Section 3.4 will discuss weak and strong in more detail, at this point it suffices to say that the trial function can be thought of as an enforcer: whatever it is multiplied by is enforced to 0 by its arbitrariness (Fish & Belytschko 2007).

The last integral term in equation is a consequence of the contact condition. Applying the same procedure as described by (De Vuyst 2003) we get:

$$\int_{\Omega} \rho H^T H dV d + \int_{\Omega} B^T \sigma dV d\sigma - \int_{\Omega} H^T f^b dV - \int_{\Omega} H^T b_c dV - \int_{\Gamma_t \cup \Gamma_u} (H^T \sigma) \cdot n d\Gamma \quad (49)$$

With H the array of shape functions and B the differential of the shape functions which acts as the strain displacement matrix. This will be expanded upon in further chapters.

The 4th term of equation (49) is the contact force. b_c is given as:

$$f_{ij} = \frac{W(r_{ij})}{W(\Delta p)} \quad (50)$$

Where (Δp) is the average particle spacing in the neighbourhood of i. W is the smoothing kernel, r the distance between a particle i and its neighbour j. Equation (49) is Monaghans repulsive force (Monaghan 2000) and is added to the SPH momentum equation in the form of Rf_{ij}^N as an artificial repulsive force. This is used as it satisfied the contact requirements (equations 46 and 47) and provides a repulsive force. As force is the gradient of the contact potential, the contact potential is the integral of force, hence defined as:

$$\varphi = \int_{CBL} Q \left(\frac{W(r_{ij})}{W(\Delta p)} \right)^n \quad (51)$$

Q is a user defined scalar contact stiffness penalty parameter and CBL is the intersection between the kernel support centred at a particle in contact with the domain of the body that it does not belong to (De Vuyst 2003).

The magnitude of the repulsive force depends on the stiffness factor Q , which is multiplied by equation (51). An illustration of the effect the stiffness factor Q has on particle penetration is shown.

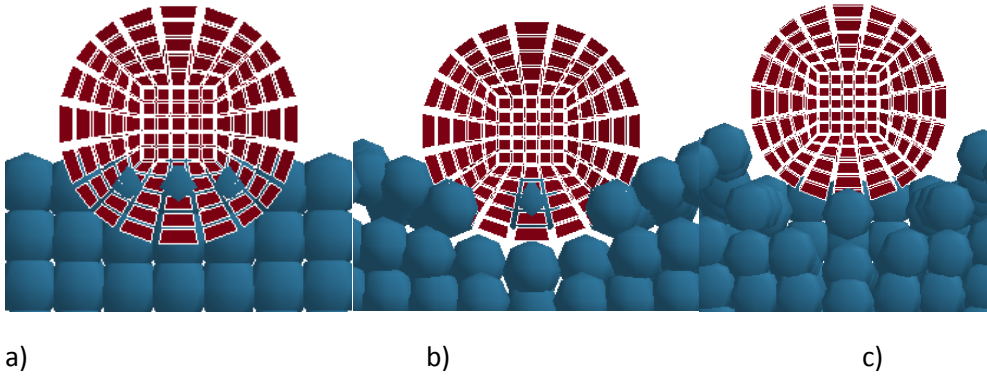


Figure 2: Illustration of effect that different values of stiffness Q has on penetration. a) has a value of 0.01, b) 0.1, c) 1

This illustrates the less stiff a material is, the more penetration occurs. The balancing act is obtaining the right contact stiffness in simulations to give the correct physical behaviour when contact occurs between materials.

Contact is implemented into MCM by penalisation of the momentum equation in the form of:

$$\langle \dot{v}_i \rangle = \sum_{j=1}^n m_j \left(\frac{\sigma_i}{\rho_i^2} + \frac{\sigma_j}{\rho_j^2} \right) \cdot \nabla W_{ij} - \sum_{j=1}^n m_j (K \cdot f_{ij}) \cdot \nabla W_{ij} \quad (52)$$

Another contact option is using pressure contact. This acts as a repulsive force but is a function of pressure and density.

$$PS \left(\frac{p_i}{(\rho_i)^2} - \frac{p_j}{(\rho_j)^2} \right) \quad (53)$$

Where PS acts as a user defined stiffness factor and this is subtracted from equation (52) instead of the contact potential.

3.4 Mixed element approach

One of the main areas of novelty in this thesis is the development of the mixed element formulation in the SPH method. As the literature review discussed, using mixed element formulation in finite element is common. This section shall illustrate the mathematics behind the development of the finite element approach to solve idealised problems for a single field using the concept of virtual work. Then the work will show how mixed formulation expands upon the single field finite element formulation to develop an assembly of elements for multiple fields that can then be solved. The proofs are taken from (Bathe 1996) with other contributions referenced if used.

3.4.1 Single field approach

The finite element formulation is a way of solving complex problems by idealising the problem as an assembly of interconnected elements, where force balance equations are developed for each element. The method is a numerical method, in that the solutions found are approximate. As the solutions found are approximate as opposed to exact, it is vital that the best solution is found, the one that minimises the error that comes because of a numerical solution.

The mathematical field that deals with minimisation problems are called variational calculus and the process of finding a solution to the finite element assembly of equations is a variational problem. A typical finite element problem is to calculate unknown kinematic quantities (displacement, velocity, acceleration) and associated stresses and strains (using constitutive relations) from a given (known) geometry, applied loads, governing equation, constitutive laws and initial conditions. The first step in doing this is to assemble the finite element equations.

The governing equation of a system is a differential equation that describes the evolution of the system. A general governing equation of a system looks like this.

$$\sigma_{ji,j} + f_i = \rho a_i \quad (54)$$

This is no more than conservation of momentum ($f=ma$). This will have different forms depending on the nature of the problem you are trying to solve. For example, if there are no external forces in the problem f_i is equal to 0, while for static problems acceleration is equal to 0. A problem in this form is called a strong form problem as it contains second derivatives. The finite element method transforms a strong form problem to a weak form problem, which is a problem containing only first derivatives. The reason behind this is that by using this approach, the continuity requirements are weakened, so the problem only has to be 1st order continuous. Continuity is an important part of a stable solution and this step makes it easier to develop elements that are 1st order continuous. Formulation of a weak form finite element problem is as follows:

Starting from the equilibrium equation:

$$\sigma_{ji,j} + f_i = 0 \quad (55)$$

With boundary conditions:

$$\sigma_{ij}n_j = f_i^{\Gamma f} \quad (56)$$

$$u_i = u_i^{u\Gamma} \quad (57)$$

To develop the FE equations, equation (55) must be restated in a ‘weak’ form. This is done by integrating (55) and multiplying by an arbitrary virtual displacement $\bar{u}_i$. This virtual displacement must satisfy the geometric constraints of the system, that is satisfy the essential boundary condition. For this to occur $\bar{u}_i$ must be 0 at the displacement boundary condition.

$$\bar{u}_i = 0 \quad (58)$$

This gives equation (55) as:

$$\int \bar{u}_i (\sigma_{ji,j} + f_i) dV = 0 \quad (59)$$

Where $\bar{u}_i$ is the virtual displacement. As this is arbitrary, that is $\bar{u}_i$ can take any form. Equation (59) is only satisfied if and only if

$$\sigma_{ji,j} + f_i = 0 \quad (60)$$

This comes from the fundamental theorem of calculus that states

$$\int_x f(x)g(x)dx = 0 \quad (61)$$

Then for all f(x) where f(x) is continuous then g(x) is identical to 0.

Therefore equation (55) and (60) are equivalent due to fact that $\bar{u}_i$ are arbitrary and the fundamental theorem of calculus (61) showing us that one function is identical to 0 if the other is continuous.

Using the identity

$$(\sigma_{ij}\bar{u}_i)_j = \sigma_{ji,j}\bar{u}_i + \sigma_{ij}\bar{u}_{i,j} = 0 \quad (62)$$

We get be substitution of (62) into (59)

$$\int_V \left[(\sigma_{ij} \bar{u}_i)_j - \sigma_{ij} \bar{u}_{i,j} + f_i \bar{u}_i \right] dV = 0 \quad (63)$$

By divergence theorem, the 1st term of (62) is written as:

$$\int_V -\sigma_{ij} \bar{u}_{i,j} + f_i \bar{u}_i dV + \int_{\Gamma} (\sigma_{ij} \bar{u}_i) n_j d\Gamma = 0 \quad (64)$$

By substitution of boundary conditions and symmetry of the stress tensor we get:

$$\sigma_{ij} \bar{u}_{i,j} = \sigma_{ij} \left[\frac{1}{2} (\bar{u}_{i,j} + \bar{u}_{j,i}) \right] = \sigma_{ij} \epsilon_{ij} \quad (65)$$

This gives:

$$\int_{\Gamma_f} f_i^{\Gamma_f} \bar{u}_i^{\Gamma_f} d\Gamma + \int_V f_i u_i dV = \int_V \sigma_{ij} \epsilon_{ij} dV \quad (66)$$

Equation (66) is defined as the principle of virtual work. This states that for small displacements that satisfy (66). Total internal virtual work = Total external virtual work. This shows the link between strong form momentum equation and its boundary conditions to a weak form expression in terms of virtual work. This procedure is the same approach used to develop the SPH momentum equation earlier on in the chapter.

The process is reversible, i.e. weak to strong. Consider that total work done by a force moving a particle from point A to point B is given by:

$$W = \int_A^B F \cdot du \quad (67)$$

Virtual work is simply the work done by a force moving a particle through a virtual displacement (or a virtual force through a real displacement). The terms in the principle of virtual work are simply different descriptions of equation (66). The internal virtual work term is simply internal forces moving through a virtual displacement and the same principle applies to the external virtual work

terms for both a surface and a volume, depending on whether a body or a surface force is applied. This gives rise to another way of obtaining the virtual work principle. Given a deformable body of volume V and surface area S , simply consider both the internal and external forces on the problem (internal stress, body force, surface force) and then multiply by an arbitrary virtual displacement. This then gives the forces in virtual work form. Equate the internal virtual work to the external virtual work to obtain the virtual work principle.

From the virtual work principle, reversing this (i.e. weak to strong) generates the momentum equation and the natural boundary condition, hence the description natural boundary condition as it arises naturally from the process. The displacement boundary condition is known as the essential boundary condition, as it is required to complete the problem. If it was not there, then $\bar{u}_i$ would not be required to equal 0 at the displacement boundary, and hence the geometric constraints of the system would be violated.

This illustrates the virtual work principle. The variation of $\bar{u}_i$ is arbitrary apart from at $\bar{u}_i = u_i^{\Gamma u}$ where it vanishes. The essential boundary condition is required to ensure the geometric constraints of the system are satisfied. The $\bar{u}_i$ that satisfies the natural boundary conditions and the equilibrium equation is the solution required. From this all other variables are calculated.

The formulation of the virtual work principle from the equilibrium equation was done using what is called a pure displacement approach. This means that the system was minimised subject to displacements. When it comes to the next step of discretising the integrals to a summation form, only displacements are interpolated with other quantities calculated from the interpolated displacements.

This approach is sufficient for most finite element problems, however as discussed in the literature review, the finite element does suffer from problems and so research has been and continues to be done in deriving and applying finite element equations that considers independent interpolation of more than one variable. This method is called the mixed element formulation.

3.4.2 Mixed formulation (MEF) introduction

The mixed formulation approach uses the Hu-Washizu functional. This was devised independently by Hu and Washizu and is a multi-field version of the virtual work principle that allows simultaneous variations of more than one variable. In fact, it can be viewed simply as a Lagrange multiplier form of the single field weak form of virtual work (or power).

A generic example of the Hu-Washizu functional is given below (Bathe 1996).

$$\pi(u, \varepsilon, \lambda) = \pi - \int_V \lambda (\varepsilon - \partial_\varepsilon u) dV \quad (68)$$

π is the principle of virtual work given by equation (66), λ is a Lagrange multiplier and is unknown, while $\varepsilon - \partial_\varepsilon u$ is the displacement-strain relation. What is evident is that the problem described by the pure displacement formulation has now been restated. Whereas before a generic problem would be along the lines of using the finite element method to solve the equilibrium equation using

the displacement-strain relation by substitution, now this relation is now a constraint on the problem. This is just another optimisation problem, but instead of substitution, the method of Lagrange multipliers will be used to optimise the solution subject to a given constraint.

The type of constraint will depend on the formulation used. The Lagrange multiplier method is to optimise the function f subject to the constraint o , this mathematically looks like: $\nabla f(x, y, z) = \lambda \nabla o(x, y, z)$.

Therefore, if using a displacement strain formulation, the constraint must be a function of displacement and strain as well. This same principle applies to all the formulations and will be shown as alternate formulations are developed.

A final point to note that as in (Bathe 1996) invoking the stationarity of π is equivalent to using the principle of virtual displacements. Hence $\delta u = \bar{u}$, $\delta \varepsilon = \bar{\varepsilon}$ and so on. This notation will be used from now on.

3.4.3 Finding the Lagrange Multiplier

Before we start the process, what is known to us are the following relationships $\sigma = C\varepsilon$, f^b = body force, f^{Γ_f} are tractions applied to Γ , the force applied to the surface. In the same manner as before, $\Gamma = \Gamma_f \cup \Gamma_u$, $\Gamma_u \cap \Gamma_f = \emptyset$, $u = \bar{u}$ is the essential boundary condition.

Virtual work is a displacement based approach. In a mixed approach, there are several variables that can be interpolated independently such as stress, strain or pressure. Strain is chosen in this case simply as a validation of the derivation as the results are known in literature (Bathe 1996).

$$\pi^*(u, \varepsilon, \lambda) = \frac{1}{2} \int_V \varepsilon^t C \varepsilon dv - \int_V u^t f^b dv - \int_{\Gamma_f} u^{\Gamma_f t} f^{\Gamma_f} d\Gamma - \int_V \lambda^t (\varepsilon - \partial_\epsilon u) dV \quad (69)$$

Applying stationarity in the same manner as in the single field approach.

$$\begin{aligned} \delta \pi^* = & \frac{1}{2} \int_V \delta \varepsilon^t C \varepsilon dV - \int_V \delta u^t f^b dV - \int_{\Gamma_f} \delta u^{\Gamma_f t} f^{\Gamma_f} d\Gamma - \\ & \int_V \delta \lambda^t (\varepsilon - \partial_\epsilon u) dV - \int_V \lambda^t (\delta \varepsilon - \delta \partial_\epsilon u) dV \end{aligned} \quad (70)$$

Performing volume integration by parts on $-\int_V \lambda^t \delta \partial_\epsilon u$ gives:

$$-\int_V \lambda^t \delta \partial_\epsilon u = -\int_{\Gamma} \delta u^{\Gamma} \lambda^t \cdot n d\Gamma + \int_V \delta u^t \lambda^t_{,j} dV \quad (71)$$

Substitution back into equation (70) and collecting terms gives:

$$\delta u^t: \lambda^t_{,j} - f^b = 0 \text{ in } V \quad (72)$$

$$\delta \varepsilon^t: C\varepsilon - \lambda^t = 0 \text{ in } V \quad (73)$$

$$\delta \lambda^t: \varepsilon - \partial_\varepsilon u = 0 \text{ in } V \quad (74)$$

Recalling the assumption that:

$$\Gamma = \Gamma_1 \cup \Gamma_2, \Gamma_1 \cap \Gamma_2 = \emptyset \quad (75)$$

And the arbitrariness of $\delta u^t, \delta \varepsilon^t, \delta \lambda^t, \delta \mu^t$ we get:

$$\delta u : \lambda^t \cdot n - f^{sf} = 0 \text{ on } \Gamma_f \quad (76)$$

$$\delta u: \lambda^t \cdot n - \mu^t = 0 \text{ on } \Gamma_u \quad (77)$$

Hence $\lambda^t = \sigma^T$ and $\mu^t = f^{\Gamma_f}$, where f^{Γ_f} is surface traction.

In the same manner as previously, plugging in the Lagrange multiplier values gives us the momentum equation, constitutive relation, displacement-strain relation and boundary conditions.

The differences between the variables that are interpolated in the virtual power and virtual work approach come from the fact that the virtual work is a displacement based approach and the virtual power is a velocity based approach. As velocity is simply a rate of change of displacement with respect to time, virtual power is simply a rate based approach of virtual work, so the variables that are functions (or functional) of the virtual power based approach are simply rate versions of the variables that are functionals of the virtual work approach (u, v) and $(\varepsilon, \dot{\varepsilon})$.

Note also that what I have done starts from the Weak form and gives us the strong form of momentum, constitutive relations and boundary conditions. This process is reversible, in that you can start with the strong form of these relations and obtain the weak integral form in the same way as in the pure displacement method.

3.5 Displacement/pressure based MEF formulation

The next stage of this process is to illustrate the theory behind a popular two field approach. This is the displacement-pressure approach.

To include pressure in the formulation, the virtual work principle is rewritten to include pressure by splitting stress and strain vectors into volumetric (subscript V) and deviatoric (dash) parts.

$$S = \sigma + p\delta \quad (78)$$

$$\epsilon' = \epsilon - \frac{1}{3}\epsilon_V\delta \quad (79)$$

Where δ is the kronecker delta function.

$$\int_V \epsilon'^t S - \int_V \epsilon_v p dV = \int_V u^t f^b dV - \int_{\Gamma_f} u^{\Gamma_f t} f^{\Gamma_f} d\Gamma \quad (80)$$

The Hellinger-Reissner functional is obtained from (80) as:

$$\pi(u, \epsilon) = \frac{1}{2} \int_V \epsilon^t C \epsilon dV + \int_V \epsilon^t C \partial_\epsilon u dV - \int_V u^t f^b dV - \int_{\Gamma_f} u^{\Gamma_f t} f^{\Gamma_f} d\Gamma \quad (81)$$

This looks quite different from (66); the reason being is that a number of assumptions have been made such as:

- $\sigma = C\epsilon$, with C being the stress-strain matrix of the material as defined in (Bathe 1996)
- Displacement boundary conditions are satisfied exactly and the displacement variations are 0 on the surface of the prescribed displacements. Hence $\partial_\epsilon u = \epsilon$ and $\int f^{\Gamma_u} (u^\Gamma - u_p) dV = 0$.

This form is displacement/strain formulation. To get into displacement pressure formulation, the strain is split into deviatoric and volumetric, with the deviatoric assumed to be from the displacement. Following the same steps outlined from (61) to (67) we get:

$$\begin{aligned} \pi^* = & \int_V \varepsilon'^t C \varepsilon' dV + \int_V \frac{p^2}{k} dV - \int_V u^t f^b dV - \\ & \int_{f\Gamma} u^{\Gamma t} f^{\Gamma f} d\Gamma - \int_V \lambda \left(\varepsilon_v + \frac{p}{k} \right) dV \end{aligned} \quad (82)$$

The last term illustrates that the problem is subject to the constraint $p = -k\varepsilon_v$, the pressure in the body.

The corresponding governing finite element interpolations are:

$$u = H\hat{u}, p = H\hat{p} \quad (83)$$

$$\varepsilon' = B_d \hat{u}, \varepsilon_v = B_v \hat{u} \quad (84)$$

Substituting the governing finite equations into the above equation gives:

$$\begin{bmatrix} K_{UU} & K_{PU} \\ K_{UP} & K_{PP} \end{bmatrix} \begin{bmatrix} \hat{u} \\ \hat{p} \end{bmatrix} = \begin{bmatrix} R \\ 0 \end{bmatrix} \quad (85)$$

Where

$$K_{UU} = \int_V B_d^T C' B_d dV \quad (86)$$

$$K_{UP} = K_{PU}^T = - \int_V B_v^T H_p dV \quad (87)$$

$$K_{PP} = - \int_V H_p^T \frac{1}{k} H_p dV \quad (88)$$

This section has illustrated how from a physical problem, the finite element solution leads to the principle of virtual work. From there it has shown that to apply to a mixed element approach, the Hu-Washizu (69) is required, which is an extension of the virtual work.

The displacement-pressure formulation for a solid body in equilibrium is given by:

$$\begin{aligned} \pi(u, p)^* = & \int_V \frac{1}{2} \varepsilon'^t C \varepsilon' dV + \int_V \frac{1}{2} \frac{p^2}{k} dV - \int_V u^t f^b dV - \\ & \int_{\Gamma_f} u^{\Gamma_f t} f^{\Gamma_f} d\Gamma - \int_V \lambda \left(\varepsilon_v + \frac{p}{k} \right) dV \end{aligned} \quad (89)$$

With $p = -K \varepsilon_v$

- Internal and external work written in terms of displacement and pressure.
- Constraint connects displacement and pressure, as volumetric strain is written in terms of displacement.
- The Lagrange multiplier has been verified to be pressure.
- The final term in (89) links pressure to volumetric strain. This will change depending on the material assumptions of the problem you wish to solve. In this case, it shall be assumed pressure has a linear relationship to volumetric strain.

The formulation will change depending on the nature of the material as well. Equation (89) considered a static body in equilibrium but for a non-viscous fluid, the displacement pressure formulation looks like this (Wang & Bathe 1997).

$$\Pi = \int_V \frac{p^2}{2\beta} dV - \int_V u \cdot f^B dV - \int_V p \left(\nabla \cdot u + \frac{p}{\beta} \right) dV + \int_{\Gamma_f} p u_n^{\Gamma_f} d\Gamma \quad (90)$$

The first two terms are simply a restatement of the strain energy and potential of external forces written in pressure form, the third term is the constitutive relation.

The first difference between equation (89) and (90) is that fact that equation (90) represents a non-viscous fluid, so deviatoric strains are 0 and hence the $\frac{1}{2} \varepsilon'^t C \varepsilon' = 0$ in this case. Secondly, as equation (96) represents a fluid, the equation of state is changed to reflect the relationship between pressure and bulk modulus as opposed to pressure and stiffness. It would be ideal to develop in the code a

general displacement-pressure formulation that will apply for any equation of state and material model.

This section has outlined and explained the approach taken by (Bathe 1996) to develop single and mixed field finite element assembly using the virtual displacement approach. This will form the foundation to developing mixed field approaches in SPH.

4. Application of MLS density update to free surface modelling.

This chapter begins the work necessary for accurate FSI modelling. The first step to this is a more accurate representation of pressure in high impact free surface and sloshing water waves. The work describes the implementation of the moving least squares approach, described in literature and in equations (23)-(39) as a way to restore 1st order consistency, to the density field. This is also shown in literature (Colagrossi & Landrini 2003) and the chapter mainly focuses on the implementation and testing of the method to MCM. However, a few new modifications are researched and tested.

As outlined in the literature overview, density was calculated as a simple sum. However, truncation at boundaries leads to neighbour deficiency in the approximation of a field variable. The equation for the summation density is given below:

$$\rho_i = \sum_{j=1}^N m_j W_{ij} \quad (91)$$

From this it can be seen how if there is not a complete neighbourhood, which would be the case for particles at boundaries and/or particles that have moved away from the general neighbourhood of the fluid (for example if there is impact on a wall, the fluid may disperse). This then leads to a deficient value of density and due to the strong coupling of density to pressure due to the Murnaghan equation of state (EOS) used for fluids, given by:

$$P = B \left(\left(\frac{\rho}{\rho_0} \right)^\alpha - 1 \right) \quad (92)$$

Any errors in density will have a big influence on pressure. The following figure below illustrates a dambreak test. The dambreak models a fluid breaking dam and then impacting on a boundary. Parameters are $B=2.8E+04, \alpha=4$. This is smaller than the actual bulk modulus of water but due to the dependence of the bulk modulus and alpha constant on the timestep, the bulk modulus has been made smaller to reduce simulation time. The Courant condition is a necessary condition for convergence in a numerical scheme and in simple terms requires the maximum timestep to be inversely proportional to the speed of sound. The speed of sound is dependant of the bulk modulus of the fluid; it increases as the bulk modulus increases. Hence for a large bulk modulus, the speed of sound will be large and the maximum timestep very small which has the consequence of a large simulation time. By reducing this bulk modulus, the speed of sound will be smaller, the timestep will be larger and simulation time will be less. Because of this, it is standard practice to use a smaller bulk modulus when modelling water than its actual value. This is justified as the instability that causes severe pressure fluctuations is a numerical one not physical, hence addressing the instability at one bulk modulus will work for all if it works. The only thing that would change is the value of the pressure at individual particles, not the pressure differences that come because of density solution degradation. This small bulk modulus is also justified by literature as follows the guidelines laid out

by (Monaghan 1994). The fluid dimensions are 0.566774m^2 consisting of 5776 particles and a total density of 1000kg/m^3 . The dambreak walls (represented by symmetry planes) were located at coordinates (0,0) to (0,20), (0,0) to (0.18) and (0.18,0) to (0.18,0.20). The bars on the right-hand side illustrate pressure in pascals.

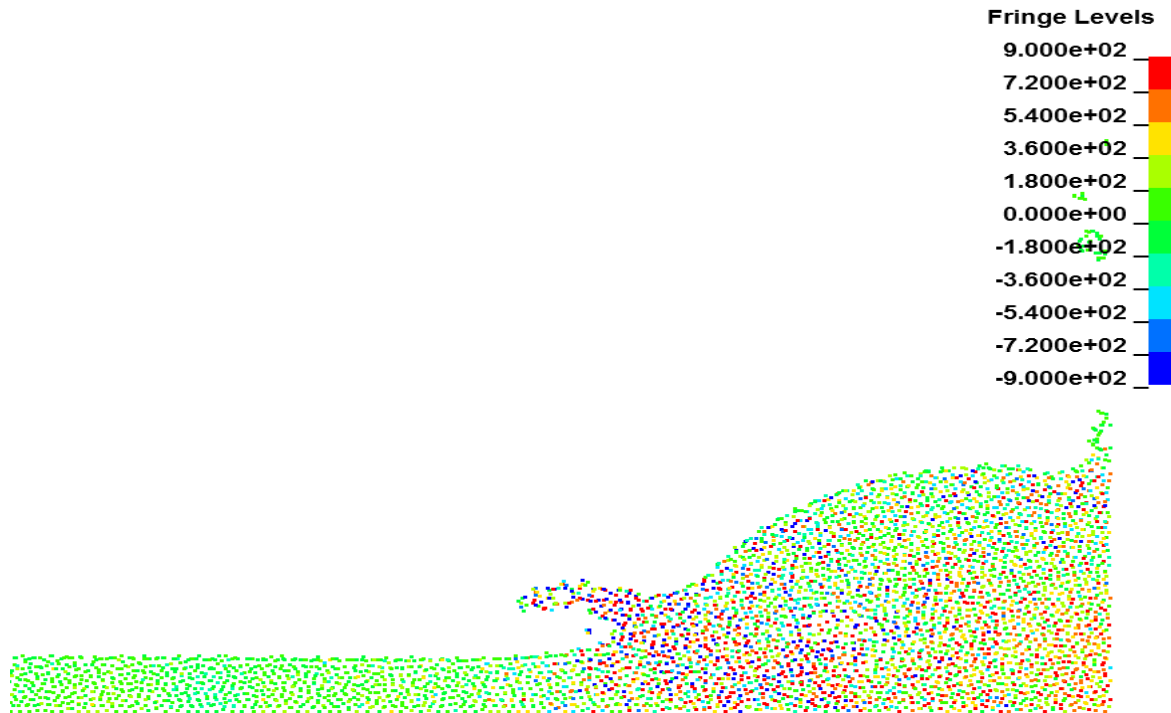


Figure 3: Illustration of pressure instability in the dambreak scenario just after wall impact.

It is clear both Figure 3 and the results from (Colagrossi & Landrini 2003) that the pressure oscillations are severe. Having used the Murnaghan equation (92) which models pressure as a function of density, it is the severe density fluctuations that lead to the pressure noise.

4.1 Density re-initialisation using MLS

As mentioned in the literature overview (Colagrossi & Landrini 2003) proposed using the moving least squares scheme developed by (Dilts 1999) on the density field. This would have the effect of re-initialising density by periodically applying the first order scheme on the density field and thus restoring 1st order consistency to irregularly scattered points. This in theory would give a far more smoothed pressure as due to the explicit link between pressure and density, a more stable density would give a more stable pressure. It is this approach that was used to develop the capability of the MCM code to reduce numerical noise in the pressure field and it will be shown how the technique used in (Colagrossi & Landrini 2003) does in fact satisfy linear consistency as outlined in (Belytschko et al. 1998).

The ability to reproduce linear functions is given as:

$$u^h(x) = \sum_i w_i(x) u_i$$

Where as shown for a 1st order complete and consistent kernel, we must have:

$$W_{ij} = b(x)^T A(x)^{-1} B(x) \quad (94)$$

Substituting $b(x) = [1, x_i - x_j, y_i - y_j]$ as the linear basis, we get for A(x)

$$\left(\sum_i W_i(x) \begin{bmatrix} 1 & x_i - x_j & x_i - x_j \\ x_i - x_j & (x_i - x_j)^2 & (x_i - x_j)(y_i - y_j) \\ y_i - y_j & (y_i - y_j)(x_i - x_j) & (y_i - y_j)^2 \end{bmatrix} \right)^{-1} \quad (95)$$

At this point in $A(x)^{-1}$ is multiplied by a basis function that shifts the co-ordinates to the origin. This is a valid procedure and avoids ill conditioned matrices as shown in (Colagrossi & Landrini 2003) and (Dilts 1999).

$$\left(\sum_i W_i(x) \begin{bmatrix} 1 & x_i - x_j & x_i - x_j \\ x_i - x_j & (x_i - x_j)^2 & (x_i - x_j)(y_i - y_j) \\ y_i - y_j & (y_i - y_j)(x_i - x_j) & (y_i - y_j)^2 \end{bmatrix} \right)^{-1} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad (96)$$

The multiplication of a 3x3 matrix by a 3x1 matrix) gives a 3x1 matrix represented by $(\beta_0(x_i) \quad \beta_1(x_i) \quad \beta_2(x_i))^T$ Multiplication by equation(B(x)) shows the moving least squares kernel to be:

$$W_j^{MLS} = (\beta_0(x_i) + \beta_1(x_i)(x_i - x_j) + \beta_2(x_i)(y_i - y_j)) W_{ij} \quad (97)$$

Hence:

$$W_j^{MLS} \equiv w_i(x) \quad (98)$$

Equation (93) gives us the formula to approximate nodal values using a linear interpolation function. In this case, the aim is to reproduce density which gives u as the original density and u^h the approximated density, hence:

$$\rho^{MLS}(x) = \sum_i W_j^{MLS} m_j \quad (99)$$

$$\rho^{MLS}(x) = \sum_i W_j^{MLS} m_j \quad (99)$$

This was implemented in the code in the form of several subroutines which are detailed in appendix 1. The code implementation is described as follows. The program will only transition to the MLS main subroutine (and as a consequence the other subroutines) if the MLS option is on and only for a fluid modelled by the equation (92). The code works for 2D and 3D problems. Developing this approach into 3D does mean that a 4x4 matrix needs to be inverted rather than the 3x3 matrix shown in equation (95). A matrix due to the presence of the z dimension in the basis vectors. This required further code implementation of a Gauss-Jordan algorithm customised to work with SPH variables to invert the matrix as for $n > 3$ matrices, finding the inverse by formula is not possible. The MLS subroutine does not work when a particle has zero neighbours as it leads to a division by 0 error, so the MLS subroutines are only programmed to run if there are neighbours, otherwise it is skipped. This is expanded upon to deal with neighbour deficiency as well, as neighbour deficiency can lead to a singular matrix. So, there is a determinant test in place that will skip the matrix if DET TEST is equal to 0 as this tells us that a matrix will be singular. Furthermore, since pressure is a consequence of change in density, which is a function of the trace of the rate of deformation, we need to be careful that the MLS approach (which as a numerical artefact, has pressure dependent on the kernel and particle positions as shown by (97)) does not affect the physical nature of the solution. One such instance is particles that are modelling the wall of the tank. As the wall is a rigid body, there is no particle deformation and hence no pressure change. However, if the MLS algorithms were to be used on 'wall particles', due to the MLS pressure being depended on the kernel function and position as opposed to the rate of deformation, an unphysical pressure is calculated. Therefore, there is another safeguard in place in the code, that only allows the MLS algorithm to run if the tracerod is not equal to 0.

4.2 Results and testing discussion: Single Phase flow

The initial test was to compare the dambreak scenario in Figure 3 without any MLS update to a MLS update test applied every time step. Then extend this testing to cases with different intervals of MLS update. The results discussed in this these shall focus on a select few intervals as these highlight the spread in results accurately and are representative of this spread. The intervals will be MLS applied every 20,10, 1 and 0 timesteps.

The dambreak case that was modelled had used parameters are $B=2.8E+04$, $\alpha=4$ The fluid dimensions are $0.566774m^2$ consisting of 5776 particles and a total density of $1000kg/m^2$. The dambreak walls (represented by symmetry planes) were located at co-ordinates (0,0) to (0,20), (0,0) to (0.18) and (0.18,0) to (0.18,0.20).

Dambreak using MLS every 20 timesteps

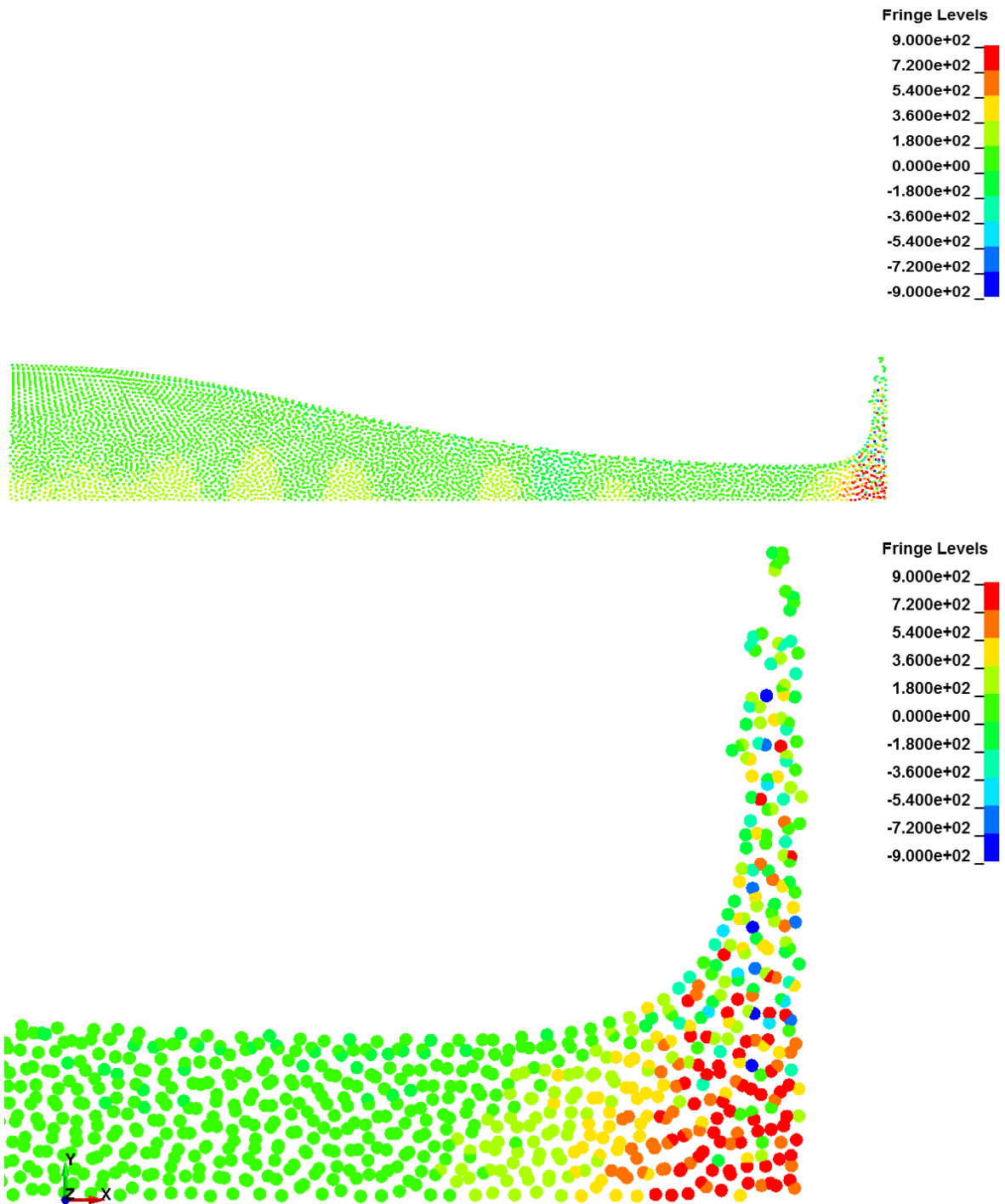


Figure 4: Illustration of pressure at time 0.16s in the dambreak case with density update applied every 20 timesteps. Figure 4 (top) shows the whole fluid. Figure 4 (bottom) shows the fluid magnified at the right-hand corner where impact against the boundary has occurred. The fringe levels indicate pressure in Pa.

While there is an improvement in reduction of pressure noise, figure 4b illustrates that is far from eliminated. Moving on to a 10 timestep update case it can be seen:

Dambreak using MLS every 10 timesteps

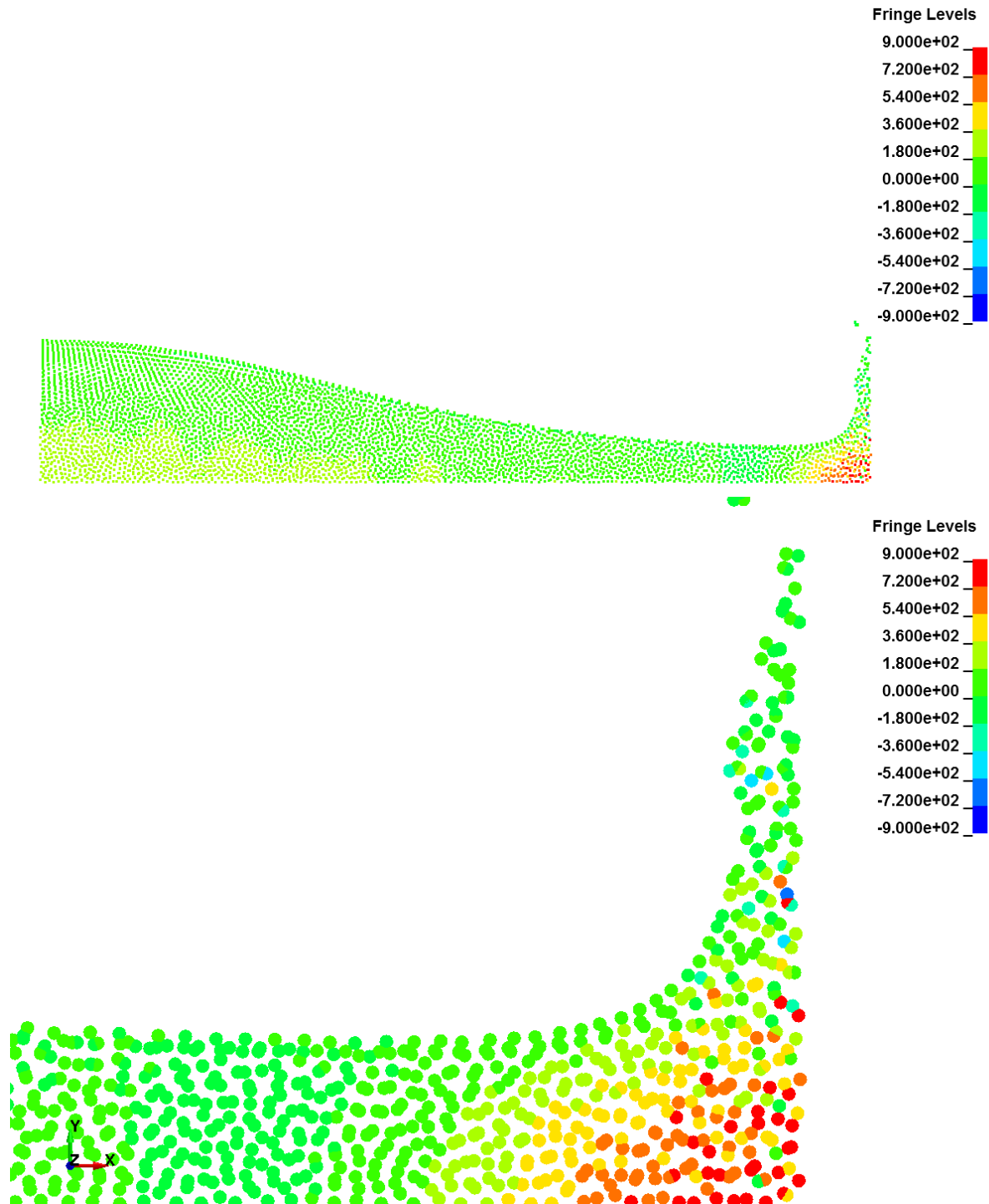


Figure 5: Illustration of pressure at time 0.16s in the dambreak case with density update applied every 10 timesteps. Figure 5 top shows the whole fluid, figure 5 bottom shows the fluid magnified at the right-hand corner where impact against the boundary has occurred. The fringe levels indicate pressure in Pa.

It is clear that Figure 5 shows further improvement in pressure distribution compared to 4a), b) Noise still exists, but the scale shows less variations in pressure. Applying the procedure every timestep it can be seen below:

Dambreak using MLS every timestep

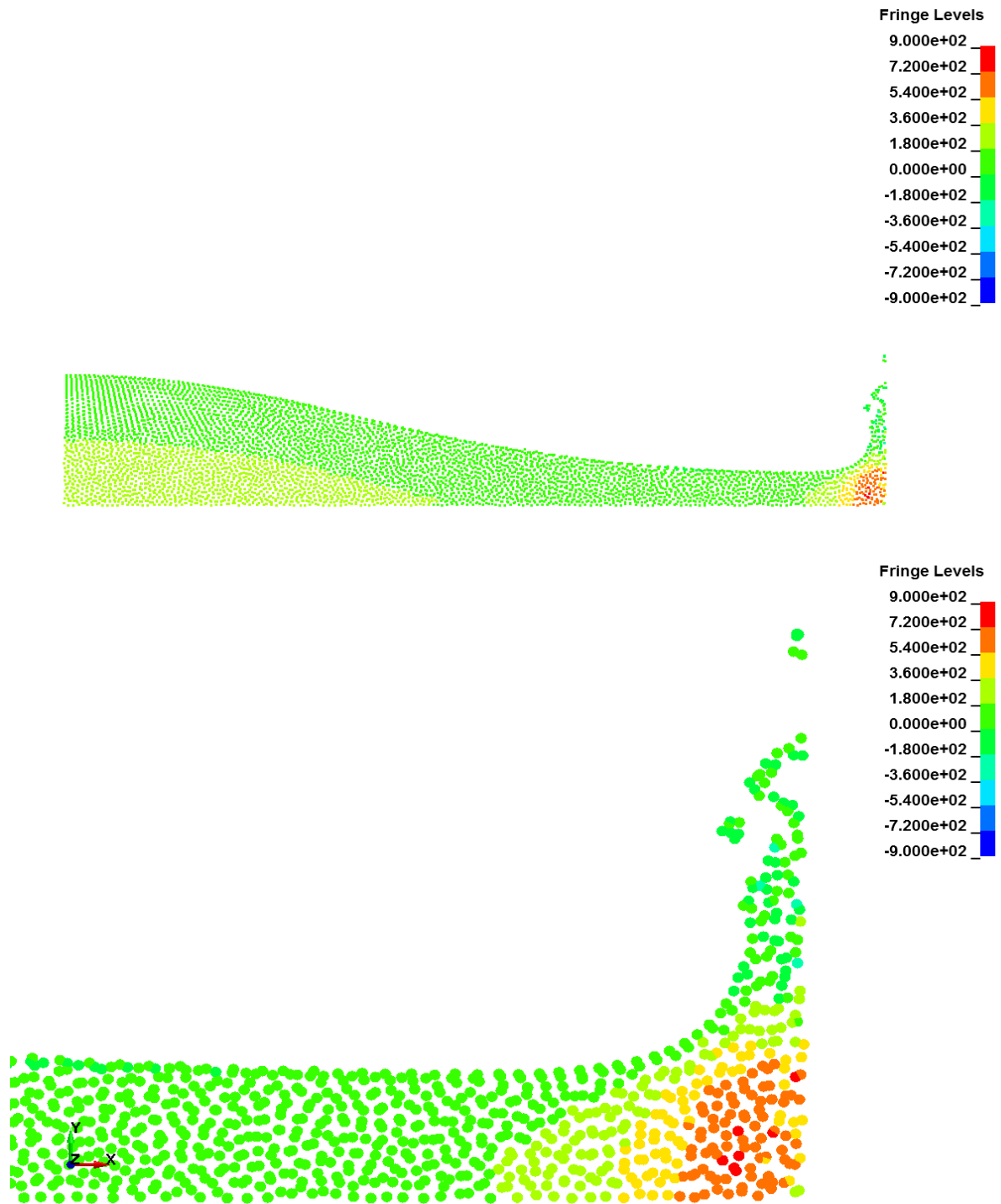


Figure 6: Illustration of pressure at time 0.16s in the dambreak case with density update applied every timestep. Figure 6 top shows the whole fluid. Figure 6 bottom the fluid magnified at the right-hand corner where impact against the boundary has occurred. The fringe levels indicate pressure in Pa.

The results show that application at every timestep gives better pressure smoothing; however, the results have shown that the improvement has come at a cost. Computational speed is one such cost but the main one that is of concern is the particle distribution of the flow.

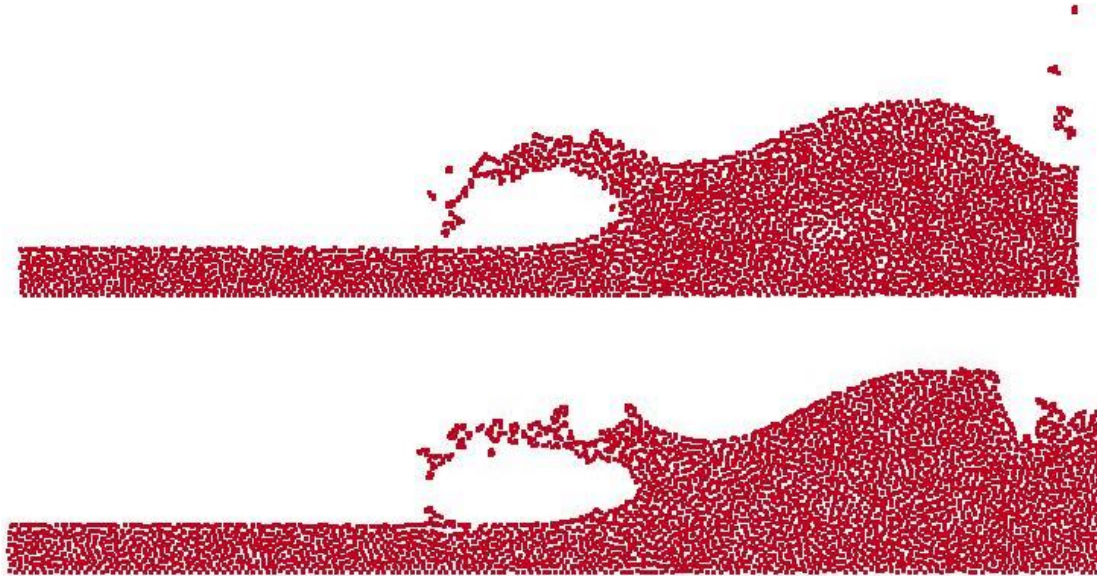


Figure 7: Comparison of profile shape at $t = 0.44$ seconds for the dambreak case. 7 (top) shows the profile for the non-MLS updated case and 7 (bottom) the profile when MLS update is applied at every timestep.

Figure 7 illustrates the differences between the profiles most notably the large gap by the wall and the curved path of the particles just before they reintegrate into the fluid. Comparison shows that the non-smoothed case has a more accurate profile.

4.3 Conclusion

The code implementation was extended to 3D with identical results. The best combination has been verified by applying the code every 20 timesteps and including bond viscosity, this same conclusion was found by (Colagrossi & Landrini 2003) which highlights that the algorithms work as they should. However, there appears to be very little discussion as to why this combination of factors gives the best results and why the MLS update does affect the profile of the wave. In hindsight, it does make sense why applying the algorithm at every timestep would lead to unphysical results, as in this situation pressure would be a numerical calculation (dependant on the Kernel sum) and not a physical calculation. However it being used every 20-50 timesteps to stabilise pressure is the right balance between a correct physical representation of pressure and other quantities which are calculated and are dependent on the pressure variable and reducing the instability inherent in the SPH method. Clearly though the presence of an artificial numerical variable despite its advantages does need to be investigated further to see if it does have a negative unphysical effect on simulations. The next section will discuss the method, implementation and results of such an investigation.

5. Investigation of MLS density update side effects.

The previous chapter has illustrated that MLS applied to density restores consistency and smoothed pressure.

The algorithm works by ‘reinitialising’ density and this can be applied every n timesteps. The more often the algorithm is applied, the smoother the pressure distribution as the results show. However, the results have shown that the improvement has come at a cost. Computational speed is one such cost but the main issue of concern is the particle distribution of the flow as shown by Figure 7.

Due to this, a compromise is usually made by updating every 20-50 timesteps. This allows a smoother pressure distribution without the expense of an inaccurate wave profile.

The previous section illustrated the potential of neighbour deficiency leading to a singular matrix in equation (96). This problem has been evidenced in (Lancaster & Salkauskas 1981) and (Duarte & Oden 1996). In general, whenever the number of neighbours of a point is less than the number of functions in p , the matrix A will be singular. This is consistent with an overdetermined system - which has more equations than unknowns - and a system like this does in general lead to a singular matrix.

Dilts tackled this singularity problem by a variable rank process (Dilts 1999). This has been proved to be computationally simple but it still ignores the singularity and furthermore as it reduces the order of the problem, it reduces the consistency. As touched upon in the previous chapter when code implementation of MLS was explained, the code would simply skip the matrix inversion if a singular matrix were to occur. However, this is at best a patch and avoids the problem rather than deals with it. One approach that would directly embrace the singularity is the theory of singular value decomposition. Singular value decomposition (SVD) allows approximation of an inverse to matrices that do not have an inverse. However, this technique is computationally expensive due to its complexity. The step by step process in implementing this is to:

- Solve a cubic
- Test to see if the cubic has solutions
- Apply synthetic division
- Solve a quadratic
- Apply upper triangular Gaussian elimination
- Build an eigenvector matrix
- Apply Gram-Schmidt process

This needs to be applied twice as the process works by approximating an upper and lower matrix.

This procedure was discussed and applied independently in (Bilotta et al. 2011) which highlighted the significant computational time increase and it was necessary to use parallel processing to achieve two orders of magnitude speed up in the code. This was confirmed when I tried to implement SVD in the code and so was aborted.

The inversion issue is a small one when considering the sheer number of particles in the system, the number of timesteps of a simulation and the fact that the MLS algorithm is only applied every 20 timesteps anyway. Even if one particle isn't say updated by MLS when all the others are, the influence from the other neighbouring particles will allow the particle to be more representative of the correct pressure anyway. That is not to be dismissive of this issue as it is known from the zero-

energy problem that one unstable particle can lead instability of the simulation but in this case the event is so rare. To put into perspective, when in the final stages of testing the MLS algorithms, it was only on timestep 2309 of a simulation of 5776 particles with MLS applied every timestep, did a 0 matrix occur for only one particle.

The bigger issue is whether the drawbacks highlighted as well as the numerical rather than physical calculation have other drawbacks. When applying this procedure to a sloshing tank which is a more complex problem than the dambreak scenario a velocity difference was shown in the sloshing water wave using MLS compared to a non-MLS updated sloshing wave. This had not been highlighted in any literature so far and so by conducting a deeper investigation than what literature using this procedure seems to have done, it has the potential to kick start further work in really assessing the drawbacks of this method. While the MLS density update procedure is not novel, the investigation in this chapter is a novel area of research.

5.1 Wave investigation

The presence of MLS clearly affects the wavespeed as illustrated below:

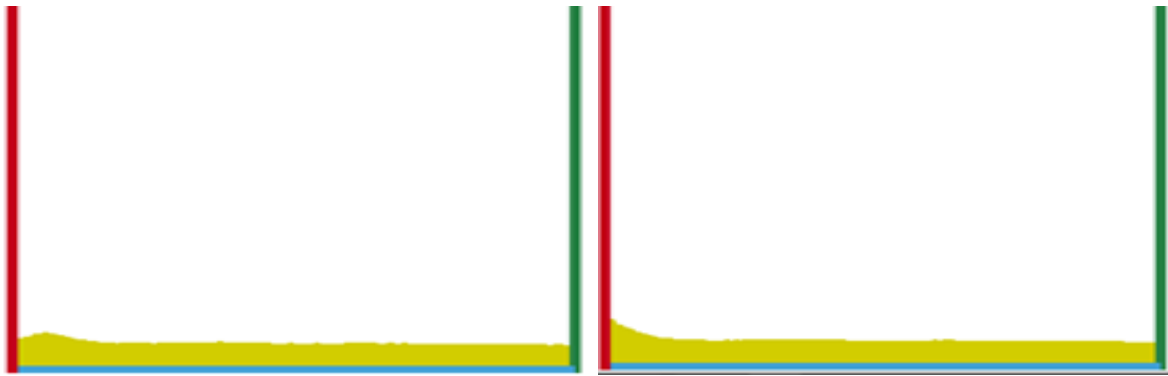


Figure 8: Illustration of wave speed difference in a linear sloshing tank at time 3.95s. The figure on the left is a non-density updated case, the figure on the right is a density update every 50 timestep case.

Figure 8 illustrates that the density updated waves travelling faster as it has reached the boundary before the non-updated case. This highlights another issue in using the density update algorithm, but it is possible that the wave velocity predicted by the algorithm is the correct one. The simulations run in Figure 8 were modelled using a basic SPH approach which has many shortcomings.

5.1.1 Differences in Density Calculation between MCM and MLS update algorithms

Density is calculated in mcm using the rho update algorithm. The density calculated is:

$$\rho_{update} = \rho_{old} (1 - tracerod * mcmdt) \quad (100)$$

Where:

MCMdt = the timestep used = $0.67 * critical\ timestep$

0.67 is the scale factor inputted by the user and the critical timestep is:

$$\Delta t = \frac{h_i}{c_i + v_i} \quad (101)$$

Tracerod is the trace of the rate of deformation tensor given by:

$$\text{Tracerod} = \frac{1}{3}(\dot{\epsilon}_{11} + \dot{\epsilon}_{22} + \dot{\epsilon}_{33}) \quad (102)$$

And ρ_{old} is the density value of an individual particle from the previous timestep. ρ_{update} is the new density calculated at the current timestep by equation (100).

The density is hence a function of velocity, speed of sound, the kernel and the strain rate. If there is no deformation, there is no density change.

Moving least squares density update has no dependence on timestep or rate of deformation as discussed in chapter 4. It is instead dependant on position vectors and the kernel of its neighbours as shown by equation (96). However, in the simulations illustrated, the update is applied only every 50 timesteps. So, the dependences of the two simulations are the same except the MLS simulation has a smoothing effect applied that re-initialises the density at every 50 timesteps. This has the effect of a smoother and more realistic pressure distribution following the $P = \rho gh$ law.

When the algorithm is activated, equation (100) is skipped.

5.1.2 Water wave investigation

To make use of linear wave theory certain assumptions need to be made. These assumptions are that the fluid is inviscid, irrotational and incompressible, however equation (92) which links pressure to density for fluids model's fluid as 'quasi-incompressible'.

Equation (92) is derived assuming a linear relationship between incompressibility (K) and pressure.

$$K = K_0 + K'p \quad (103)$$

As density is related to volumetric strain this equation of state has been proven experimentally to model pressure in fluids. The bulk modulus is derived as K/K' and α as inversely proportional to K' . K in this case defines incompressibility. In modelling the fluid with other equation of states, this equation of state was shown to give the best results for my simulations.

By modelling the fluid as quasi (or weakly)-incompressible, it means the assumption that the fluid is incompressible is not quite accurate. This is an idealisation used in many problems to make modelling of fluid simpler and less complex. Physically the difference between compressible and incompressible is that the divergence of velocity is zero when incompressible and non-zero when compressible. In a compressible flow, this has the consequence of significant density and pressure changes, which makes the modelling of such a problem more difficult and can cause behaviour such as shock waves, meaning that additional terms will need to be added in equations to represent this behaviour. By assuming the fluid is incompressible, the divergence free governing equation can be

used to represent the flow. However, in making this assumption, it implied that there are no density changes, this is not true, so using the divergence free governing equation to describe the flow would be incorrect also.

To solve this problem, the fluid is treated as 'weakly compressible', therefore divergence of velocity occurs and hence density and pressure changes, but on small scales. For weakly compressible fluids, equation (98) is used to relate pressure and density.

It is important to note that the bulk modulus represents incompressibility. The smaller the bulk modulus is, the more compressible the fluid is. As discussed, to avoid the complexities of modelling fluid as compressible, the divergence of velocity must be small and hence the density variations must also be small. Therefore, there is a balancing act between using a bulk modulus that is small enough to not affect computational time but large enough to avoid the large density and pressure fluctuations.

The first test illustrated below involves water contained between a solid block on the left and a symmetry plane on the right. The block is moved into the water, which generates a wave which will propagate through the water and rebound off the symmetry plane. The wave was generated using prescribed displacement boundary conditions where a block is moved in the positive x direction 0.55m following a half crest sinusoidal path, this has the effect of generating a travelling sine wave. The rationale behind this test is its simplicity as other than the boundary there is nothing else that could influence the results and it also allows the option to compare results to linear wave theory.

The wave being modelled is a shallow water wave ($h \ll L$) and so the equations of mass and momentum and governing equations will be described by shallow water theory.

A shallow water wave described by depth averaged mass and momentum equations propagate with a speed independent of its wave length but dependant on its amplitude, the higher the amplitude, the faster it propagates. Potentially the moving least squares algorithm influences the amplitude and hence the speed.

All tests shall be between a non-density updated case and one updated every 50 timesteps. Further tests involving 1,20 and 100 timestep update will occur once quantifying the growth rate is done.



Figure 9: Illustration of velocity difference between a non-updated (top picture) at time 16.65s and 50 timestep density updated (bottom picture) at 16.75s.

As illustrated, there is a velocity difference as the wave crest hits the boundary at 16.65s in the non-updated case and 16.75s for a 50 timestep case. However, this may be due to the presence of boundaries. The next test highlights whether boundaries have an influence.

In the next case, the length of the water is 36.9 meters and height is 0.2m for a sine wave generated in the same manner as Figure 9. The only difference is the length and hence volume of the water. A wave is generated and propagated through the water. The reason for the long length of the water is that as shown in the previous illustration (Figure 8) the first noticeable change between the density and non-density updated cases occur as 16.65 seconds which is after the water has hit the boundary. Therefore, by defining a water length of 36.9 metres, the wave will take approximately 21 seconds to reach the symmetry plane boundary that contains the water. This test will be able to ascertain whether boundaries are the cause of the velocity difference as if at the point of the boundary impact, there is not a difference in wave position between the two cases, then clearly boundaries are the cause as the previous simulation highlighted in Figure 8 showed a wave position difference at this time. If there is still a difference, then something other than boundaries is the cause.



Figure 10: shows a single wave generated case for a largewater constrained tank illustrating velocity difference between a non-updated (top picture) and 50 timestep density updated (bottom picture) at time 22s

Clearly boundaries have no influence as the wave velocity difference occurs even before the boundary is hit. The results show the same result as the previous case, the non-updated density wave moves faster than the updated density wave. This is contrary to the result highlighted in Figure 8, indicating that it is not always the case that the density update will always give a faster wave.

5.2 Particle density investigation

The investigation begins by designing a tank based on the sloshing benchmark case described in (Vera et al. 2010). This is a rectangular sloshing tank that is shaken angularly with a period of 1.9191seconds, this will be referred to in the review as the angular sloshing tank. The tank has a length of 0.9m and the height of the fluid contained in the tank is 0.093m. Tests were conducted initially using oil with a density of 990kg/m³ and viscosity of 0.045. There was no noticeable difference between the non-density updated and density updated case. Running the simulations with water (density 998kg/m³, viscosity 0.000894) also showed no difference. The particle density of this simulation was 38698 *particlesm*⁻³

The initial simulation was run with 3239 particles in water, this gives a particle density of:

$$\text{Particle density} = \frac{3239}{0.0837\text{m}^3} \approx 38698\text{particlesm}^{-3} \quad (110)$$

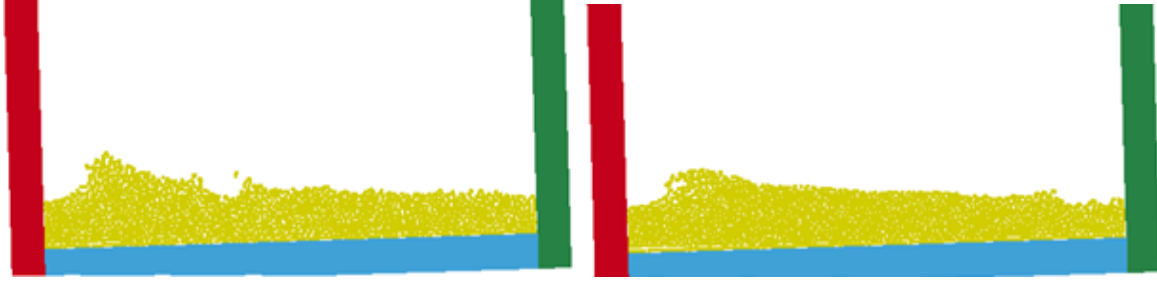


Figure 11: Illustration of wave profile position at time 5.45s for the angular sloshing tank described in (Vera et al. 2010) The picture on the left is a 50 timestep density update case, the picture on the right is a non-density update case.

As highlighted, there appears to be no significant difference in the position of the water wave at time 5.45s for the sloshing benchmark case, this is true throughout the simulation. However, the particle density in this case is different to the particle density of the water wave test, which did highlight the wave velocity difference.

Particle density is calculated as:

$$\text{Particle density} = \text{number of particles/volume} \quad (105)$$

The water wave particle density depicted is:

$$\text{Particle density} = \frac{73900}{7.38\text{m}^3} \approx 10012\text{particlesm}^{-3} \quad (106)$$

Applying this particle density to the sloshing test outlined in figure 11 means that the water must contain 838 particles due to the differing volumes of the cases.

$$\text{Particle density} = \frac{838}{0.0837\text{m}^3} \approx 10012\text{particlesm}^{-3} \quad (107)$$

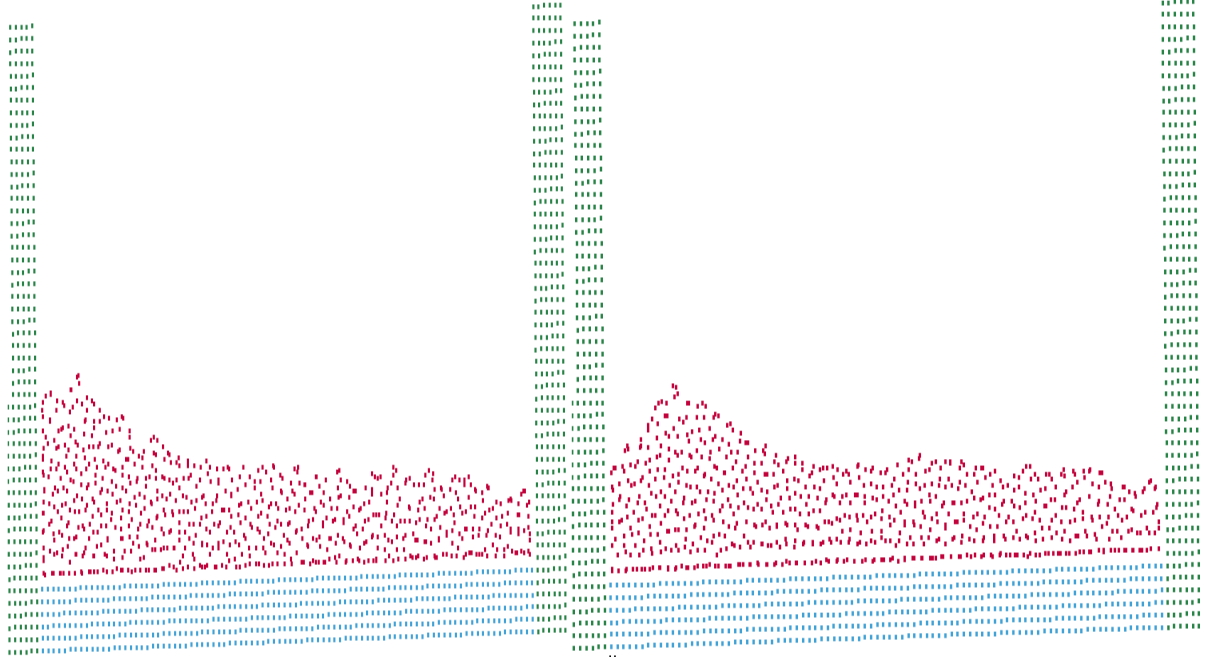


Figure 12: Illustration of wave profile position at time 5.5s for the angular sloshing tank. This test has a particle density of $10012 \text{ particles m}^{-3}$. The picture on the left is the non-density updated wave, on the right a 50 timestep density update case.

At time 5.5 seconds, the non-MLS updated wave is ahead of the MLS 50 updated wave. This highlighted that particle density was a factor in the wave difference. Interestingly for the linear sloshing tank depicted in Figure 8 the MLS updated case is in fact faster than a non-updated case, contrary to all the results that have been found so far.

Calculating particle density for the linear sloshing tank (Figure 8) gives:

$$\text{Particle density} = \frac{7859}{0.0177 \text{ m}^3} \approx 444011 \text{ particles m}^{-3} \quad (108)$$

Based on the tests so far; the results indicate that:

$$\begin{aligned} (\text{MLS UPDATE } v < \text{no MLS update } v) &< 38698 \text{ particles m}^{-3} \\ &< (\text{MLS UPDATE } v > \text{no MLS update } v) \end{aligned}$$

In words this tells us that when the particle density is below $38698 \text{ particles m}^{-3}$, the density update wave is slower than the non-density update wave as evidenced by the large water case (Figure 9 and Figure 10) and the angular sloshing (Figure 12). But when the particle density is

above $38698 \text{ particles m}^{-3}$, the density update wave is faster than the non-density update wave as evidenced by the linear sloshing tank (Figure 8).

However, there is a magnitude of difference between the slower and faster waves particle density. Additionally, tests have been conducted on different cases, so the next step is to test on a single case and try different particle densities to quantify this wave speed growth and reduction rate.

Running the rotational sloshing tank with the same particle density as the linear sloshing tank to confirm the hypothesis presented gives the number of particles as 37200, given by equation (109)

$$\text{Particle density} = \frac{37200}{0.0837\text{m}^3} \approx 444444 \text{ particles m}^{-3} \quad (109)$$

Based on results so far, this should generate a faster wave in comparison to the rotational sloshing results so far. To confirm this, comparison to the results illustrated in Figure 11, which has a particle density of $38698 \text{ particles m}^{-3}$ will occur. Once this is shown, there will be a uniform set of cases to for the rotational sloshing tank to make comparisons with.

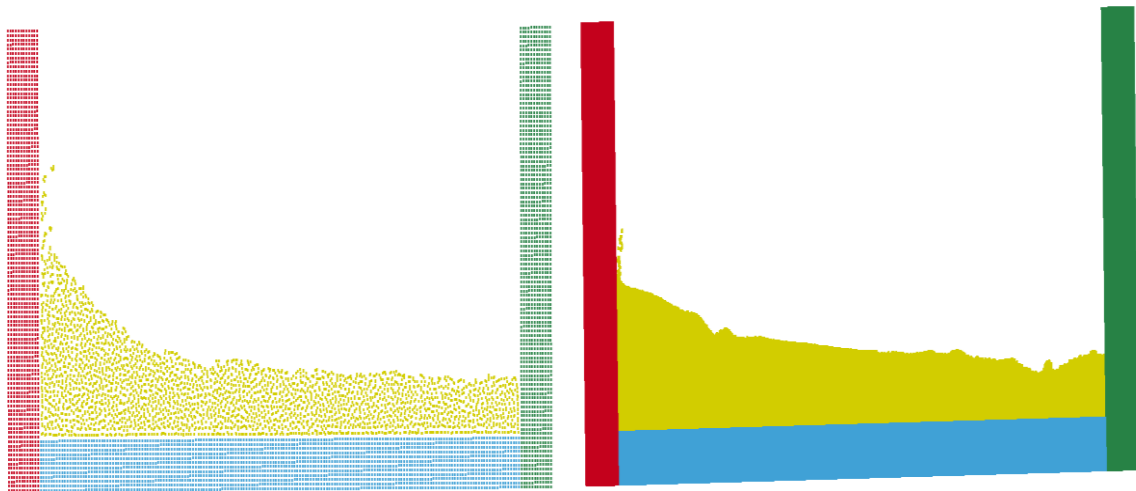


Figure 13: Comparisons of wave speed at 5.5 seconds between the rotational sloshing tank with different particle densities. On the left the tank has a particle density of 38698 m^{-3} , the right 444444 m^{-3} .

As predicted the denser case is faster than the smaller particle density case. This would imply that the more accurate value of velocity is faster than predicted in the less dense simulations for both MLS and non-MLS cases. This is since a denser particle simulation would, in theory, be more accurate than a less dense case as fewer particles mean less likely to capture all the behaviour necessary, particularly in a complex sloshing scenario. Clearly MLS at a lower particle density does not correct this; in fact, the MLS wave speed is predicted slower in the lower particle density cases.

5.3 Linear water tests

The use of different cases has given contradictory results, indicating dependence on more than particle density. To test more accurately, a uniform test should be used with different particle densities. This will enable both a more scientifically accurate testing process and will allow growth rate to be quantified. This will be done by considering a tank of water which is impacted upon in a

similar manner to what was shown in Figure 9 and Figure 10. The difference will be how the wave is generated. The wave generated in Figure 9 and Figure 10 was a single wave forced by the forward movement of the block. A more accurate way to generate waves is via a periodic oscillation of a flexible beam. This will give a continuous generation of waves in which to observe the wave behaviour and gives better representation of sinusoidal wave behaviour than the moving block generation

An initial test was done using a length of water of 30.4m and a height of 0.4m. The particle density is given as approximately 10514 particles per metre cubed.



Figure 14: Illustration of a constrained water tank with airy waves generated by the flexible beam.

From here, the waves generated are airy waves.

To determine the velocity difference of the 2 cases, checkpoints are used that determine the wave height at a point. Check points have been introduced at 0,10,20,30m. The results also show the peaks and troughs are lower for the MLS cases.

Table 1: Illustration of wave height and speed differences taken at the 20-meter checkpoint for the tank given in Figure 14.

	No density update wave height (m)	No density update time of peak (s)	50 timestep density update wave height (m)	50 timestep density update time of peak(s)
1 st wave peak	0.422	11.18	0.421	11.17/11.18
1 st wave trough	0.394	13.2/13.3/13.4	0.394	13.2/13.3/13.4
2 nd wave peak	0.439	14.4/14.5	0.437	14.4
2 nd wave trough	0.381	15.7/15.8	0.381	15.7/15.8

The results show the peaks are lower for the density updated cases and the density updated wave is marginally faster than the non-updated case. Based on previous links with particle density, this would indicate that the case shown in Figure 14 has a very high particle density (Greater than $38698 \text{ particles m}^{-3}$) This is not the case, as the particle density in this case is approximately 10514, which based on the particle density tests should be the opposite. This conclusively eliminates particle density as a meaningful factor in this velocity difference.

Applying the oscillation of the beam to the single wave generation test described in Figure 10, the non-density updated wave is slightly ahead, which is different compared to the previous case illustrated. This, like the last case is determined by when the peaks pass through the wave height checkpoints. Additionally, the peaks are lower for the density update test cases.

Table 2: Illustration of wave height and speed differences taken at the 20-meter checkpoint for the largewater case given in Figure 10

	No density update wave height (m)	No density update time of peak (s)	50 timestep density update wave height (m)	50 timestep density update time of peak(s)
1 st wave peak	0.210	14.6/14.7	0.208	14.6/14.7
1 st wave trough	0.192	15.7	0.192	14.6/14.7
2 nd wave peak	0.203	16.6/16.7	0.201	16.7/16.8
2 nd wave trough	0.189	17.4	0.190	17.4
3 rd wave peak	0.203	18.0/18.1	0.201	18.1
3 rd wave trough	0.186	18.9	0.186	18.9

Based on this result and the previous results, it can be concluded that the moving least squares algorithm acts as a damper to energy, and it is this damper that has far more influence on the velocity difference than particle density. That is, the energy of the system of interest has more influence on the magnitude of the velocity difference than the particle density. This is illustrated by the difference in amplitude in the updated and non-density updated cases.

As particle density is now ruled out as a significant factor, the final step is to test the block generated single wave test as in figure 10, but test different density update cases to further establish the link between density update and energy dissipation. A final difference is introduced in that all cases will have the same initial conditions, that is all cases will begin from a 50 density timestep updated relaxed water tank as opposed to a non-density updated case being run from a non-density updated relaxed case, a 20 timestep updated case from a 20 timestep relaxed case and so on. The aim of this is to see if the initial energy of the system has an effect, as now it is conclusive that energy, rather than particle density is the main factor in this velocity difference.

Table 3: Time taken for the wave crest to reach the barrier

Number of timesteps updated	Time at which crest reaches the barrier
1	24.2s
20	22.6s
50	22.5s
100	22.5s
None	22.4s

Table 4: Wave-height of the wave crest at 30 metres from the origin

Number of timesteps updated	Waveheight 30meters from origin
1	0.0209m
20	0.0255
50	0.0256m
100	0.0256m
None	0.0258m

Visual comparison shows that the velocity difference between the 50 timestep density update and the non-density update case is about 0.1s which is shorter than illustrated in Figure 10. The case in Figure 10 shows a velocity difference of 0.25s. As everything else is the same, it is reasonable to conclude that the initial energy does have an effect. This is illustrated in the next figures:

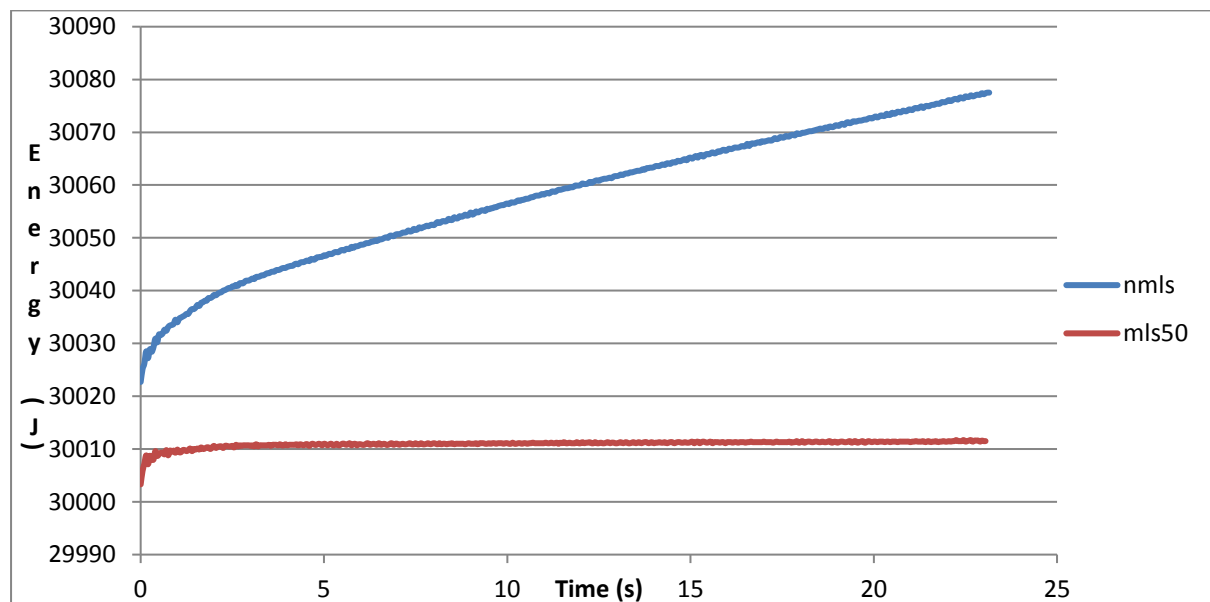


Figure 15: Single wave generation kinetic energy profile for Figure 10 where 0 timestep updated case is relaxed using 0 timestep density update and the 50 timestep density update case is relaxed using a 50 timestep density update.

The system is increasing in energy for the non-updated case, while the 50 MLS case has almost constant energy. In this case there is no gravity in the system.

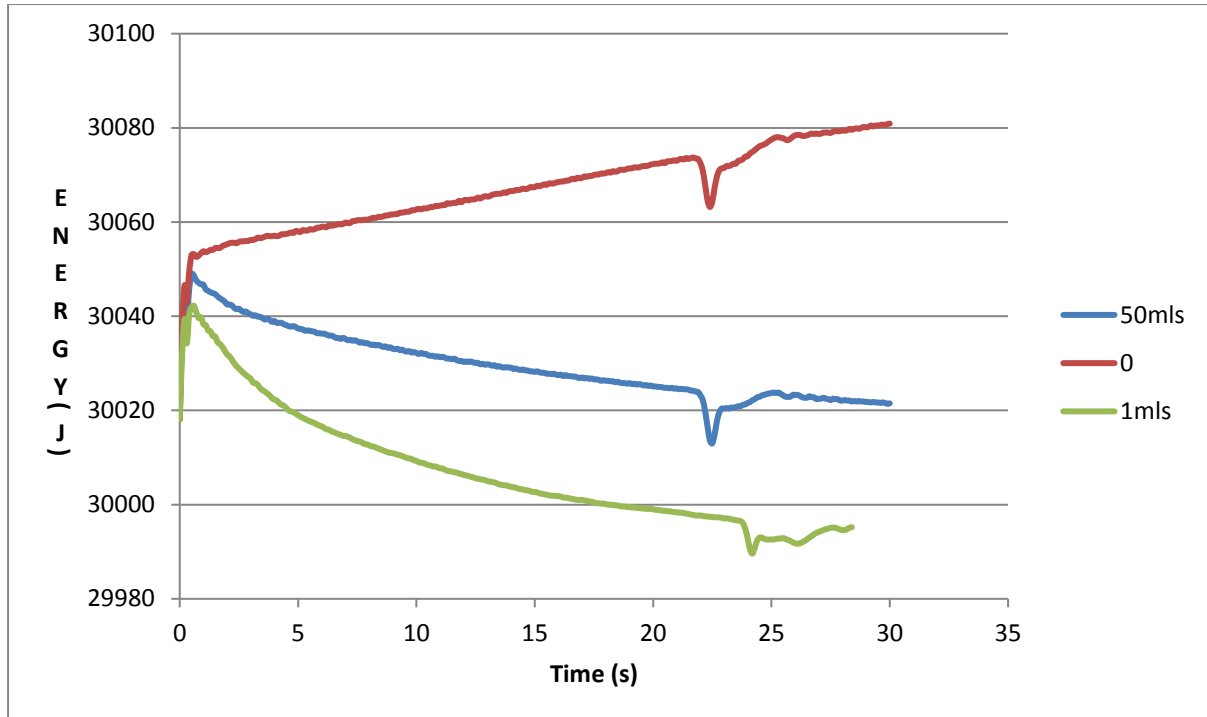


Figure 16: Kinetic energy profile describing 0,1 and 50 timestep density update cases for the case depicted in Figure 14 are relaxed using the 50 timestep density update.

Figure 15 shows that while there is no energy growth, the behaviour isn't quite correct as you would expect some energy loss. This is due to the fact in that case, the wave is generated by the movement of the block which is then stationary; therefore no additional energy should be entering the system. As the block is then stationary, the forced oscillation that occurs should lose energy due to the resistance of gravity which will be acting against the wave motion. Interestingly, this behaviour is captured in both cases.

Table 1 shows a decrease in amplitude for the airy wave test. As energy is proportional to the root of the amplitude, this would imply correct behaviour is followed. The energy profiles would suggest otherwise. The growth in energy is solely due to the unphysical growth of internal energy, the kinetic energy profiles oscillate back and forth due to the continual exchange of kinetic and potential energy which as the wave generated in all cases are harmonic waves, this is to be expected. The unphysical growth of internal energy is an example of the so called tensile instability problem in SPH which will be covered in more detail in the mixed formulation chapter.

Of further interest is the energy profile in Figure 16. In this case, the 50MLS case gives a more realistic energy profile, indicating dependence on initial conditions as the only difference in the cases was how the simulation was relaxed. Furthermore, the comparison between this and the 1MLS case shows the more updates used, the more energy is lost. Certainly, using the MLS update every timestep is not good practice as you are severely weakening the link between density and pressure, which would then lead to the system not being physically representative since pressure will be governed by a numerical equation rather than a physical one.

5.4 Conclusion

The density update algorithm has been shown to be very effective in achieving pressure smoothing. This, however, comes at a cost as illustrated in terms of the wave profile. This investigation has highlighted another cost, namely representation of wave velocity.

The initial conclusion of relation to particle density was since the sloshing tanks initially showed a pattern that below a certain particle density, the 50 timestep density update case was slower than the non-updated case, above this particle density it was faster. This turned out to not be the case and there was no relationship between the two. By simplifying the tests to linear wave propagation in a tank, it could be determined that energy damping was the cause of this velocity difference. Further tests showed that the velocity difference is influenced by the initial energy of the system. However, perhaps energy damping is the wrong term to use. Basic SPH is non-conservative but the density updates due to its re-initialisation of density restore consistency and hence achieves energy conservation of the system. Clearly, the smoothing of pressure leads to momentum conservation as the smoothed pressure is used in the momentum equation and hence leads to the system being energy conserved. What is also of interest is that the energy conservation only applies within the 20-50 timestep range just like the best results required for the pressure smoothing. This also makes sense as applying the update too little means that the density update will not have enough influence and be lost in the time evolution of the system and too much means that the density update dominates which means a non-physical numerical artefact will dominate results rather than physical density based on time evolution of conservation equations.

The lack of energy conservation is due to the unphysical growth of the internal energy due to tensile instability, however, while MLS gives better energy representation, this is more of an accident and doesn't address the tensile instability problem. What it does do, however, is that due to the extra smoothing -because of the presence of more kernel terms- weaken the link between volumetric strain and pressure which is the direct cause of the internal energy growth and thus acts as a dampener. This then explains the velocity difference as the energy will directly influence the velocity.

The velocity difference may explain the breaking of waves that occur when using this algorithm. Breaking waves occur when the crest of the wave overtakes the trough and is particularly prevalent in shallow waves such as the experiment showed in (Colagrossi & Landrini 2003). Thus, the breaking phenomenon is likely a consequence of the MLS algorithm giving different velocities, particularly as this behaviour was more prevalent the more timesteps the algorithm was used, which meant that despite the pressure being more smoothed, the velocity was less physically dependant on the system and more a numerical consequence of the algorithm. An incorrect velocity may explain why the waves break.

The finding of the influence of MLS on the tensile instability problem will be investigated further in the mixed formulation chapter.

6. Benchmark FSI problem modelling using mixed Eulerian and Total-Lagrangian approach

The density update algorithm and subsequent investigations are the first steps to establishing a working fluid-structure interaction model. The next step is to understand and represent the phenomenon of sloshing, which was illustrated in the previous chapter as a test case for the MLS investigation.

(Moiseyev & Rumyantsev 1968) defines sloshing as slosh refers to the movement of liquid inside another object. However, this is quite simple as a liquid must have a free surface to slosh. A free surface is a liquid that is subjected to constant normal stress and zero shear stress. This is a necessary component of a slosh problem as the hydrodynamic pressure of liquids in moving rigid containers has 2 distinct components. One is proportional to the acceleration of the tank and is caused by the part of the fluid moving with the same tank velocity. The 2nd pressure component represents the free-surface liquid motion.

Sloshing is an extremely complex natural phenomenon due to its non-linearity. By shaking a partially filled tank and inducing sloshing, the liquid will move at distinct natural frequencies. To gain a more scientific definition of sloshing, it must contain information about the natural frequency oscillations. So, sloshing is defined as low-frequency oscillations of liquid (Gradinscak 2009). When excitation frequency is close to the natural frequency of a sloshing tank, the sloshing is critical.

Being able to predict this phenomenon is vitally important in marine industry. This is explained in (Gradinscak 2009) and (Colagrossi 2005).

As the literature shows, modelling a complex fluid-structure interaction problem with the SPH method and with no coupling to a different numerical model has not been done before. Only small scale FSI models -detailed in the literature review- have been done. Furthermore, the FSI model in question involves the interaction of a non-linear sloshing liquid and a highly deformable beam (S R Idelsohn et al. 2008; Vera et al. 2010; Degroote et al. 2010), which is hugely expanding the capability of the SPH method. Finally, the modelling of this problem is also novel as the work in this these will be using a mixed Eulerian-total Lagrangian scheme to model this problem, with repulsion contact simulation contact between the fluid and structure. The strengths and novelty of the Total-Lagrange approach are shown in (Rade Vignjevic et al. 2006) and repulsion contact by (R. Vignjevic et al. 2006; De Vuyst 2003). This work is a continuation of the work in these papers by expanding the capability of the approaches to FSI. If successful, this work has the potential to show SPH as a major player in FSI simulations. Because this will be the first body of work in SPH ever to model a complex FSI problem without the need of coupling to another method.

While this will be the first body of work in SPH to model such a complex FSI scenario without coupling to another solver, this is not the case for the FE method. LS-Dyna, for example, has many different types of contact methods. While MCM has 3 contacts which are kernel contact, which basically has the effect of particles sticking together, repulsive contact and pressure contact. Kernel contact is the simplest form of contact as it is contact inherent in the method. If particle j is a neighbour of particle I then they are in kernel contact. However, this has been shown (R. Vignjevic et al. 2006) that it is insufficient to capture correct physical contact behaviour. Repulsion contact and pressure contact has been discussed in chapter 3. Ls-Dyna, on the other hand, has 8 ways of representing contact. The first is the general 3D contact algorithms. The second provides a means of coupling to deformable surfaces. The third treats contact using mathematical functions to describe the surface geometry of the master surface. The fourth is a specialised form of the contact entity for use with the rigid body dummies. The fifth is under development and is used with soft foams where element inversion is sometimes a problem. Contact between layers of brick elements is treated to eliminate negative volumes. The sixth is for modelling road surfaces for durability and NVH calculations. The seventh, in LS-DYNA for historical reasons, and is sometimes still used to model rebars which run along edges of brick elements. The last is the general 2D contact algorithm based on those used previously in LS-DYNA2D (Livermore Software Technoogy Corporation 2015). While Abaqus and Ansys provide many different models for specific situations, a few examples are:

- Coupled acoustic-structural medium analysis
- general frequency-dependent complex bulk modulus and complex density
- Craggs model for dynamic equilibrium

While MCM has the capability to model different fluids and structures at the constitutive level (see appendix), the solution loop is the solution to the general governing momentum equation. Where, as each of the commercial software packages mentioned have specific solutions for specific cases (such as the Cragg model for dynamic equilibrium).

These further highlights not only the need of the SPH method but the capability of MCM to develop and really does show the commercial need of the work this thesis is undertaking to model FSI. By making this start, it will encourage further work in developing more ways to model contact and development of specific modelling loops.

6.1 Problem description

The benchmark problem considers a clamped elastic beam in the centre of a tank filled with fluid up to the same height as the beam so that the tip of the beam is at the liquid- gas interface. The problem dimensions and material properties are taken from (Degroote et al. 2010). In this paper, they attempt to simulate the benchmark cases described in (Vera et al. 2010), using a coupled finite volume and FE solver. This approach is unique in that it uses a partitioned approach- an approach that solves the equation of each subproblem separately and the interaction between the bodies solved using a coupling algorithm- as opposed to the monolithic approach which solves all equations simultaneously. The FSI problems are used to test two coupling algorithms. Their results are generally in good agreement with the experiment from a visual perspective but in the case of beam deflection in the fluid, the amplitude is overestimated and slightly out of phase. The work done in this paper makes it ideal to use as validation for our results as not only is experimental data available, but it allows comparison to another numerical method.

Table 5: Dimensions of tank

Parameter	Value (m)
Tank Width	0.609
Tank Height	0.3345
Liquid height	0.0574
Beam height	0.0574
Beam width	0.004

Table 6: Material properties of elastic beam

Parameter	Value
Density	1100 kg/m ³
Young's modulus	6x10 ⁶ Pa
Poissons ratio	0.49

Table 7: Material properties of fluid modelled using Murnaghan EOS (Equation 92)

Parameter	Value
Density	998.2 kg/m ³
Bulk Modulus	28000 Pa
Gamma	4

Rolling movement is rotational, where by the tank rotates about the midpoint of the bottom of the tank at the location where the beam is clamped.

The angular frequency of the rolling motion imposed on the tank is given by the fundamental frequency of gravitational waves in a liquid of shallow depth, given by:

$$w = \sqrt{\frac{\pi g}{L} \tanh\left(\frac{\pi H}{L}\right)} \quad (110)$$

Where H is the height of the liquid and L the width of the tank. Inputting, the problem dimensions gives a period of 1.65s for the motion.



Figure 17: Illustration of experimental set-up of the rotational sloshing tank (Vera et al. 2010)

Assumptions made in the modelling of this problem are:

- The fluid is incompressible and inviscid (when modelling water not oil)
- The small height in relation to width of the fluid means that fluid behaviour can be described by small amplitude wave theory
- The beam is linear elastic
- The Bulk modulus is over 1000 times smaller than a water case.
- Fluid is not turbulent

6.2 Problem Modelling

The FSI SPH solver used is Cranfield's in-house Meshless Continuum Mechanics code (MCM). In running a simulation using MCM, a user will generate an input file which contains problem dimensions, material properties, control parameters, boundary conditions and applied loads. However, due to the complexity of the benchmark problem, two additional things need to be considered to complete the problem description.

The first is the description of motion. Generally, if a fluid is the problem of interest, a Eulerian (or Updated Lagrangian as SPH is a Lagrangian method) is used. If structure deformation is of interest then the total Lagrangian approach is used to describe the motion. As discussed at the beginning of this chapter and in the literature review, the SPH method generally only models' fluids with structures using other approaches such as finite element and then the two are coupled. Therefore, despite SPH being a Lagrangian method, the motion approach used is that of Eulerian, hence the novelty of the total Lagrange approach and the further novelty of this work in combining them.

To further explain why this is, an understanding of the difference between the 2 approaches is required.

A Eulerian approach describes motion or any other property of interest such as density, velocity etc at a point in space, with changes at that point observed as time evolves. This is called the spatial description for that reason, as observation is restricted to changes in the state of the system at that point or section in space. This means that any property such as density, velocity or displacement is a function of current position and time.

A Lagrangian approach describes motion or any other property of interest by following individual points or particles as they evolve in time. Essentially, while the Eulerian approach focuses attention on a point in space, a Lagrangian approach tracks particles over time, so observation is focused on what happens to individual particles as they move. This is known as the material description for that reason as material points are followed in time. Mathematically, any properties of a particle or point in space with this description of motion are a function of initial position and time.

For a fluid, describing motion with respect to its initial undeformed state is not only impossible but not required. The history of the fluid is not important; the interest in a fluid dynamics problem is normally to do with changes in the fluid at points in space such as wave impact or breaking. For materials, there exists a clear undeformed state, so for problems involving structure change or impact, interest will be in the history of this process. Knowing how this structure looks at a certain point in space is not of use, how the structure gets from the undeformed state to the deformed state- the time history- is of use.

It is important to note that these are very general situations and there will be occasions where structure deformation properties are required to be written in the current configuration and the same applies to fluid proper ties in the initial configuration. Therefore, benchmark testing was not restricted to using a Eulerian approach for the fluid and Lagrangian for the structure.

6.2.1 Difference between Eulerian and Lagrangian SPH conservation equations

The 2 different descriptions of motion give rise to different formulations of the SPH equations of motion. Conceptually, in SPH the Lagrangian Kernel for each particle is calculated just once at the beginning of the simulation and does not change throughout, which has the consequence of the neighbourhood of each particle not changing as the simulation evolves. An Eulerian kernel however needs to be recomputed for each particle at every timestep and has a variable neighbourhood.

The Eulerian SPH equations of motion are hence given by (Rade Vignjevic et al. 2006).

$$\langle \dot{\rho}_i \rangle = \rho_i \sum_j^n \frac{m_j}{\rho_j} (v_j - v_i) \cdot \nabla W_{ij} \quad (111)$$

$$\langle \dot{v}_i \rangle = \sum_{j=1}^n m_j \left(\frac{\sigma_i}{\rho_i^2} + \frac{\sigma_j}{\rho_j^2} \right) \cdot \nabla W_{ij} \quad (112)$$

$$\langle e_i \rangle = -\frac{\sigma_i}{\rho_i^2} \sum_j^n m_j (v_j - v_i) \cdot \nabla W_{ij} \quad (113)$$

The Lagrangian description of the SPH conservation equations are given by(Rade Vignjevic et al. 2006):

$$\rho(X, t) = J^{-1}(X, t) \rho_0(X) \quad (114)$$

$$\langle \dot{v}_i \rangle = - \sum_{j \in S} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \cdot \nabla_{X_j} W(X_I - X_j, h_o) \quad (115)$$

$$\langle \dot{e}_i \rangle = -\frac{P_i}{\rho_i^2} : \sum_j^n m_j (v_j - v_i) \otimes \nabla_{X_j} W(X_I - X_j, h_o) V_j \quad (116)$$

One of the key differences in the conservation equations between the Eulerian and Lagrangian descriptions is that of the Kernel. In the Eulerian approach, the kernel is a function of current position and so the kernel and its derivatives are calculated with respect to current positions, which is consistent with the Eulerian approach. The consequence of this is that the number of neighbours of a particle can vary and hence particles can enter and leave kernel sums (De Vuyst 2003). This approach does lead to the aforementioned tensile instability problem.

The Lagrangian kernel is a function of initial position and initial smoothing length. As a function of initial position, this means that the number of neighbours is fixed as the initial position does not change. This has been shown to cure the tensile instability problem but at the cost of not being able to extreme material deformations (Rade Vignjevic et al. 2006). The Lagrangian SPH results will be used as a comparison when testing mixed formulation in the next chapter.

The second consideration is contact between boundaries. This work will use the MCM contact algorithm outlined in chapter 3

6.3 Benchmark case testing

Testing was done methodically, starting from a very simple case of 2 blocks impacting on each other and increasing in complexity with each phase. The passing criterion was the simulation illustrating expected physical behaviour. Once this was achieved, then another layer of complexity was added.

6.3.1 2 block impact case, no initial contact

This case was a simple 2 block impact case with same density of 1000kg/m^3 and the same mass and volume. An initial velocity of 0.1m/s was applied to the left block with the right stationary.

Properties varied in testing were:

- Contact type
- Contact stiffness
- Young's modulus
- Poissons ratio
- Discretisation type
- Material properties

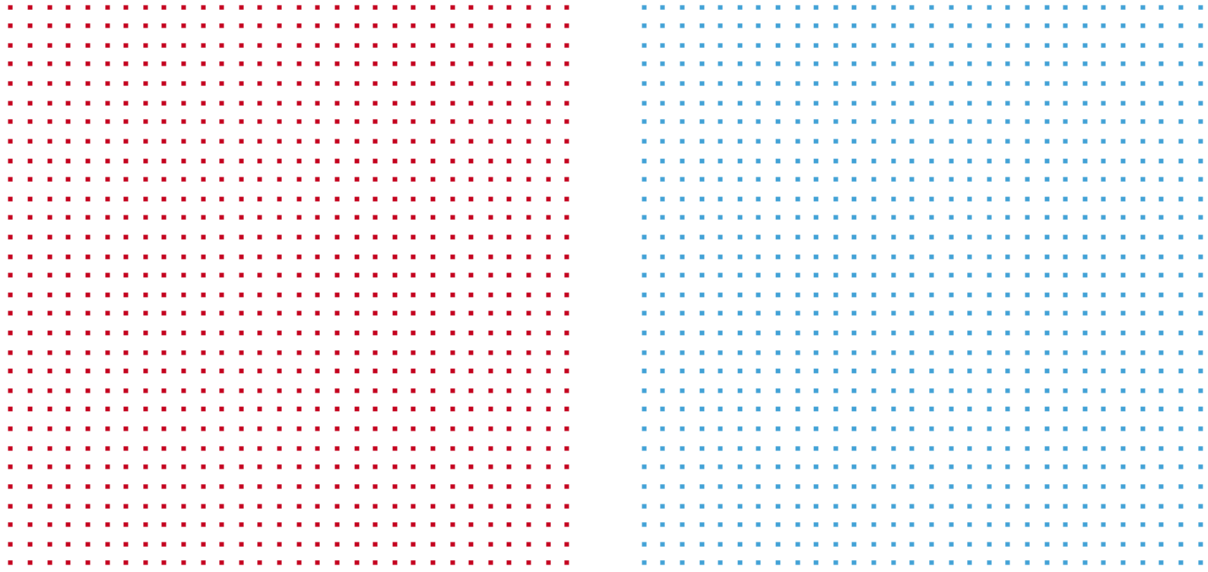


Figure 18: Simple 2D block test

6.3.2 Summary of 2D block testing

Fluid to fluid impact for differing bulk modulus, elastic to elastic impact with different Young's modulus's and fluid to elastic with a bulk modulus of $1\text{E}+07$ Pa passed as they gave expected behavioural results, namely impact without particle penetration, propagation of the pressure wave upon impact and the movement of the right block due to momentum conversation. This was expected due to the simplicity of the tests but 2 things occurred of note. One was that at a bulk modulus of $1\text{E}+04$ Pa, the fluid collapsed when impacted with the structure. The second was the different contact behaviour when using either a repulsive or pressure contact. When 2 repulsive blocks met, the left block would bounce of the right one and move in the opposite direction. This effect was less prevalent in the pressure contact scenario. The tests also revealed a limit at which the stiffness of both the pressure and repulsion gave effective results. Too little, and particle penetration occurred, too much, and exploding of particles would occur.

$$0.01 < Q < 1000 \text{ for repulsive contact}$$

$$0.0001 < Q < 10 \text{ for pressure contact}$$

6.3.3 Blocks with initial contact

The blocks, properties, dimensions and initial velocities were identical to the previous case except they were in initial contact. By this it is meant that they were less than 2 times the smoothing length away from each other. In fact, they were only a particle spacing distance from each other.

The testing results for the elastic to elastic test showed that only pressure contact with a Lagrangian approach passed. Extended to a fluid-structure case with a mixed approach (fluid as Eulerian, structure as Lagrangian) also showed a pass.

6.3.4 Extension to 3 and 4 blocks

The results showed that pressure contact with stiffness between 0.001 and 1 were the only acceptable results, with particle penetration or explosions occurring in the other cases. This also

failed when application of constraints to clamp the beam into place were added. It was clear that although it was good that a mixed discretisation approach (fluid as Eulerian, structure as Lagrangian) seemed to work and contact possibilities for the simulation had been isolated to only a few, thus reducing a long set of additional possibilities, a more realistic description of the beam was required to see if the benchmark case was feasible.

6.4 Beam testing

Testing of the elastic beam was more successful. A beam was designed using the parameters given in (Groenenboom n.d.). This paper compares an SPH simulation of an elastic beam to a FE LS-Dyna modelled beam of identical properties and dimensions, subject to a varying gravitational load. The paper aimed to assess whether the addition of artificial stresses in the momentum equation enabled better representation of elastic beam behaviour. The results indicated the same problem as highlighted in (Antoci et al. 2007) and (Paredes & Imas 2011), the overestimation of deflection and additionally highlighted differing behaviour depending on whether an odd or even number of particles were used in the vertical axis of construction of the beam.

The test case is an elastic beam with a width of 5mm and length of 79mm. The young's modulus of this material is 12MPa. In this case, a x direction load is applied linearly for 0.1s where it reaches its maximum of 200m/s^2 . At this point in time, the load is kept constant for 0.3s, then is linearly decreased back to 0, which occurs at 0.5s. The simulation continues to run until 0.8s where it is then terminated.

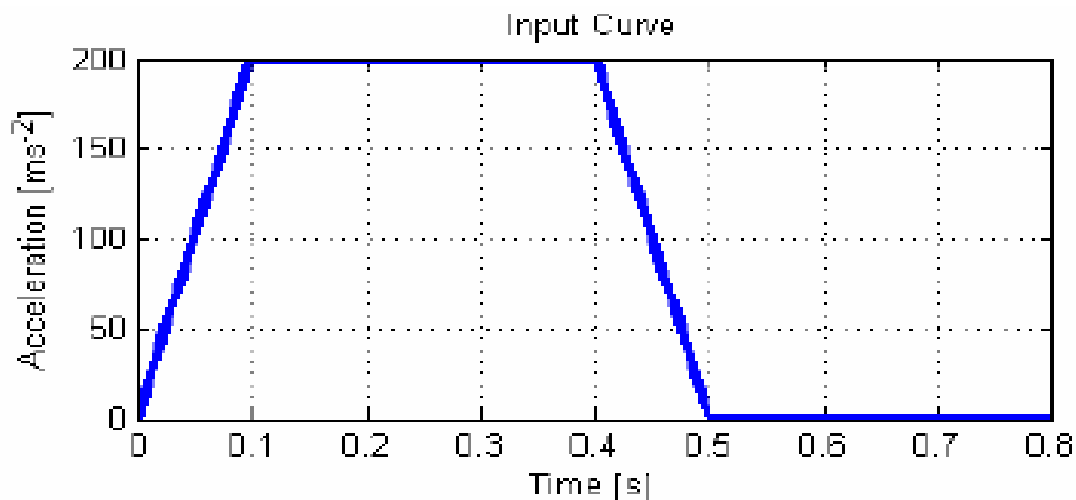


Figure 19: Load curve of acceleration applied to the beam.

The aim of these tests is to validate the MCM SPH modelled beam by comparison with the LS-Dyna beam and compare the accuracy of the simulation with the SPH beam described in (Degroote et al. 2010). To achieve validation mesh independence must also be proved.

6.4.1 Deflection result comparisons between MCM and finite element modelled beam

Deflection comparison is done by comparing the outmost particle and node at the top right of the beam. The FE solver used is LS-Dyna with Belytschko-Tsay element formulation. The MCM SPH beam is modelled with a Total Lagrangian approach and in some cases a Normalised Total Lagrange

approach. Normalised Total Lagrangian involves invoking first order consistency to the Total Lagrange approach. The proof is outlined in (Rade Vignjevic et al. 2006). The cases tested are a 0.1, 0.05, 0.033 and 0.025cm particle spacing case which corresponds to a 5,10,15 and 20 particle width respectively. This corresponds to an FE mesh spacing of 0.1, 0.05, 0.033 and 0.025cm. Both are accelerated under the applied load illustrated in Figure 19

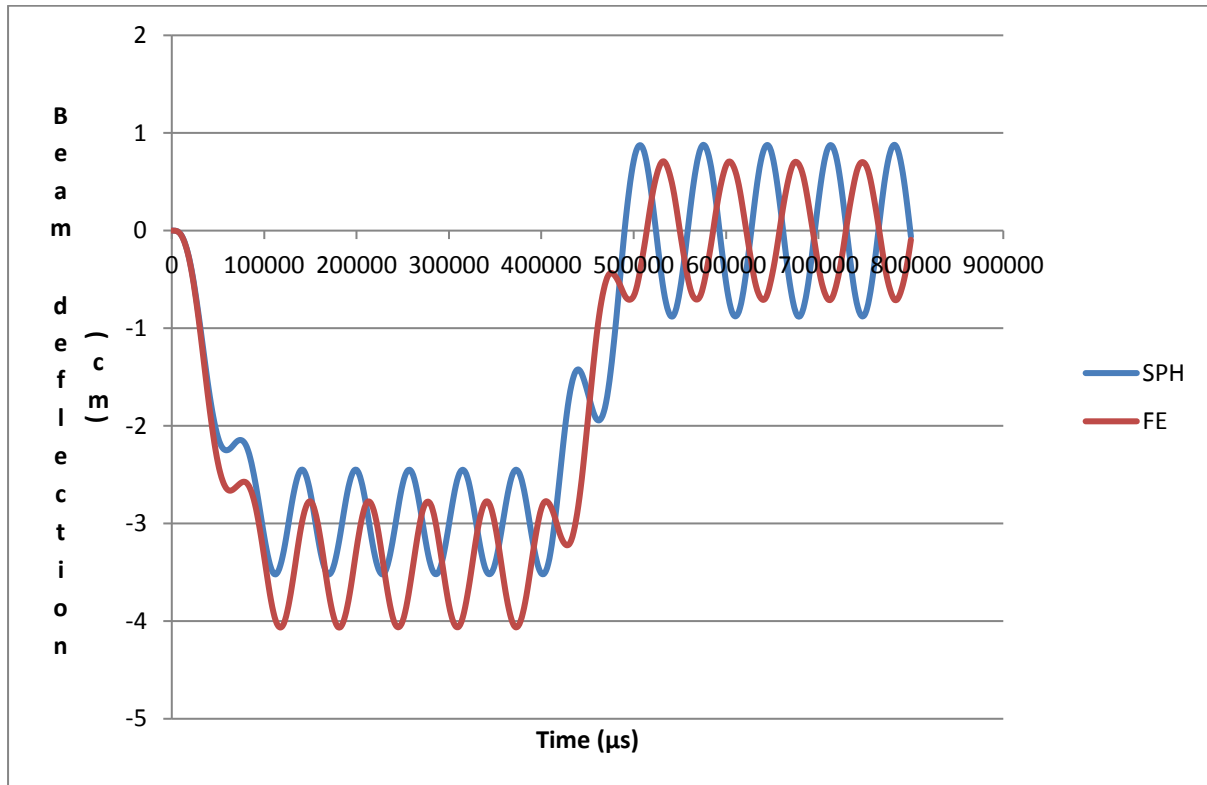


Figure 20: Deflection comparison of an MCM (SPH) and LSDyna(FE) modelled beam. The beam is 5mm wide and consists of 5 particles across its diameter

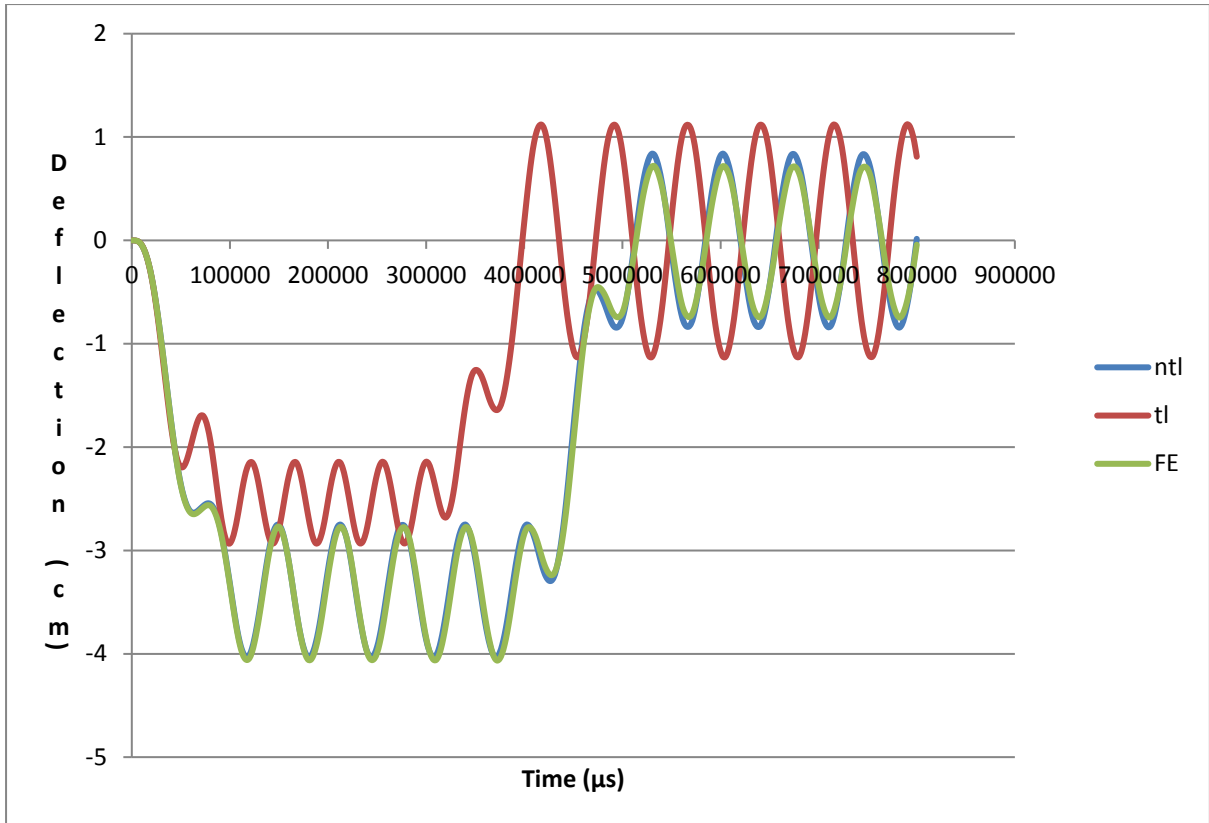


Figure 21 Deflection comparison of an MCM Total Lagrange case(TL), MCM corrected total Lagrange case (NTL) and LSDyna modelled beam(FE). The beam is 5mm wide and consists of 10 particles across its diameter.

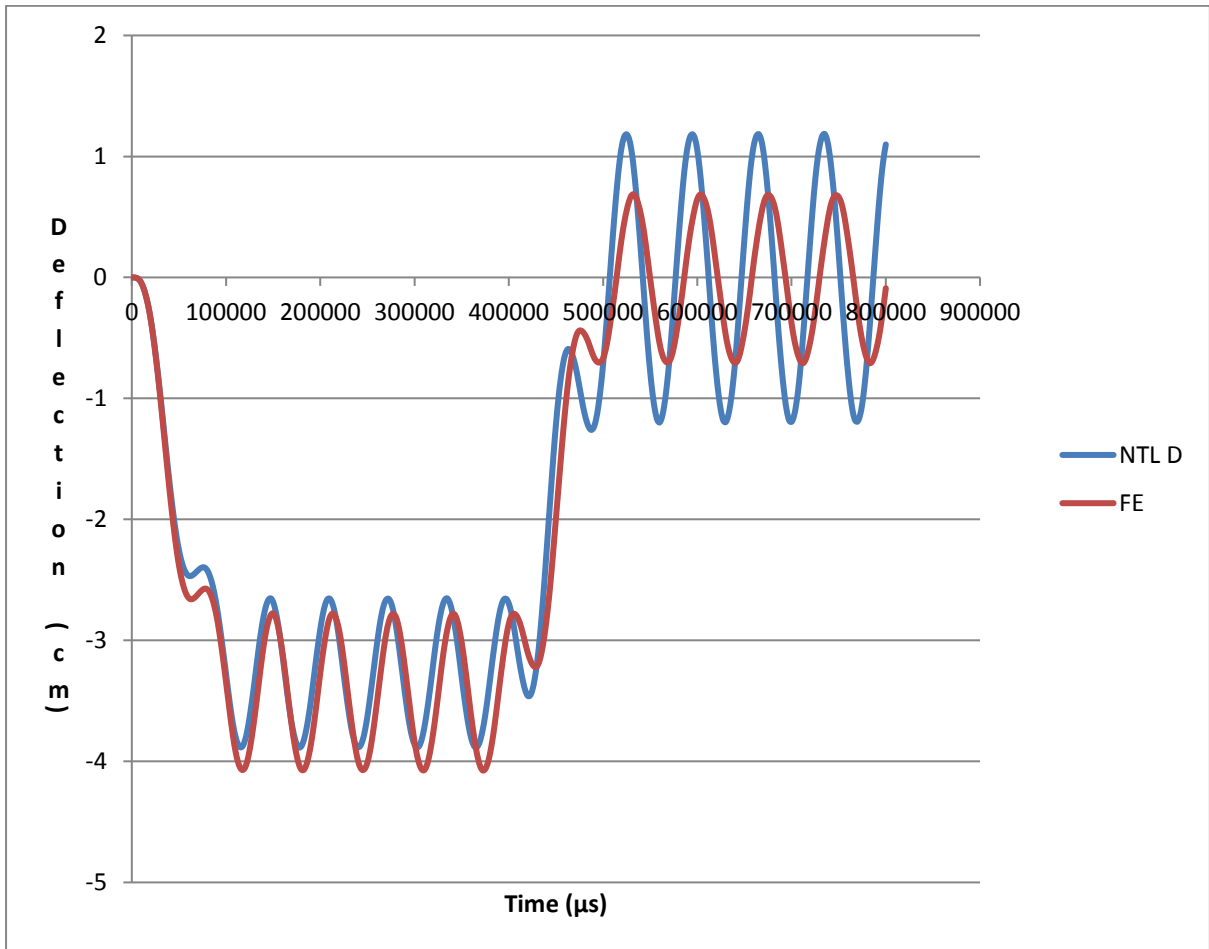


Figure 22: Deflection comparison of an MCM corrected Total Lagrange case (NTL) and LSDyna (FE) modelled beam. The beam is 5mm wide and consists of 15 particles across its diameter.

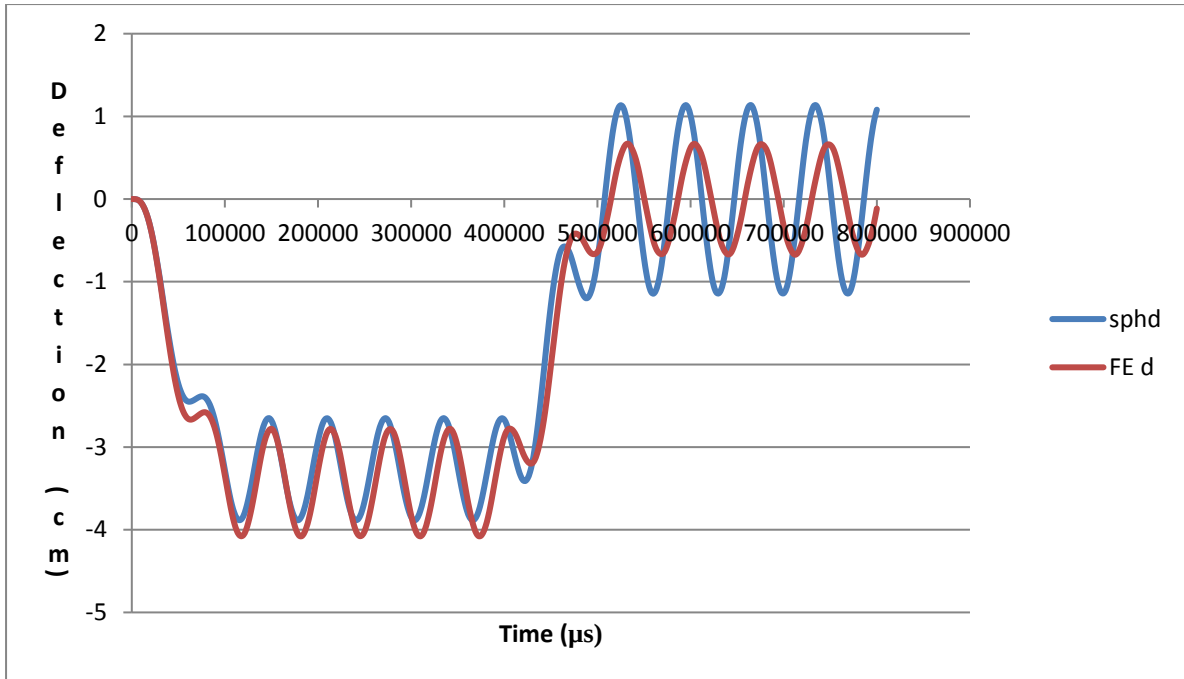


Figure 23: Deflection comparison of an MCM Total Lagrange case(TL) and LSDyna (FE) modelled beam. The beam is 5mm wide and consists of 20 particles across its diameter.

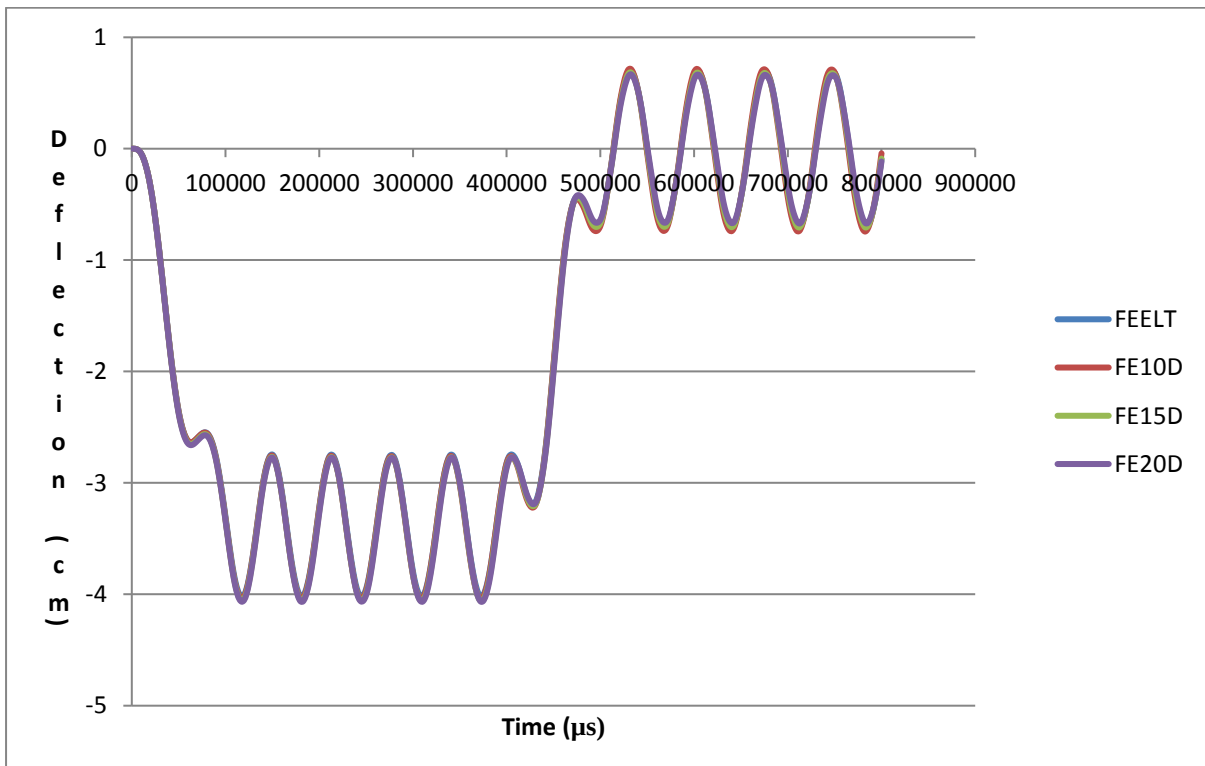


Figure 24: Mesh independence test for the LSDyna beam.

The deflection behaviour of the beam agrees up to a point with the LS-DYNA equivalent. Where things do differ significantly is at the point of gravitational release, where the motion of the beam rotates about its equilibrium. The amplitudes and frequencies differ more than what is desirable. The difference in the estimate of the amplitude of displacement is 50%. The exception to this occurs at the 10 particle case shown in Figure 21 where the corrected Total Lagrange case (which is a 1st order consistent version of the Total Lagrange formulation) matches the FE modelled beam.

6.4.2 Reasons for difference in results

This could be for many reasons. Firstly, these are two different numerical methods at which this problem is being simulated, there are bound to be differences between the two as they are two different techniques. Another possibility is load curve interpolation. Although in both cases the gravity is specified at certain times, the gravity at times in between needs to be interpolated, and this will yield slightly different values which may amplify as the problem develops.

There is also the fact that SPH particles are specified at different positions to LS-Dyna nodes, this may influence the neutral axis of the beam. The neutral axis of the beam is where there exists no strain or stresses as at that axis, tension and compression are balanced. This is normally located at the centre of the beam. However, as the dimensions of the problem do not change, only the number of particles that model it, therefore if the number of particles making up the x component of the beam is odd, there may not be any particles on the neutral axis, whereas for an even number of particles there would be, or vice versa. This could have an effect as unphysical strain and stresses may be produced on the neutral axis in one of these situations. This difference in behaviour depending on whether there was odd or even number of particles composing the x component of the beam was shown in (Groenenboom n.d.) with an odd number of particles leading to overestimation of deflections and even number of particles and even number of particles reducing the strength of the material.

The overestimation of deflection is a common problem in all SPH modelling cases as discussed earlier, so this could be inherent to the method. As the 10 particle case seems to be the most successful, the beam in the FSI case will be constructed with a width of 10 particles.

6.5 Shaking motion testing of beam and fluid tank

Despite room for improvement in comparison to the LS-DYNA beam, this can be considered a working beam. Extending to FSI testing, the same step by step methodical approach was used as before.

The first step was to test the beam under different, more representative conditions. So far it had only been tested under a variable x direction gravitational force. For a sloshing and/or rolling tank, it needs to be proved that the beam will not break, collapse or explode under sloshing/rolling tank conditions. Instead, the beam should show its same flexible behaviour.

To achieve this first validation, the beam was subjected to a shaking motion. The frequency of shaking motion comes from (Reed et al. 1998), where the behaviour of tuned liquid dampers was investigated under large amplitude excitation. The frequency of the shaking of the tank corresponds to the natural frequency of the water sloshing motion predicted by linear water wave theory (Falnes 2005). This is given by:

$$f = \frac{1}{2\pi} \sqrt{\frac{\pi g}{L} \tanh\left(\frac{\pi H}{L}\right)} \quad (117)$$

Where H is the water depth, L the length of the tank. The water depth H is 0.03m and the Length L 0.59m. This corresponds to a frequency of 0.458Hz. All tests will be tested using this frequency of shaking motion unless otherwise specified.

The application of this shaking motion to the beam was achieved by creating another material of identical properties at the base of the beam, thus acting as a piece of the tank that the beam will be connected to. Kernel contact is introduced between the 2 materials, this has the effect of treating the whole system as 1 material as kernel contact between 2 materials is essentially the same as no contact between the materials, so any interpolation between a particle and its neighbours is treated as if it is from the same material. This 'connects' the 2 materials and is an example of the neighbour contact as discussed before.

The particles that make up the base (shown in red in Figure 25) are then subjected to displacement load curves of a period corresponding to the frequency given in equation (117). This induces the same shaking motion, but only at the base. If the test is successful, the beam as it is connected to the base, should move along with it and not break off or fall apart. This was achieved.



Figure 25: Illustration of the beam

Physically this test was an example of forced oscillating motion. The beam displacement frequency should correspond to the frequency of the shaking and be in phase as there is no lag between movement of the base and the beam. This is shown in Figure 26.

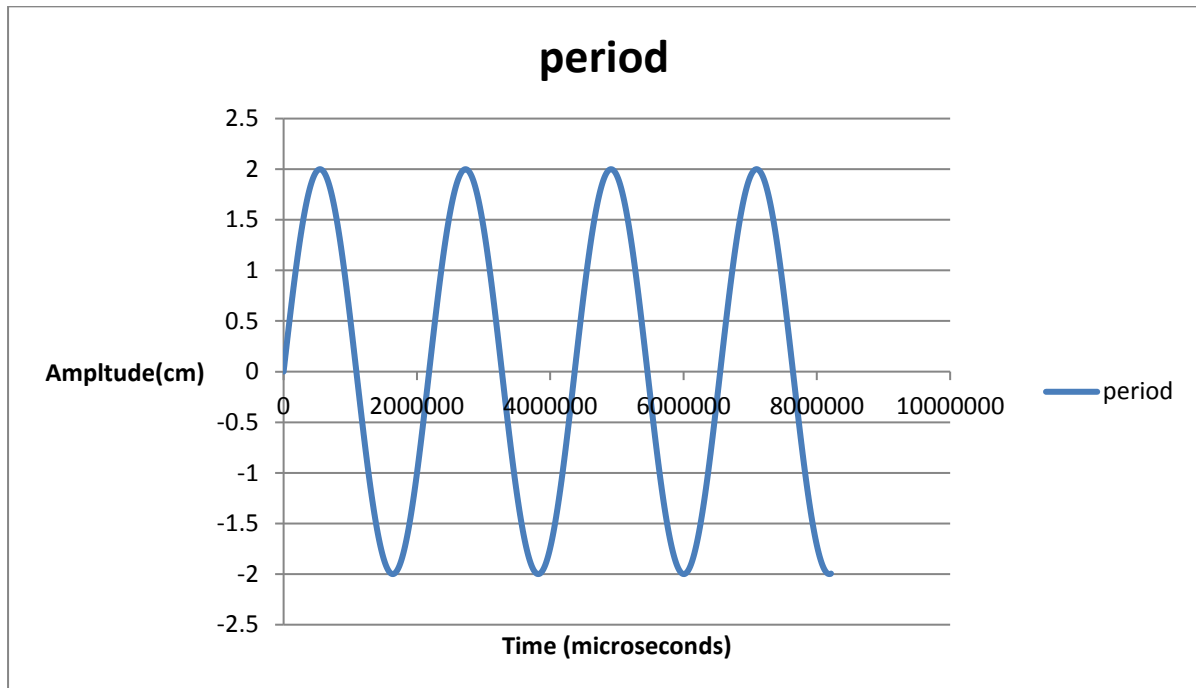


Figure 26: Illustration of frequency of oscillation of the forced shaking of the beam

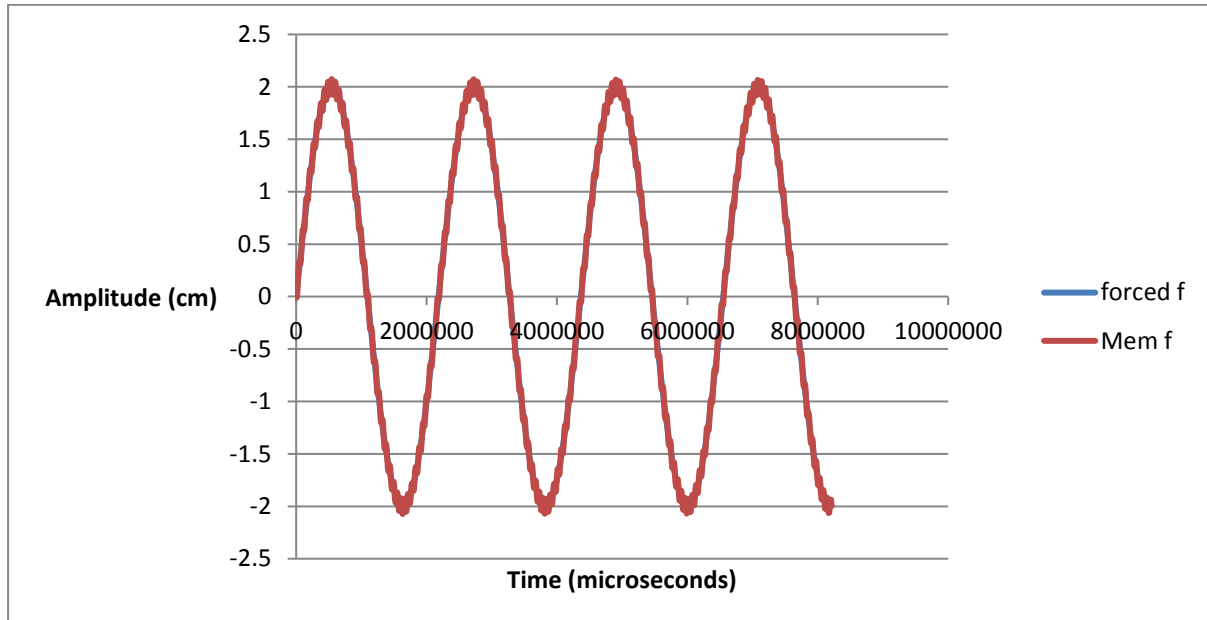


Figure 27: Illustration of forced oscillation (forced f) against subsequent beam oscillation (Mem f)

The success of the beam test means that FSI modelling can be considered. The next test is extension to a tank case whereby the walls were modelled with the same properties as the beam, and fluid of differing bulk modulus' were added in between the beam and the walls. This was shaken in the same manner as in Figure 26. This was successful for pressure contacts within the ranges described by the 2D block testing. There was a slight concern with a few particles penetrating the boundary and the

fluid trying to escape, but this was not a surprise given that the fluid was not relaxed and so had 0 pressure at the beginning of the simulation. A more realistic test is shown below.

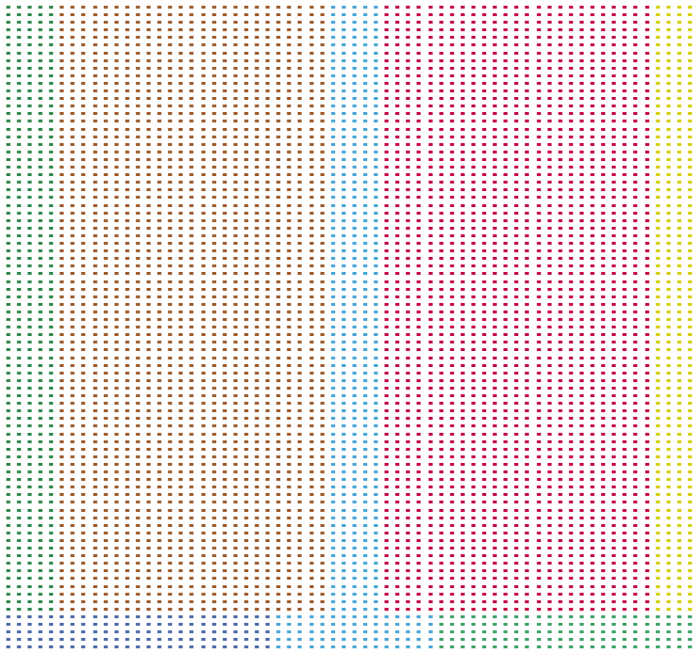


Figure 28: Sloshing tank test with elastic clamped beam.

This test models the walls as solid boundaries. The testing parameters have been significantly reduced due to failure of simpler tests using repulsive contact and small bulk modulus' for water.

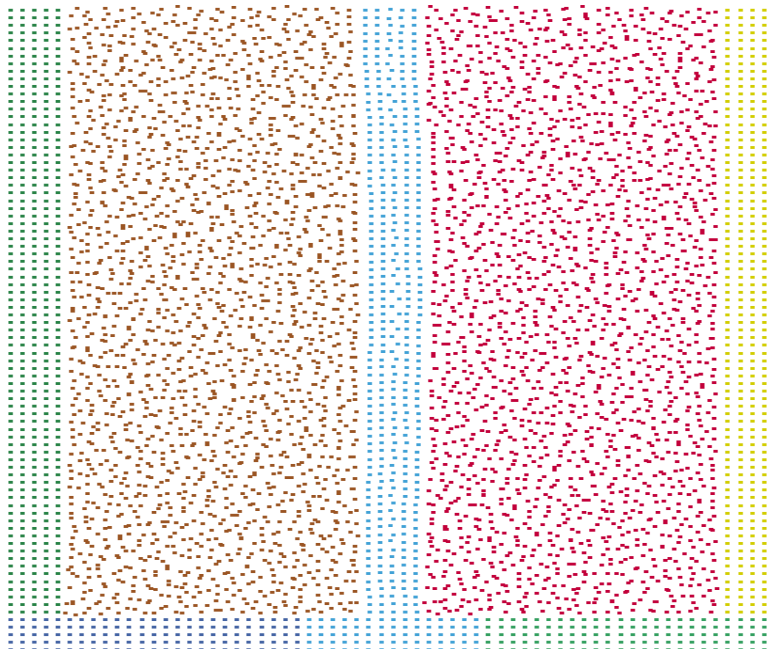


Figure 29: Sloshing tank at 4 seconds with a pressure contact of stiffness 1.

The beam shows flexible behaviour and there is no particle penetration.

The next step was to extend the FSI testing. This was done by simulating a tank with the same geometry as outlined in Table 1 and Table 2 and shaking with the same frequency as the previous tests. All other properties remain the same as they were taken from Table 5 and Table 6.

since the testing so far has been done with a beam of height 7.9cm and been successful. Once success of this test is complete, the final step will be to make the water and beam height the same as (Vera et al. 2010) and then compare the behaviour.

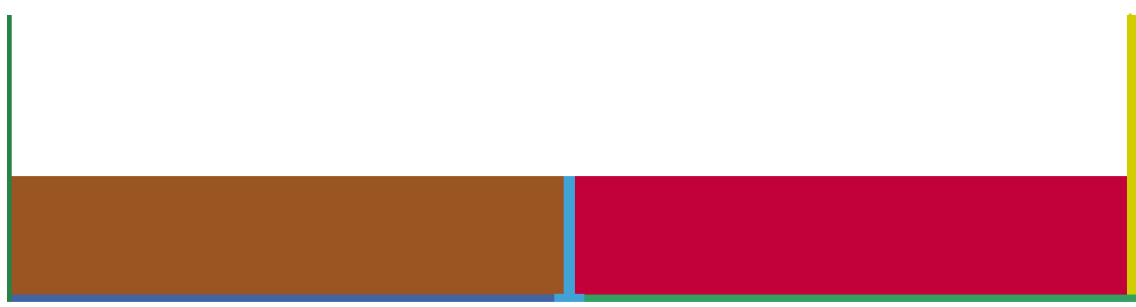


Figure 30: Illustration of tank test with dimensions given in (Vera et al. 2010)

The water was initially relaxed to achieve realistic initial conditions for the water. This is shown in Figure 31.

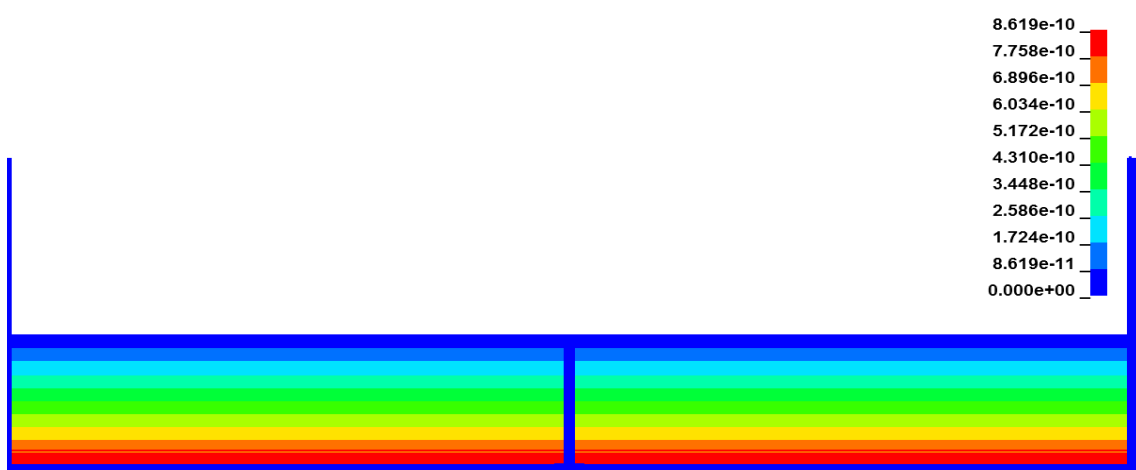


Figure 31: Illustration of relaxed tank

The fringe levels on the right of the tank is the pressure given in $\text{gcm}/\mu\text{s}^2$ and follows the $P = \rho gh$ law. To test the accuracy of the pressure calculation, the height of the tank was given as 57.4mm, which in cm is 0.574cm. gravity in the units used was $9.81 \times 10^{-10} \text{cm}/\mu\text{s}^2$ and density in the units used was $0.99 \text{g}/\text{cm}^3$. Using $P = \rho gh$, and $h = 0.56$ so pressure calculated is just before the tank bottom, we get an analytical pressure value of approximately $5.48 \times 10^{-10} \text{gcm}/\mu\text{s}^2$. Using a height of 0.1, we get approximately $9.79 \times 10^{-11} \text{gcm}/\mu\text{s}^2$. The numerical values give slightly higher values of approximately $8 \times 10^{-10} \text{gcm}/\mu\text{s}^2$ and $2 \times 10^{-10} \text{gcm}/\mu\text{s}^2$ respectively but what this does prove is a) The pressure distribution is correct and b) Using the bulk modulus of 2.8×10^4 has not had a negative effect on the magnitude of the pressure. In fact, the magnitude is in the correct ballpark, the difference between numerical and analytical will be more down to the numerical method rather than the value of Bulk Modulus.

6.6 Code additions and testing of 2D rotational boundary conditions

To model the tank rolling movement necessary for validation with the capability of forced angular motion as described by equation (117) was required. Mathematically, this is modelled by the following co-ordinate transformation:

$$\begin{bmatrix} x' \\ y' \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \quad (118)$$

Equation (118) is only valid for a 2d case rotation case and rotates at the origin. This is sufficient for experimental comparison as (Degroote et al. 2010) assumes 2d behaviour.

Equation (118) maps current co-ordinates $[x \ y]^T$ to new co-ordinates $[x' \ y']^T$ via the rotation matrix. This achieves the rotation effect in 2D without changing co-ordinate systems as the co-ordinate system has not changed. The problem of interest is still in the Cartesian co-ordinate system and all the equations that govern it are in Cartesian form. This makes using the rotation matrix ideal as the mapping rotates the particle at (x,y) by θ degrees but gives its new position in Cartesian co-ordinates.

MCM did not have the capability of rotational boundary conditions, so additional coding and testing needed to add. Boundary conditions are modelled as a prescribed displacement, so rotational boundary conditions were also described as a prescribed angular displacement, with interpolation between load curve points done in the same manner as the prescribed displacement routine. User input is simple; the user inputs desired times and the angle of rotation in degrees desired at that time. Testing has occurred by using the benchmark test case illustrated in (Degroote et al. 2010). Oil and water were tested to ensure that particle penetration did not occur.

The prescribed angular displacements were applied on the walls of the structure in a periodic manner as shown below.

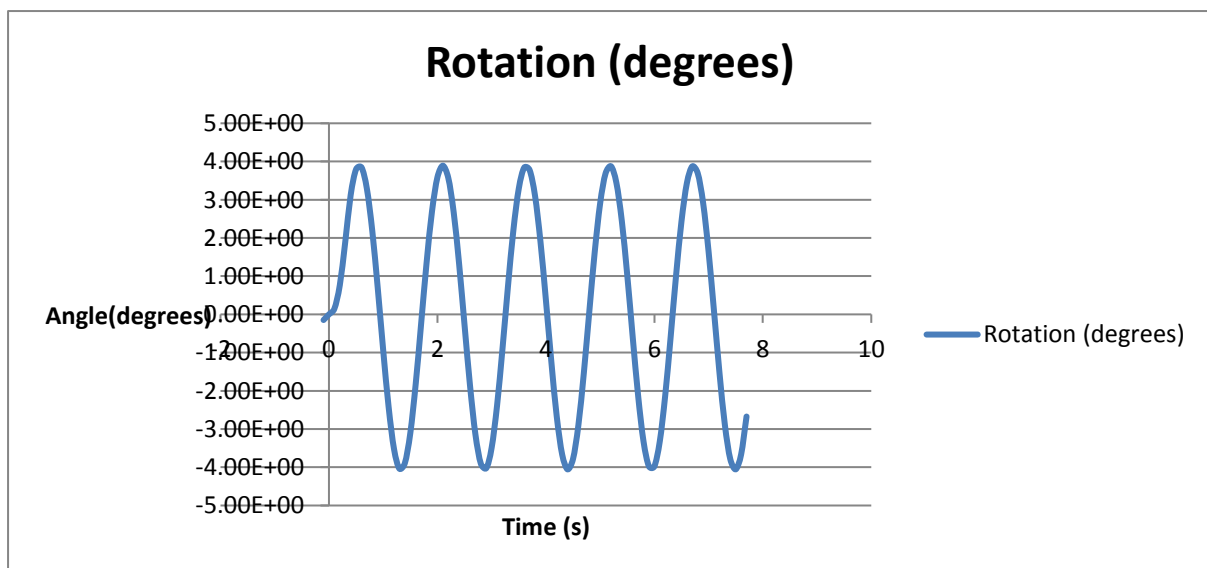


Figure 32: Plot of angle of rotation over time.

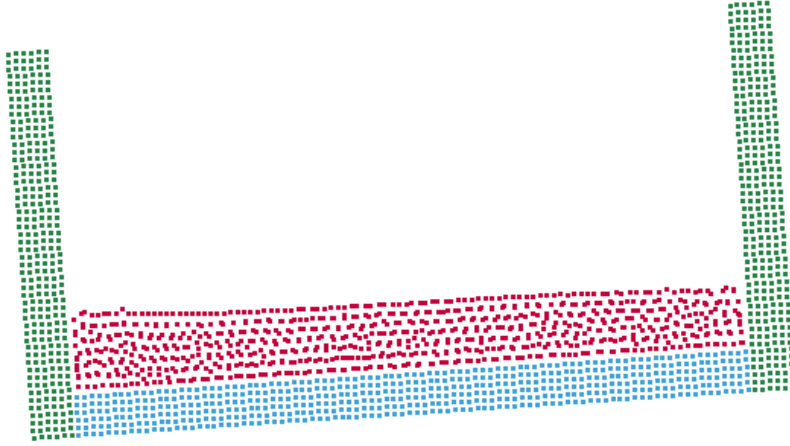


Figure 33: Rotation of tank at 0.6s

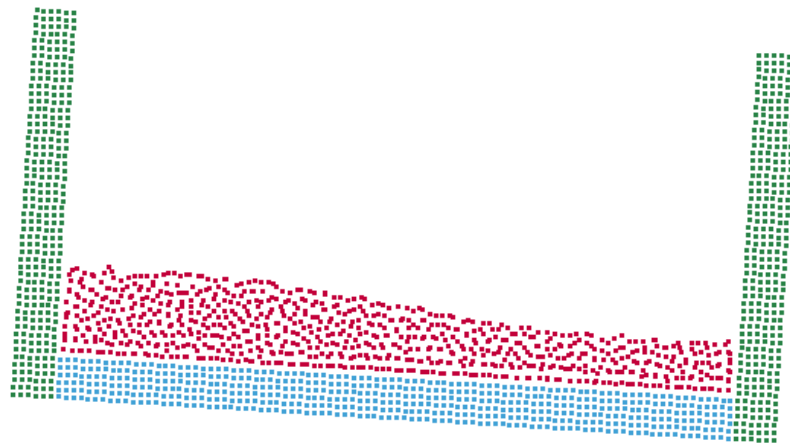


Figure 34: Rotation of tank at 1.2s

Figure 33 and Figure 34 illustrate the rotation effect on the sloshing tank because of the periodic rotation applied. The tank is rotating and particle penetration is not occurring. To validate the accuracy of the rotation, results are compared to the analytical solution of the arc length of a circle as the rotation is of a circular manner.

The arc length of a circle is given by:

$$s = r\theta \quad (119)$$

S is the arc length, r the radius and θ the angle of rotation in radians.

Picking particle 3420, the bottom right particle of the tank for analysis at co-ordinates (0.5075,0), adjacent to the rotational point (0,0), the radius can be defined as 0.5075m. The resultant displacement of the particle can be considered as the arc length as it represents the same thing, the displacement of the particle from the point of origin subtended by an angle to its current position. However, where this fails is that the resultant displacement is always positive, the arc length is not. The arc length will be negative when the angle is negative. This problem is solved by multiplying the resultant displacement by -1 when the angle is negative. This now allows us to relate the resultant displacement to the arc length.

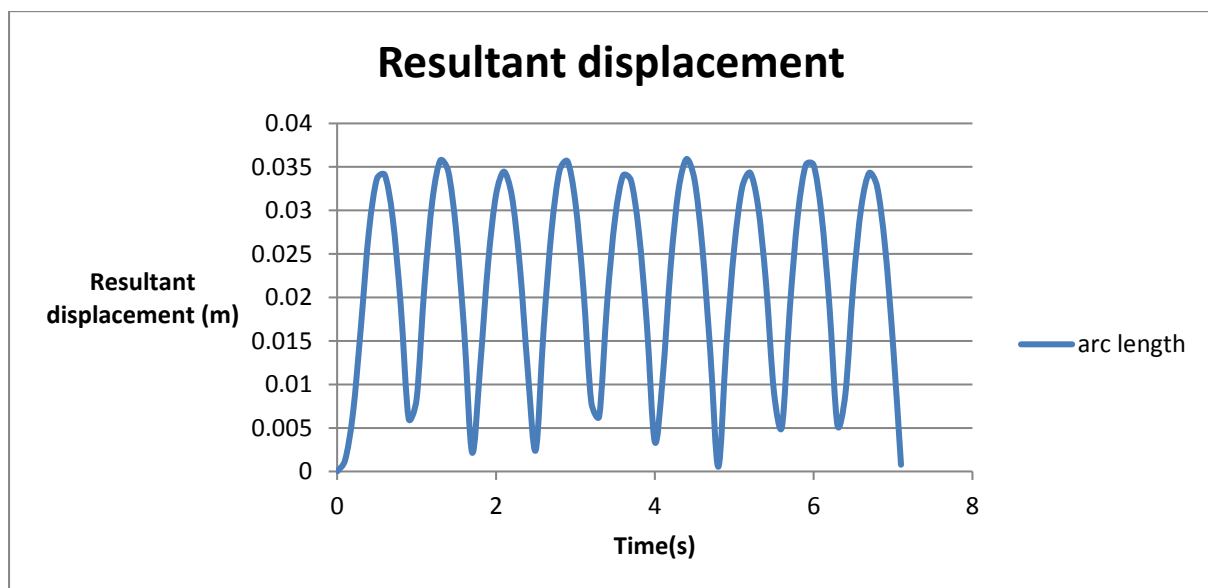


Figure 35: Resultant displacement of particle 3420 over time.

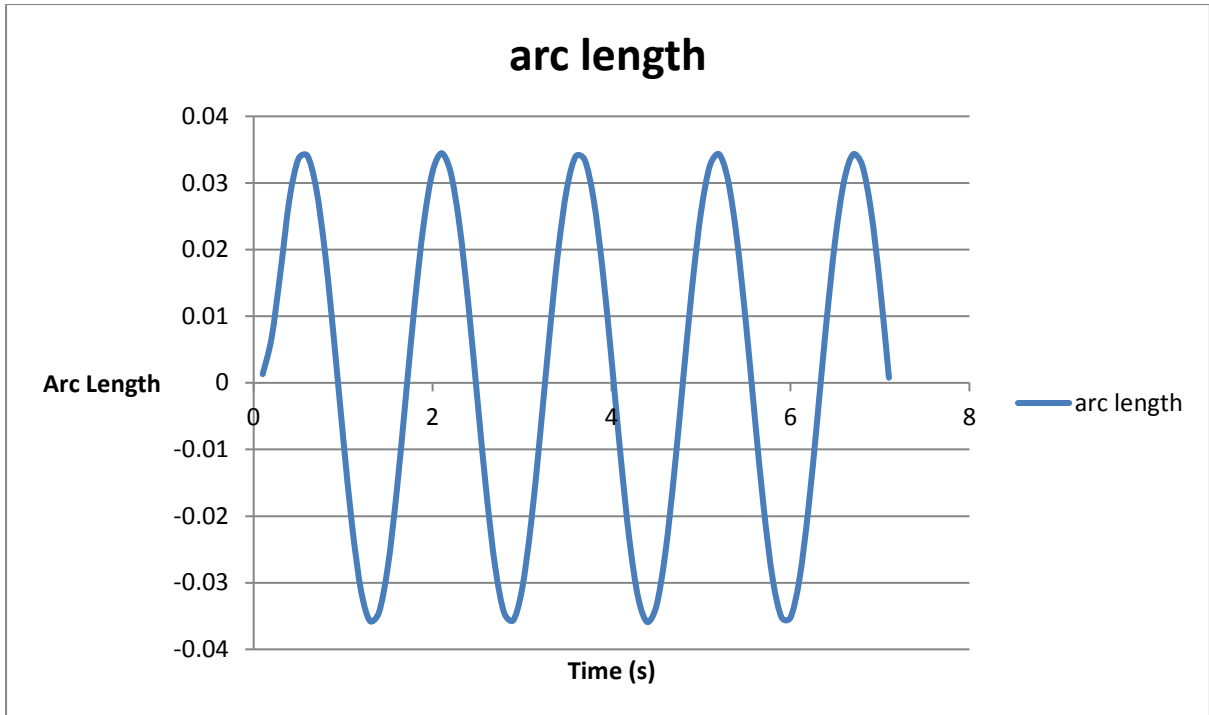


Figure 36: Arc length of particle 3420 over time.

As the arc length of the particle distance is now known and the radius is also known, the angle can be found by dividing the arc length over the radius (s/r) and compared to the actual input values.

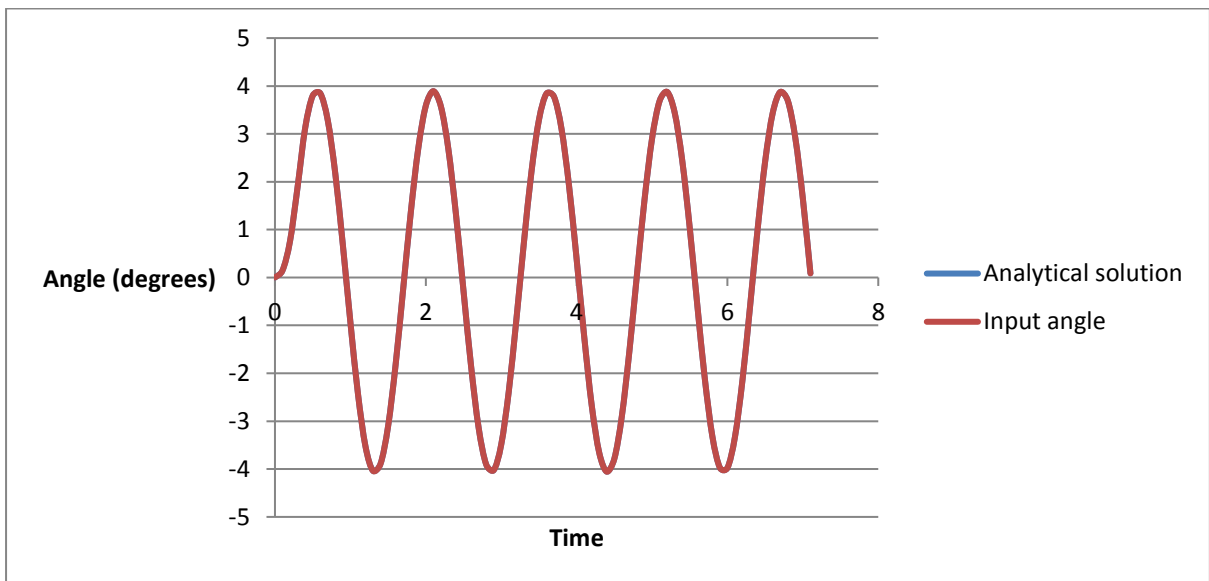


Figure 37: Comparison between analytical solution of angle and input angle.

Figure 37 shows that the analytical solution and the input angle are identical. This achieves validation of the code as it has been proven that the angle of rotation seen in the simulation matches the user input. The code does as it should.

6.7 3D testing of rotational boundary condition algorithms

The previous results show the accuracy of the implementation but not the versatility. The next tests shall show this by testing on a tensile bar in 3D. This will show that the implementation can work in

3D and with other materials and engineering situations. The simulation completed a rotation of 360 degrees in 6 seconds.

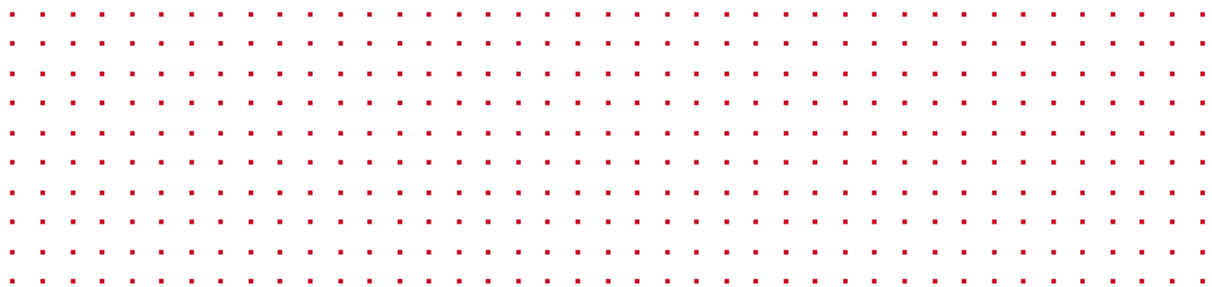
The equation for 3D rotation is given by

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad (120)$$

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \cos \theta & 0 & -\sin \theta \\ 0 & 1 & 0 \\ \sin \theta & 0 & \cos \theta \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad (121)$$

$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad (122)$$

With the code implementation shown in appendix 1.2



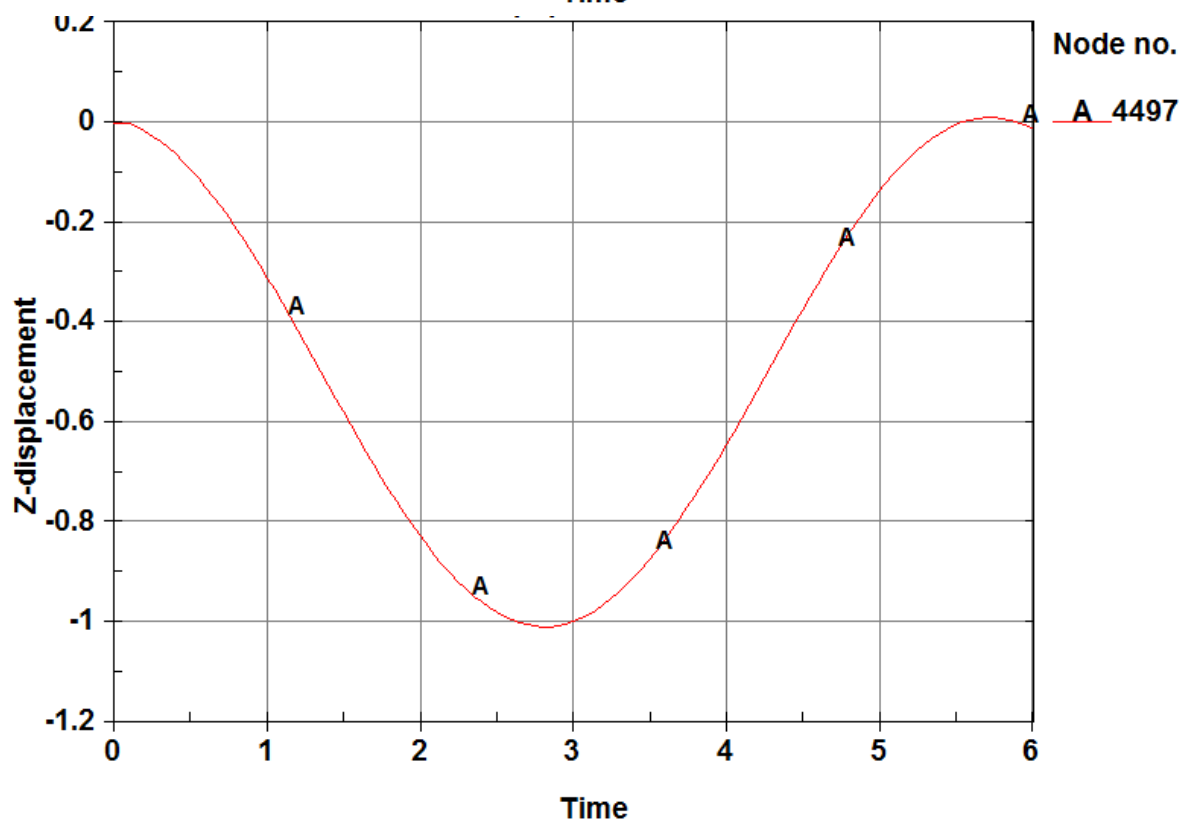
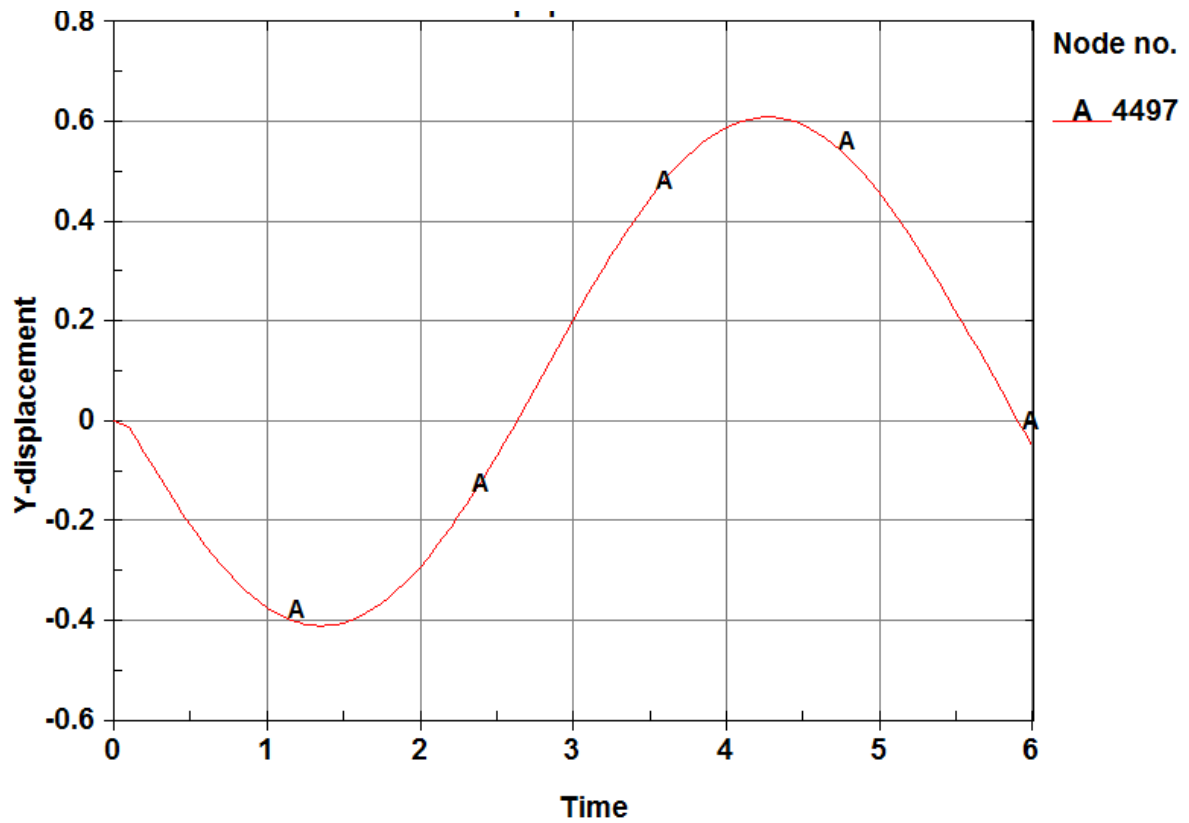


Figure 38: X and z displacement rotations (cm)for 3D block rotated 360 degrees in the y direction. The block has a density of 1100kg/m^3 , Youngs modulus of $1.2\text{E}+07$ and passions ratio of 0.4. Dimensions were $1\text{m}\times 1\text{m}\times 1\text{m}$.

The results show that the implementation of rotational boundary conditions is analytically correct. The next section shall detail the testing of the FSI problem.

7. FSI testing of the benchmark cases

The previous chapter illustrated the steps required, testing and results for each component of the FSI simulation in order to develop a model capable of the FSI problem models described in (Degroote et al. 2010; Vera et al. 2010). This chapter is a continuation of the work in chapter 6 by putting together the individual components tested in chapter 6 and putting them together for large scale testing of the FSI models described above. The two FSI models this work will be focussing on are a rolling tank with two different beam configurations. One was a small beam in shallow water, the second a larger beam in oil. Both were immersed in water with the tip of the beam at the same position as the free surface of the fluid. The results of the simulations detailed visual comparison of the fluid at certain times and beam deflection. This section shall compare results with the experimental data outlined in (Vera et al. 2010) tests described in (Degroote et al. 2010).

7.1 Visual comparison of flow profile between MCM testing, experimental results and another numerical solver for shallow fluid

The best results for all cases were using a repulsive contact parameter of 1 between all materials. Pressure contact achieved no discernible results due to the significant variation of pressure when shaking of the tank. The constant pressure variation and noise meant that pressure contact was unreliable leading to unphysical particle penetration. For the following figures, the top pictures that contain the real life model are from (Vera et al. 2010) titled 'experiment'. The simulations of the experiment from Degroote from their interface quasi-Newton algorithm with the approximation of the inverse of the jacobian from the least squares model (IQN-ILS) algorithm (Degroote et al. 2010) are titled 'simulation' and this thesis' work is titled MCM in the figure captions.

For the shallow water case, the best results were:

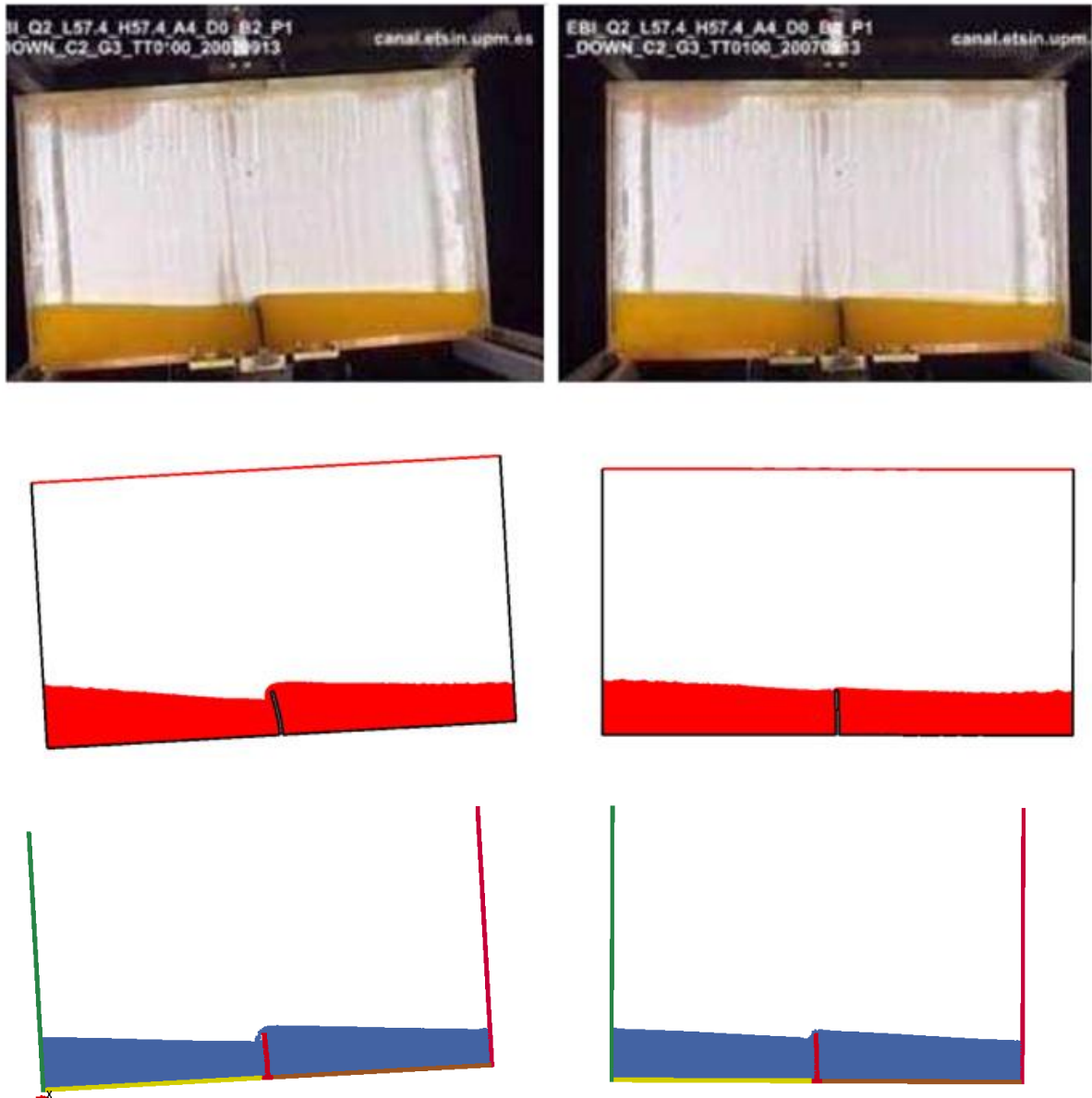


Figure 39: Visual comparison for shallow water case between experiment (top), simulation (middle) and MCM simulation (bottom). The left-hand side is recorded at 0.9s, the right-hand side at 1.2s.

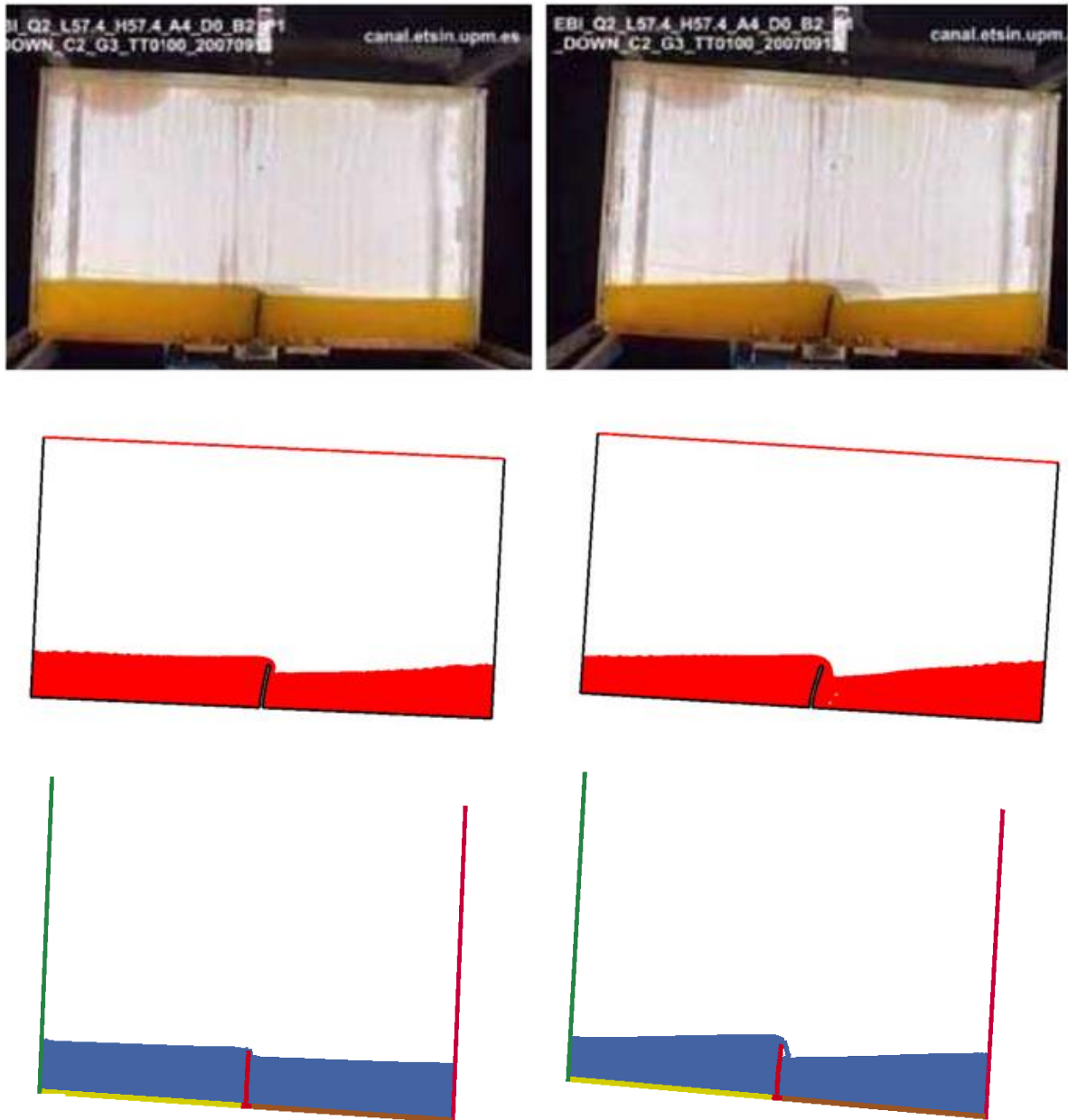


Figure 40: Visual comparison for shallow water case between experiment (top), simulation (middle) and MCM simulation (bottom). The left-hand side is recorded at 1.4ss, the right-hand side at 1.68s.

It can be seen from Figure 40 that there are significant gaps in the fluid and the free surface at certain points is not correctly defined. This is part could be down to the bulk modulus being significantly lower than simulations than in practice. A lower bulk modulus means more compressible which may explain the gaps as the gaps are due to the fact the water profile is lower than it should be by the beam.

Another potential issue is the nature of the contact algorithm. The contact algorithm only represents repulsion and has a dependency on the neighbours, hence it would have the same neighbour deficiency issue that SPH is plagued with.

Investigating the gap issue further, another test began with a fluid with bulk modulus of order of magnitude of 4 and contact 1 under dynamic relaxation. Focusing on particle 92936 which is a particle located at the top middle of the tank, it can be seen that under dynamic relaxation the fluid slightly compresses. The next three figures detail the particles under observation with time in seconds and y coordinate in cm.

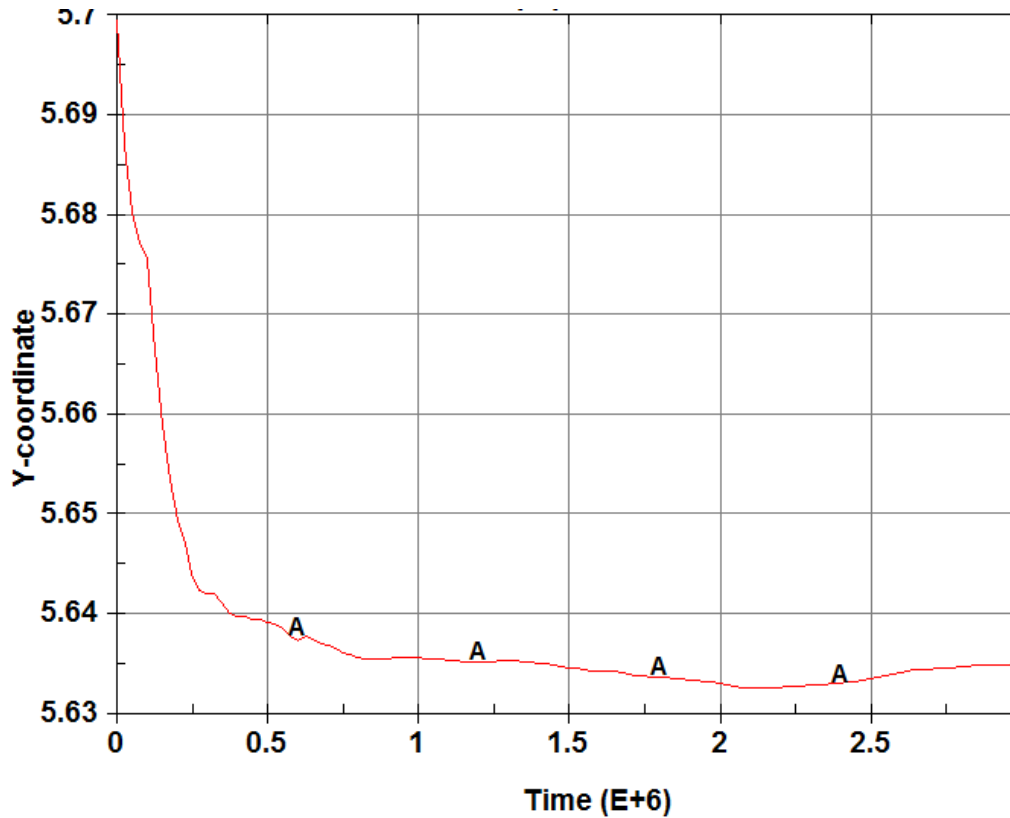


Figure 41: Particle 92936 movement under dynamic relaxation.

What was of interest and relevant to the 'gap' issue in the simulations is that the gaps occur near boundaries. Comparing particle 92936 to particle 93378, which is a particle near a boundary for water and oil it can be seen that the boundary particle compressed more.

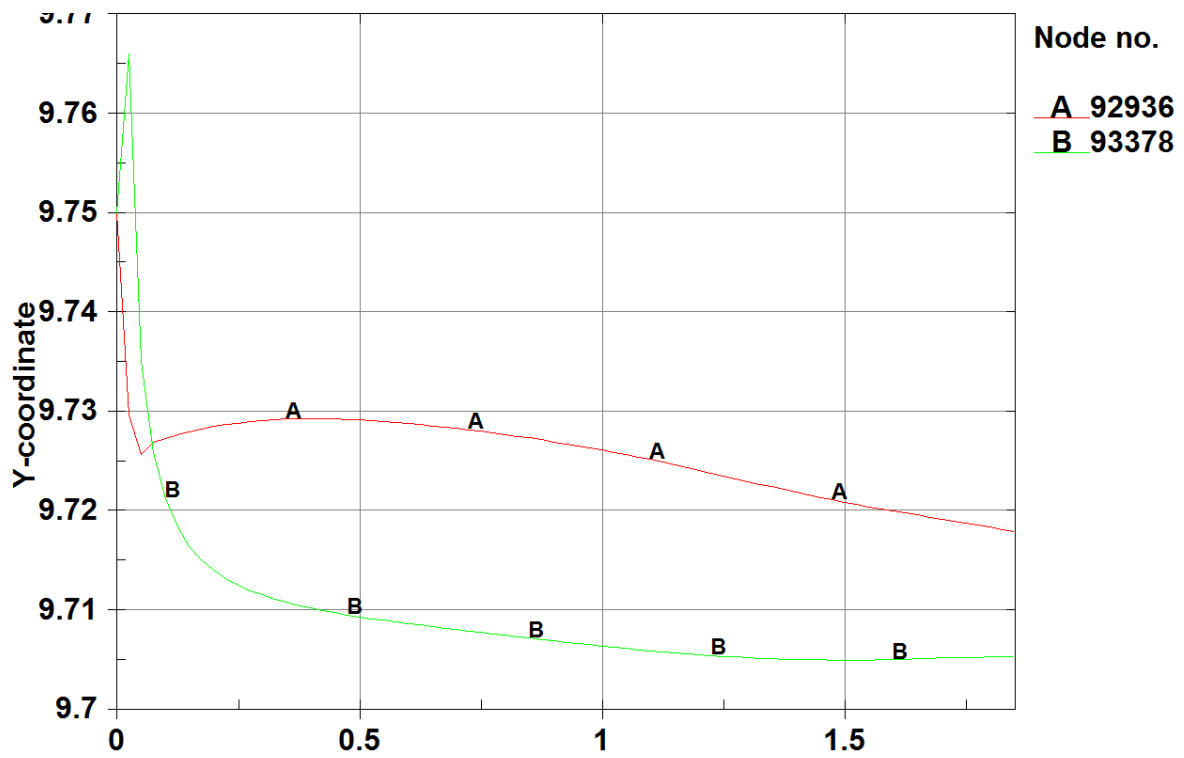


Figure 42: Comparison between 'centre' and 'boundary' particle for water.

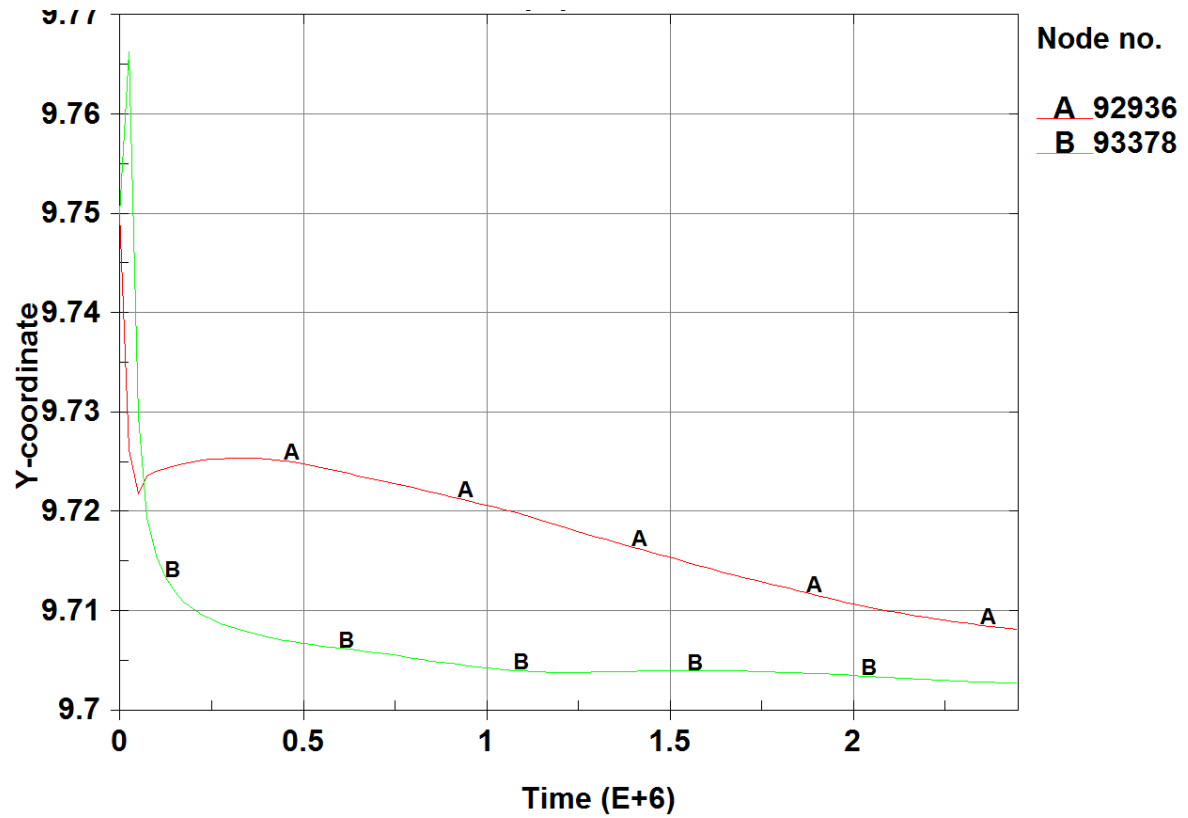


Figure 43: Comparison between 'centre' and 'boundary' particle for Oil simulation.

What was of further interest is the representation of contact as the repulsion is more prevalent nearer the top of the water than the bottom. This is highlighted in the figure below where it can be seen that the fluid (in blue) and the wall (in red) has more repulsion the closer to the free surface.

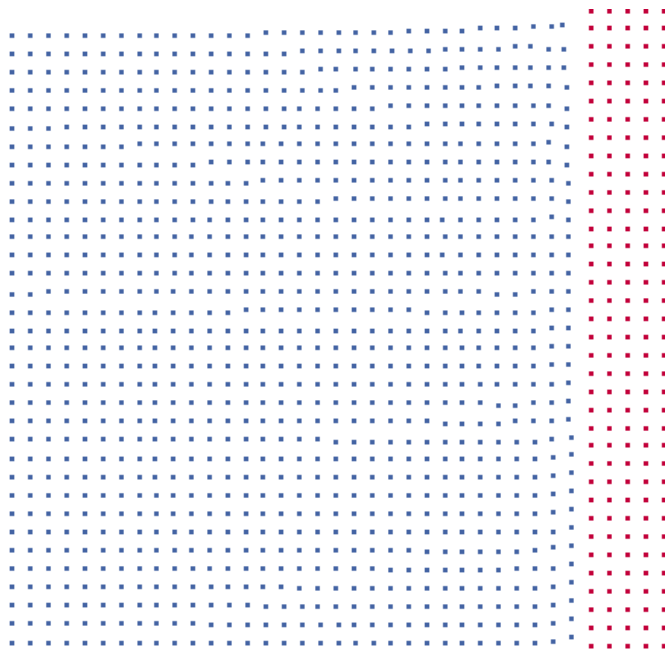


Figure 44: Visual illustration of the gap issue.

The results show that both the issues discussed are relevant to the accuracy of the simulation. A low bulk modulus clearly affects the compressibility and so even before the simulation is run, the initial conditions for a low bulk modulus mean that the fluid is more compressed than it should be. The other figures clearly illustrate how neighbour deficiency affects contact as well.

The next figure compares three fluids. Two have the same bulk modulus and the third one with three magnitudes higher. Using particles of equivalent position, the following figure illustrates the result.

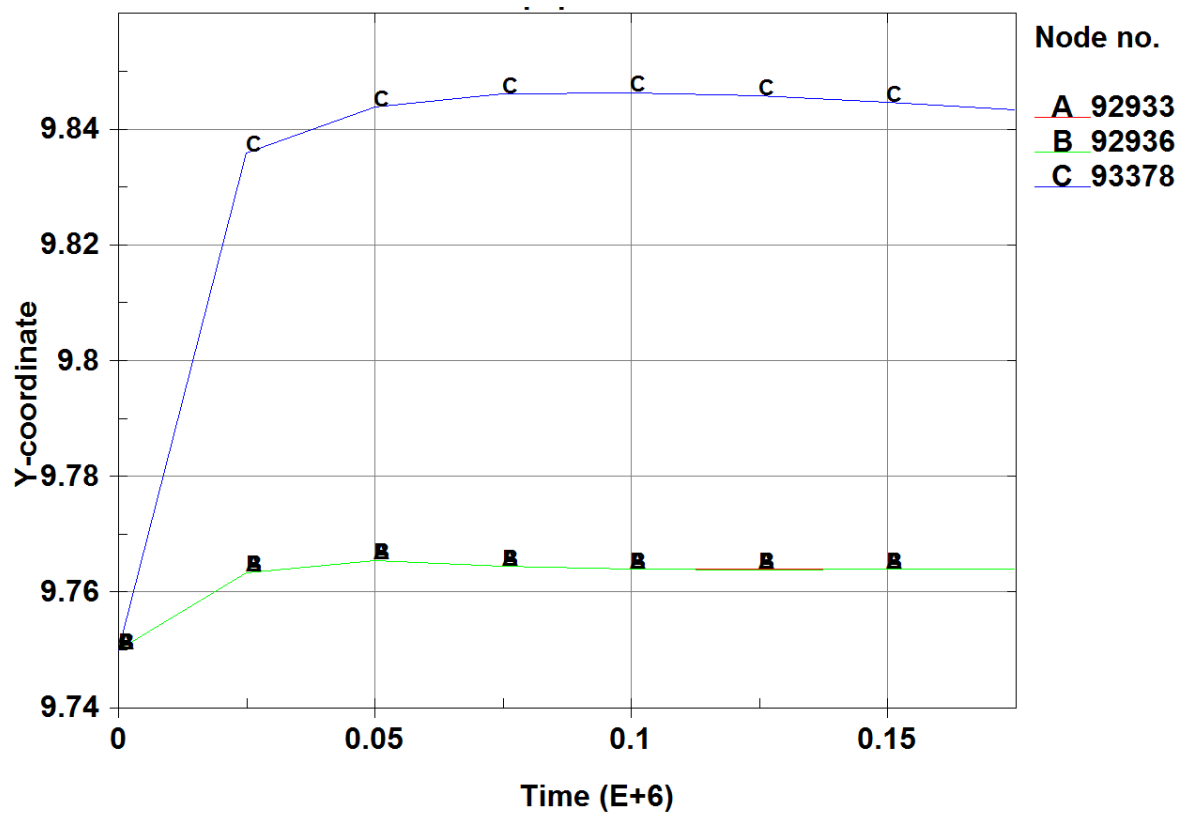


Figure 45: Comparison between three particles under dynamic relaxation. Time is in seconds and y co-ordinate in cm.

Clearly it can be seen that the Bulk Modulus this does have an influence on free surface position. Moving on to investigate the repulsion gap issue further, the contact was lowered to $Q = -02$ for the walls. This gives the following result

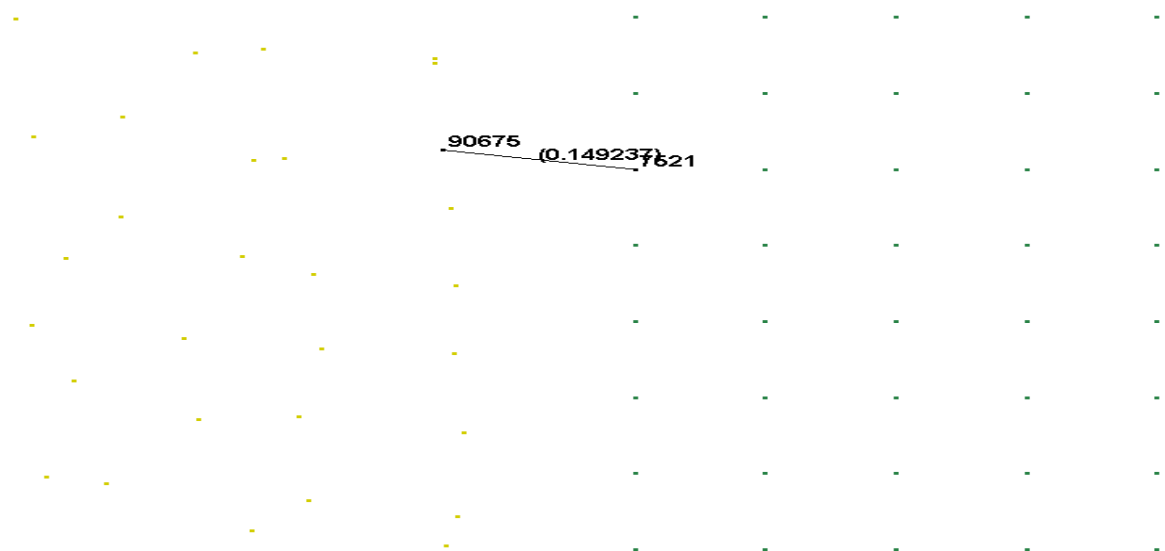


Figure 46: Contact at $Q=-02$ at the wall. The yellow particles are fluid particles, the green more ordered particle are wall particles.

While with $Q=-04$ at the walls, the particles are slightly closer.

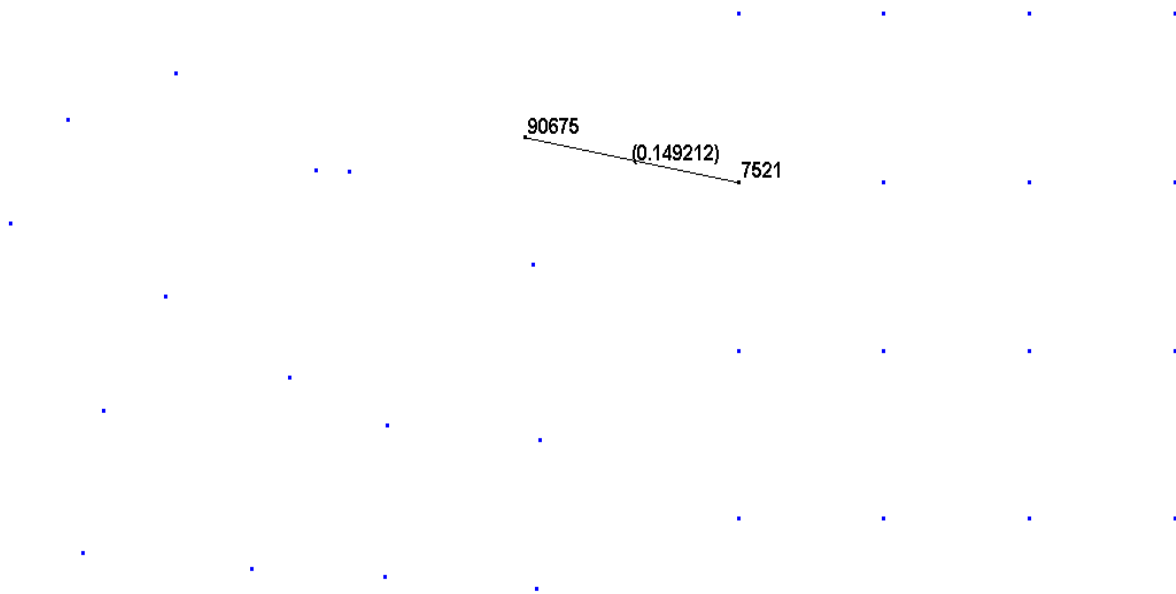


Figure 47 Contact at $Q=-04$ at the wall. The yellow particles are fluid particles, the green more ordered particle are wall particles.

7.2 Modified repulsive contact testing

The results above clearly show that the contact algorithm is affected the closer to the surface the contact is. I believe this is due to contact neighbour deficiency as at the surface, a particle will have fewer contact neighbours than at the bottom of the tank; this will then result in a different value.

In real life, contact does not work like this. When you have a cup of water, the contact between the water and cup is the same at the top as at the bottom (there is no gap between the water and the cup at the top for example)

To get around this, a modification is added which occurs when there are fewer contact neighbours. Initially this was done at the neighbour level, however, it is theorised that the contact gap is due to influence of pressure rather or as well as neighbour deficiency. This is a logical deduction as the contact gap increases as the pressure of the fluid decreases (following $P=\rho gh$ law). The proposed modification is a factor that is a function of pressure so as pressure decreases, the factor increases which corrects the neighbour deficiency of the contact algorithm. The factor is multiplied at the contact algorithm level. Results of a relaxed simulation of the simulation in Figure 40 are shown below.

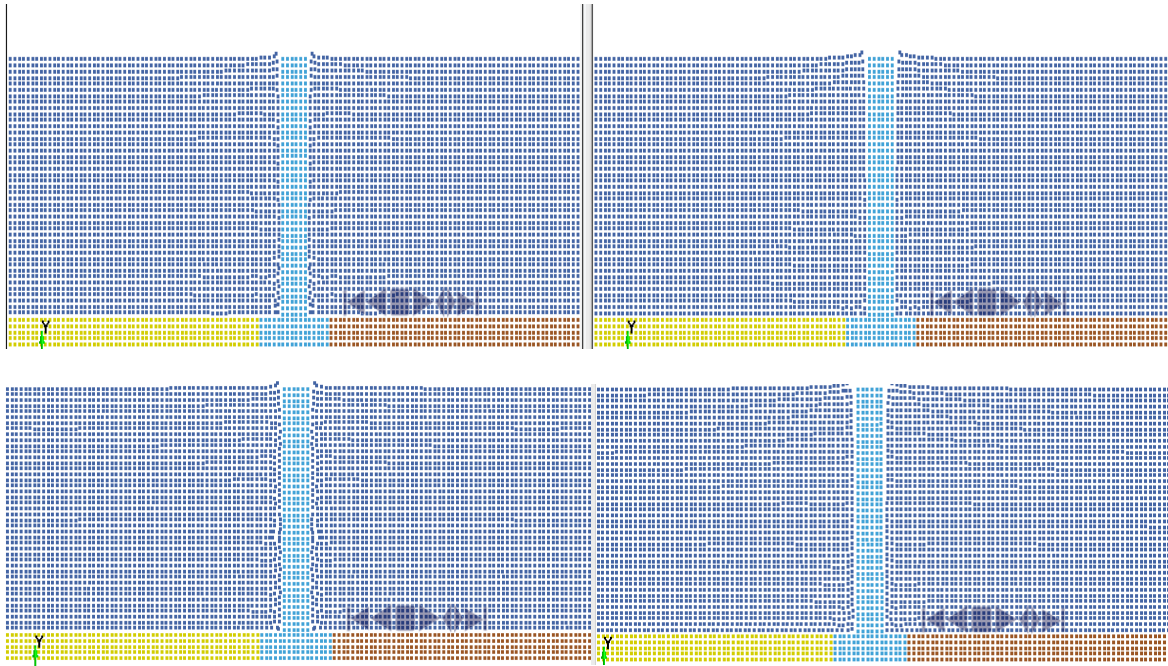


Figure 48: Contact comparison between the artificially modified contact (left) and normal contact (right).

Clearly, it can be seen that the contact is tighter on the left, showing the modification works.

However, when this modified contact is applied to the rotating tank, a huge amount of particle penetration occurs. This implies that the factor is too high, that is when the repulsive force is multiplied by the factor, the repulsion is too weak.

This is likely due to the noise of the pressure, for example pressure early in the rotation looks like this:

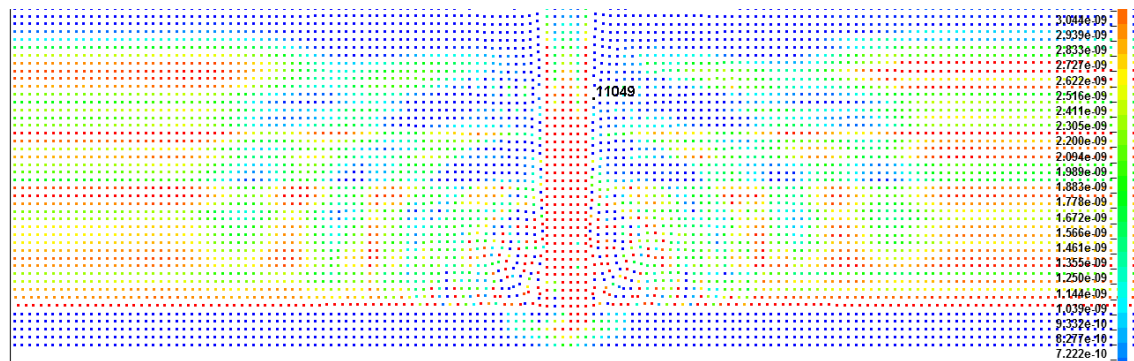


Figure 49: Pressure distribution for the tank in Figure 48 using modified contact just after start of rolling motion.

As this shows, the pressures of the fluid particles by the beam does not follow the $P=pgh$ law. This means at places there will be too much penetration, at others too much repulsion. For example, the pressure at the middle of the tank is lower at the interface than predicted by $P=pgh$, therefore the factor it will be multiplied be will be smaller and hence will output a lower repulsion, leading to penetration. Even with MLS used, there is still noise when rotated.

At this point, the noise and limitations of the pressure factor are accepted and instead use the previous factor that used many neighbours as a factor of repulsion. This has the same effect as the

number of contact neighbours is less at the top than the middle, but also the middle contact neighbours is less than the bottom. This is equivalent to the $P=\rho gh$ law as a number of neighbours also increases with depth.

7.3 Visual comparison of flow profile between MCM testing, experimental results and another numerical solver for deep fluid

The second case is a beam in deep fluid, in this case oil. Due to the viscosity, turbulent effects are negligible and the physics of deepwater apply since:

Criteria for deep water is given as (Falnes 2005)

$$h > \lambda/4 \quad (123)$$

Using the value of the height given in Table 5 for the large case, it can be verified this is a deepwater case.

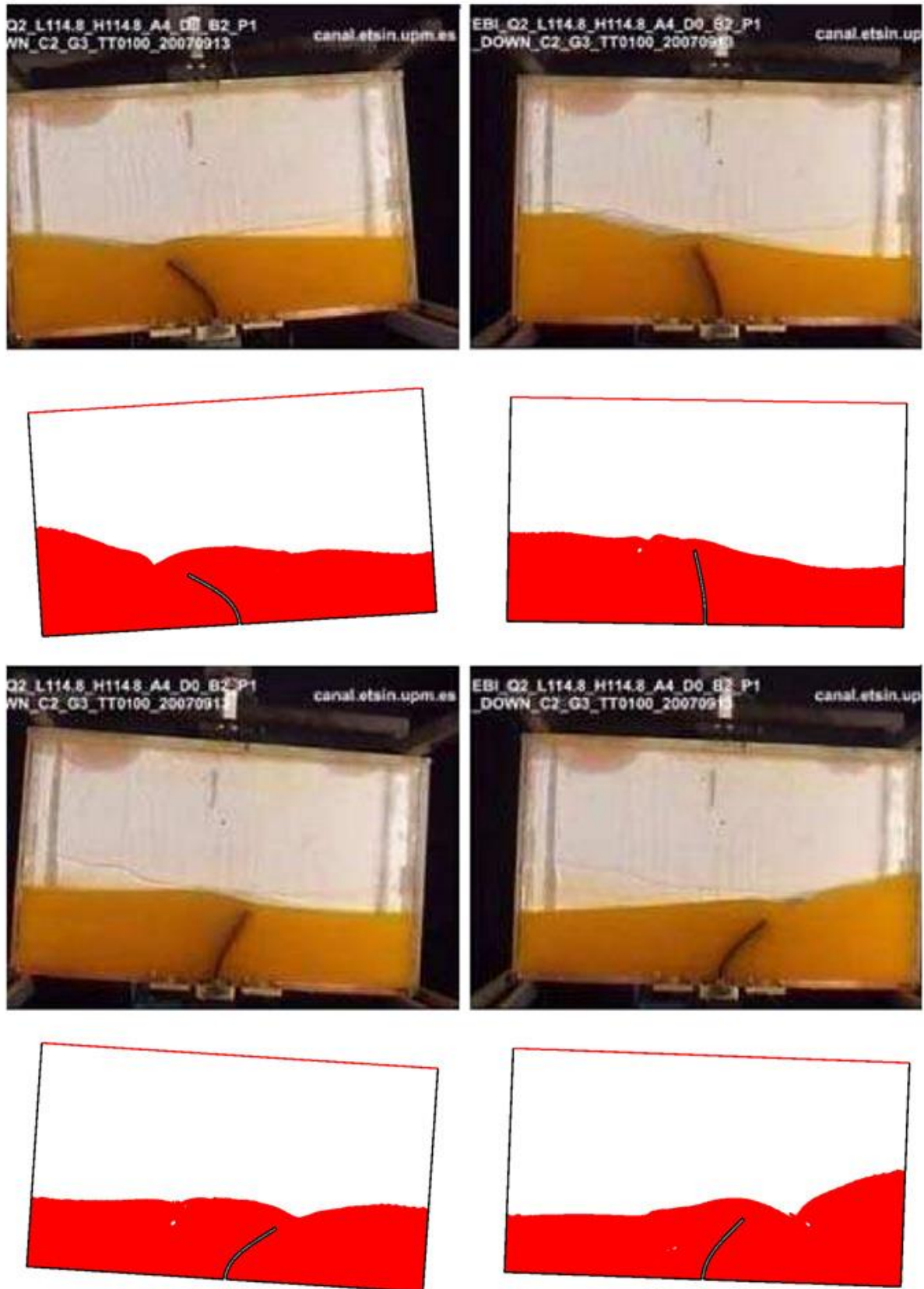


Figure 50: Comparison of deep oil sloshing tank with standing beam in between experiment and numerical results of (Vera et al. 2010; Degroote et al. 2010).with their IQN-ILS algorithm at time 1.84,2.12,2.32,2.56s.

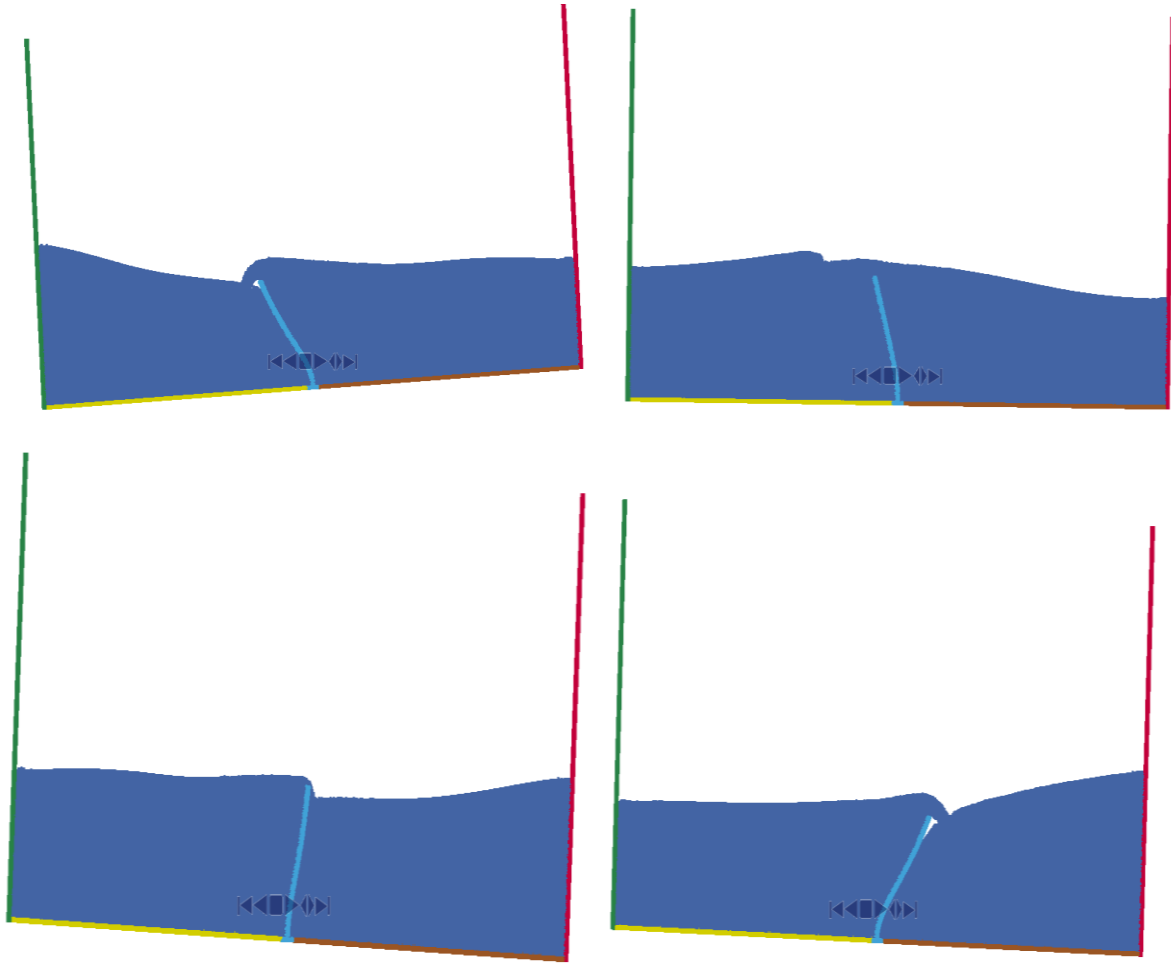


Figure 51: FSI SPH simulation of the same tank with modified contact and Bulk modulus $2.8\text{E}+07$. Other properties are illustrated in Table 5 and Table 6.

Even with the bulk modulus and contact modifications, there are still gaps and in extreme rotation the free surface by the boundary is still not correct in the centre by the beam, which contributes to the gap issue. It can also be seen that the beam behaviour is not quite correct at extreme rotations.

7.4 Beam deflection comparison between MCM testing, experimental results and another numerical solver

The shallow water deflection is given below:

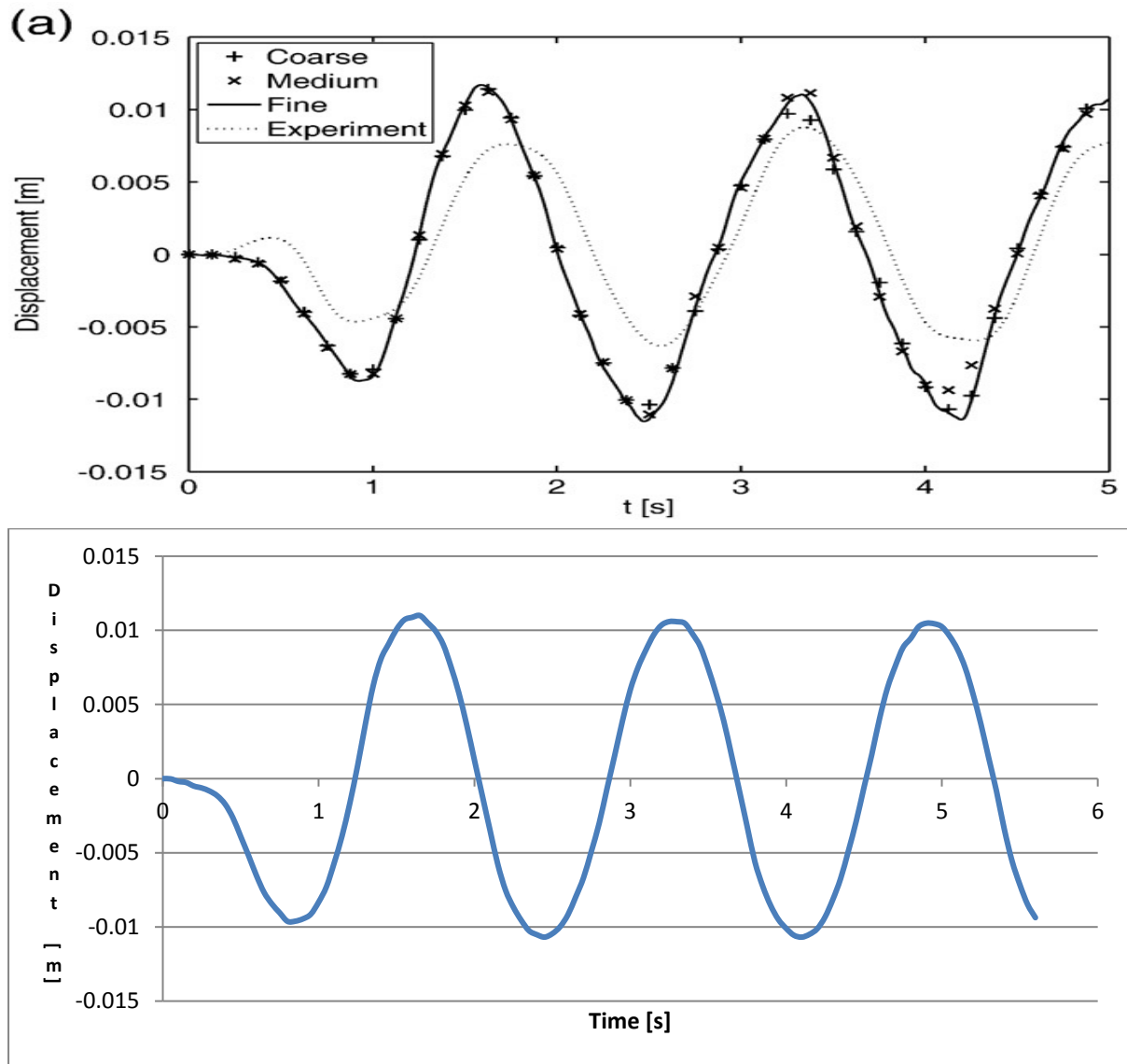


Figure 52 Comparison of beam deflection measured at the tip of the beam, parallel to the bottom of the tank between the experiment (Vera et al. 2010) and numerical results displayed in (Degroote et al. 2010) for the shallow water beam with modified contact.

It can be seen that the beam deflection matches the results in (Degroote et al. 2010) in amplitude and phase. However, this does not quite conform to the experiment.

Looking at the beam deflection for the deepwater case for normal contact $V = -0.5$ and modified repulsion factor contact (VP2Run 0.001), a similar trend of underprediction of beam deflection is observed. The beam deflection is measured at the tip parallel to the bottom of the tank. The x axis is the beam deflection in cm and y axis is time in seconds

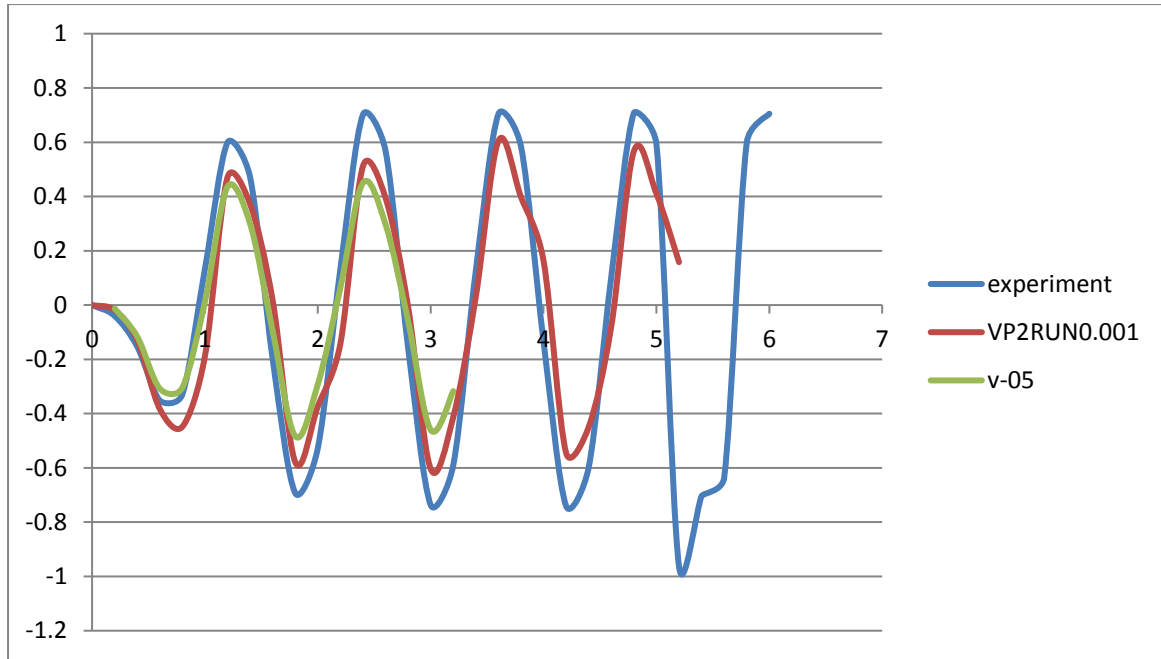


Figure 53: Comparison of beam deflection for the deepwater beam between the experiment (Vera et al. 2010) SPH modified contact and SPH non modified. The beam deflection is measured at the tip parallel to the bottom of the tank. The x axis is the beam deflection in cm and y axis is time in seconds.

Comparison to the amplitude in Figure 52, Figure 51 shows that the beam deflection is over predicted rather than under predicted, corroborating the fact that the gap is responsible for this. This makes sense as if the gap was not present, there would be contact between the fluid and the beam leading to more pressure being applied on the beam and therefore a greater deflection. Furthermore, the over prediction in this case also makes sense, as by immersing the beam, there is a greater force on the beam as it is surrounded by fluid, as opposed to the free-surface behaviour that occurs otherwise.

Figure 53 further strengthens this argument. Running the deepwater case for both non-modified and modified contact shows the modified contact is closer in amplitude to the experiment, this is only a slight improvement, due to the only minor effect this modified contact has on the gap. The modified contact does address some issues but something more robust is needed.

By only simulating repulsion, the correct behaviour between particles is not representative. One of the reasons the gaps occur is because of the lack of 'sticking' or adhesion between the particles. If the particles are just repulsing there will be gaps. The fact that the modification made to correct the neighbour deficiency does improve beam deflection and reduce gaps shows that a more robust representation of the intermolecular force between particles should improve results.

Equation (51) shows the potential based on (De Vuyst 2003) with n equal to four as the best factor to use for the repulsion factor (Monaghan 2000; De Vuyst 2003). This gives a repulsion factor that decreases with increased distance between particles and at smoothing length $2h$ becomes 0. Figure 54 shows the repulsive force profile of equation (51). The x axis shows the radius in cm between 2 particles and the y axis the strength the potential in J

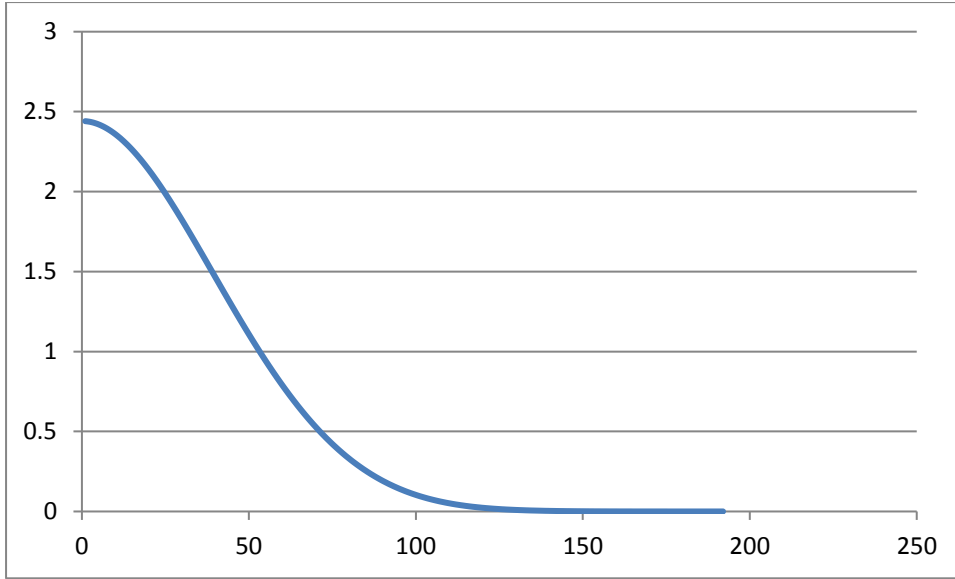


Figure 54: Repulsive force profile as a function of position.

The Leonard Jones force follows the following pattern. Axis and units are the same quantities and values as in Figure 54.

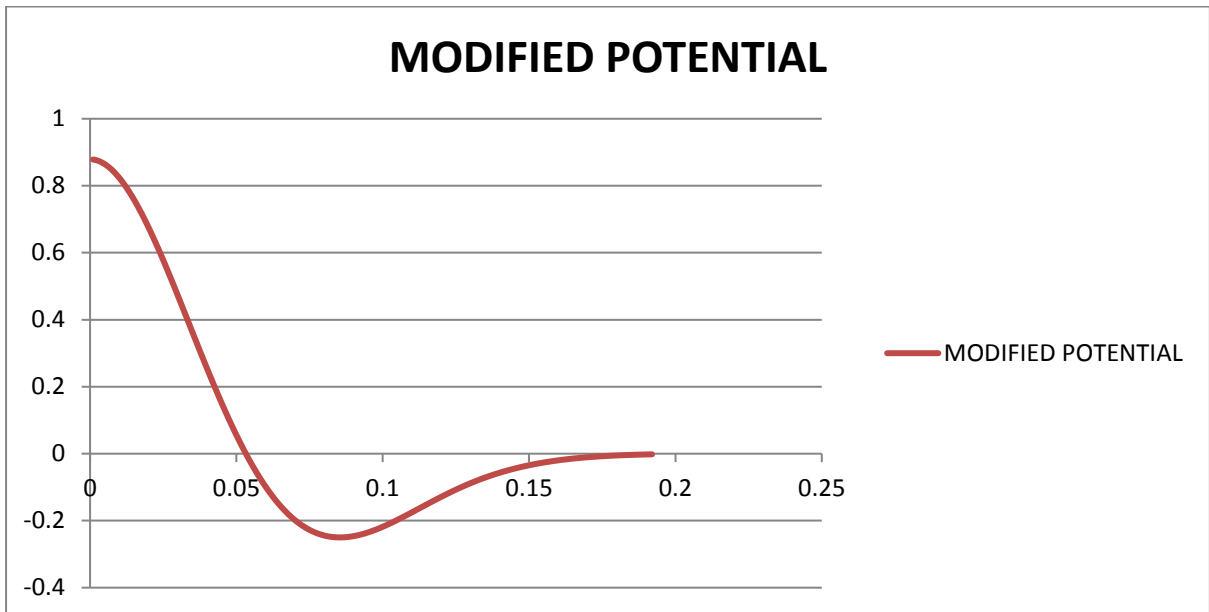


Figure 55: Leonard Jones potential between 2 interacting particles.

An SPH Leonard Jones potential would include the attractive component of a force. Hence in SPH form this would be written as:

$$\varphi = \int_{CBL} K \left(\frac{W(r_{ij})}{W(\Delta p)} \right)^4 - \left(\frac{W(r_{ij})}{W(\Delta p)} \right)^2 \quad (124)$$

With $\left(\frac{W(r_{ij})}{W(\Delta p)}\right)^2$ simulating the attractive component of the force.

This gives the force profile as:

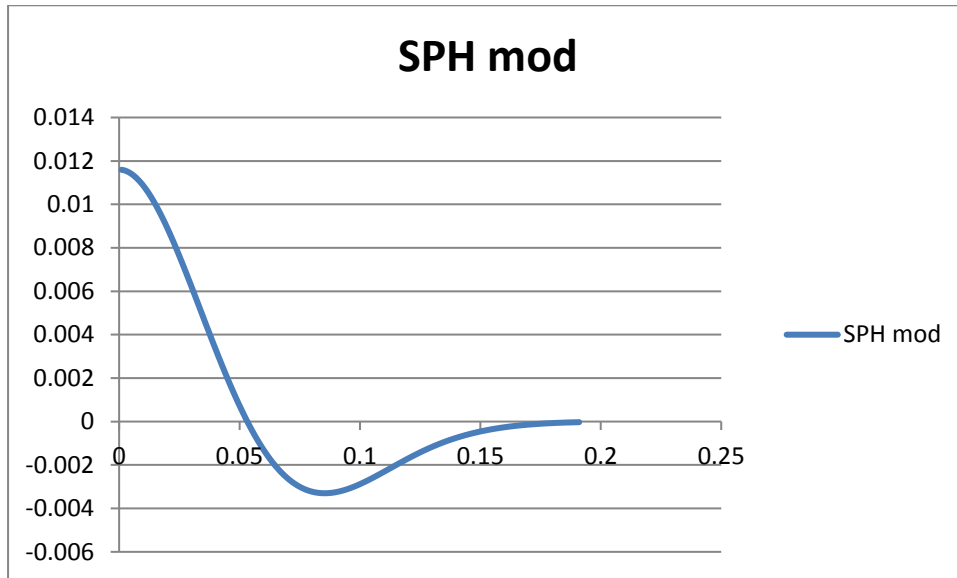


Figure 56: SPH Leonard Jones potential based on equation 124.

7.5 Summary and future work

This work is the most complex FSI simulation using non-coupled code in SPH to date. It is also the first to use a mixed Eulerian and Lagrangian scheme to achieve this. The results shown are similar in profile and beam deflection to published work in this field which is encouraging. It also highlighted that work needs to be done to develop our contact algorithm to consider friction and adhesion for deformable bodies. Future work should focus on this and begin from the development of a more complete contact algorithm that considers attraction. The research does show work in this area but results are limited in scope.

8. Mixed formulation application and implementation to the SPH method

Despite the success of mixed formulation of addressing FE shortcomings as highlighted by the literature overview, there is no evidence that this approach has been used in meshless methods despite the similarity in the derivation of the governing equations. This is a whole new area of research and for that reason has novelty. SPH suffers from many shortcomings as discussed and research in these areas tends to focus on short term fixes such as adding artificial forces which treat the symptom but does not address the underlying cause or provide mathematical rigour. Never has the mixed formulation approach been used to tackle the SPH shortcomings. Therefore, the research in this section is to see if mixed formulation-because of its success in other fields as highlighted in the literature review- could be used to reduce or eliminate particle clumping or at the very least, even if not then one potential avenue of research in this field has been eliminated. In theory, the extra terms that come out of the development of the mixed method compared to the single field finite element method could be the artificial force terms necessary to suppress particle clumping. While the three-field approach could, in theory, decouple stress and strain and therefore eliminate the kernels derivatives influence on the stress-strain relationship leading to the reduction of tensile instability. There is also the potential to use the displacement-pressure approach in dealing with incompressible media. Basically, as the literature shows for FE, there is a whole range of applications mixed formulation can be used for.

As discussed in the introduction, two of the main shortcomings in SPH are zero-energy modes and tensile instability. Zero energy modes are analogous to hourglassing in the finite-element method. The next part will expand on the nature of these issues a bit more.

In the finite element method, if only one central Gaussian point is used to determine the stiffness, hourglass modes can occur. This occurs when there are no forces generated to resist deformation, due to there being no strain energy predicted in the computational model. Therefore, deformation occurs under no strain energy even though the body is not rigid.

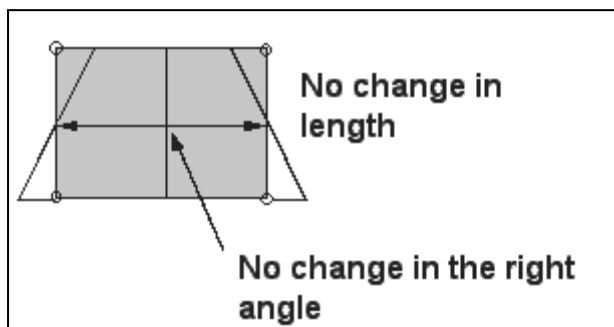


Figure 57: Illustration of the zero-energy issue in the finite element method.

Consider the 4-node quad in Figure 57 in its un-deformed state (the shaded square). When deformation occurs, the node will look more like the triangle superimposed on the square in Figure 57. This deformation has led to the particles at the lower part of the square moving further apart from each other, and on the upper edge closer together by the same amount. What you now have is a deformed element. However, in this example, the Gaussian integration point is in the middle of the element, and was not influenced by the deformation. As Figure 57 shows; there is no vertical or horizontal deformation, therefore you have a deformation which produces no strains. No strains

mean no forces to resist deformation and consequently the node looks like an hour-glass. In the SPH method, this represents itself as particle clumping for the same reason, the lack of resistance to deformation means that the particles will continue to un-physically attract to each other, leading to the clumping phenomenon.

The logical solution to this problem in the finite element method is to simply use more elements. The problem described where only one element is used is called under-integration, so by using more elements, the node is no longer under integrated. However, the consequence of this is that of computational time, this computational issue –in particular- is highlighted in the volumetric locking issue, where for the analysis of near or incompressible materials, stresses are inaccurately predicted, leading to a higher value of stiffness than what is expected and hence ‘locking’ occurs (Bathe 1996). One solution to this is again to use more elements, but this will lead to huge computational expense. Furthermore, adding more elements to the problem does not solve the underlying issue of why this occurs.

In the SPH method, the equivalent zero energy problem comes from the fact that field variables and their derivatives are evaluated at the same point, therefore an alternating field variable will have a zero gradient at the particles. Given a particle at position i , the derivative of this field when approximated with a central difference we would get:

$$\frac{\partial f}{\partial x} = \frac{f(x_{i+1}) - f(x_{i-1}))}{x_{i+1} - x_{i-1}} \quad (125)$$

Which would give:

$$\frac{\partial f}{\partial x} = 0 \quad (126)$$

Therefore, this mode cannot be detected and can grow unhindered until it dominates the solution. This then leads to the aforementioned zero energy mode problem as a zero kernel gradient will give a zero strain energy which like in the finite element equivalent problem, leads to unphysical clumping as there is no forces to resist the strain.

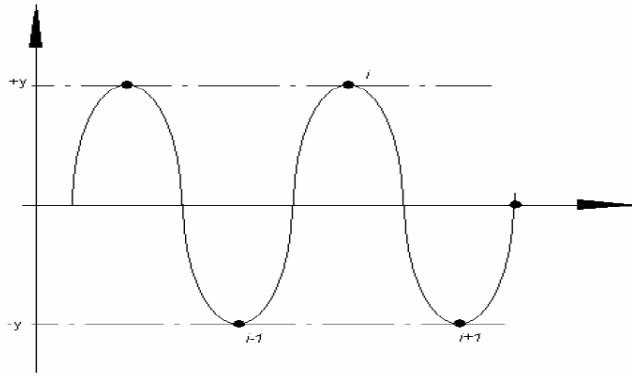


Figure 58: Illustration of the SPH zero energy issue

To solve the zero-energy issue in the finite element method, artificial internal forces are added to compensate for the lack of opposing force to resist deformation. Often this is of a heuristic nature, though research is focused on deriving these internal forces from mathematical proof or redeveloping finite element equations that will output extra terms that represent these forces, thus adding more credibility to the theory as opposed to just adding terms to make it work. One such approach is the mixed element formulation approach and it is this area of research that this chapter shall focus on.

The other issue in SPH which manifests itself the same way as the zero energy modes of particle clumping is tensile instability. While it looks the same as zero-energy modes, the mechanism in which this occurs is very different.

While zero energy modes occurring are due to the lack of resistance to deformation, tensile instability has been shown by¹ to occur because of the relationship between stress and strain in SPH.

As highlighted in the literature overview, Swegle's Von Neumann analysis showed SPH to be unstable in tension. The Von Neumann analysis is a standard test in numerical methods to analyse the stability of a particular method, this is due to the fact it is a test of the stability of the method, which the Lax-Richtmyer theorem tells us that stability and convergence is equivalent and hence for a scheme to converge, it must be stable. The cause of the instability was shown by which was that effective stress was proportional to $-\sigma W'$ in the SPH method. The consequence of this relationship is highlighted in this diagram.

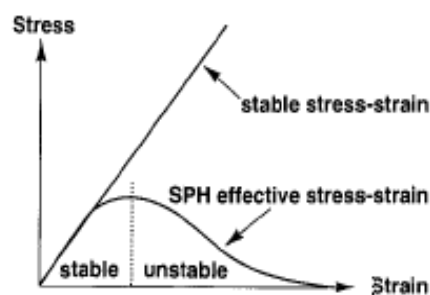


Figure 59: Illustration of tensile instability issue(J.Swegle, D.Hicks, S.Attaway 1995)

The above figure illustrates the tensile instability problem. For a fluid or elastic problem where failure is not expected to occur, stress is proportional to strain. However-as stated in the previous paragraph- in SPH the proportionality relationship is multiplied by the negative kernel derivative. Figure 59 shows the Gaussian kernel, which is bell shaped and tells us that the linear relationship between stress and strain will break down at a certain critical point and mean that stress will *decrease* as strain decreases and will eventually go to zero. Furthermore Figure 59 shows us that the change in relationship between stress and strain is dependent on the smoothing length of the kernel and particle positions as the kernel itself is a function of these parameters.

The smoothing length is a key reason why the problem was called tensile instability. In tension, stress is positive, so when the slope of the kernel gradient is positive, the stress will output as negative, since stress is proportional to the negative of the kernel gradient, which leads to the instability. The minimum value of the kernel derivative is at $2/3h$, anything greater than $2/3h$ is a positive slope, therefore in tension the instability will occur only if the particle spacing is greater than $2/3h$ which in simulations it invariably is. Hence the name tensile instability is a misnomer as this problem can occur in compression, but only if particle spacing is less than $2/3h$, which is generally not the case in SPH simulations.

8.1 Commercial code use of mixed approaches

The introduction highlighted that mixed formulation is a big part of finite element research in dealing with the methods shortcomings. This is reflected in the FE commercial codes. Even without mixed formulation, there are suppression algorithms that can deal with hourglassing by viscous damping of hourglass modes but leaving all other elements alone. The models in LS-Dyna are based (Kosloff & Frazier 1978) and (Wilkins et al. 1975). While in Abaqus, it is dealt with by artificial stiffness and damping procedures (Flanagan & Belytschko 1981), however, it does mention that the procedure breaks down for most non-linear problems (Hallquist 2006). A comparison between Nastran, Abaqus and Ansys by (Sun 2006) showed that both Abaqus and Ansys performed on the same level when trialling the hourglassing approach for a beam and composite beam by reduced integration.

With regards to the mixed formulation, LS-Dyna has an option that uses an assumed transverse shear strain field (Bathe & Dvorkin 1985) in hourglass control of the Belytschko-Lin Tsay Shell.

Moving on to Abaqus, where there are plenty of examples of the development of mixed element formulation in the code to deal with situations such as incompressible materials. For this case, a mixed (hybrid) formulation is required, where the displacement field is augmented with a hydrostatic pressure field. The hydrostatic pressure field plays the role of a Lagrange multiplier field enforcing the incompressibility constraints. This is no more than the 2-field displacement-pressure formulation illustrated in chapter 3 but applied to Lagrangian equations since the procedure is for incompressible solid elements. This volumetric locking issue has been discussed in the literature overview. Furthermore, Abaqus provides the option for a virtual velocity- virtual rate of deformation to develop the equilibrium condition for modelling of a porous medium.

Ansys has the capability of the mixed displacement-pressure formulation (Bhashyam 2002) which again is used in the analysis of incompressible or near incompressible media.

So, by showing this is a viable avenue of research in SPH, it really could be the beginning of a whole host of research and application for this method not just for addressing particle clumping. The focus shall be on the derivation, coding, research and analysis on the various formulations in the SPH method to assess if the mixed formulation approach does provide a solution to any of these problems.

The next sections shall outline the SPH derivation of the mixed formulation method for displacement-pressure formulation and velocity-rate of the deformation-stress formulation.

8.2 SPH derivation of displacement-pressure formulation

The main steps in developing the displacement-pressure formulation into SPH form are as follows:

Invoke stationarity of Hu-Washizu.

Write kernel approximation of dependant variables and then discretise.

Write resulting equations in matrix form.

It is shown in (Wang & Bathe 1997) that the spurious non zero frequencies are in the use of displacement based FE and in mishandling of FSI. They propose u-p (displacement and pressure independently interpolated) formulations with elements that satisfy the inf-sup condition. The spurious pressure modes have no relationship to the spurious zero energy modes, which are a result of using reduced numerical integration in the evaluation of element stiffness matrices. Since displacement and pressure are in phase and using pressure rather than stress or strain will reduce the computational time, it is this formulation that will initially be developed in SPH form

A general u-p formulation equation is given by:

$$\Pi(u, p) = - \int_V \frac{1}{2} \varepsilon' C \varepsilon' dV + \int_V \frac{p^2}{2k} dV - \int_V (u \cdot f^B) dV - \int_V \left[p \left(\nabla \cdot u + \frac{p}{k} \right) \right] dV \quad (127)$$

= 0

Using $u = H\hat{u}$, $\varepsilon' = B_d \hat{u}$, $\varepsilon_v = B_v \hat{u}$, and the additional pressure interpolation assumption $p = H\hat{p}$, we substitute into (127)

$$= - \int_V \frac{1}{2} B_d \hat{u} C B_d \hat{u} dV + \int_V \frac{H\hat{p}H\hat{p}}{2k} dV - \int_V H\hat{u} \cdot f^B dV - \int_V H\hat{p} \left(B_v \hat{u} + \frac{H\hat{p}}{k} \right) dV \quad (128)$$

$$= - \int_V \frac{1}{2} B_a \hat{u} C B_a \hat{u} dV + \int_V \frac{H \hat{p} H \hat{p}}{k} dV - \int_V H u \cdot f^B dV - \int_V H \hat{p} B_v \hat{u} dV \quad (129)$$

Invoking stationarity gives us:

$$= - \int_V B_a \hat{u} C B_a \delta \hat{u} dV + \int_V \frac{H \hat{p} H \delta \hat{p}}{k} dV - \int_V H \delta u \cdot f^B dV - \int_V H \hat{p} B_v \delta \hat{u} dV + \int_V H \delta \hat{p} B_v \hat{u} dV = 0 \quad (130)$$

Where:

$$f^B = -\rho \ddot{u} \quad (131)$$

The above will be written using kernel approximation, in which the value of a function at position x is written in continuous form as:

$$\langle f(x) \rangle = \int f(x') W(x - x', h) d\Omega' \quad (132)$$

Where $W(x - x', h)$ is the kernel function of the spatial position centred at x and a smoothing length h . The change of notation from dV to $d\Omega'$ is a necessary change which will become clear moving forward.

Providing the kernel function has compact support, the above can be written in summation form spanning only the neighbouring particles defined by the smoothing length.

$$\langle f(x) \rangle = \sum_{j=1}^{nnbr} f(x_j) W(x_i - x_j, h) \frac{m_j}{\rho_j} \quad (133)$$

The above could also be written in terms of shape functions:

$$\langle f(x) \rangle = \sum_{j=1}^{nnbr} f(x_j) H_j(x) \quad (134)$$

In which the shape function can be compared to the SPH kernel where (De Vuyst 2003):

$$H_j(x) = W(x_i - x_j, h) \frac{m_j}{\rho_j} \quad (135)$$

$$B_j(x) = \nabla W(x_i - x_j, h) \frac{m_j}{\rho_j} \quad (136)$$

Now writing the following interpolations, where the triangular brackets denote an SPH approximation of the dependant variable at position i . j are the neighbouring particles defined by the smoothing length.

$$\langle u_i \rangle = \sum_{j=1}^{nbr} u_j W(x_i - x_j, h) \frac{m_j}{\rho_j} = H\hat{u} \quad (137)$$

$$\langle p_i \rangle = \sum_{j=1}^{nbr} p_j W(x_i - x_j, h) \frac{m_j}{\rho_j} = H\hat{p} \quad (138)$$

$$\langle \delta u_i \rangle = \sum_{j=1}^{nbr} \delta u_j W(x_i - x_j, h) \frac{m_j}{\rho_j} = H\delta\hat{u} \quad (139)$$

$$\langle \delta p_i \rangle = \sum_{j=1}^{nbr} \delta p_j W(x_i - x_j, h) \frac{m_j}{\rho_j} = H\delta\hat{p} \quad (140)$$

And substituting the SPH interpolations term by term into (130) we get:

$$\begin{aligned} - \int_V B_d \hat{u} C B_d \delta \hat{u} dV &= \left[- \int_V \delta \hat{u} \nabla W(x - x', h) d\Omega C \int_V \hat{u} \nabla W(x - x', h) d\Omega \right] dV \\ &= \int_V \left[\sum_{j=1}^{nbr} u_j \nabla W_{ij} \frac{m_j}{\rho_j} \sum_{k=1}^{nbr} \delta u_k \nabla W_{ik} \frac{m_k}{\rho_k} \right] dV \\ \delta u_k \int_V &\left[\frac{1}{\beta} \sum_{j=1}^{nbr} \sum_{k=1}^{nbr} u_j \nabla W_{ij} \nabla W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] dV \end{aligned} \quad (141)$$

$$\begin{aligned} &\int_V H \delta \hat{p} H \hat{p} dV = \\ \int_V &\left[\frac{1}{\beta} \int_V \delta \hat{p} W(x - x', h) d\Omega \int_V \hat{p} W(x - x', h) d\Omega \right] dV \end{aligned} \quad (142)$$

$$\int_V \left[\frac{1}{\beta} \sum_{j=1}^{nbr} \delta p_j W_{ij} \frac{m_j}{\rho_j} \sum_{k=1}^{nbr} p_k W_{ik} \frac{m_k}{\rho_k} \right] dV =$$

$$\begin{aligned}
& \delta p_j \int_V \left[\frac{1}{\beta} \sum_{j=1}^{nbr} \sum_{k=1}^{nbr} p_k W_{ij} W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] dV \\
& \int_V H \delta \mathbf{u} \cdot \mathbf{f}^B dV = \\
& \int_V \left[\int_V \delta \hat{\mathbf{u}} W(\mathbf{x} - \mathbf{x}', h) d\Omega \int_V \hat{\mathbf{p}} W(\mathbf{x} - \mathbf{x}', h) d\Omega \ddot{\mathbf{u}} \right] dV = \\
& \int_V \left[\sum_{j=1}^{nbr} \delta u_j W_{ij} \frac{m_j}{\rho_j} \cdot \sum_{k=1}^{nbr} \rho_k W_{ik} \ddot{u}_i \frac{m_k}{\rho_k} \right] dV = \\
& \delta u_j \int_V \left[\sum_{j=1}^{nbr} \sum_{k=1}^{nbr} W_{ij} W_{ik} \frac{m_j m_k}{\rho_j} \ddot{u}_i \right] dV \\
& \int_V H p B \delta \mathbf{u} dV = \\
& \int_V \left[\int_V \hat{\mathbf{p}} W(\mathbf{x} - \mathbf{x}', h) d\Omega \int_V \widehat{\delta \mathbf{u}} \nabla W(\mathbf{x} - \mathbf{x}', h) d\Omega \right] dV =
\end{aligned} \tag{143}$$

$$\begin{aligned}
& \int_V \left[\sum_{j=1}^{nbr} p_k W_{ij} \frac{m_j}{\rho_j} \sum_{k=1}^{nbr} \delta u_k \nabla W_{ik} \frac{m_k}{\rho_k} \right] dV = \\
& \delta u_k \int_V \left[\sum_{j=1}^{nbr} \sum_{k=1}^{nbr} p_k W_{ij} \nabla W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] dV
\end{aligned} \tag{144}$$

$$\begin{aligned}
& \int_V H \delta \hat{\mathbf{p}} B_v \hat{\mathbf{u}} dV = \int \left[\int_V \delta \hat{\mathbf{p}} W(\mathbf{x} - \mathbf{x}', h) d\Omega \int_V \hat{\mathbf{u}} \cdot \nabla W(\mathbf{x} - \mathbf{x}', h) d\Omega \right] dV \\
& \int_V \left[\sum_{j=1}^{nbr} \delta p_j W_{ij} \frac{m_j}{\rho_j} \sum_{k=1}^{nbr} \mathbf{u}_k \cdot \nabla W_{ik} \frac{m_k}{\rho_k} \right] dV \\
& \delta p_j \int_V \left[\sum_{j=1}^{nbr} \sum_{k=1}^{nbr} \mathbf{u}_k W_{ij} \nabla W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] dV
\end{aligned} \tag{145}$$

The next section puts equations (140)-(145) into a more compact matrix form.

Writing the resulting equations in matrix form we get:

$$\begin{bmatrix} \mathbf{M} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{U}} \\ \hat{\mathbf{P}} \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{up} \\ \mathbf{K}_{pu} & \mathbf{K}_{pp} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{U}} \\ \hat{\mathbf{P}} \end{bmatrix} = \begin{bmatrix} \mathbf{R} \\ \mathbf{0} \end{bmatrix} \tag{146}$$

The volume integrals can be written as a summation over the entire volume. The equivalent FE and SPH forms in the above are:

	SPH	FE
$\mathbf{M}$	$\sum_{i=1}^{np} \left[\sum_{j=1}^{nnbr} \sum_{k=1}^{nnbr} W_{ij} W_{ik} \frac{m_j m_k}{\rho_j} \right] \frac{m_i}{\rho_i}$	$\int_V \rho H^T H dV$
$\mathbf{K}_{uu}$	$\sum_{i=1}^{np} \left[\sum_{j=1}^{nnbr} \sum_{k=1}^{nnbr} W_{ij} \nabla W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] \frac{m_i}{\rho_i}$	$\int_V (B_d^t C B_d) dV$
$\mathbf{K}_{up}$	$\sum_{i=1}^{np} \left[\sum_{j=1}^{nnbr} \sum_{k=1}^{nnbr} W_{ij} \nabla W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] \frac{m_i}{\rho_i}$	$-\int_V B^T H_p dV$
$\mathbf{K}_{pu}$	$\sum_{i=1}^{np} \left[\sum_{j=1}^{nnbr} \sum_{k=1}^{nnbr} W_{ij} \nabla W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] \frac{m_i}{\rho_i}$	$-\left(\int_V B^T H_p dV \right)^T$
$\mathbf{K}_{pp}$	$\sum_{i=1}^{np} \left[\frac{1}{\beta} \sum_{j=1}^{nnbr} \sum_{k=1}^{nnbr} W_{ij} W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] \frac{m_i}{\rho_i}$	$-\int_V \frac{1}{\beta} H_p^T H_p dV$

Now as there are two equations with two unknowns, the system can be solved by variable elimination.

The solution procedure is as follows:

Solve for p using

$\mathbf{K}_{pu}\mathbf{u} + \mathbf{K}_{pp}\mathbf{P} = 0 \rightarrow \hat{\mathbf{P}} = \mathbf{K}_{pp}^{-1}(\mathbf{K}_{pu}\hat{\mathbf{u}})$. The substitute into $\mathbf{M}\hat{\mathbf{U}} + \mathbf{K}_{uu}\mathbf{u} + \mathbf{K}_{up}\hat{\mathbf{P}}$ to give a corrected acceleration. This corrected acceleration would in theory contain extra terms that may penalise the error prevalent in the SPH acceleration equation. However, this process is dependent on $\mathbf{K}_{pp}$ being invertible.

However, $\mathbf{K}_{pp}$ is not invertible. Take a four particle problem, where all particles are neighbours of each other. For a given particle $i = 1$, with four neighbours. $\mathbf{K}_{pp}$ would look like this:

$$\int_V \frac{1}{\beta} \begin{bmatrix} \sum H_1^1 \sum H_1^1 & \sum H_1^1 \sum H_2^1 & \sum H_1^1 \sum H_3^1 & \sum H_1^1 \sum H_4^1 \\ \sum H_2^1 \sum H_1^1 & \sum H_2^1 \sum H_2^1 & \sum H_2^1 \sum H_3^1 & \sum H_2^1 \sum H_4^1 \\ \sum H_3^1 \sum H_1^1 & \sum H_3^1 \sum H_2^1 & \sum H_3^1 \sum H_3^1 & \sum H_3^1 \sum H_4^1 \\ \sum H_4^1 \sum H_1^1 & \sum H_4^1 \sum H_2^1 & \sum H_4^1 \sum H_3^1 & \sum H_4^1 \sum H_4^1 \end{bmatrix} dV \quad (147)$$

Where $H_j^i = W(x_i - x_j, h) \frac{m_j}{\rho_j}$

Equation (147) does not have inverse due to the linear dependence of the rows and columns. That is, each row is a linear combination of the first row. Hence the matrix does not have an inverse.

Even though the matrix does not have an inverse, this in isolation would not be the problem as you could approximate an inverse by a pseudo-inverse. Or, as using shape functions, find a way to orthogonalise them. That way, the product of different element shape functions would always be 0, hence giving us a diagonal matrix. It is for this reason why this issue does not occur in the finite element implementation of this as the shape functions have the property of strict interpolants. The pros to using the orthogonalisation approach compared to a pseudo-inverse as not only would accuracy be not affected, it would also solve the second problem of inverting a matrix; the computational time.

There are different ways to achieve the orthogonal criteria. One way is to use different shape functions that are naturally orthogonal in the first place. Another way is to apply an orthogonalisation procedure to the existing SPH shape functions. However, this highlights a potential negative to this approach in the sense that by orthogonalising the shape functions, the nature of the SPH approach is changing and this could have unforeseen side effects. Furthermore, if different results are yielded using the mixed formulation approach with the orthogonalised shape functions, it would be difficult to prove that the result is solely down to the mixed formulation. Changing the nature of the shape functions is worthy of its own separate area of research and is beyond the scope of this work.

The most desirable way to solve this inverse issue is to use the Brezzi correction. This is an extra term dependant on the second derivative and is used to stabilise the matrices in the finite element version of the mixed element. This is used in incompressible materials where the KPP term is 0 and hence the matrix of equations is not symmetric. This is useful in our problem as the parameter can be refined to only apply to the diagonal terms and give only a slight 'shift' from the original non-invertible matrix. In essence, a user would have more control over the correction than the SVD approach and it will be less computationally expensive. The correction is given by:

$$\tau \nabla^2 p, \text{ where } \tau = \frac{\alpha(h)^2}{2\mu} \quad (148)$$

α is a dimensionless parameter needing to be calibrated, h is the element spacing and μ the shear modulus of a material. This term is added to the pressure-volumetric strain relationship terms and has the following effect on matrix $\mathbf{K}_{pp}$

$$\mathbf{K}_{pp} = - \int_V \frac{1}{\beta} H_p^T H_p dV + \int_V \frac{1}{\beta} \nabla H_p^T \tau \nabla H_p dV \quad (149)$$

However, in this form, this would have no effect on the inverse problem. All it would do is shift K_{pp} . The underlying row dependence problem would not be solved unless it was diagonalised. This is done by adding a Kronecker delta term to the correction, thus ensuring that the correction would only apply to the diagonal terms, thus making it invertible. The task is to find the right balance between applying this correction to solve the inverse problem, and not shifting the matrix too far from the correct non-shifted value of pressure.

The approach used so far has assumed that it is reasonable to just eliminate the pressure unknowns from the system of equations. This is known as static condensation and is used to eliminate pressure degrees of freedom. In the finite element method, this can only be done if the pressure variables apply only to the specific element being considered and none other. This would not be the case in SPH as in the equivalent situation; particles will share the same neighbours. From what I tell, there are two reasons why static condensation can only be used in this instance. The first is inter element continuity, in that continuity of pressure would not be enforced if the pressure variables are condensed out. The second is that there will be no unique solution for pressure variables if they are used within different elements. For example, how could we have a unique value for say pressure node two if it for one element, it is dependent on nodes one,three and four, for another five and six? In the SPH method, the first reason is irrelevant as the theory is meshless so continuity between elements is not required. The second reason gives cause for concern.

8.3 Code application of U-P formulation

For a general displacement-pressure mixed element scheme, the equations to be solved look like:

$$\begin{bmatrix} \mathbf{M} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{u}} \\ \hat{\mathbf{p}} \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{up} \\ \mathbf{K}_{pu} & \mathbf{K}_{pp} \end{bmatrix} \begin{bmatrix} \hat{\mathbf{u}} \\ \hat{\mathbf{p}} \end{bmatrix} = \mathbf{0} \quad (150)$$

Which gives us:

$$\begin{aligned} \mathbf{M}\hat{\mathbf{u}} + \mathbf{K}_{uu}\hat{\mathbf{u}} + \mathbf{K}_{up}\hat{\mathbf{p}} &= \mathbf{0} \\ \mathbf{K}_{pu}\hat{\mathbf{u}} + \mathbf{K}_{pp}\hat{\mathbf{p}} &= \mathbf{0} \end{aligned} \quad (151)$$

With the familiar notation given below:

$\mathbf{M}$	$\int_V \rho \mathbf{H}^T \mathbf{H} dV$
$\mathbf{K}_{uu}$	$\int_V (\mathbf{B}_d^T \mathbf{C} \mathbf{B}_d) dV$
$\mathbf{K}_{up}$	$-\int_V \mathbf{B}_v^T \mathbf{H}_p dV$

K_{pp}	$-\int_V \frac{1}{k} H_p^T H_p dV$
----------	------------------------------------

Dimensionally, the problem looks like this:

$\mathbf{H}$ has dimensions $2 \times 2NP$, hence $\mathbf{M}$ has dimensions $2NP \times 2NP$

B_V has dimensions $1 \times 2NP = 1 \times 16$ and H_p has dimensions $1 \times NP$ as it is a scalar, hence

K_{up} has dimensions $2NP \times NP$ and consequently the transpose of

K_{up} has dimensions $NP \times 2NP$

K_{pp} has dimensions $NP \times NP$

With NP being the number of particles.

For the pure displacement approach, the governing equation is given by:

$$\mathbf{M}\hat{\mathbf{u}} + \mathbf{K}\hat{\mathbf{u}} = 0 \quad (152)$$

The MCM time integration loop designed to solve this equation is based upon a pure displacement approach, therefore in order to make it applicable for mixed problems, a solution loop needs to be developed that will not only obtain solutions for problems using a displacement pressure formulation, have generality, BUT will be computationally efficient. This efficiency is vital, given that the mixed equations contain more terms and requires inversion of matrices at every timestep.

In order to do this, a MCM mixed displacement-pressure formulation loop will be developed that utilises what has already been done for the pure-displacement MCM code, but just with the extra terms that comes as a consequence of the mixed derivation.

Side by side the pure displacement and the mixed displacement pressure formulation look like this (assuming elimination of pressure)

$$Pure = \int_V \rho H^T H dV \hat{\mathbf{u}} + \int_V (B^t C B) dV \hat{\mathbf{u}} \quad (153)$$

$$Mixed = \int_V \rho H^T H dV \hat{\mathbf{u}} + \int_V (B_d^t C B_d) dV \left(- \int_V \frac{1}{k} H_p^T H_p dV \right)^{-1} \int_V B_V^T H_p dV \hat{\mathbf{u}} \quad (154)$$

With $B = B_d + B_V$

From this, it can be seen that a lot of the terms calculated in the pure displacement scheme will be calculated in the mixed scheme as well, therefore the mixed solution loop can use what has been done in the pure displacement loop. Details of the loops are in appendix 1.

8.4 Investigation into uses of other EOS

Displacement (or velocity) –pressure formulation is used to cure volumetric locking and better represent incompressible behaviour in materials. Volumetric locking is a problem not relevant in SPH but incompressibility is. It is proposed that this scheme is used for incompressible or near-incompressible problems. However, it should be noted that if the material is totally incompressible, K_{pp} will be equal to 0, which will need to be considered in the solution procedure.

In addition, so far the scheme is only applicable to materials with a linear relationship between pressure and volumetric strain, such as fluids using polynomial equation of state or elastic materials.

For example:

The polynomial equation of state used to relate volume to pressure is given as:

$$P = c1mu, \text{ where } mu = \frac{\rho}{\rho_0} - 1 \quad (155)$$

Note that the polynomial eos normally has more terms, but the coefficients other than c1 are all 0.

The constitutive relation used for the derivation of the u-p formulation for fluids, of which my derivation is based on, relates divergence of displace to pressure. This is given as:

$$\nabla \cdot u = \frac{P}{\beta} \quad (156)$$

We can relate the two equations of state by the following:

$$\frac{\rho}{\rho_0} = (1 - \nabla \cdot v)dt \quad (157)$$

Hence P can be written as:

$$P = c1\left(\frac{\rho}{\rho_0} - 1\right) \rightarrow c1((1 - \nabla \cdot v)dt - 1) \quad (158)$$

As velocity is simply the time derivative of displacement, the dts cancel out and we are left with:

$$P = c_1 \nabla \cdot u \quad (159)$$

Hence the only difference between the two is that $c_1 = \beta$

However, when using the Murnaghan equations of state, problems are encountered as pressure is related to density change as:

$$P = \beta \left(\left(\frac{\rho}{\rho_0} \right)^\alpha - 1 \right) \quad (160)$$

Substituting

$$\frac{\rho}{\rho_0} = (1 - (\nabla \cdot v) dt) \quad (161)$$

Into the Murnaghan equation gives:

$$P = \beta \left((1 - \nabla \cdot u)^\alpha - 1 \right) \quad (162)$$

Which would give a α polynomial to solve.

It is clear from this that mixed element can only be used for interpolation of variables that have a linear relationship.

8.5: Different mixed approaches

This section outlines the procedure in finding the Lagrange multiplier and developing the SPH equations for other mixed approaches. This is done to show uniformity of the method and to research different possibilities and uses for two or three field approaches. Certainly, in all the literature as discussed at the beginning of the chapter, there are many examples of application of multi-field approaches.

8.5.1 Virtual velocity formulation

Virtual power subjected to an infinitesimal variation is given by (Belytschko et al. 2014).

$$\delta P = \delta P^{int} - \delta P^{ext} + \delta P^{kin} = 0 \quad (163)$$

Where:

$$\delta P^{int} = \int_V \delta D_{ij} \sigma_{ij} dV \quad (164)$$

$$\delta P^{ext} = \int_V \delta v_i \rho b_i dV + \int_{\Gamma_t} \delta v_j t_j d\Gamma \quad (165)$$

$$\delta P^{kin} = \int_V \delta v_i \rho \dot{v}_i dV \quad (166)$$

In the Lagrange multiplier method, a functional say $F(u,v)$ is minimised subject to a given constraint $G(u,v) = k$. The constraint should be a function of those variables. In the principle of virtual power, P is a function of v . As a multifield principle, another variable as well as the lagrange multiplier needs to be determined as the variable that will be independently calculated of V . This choice is the strain rate (rate of deformation). This choice has been corroborated in textbooks (Bathe 1996; Belytschko et al. 2014) that illustrate this approach.

Hence the constraint is:

$$\lambda_{ij} (D_{ij} - v_{i,j}) \quad (167)$$

And the H-W principle in virtual power form is given as:

$$\pi = P^{int} - P^{ext} + P^{kin} - \lambda_{ij} (D_{ij} - v_{i,j}) \quad (168)$$

This is dimensionally correct and the fact that the 2 choices, D_{ij} and $v_{i,j}$ are independent means that they will be calculated differently, hence this constraint will illustrate the 'error' between the two methods of calculation and it is that error which will penalise the result. As the Lagrange multiplier is unknown, the aim is to find the solution of the Lagrange multiplier to determine the magnitude of this correction.

Applying variations to:

$$\begin{aligned} \delta\pi(v_i, D_{ij}, \lambda_{ij}) = & \int_V \delta D_{ij} \sigma_{ij} dV - \left(\int_V \delta v_i \rho b_i dV + \int_{\Gamma_t} \delta v_j t_j d\Gamma \right) + \int_V \delta v_i \rho \dot{v}_i dV \\ & - \int_V \delta \lambda_{ij} (D_{ij} - v_{i,j}) dV - \int_V \lambda_{ij} (\delta D_{ij} - \delta v_{i,j}) dV = 0 \end{aligned} \quad (169)$$

Taking the term $-\int_V -\delta v_{i,j} \lambda_{ij} dV = \int_V \delta v_{i,j} \lambda_{ij}$ and using the product rule we get:

$$\int_V \delta v_{i,j} \lambda_{ij} dv = \int_V \left[(\delta v_i \lambda_{ij})_{,j} - \delta v_i \lambda_{ij,j} \right] dV \quad (170)$$

For the $(\delta v_i \lambda_{ij})_{,j}$ applying gauss' theorem for Tensors and assuming $\Gamma = \Gamma_t \cup \Gamma_{t0} \cup \Gamma_v$ we get:

$$\int_V \left[(\delta v_i \lambda_{ij})_{,j} \right] dv = \int_{\Gamma_t} \delta v_i \lambda_{ij} n_j dS + \int_{\Gamma_{t0}} \delta v_i \lambda_{ij} n_j dS \quad (171)$$

Note that due to homogeneous boundary condition, $\delta v_i = 0$ on Γ_v , hence why the Γ_v is not considered. To illustrate further, any variations must satisfy the geometric boundary conditions, hence $v = \bar{v}$ and $\delta v_i = 0$. Substitute back in (169) gives:

$$\int_V \delta v_{i,j} \lambda_{ij} dv = \int_{\Gamma_t} \delta v_i \lambda_{ij} n_j d\Gamma + \int_{\Gamma_{t0}} \delta v_i \lambda_{ij} n_j d\Gamma - \int_V \delta v_i \lambda_{ij,j} dV \quad (172)$$

And

$$\begin{aligned} \int_V \delta \lambda_{ij} (D_{ij} - v_{i,j}) dV - \int_V \lambda_{ij} (\delta D_{ij} - \delta v_{i,j}) dV = & \int_V \delta \lambda_{ij} (D_{ij} - v_{i,j}) dV \\ & + \int_{\Gamma_t} \delta v_i \lambda_{ij} n_j d\Gamma + \int_{\Gamma_{t0}} \delta v_i \lambda_{ij} n_j d\Gamma - \int_V \delta v_i \lambda_{ij,j} dV + \int_V \lambda_{ij} (\delta D_{ij}) \end{aligned} \quad (173)$$

And back into (169) gives:

$$\begin{aligned}
& \int_V \delta D_{ij} \sigma_{ij} dV + \int_V \delta \lambda_{ij} (D_{ij} - v_{i,j}) dV \\
& + \int_{\Gamma_t} \delta v_i \lambda_{ij} n_j d\Gamma + \int_{\Gamma_{t0}} \delta v_i \lambda_{ij} n_j d\Gamma - \int_V \delta v_i \lambda_{ij,j} dV \\
& - \int_V \lambda_{ij} (\delta D_{ij}) - \int_V \delta v_i \rho b_i dV + \int_{\Gamma_t} \delta v_j t_j d\Gamma + \int_V \delta v_i \rho \dot{v}_i dV
\end{aligned} \tag{174}$$

Due to the fact that δv_i , δD_{ij} , $\delta \lambda_{ij}$ are arbitrary we get:

$$\delta v_i: -\lambda_{ij,j} - \rho b_i + \rho \dot{v}_i = 0 \text{ in } V \tag{175}$$

$$\delta \lambda_{ij}: v_{i,j} - D_{ij} = 0 \text{ in } V \tag{176}$$

$$\delta D_{ij}: \sigma_{ij} - \lambda_{ij} = 0 \text{ in } V \tag{177}$$

$$\delta v_i: \lambda_{ij} n_j - t_j = 0 \text{ on } St \tag{178}$$

$$\lambda_{ij} n_j = 0 \text{ on } t\Gamma_0 \tag{179}$$

s

Hence $\lambda_{ij} = \sigma_{ij}$ and plugging in (175) gives us:

The momentum equation:

$$\frac{\partial \sigma_{ij}}{\partial x_j} + \rho b_i = \rho \dot{v}_i \tag{180}$$

Strain measure:

$$\text{sym}v_{i,j} = D_{ij} \quad (181)$$

Note that equation (181) is assumed symmetric as the strain rate tensor is described by the symmetric part of the velocity gradient.

Traction BC:

$$\sigma_{ij}n_j = t_j \quad (182)$$

Interior BC:

$$\sigma_{ij}n_j = 0 \quad (183)$$

8.5.2 Conversion to SPH

$$\begin{aligned} \pi(v_i, D_{ij}, \lambda_{ij}) = & \int_V \delta D_{ij} \sigma_{ij} dV - \int_V \delta v_i \rho b_i dV + \int_{\Gamma_t} \delta v_j t_j d\Gamma + \int_V \delta v_i \rho \dot{v}_i dV \\ & - \int_V \delta \lambda_{ij} (D_{ij} - v_{i,j}) dV - \int_V \lambda_{ij} (\delta D_{ij} - \delta v_{i,j}) dV = 0 \end{aligned} \quad (184)$$

Hu-Washizu three field principle is given by:

$$\Pi_{HW} = \Pi - \int_V \tau^T (\epsilon - \partial_\epsilon u) dV - \int_{\Gamma_u} f^{\Gamma_u T} (u^{\Gamma_u} - u_p) d\Gamma \quad (185)$$

$$\Pi(u) = \frac{1}{2} \int_V \epsilon^T C \epsilon dV - \int_V u^T f^B dV - \int_{\Gamma_f} u^{\Gamma_f T} f^{\Gamma_f} d\Gamma \quad (186)$$

The same steps can be followed as before.

Ignore boundary terms and invoke stationarity, take variations with respect to strain, stress and displacement, ignoring surface terms and assuming no body force.

$$\int_V \delta \epsilon^T (C \epsilon - \tau) dV - \int_V \delta \tau^T (\epsilon - \partial_\epsilon u) dV + \int_V (\partial_\epsilon \delta u)^T \tau dV - \int_V \delta u^T f^B dV = 0 \quad (187)$$

Write kernel approximation of dependant variables and then discretise.

$$\begin{aligned} & \int_V \delta \epsilon^T (C \epsilon - \tau) dV = \\ & \int_V \sum_{j=1}^{nnbr} \delta \hat{\epsilon}_j W_{ij} \frac{m_j}{\rho_j} C \sum_{k=1}^{nnbr} \hat{\epsilon}_k W_{ik} \frac{m_k}{\rho_k} - \sum_{j=1}^{nnbr} \delta \hat{\epsilon}_j W_{ij} \frac{m_j}{\rho_j} \sum_{k=1}^{nnbr} \hat{\tau}_k W_{ik} \frac{m_k}{\rho_k} dV = \\ & = \delta \hat{\epsilon}_j \left[\int_V \left[\sum_{j=1}^{nnbr} \sum_{k=1}^{nnbr} W_{ij} C \hat{\epsilon}_k W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] dV \right. \\ & \quad \left. - \int_V \left[\sum_{j=1}^{nnbr} \sum_{k=1}^{nnbr} W_{ij} \hat{\tau}_k W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] dV \right] \end{aligned} \quad (188)$$

$$\begin{aligned} & \int_V \delta \tau^T (\epsilon - \partial_\epsilon u) dV = \\ & \int_V \sum_{j=1}^{nnbr} \delta \hat{\tau}_j W_{ij} \frac{m_j}{\rho_j} \sum_{k=1}^{nnbr} \hat{\epsilon}_k W_{ik} \frac{m_k}{\rho_k} - \sum_{j=1}^{nnbr} \delta \hat{\tau}_j W_{ij} \frac{m_j}{\rho_j} \sum_{k=1}^{nnbr} \hat{u}_k \nabla W_{ik} \frac{m_k}{\rho_k} dV = \\ & = \delta \hat{\tau}_j \left[\int_V \left[\sum_{j=1}^{nnbr} \sum_{k=1}^{nnbr} W_{ij} \hat{\epsilon}_k W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] dV \right. \\ & \quad \left. - \int_V \left[\sum_{j=1}^{nnbr} \sum_{k=1}^{nnbr} W_{ij} \hat{u}_k \nabla W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] dV \right] \end{aligned} \quad (189)$$

$$\begin{aligned} & \int_V (\partial_\epsilon \delta u)^T \tau dV = \\ & \delta \hat{u}_j \int_V \left[\sum_{j=1}^{nnbr} \nabla W_{ij} \frac{m_j}{\rho_j} \sum_{k=1}^{nnbr} \hat{\tau}_k W_{ik} \frac{m_k}{\rho_k} \right] dV = \\ & \delta \hat{u}_j \int_V \left[\sum_{j=1}^{nnbr} \sum_{k=1}^{nnbr} \nabla W_{ij} \hat{\tau}_k W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] dV \end{aligned} \quad (190)$$

$$\begin{bmatrix} 0 & 0 & K_{u\tau} \\ 0 & K_{\epsilon\epsilon} & K_{\epsilon\tau} \\ K_{u\tau}^T & K_{\epsilon\tau}^T & 0 \end{bmatrix} \begin{bmatrix} \hat{u} \\ \hat{\epsilon} \\ \hat{\tau} \end{bmatrix} = \begin{bmatrix} R \\ 0 \\ 0 \end{bmatrix} \quad (191)$$

	SPH	FE
$K_{u\tau}$	$\sum_{i=1}^{np} \left[\sum_{j=1}^{nubr} \sum_{k=1}^{nubr} \nabla W_{ij} W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] \frac{m_i}{\rho_i}$	$\int_V B^T E dV$
$K_{\epsilon\epsilon}$	$\sum_{i=1}^{np} \left[\sum_{j=1}^{nubr} \sum_{k=1}^{nubr} W_{ij} C W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] \frac{m_i}{\rho_i}$	$\int_V E^T C E dV$
$K_{\epsilon\tau}$	$\sum_{i=1}^{np} \left[\sum_{j=1}^{nubr} \sum_{k=1}^{nubr} W_{ij} W_{ik} \frac{m_j}{\rho_j} \frac{m_k}{\rho_k} \right] \frac{m_i}{\rho_i}$	$\int_V E^T E dV$

8.6 Testing and results of MEF

The first test of the method shall be done using what is termed the Swegle box which is used by (J.Swegle, D.Hicks, S.Attaway 1995) to highlight instability under tensile stress in the SPH method. This is a box which is subjected to a uniform tensile stress, and the outer layer of particles that make up the box are fixed to avoid wave propagation that will relieve the initial stress. A velocity perturbation of $10^{-10} m/s$ is applied to a single particle in the box. What should occur (and what does occur under compressive stress) is that no change in the particle positions occurs as due to the extremely small velocity of the particle, it would take $10^4 s$ for the particle to move a distance to equal the particle spacing. However in tensile stress this occurs after $100 \mu s$ (J.Swegle, D.Hicks, S.Attaway 1995) This leads to particle clumping and a huge increase in the particle velocities and energy of the system, indicating instability. This is an example of tensile instability.

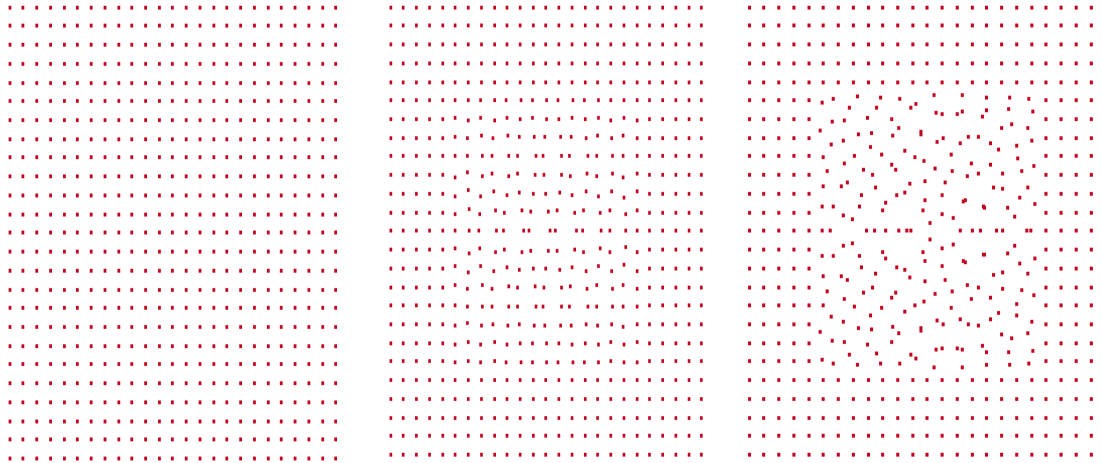


Figure 60: Illustration of tensile instability in the Swegle Box over time. The left figure is the Swegle box in its initial state. The middle box illustrates the instability occurring due to the perturbation of one particle and the right box shows blow up of the particles when the energy becomes too great.

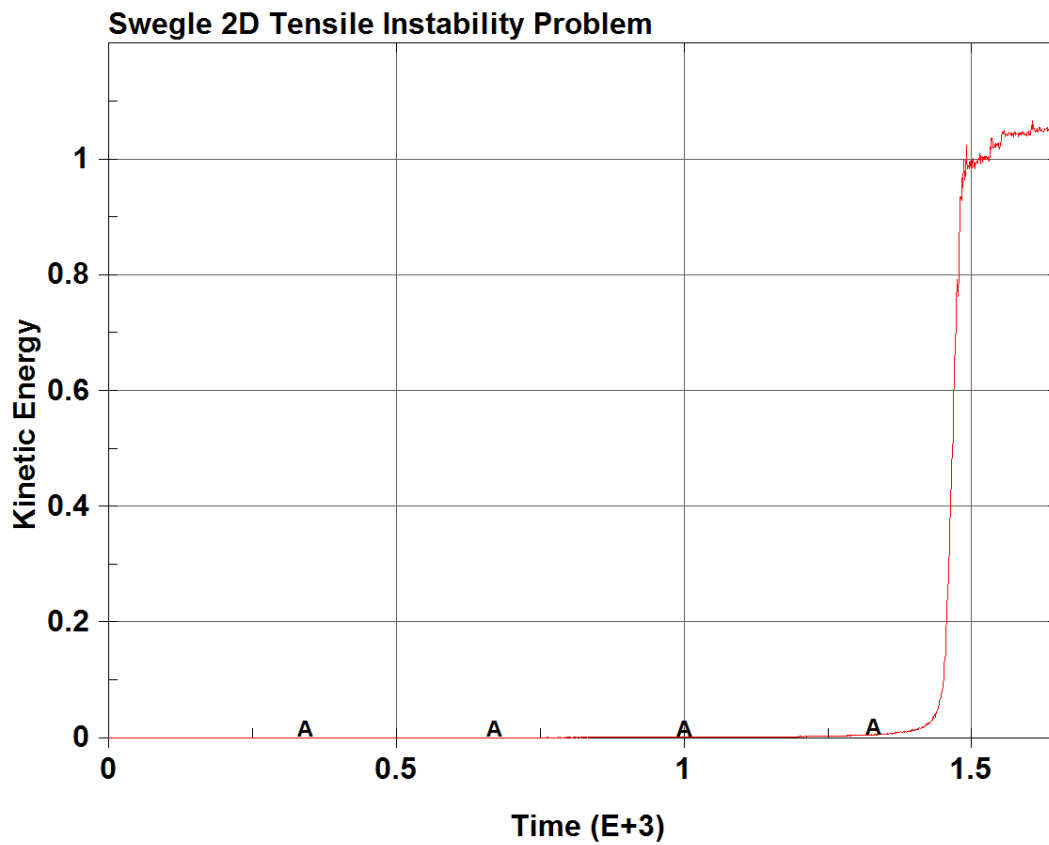


Figure 61: Kinetic energy verses time for the Swegle box.

The large unphysical energy growth leads to the explosion shown in Figure 60. This test shows that tensile instability is a consequence of the relation between the kernel derivative and stress (Figure 59). To further test this hypothesis, it is of interest to see using the moving least squares kernel highlighted in chapter 2 would influence the stability. The following results show kinetic energy in Joules over time in seconds.

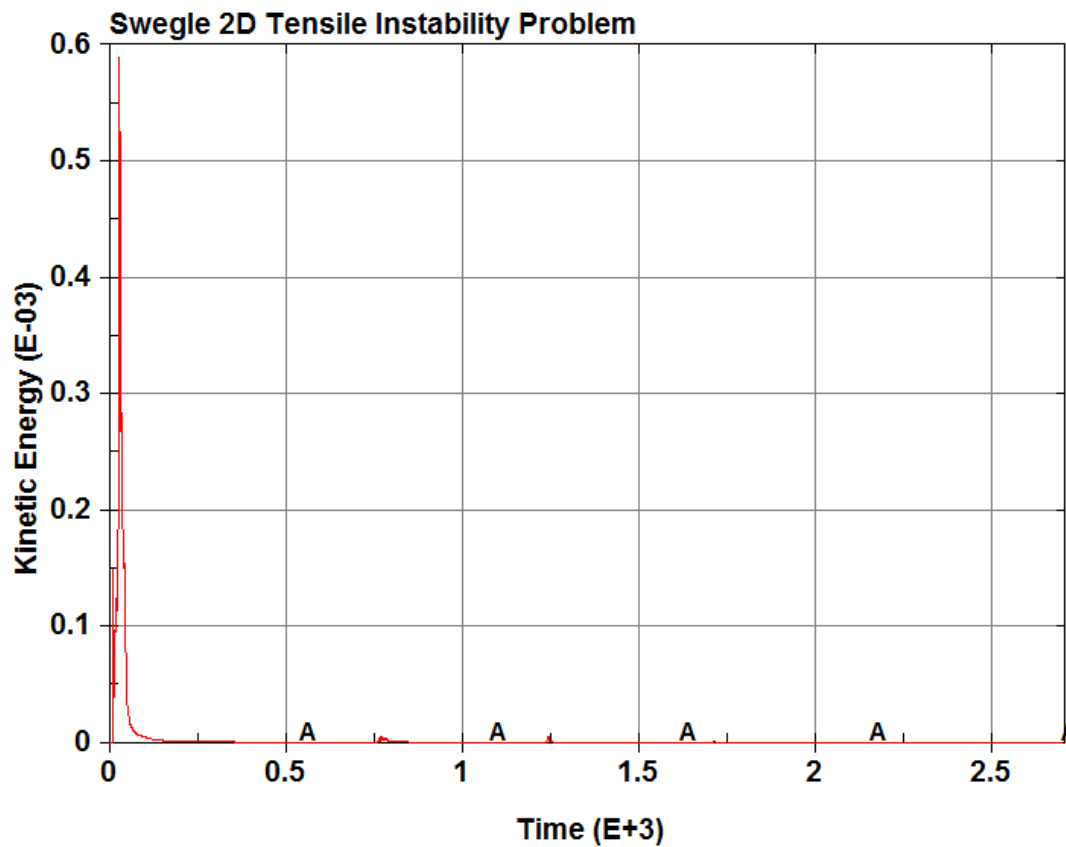
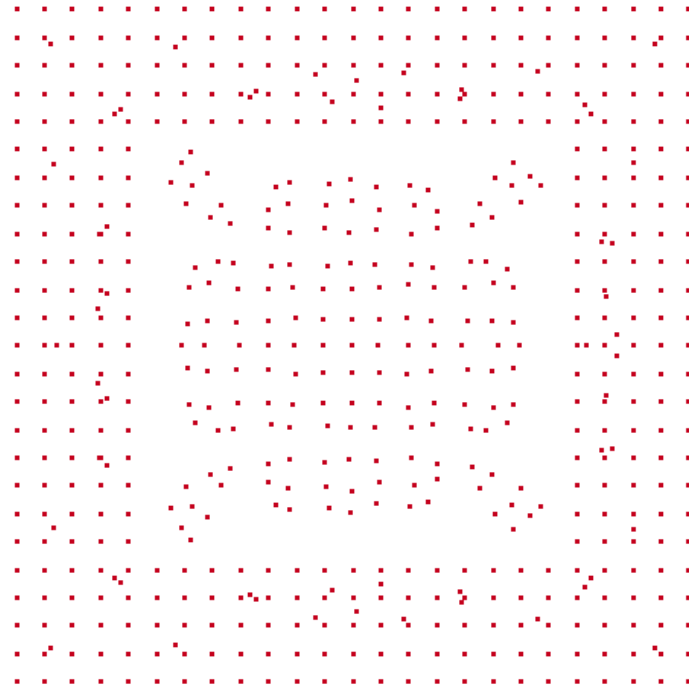


Figure 62: Illustration of the damping effect of the density update on the swegle box.

Figure 62 Shows that while the instability does still occur, even to the point of particle explosion, this explosion is stopped by the sharp reduction of kinetic energy of the system. While this has no real bearing on the validity of the mixed element approach, it does highlight the influence the moving least squares kernel has on tensile instability illustrated in section 3 and confirm the conclusions

deduced. In addition, this also justifies the decision not to use different kernels to achieve orthogonalisation of the KPP matrix as different kernel will have different gradients and different critical points, which will influence the stability. Therefore, any change in kernel will influence any results obtained and hence it would not be ideal to use different kernels as any changes in results using mixed element may be down in part or totally to the change in kernel.

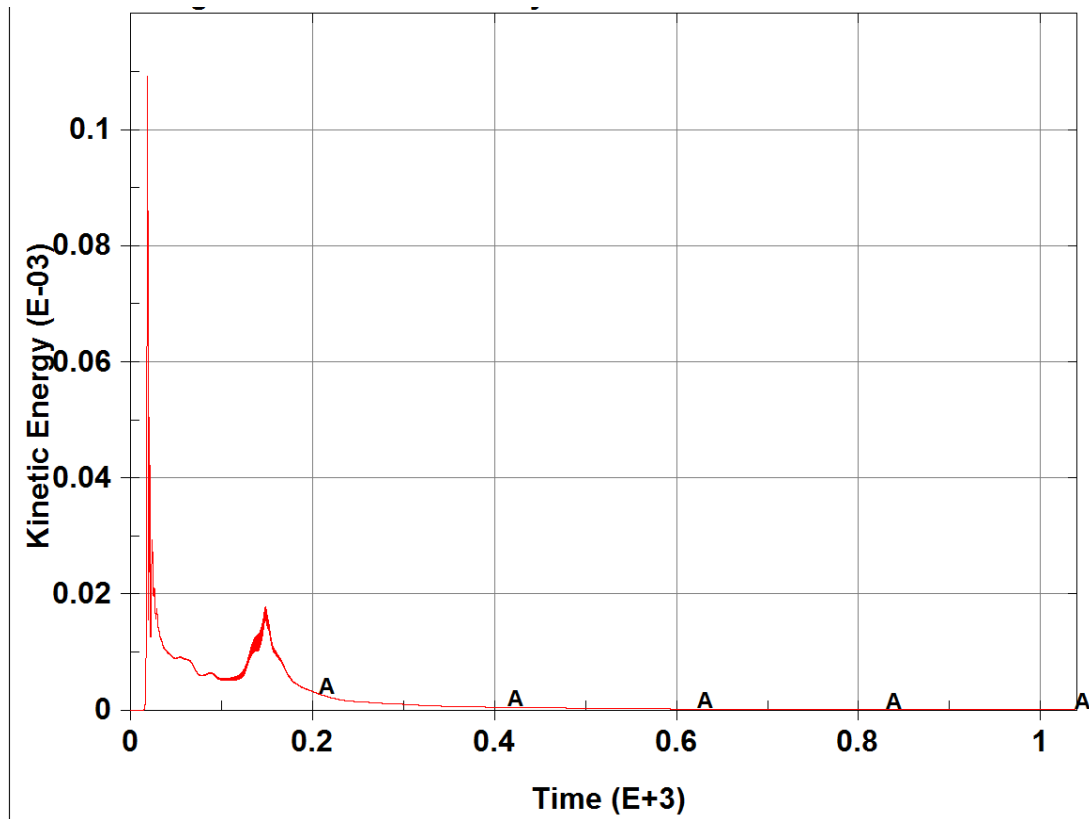


Figure 63: Kinetic energy for MLS kernel

The instability begins 20 seconds into the simulation. Stability occurs at 0.00000017J

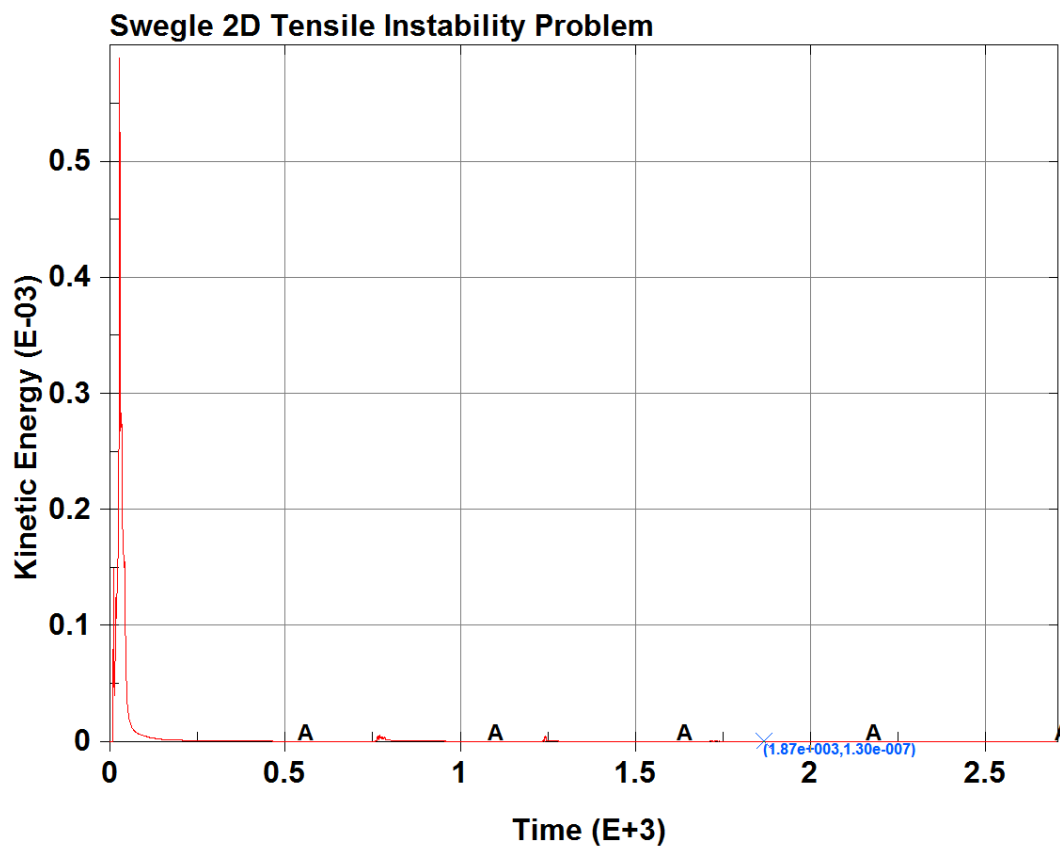


Figure 64: MLS density update every time step

The instability grows almost straight away but stabilises at 0.000000538J

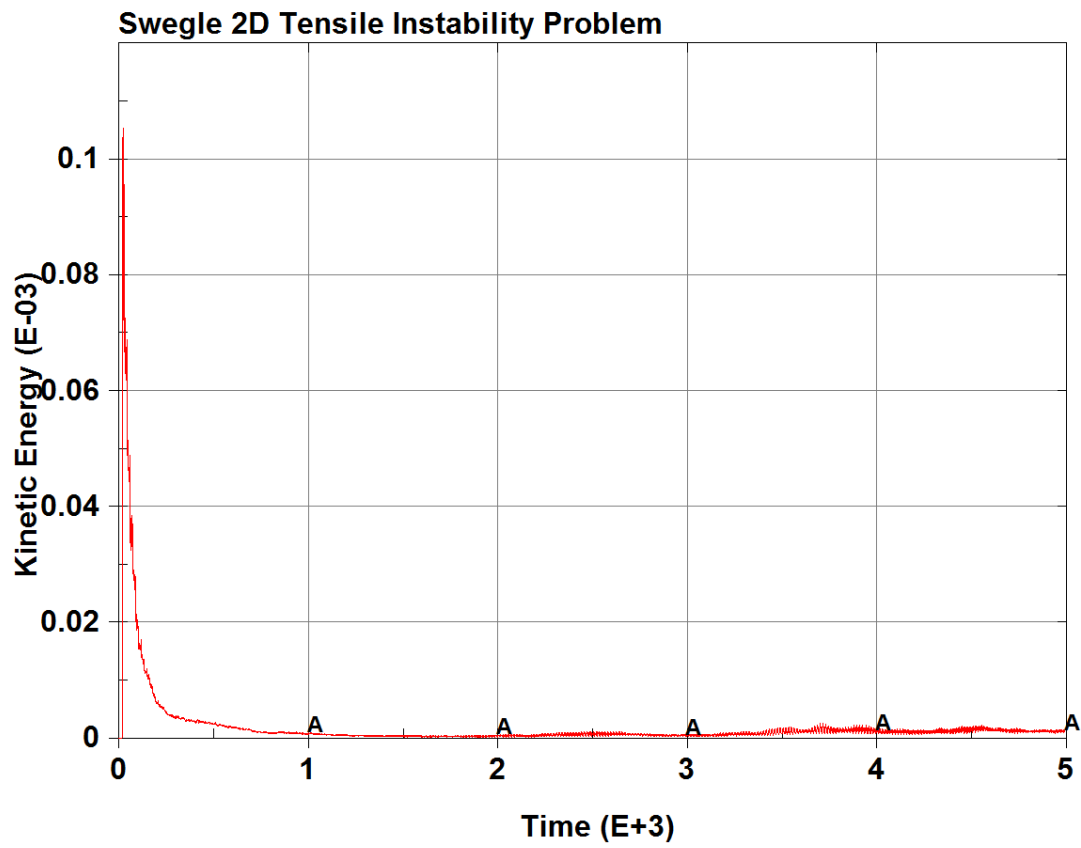


Figure 65: MLS density update every 500 timesteps. Instability occurs at 19s and stabilises at 0.0000014J

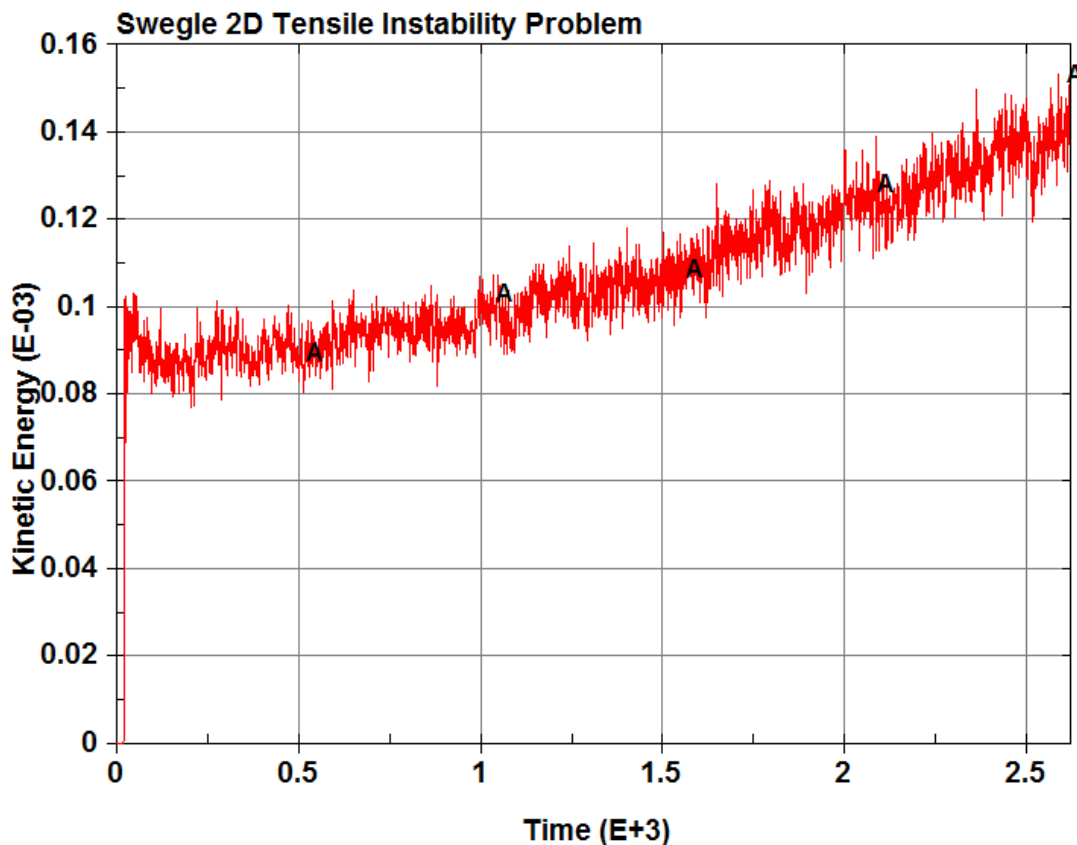


Figure 66: No MLS update case.

The growth begins at 18 seconds and stabilises at around 0.0017J

From the previous figures, the following can be concluded:

- The frequency of MLS update is related inversely to when instability occurs
- The frequency of MLS update is related inversely to the energy level at which stability occurs
- These results do not have a linear relationship

Revisiting the MLS kernel, due to the fact it is first order consistent, the Kernel will have a different form and hence a different profile than the kernel described in Figure 59. This will mean that the kernel relationship between stress and strain will be altered. The instability grows straight away then stabilises, implying that the particles move to stable positions. It is reasonable to conclude that the MLS density kernel will suffer from instability at a smoothing length smaller than conventional SPH but stabilise at a smoothing length of between 1.5 and 2h.

8.7 Displacement-pressure formulation results

The issues discussed and tests run show that static condensation is not suitable for implantation. Furthermore, the mathematics show that static condensation does nothing to tackle the core issue of the relationship between stress and strain. It does not work as does not have the effect of penalising the system; more just calculates pressure in a different way. Another approach is a

penalisation approach where the momentum equation is penalised in the same way the repulsion force is derived by penalising the momentum equation. However, this has had no effect. This would further strengthen the case that the focus needs to be weakening the dependency between strain and pressure to stop the particle clumping rather than adding artificial terms to ensure conservation of momentum. The results in the previous MLS chapter confirm this and now the focus is on solving the tensile instability consequence of particle clumping - the negative stress that occurs due to kernel interpolation of strain-

The appeal of the mixed element approach and more specifically employing static condensation was the mathematical consistency, the governing equations described by (151) are consistent and the elimination of nodal pressure gives as a governing equation in terms of displacements only. No heuristic 'leap' was made; every step was justified and derived.

By not employing static condensation, you are left 2 separate equations (151) with no link, this means it needs to be defined what nodal pressure is to solve the system. If nodal pressure is defined as the calculated pressure at the nodes, then there is little point in employing this technique as although these nodal pressures will form the neighbour particles of the smoothed particle, there is still that strong link between pressure and strain, hence the same particle clumping problem will occur.

In the finite element application of mixed formulation, nodal pressures, stresses and/or strains are defined as being 'enhanced' (Taylor 2000) or assumed (Borja 2008). What this means is that the nodal points for any of the fields considered are stable versions of the original field. For example, in (Belytschko et al. 2014) for a three-field velocity, rate of deformation and stress approach- the strain is constant as this is stable. (Borja 2008) also goes on to state that the mixed element approach will only work if the assumed strain is 'lesser' than the calculated strain, i.e something has been removed from the calculated strain. Other examples are in (Belytschko & Bindeman 1993) where the element assumed strain has the criteria that the shear strains remain 0 when deforming in an hourglass node but remain consistent with pure beam bending.

This has been shown to work in the finite element method and in fact is even more consistent than static condensation as continuity of pressure is assured (Bathe 1996). However, by removing parts of a strain (or any other) field, a careful approach is needed to ensure this does not affect the physics of the solution. The static condensation approach was guaranteed not to do this as there was no artificial changing or removing of terms to make the solution work. For this approach, it cannot be guaranteed this is the case, removing parts of fields may cure the problem you are trying to solve such as particle clumping, zero pressure modes (Bathe 1996) or rotational nodes (Wang & Bathe 1997) but it could have the negative consequence of inaccurate calculation of other variables or lack of convergence in the solution.

In addition, the nature of the pressure nodes need to be considered. How can pressure be defined in the SPH method without a strong link to strain? The key word here is 'strong' as no matter how you define the assumed or enhanced field, there still needs to be a link to the dependent variables, otherwise the whole physics is lost. For example, pressure is related to strain, if it wasn't it would not be pressure anymore. By removing parts of the field you are interpolating, this does weaken the dependency but does not eliminate it entirely. The mathematical consistency of the solution is also

ensured by the fact that the constraint (the link between pressure and strain) is enforced by the Lagrange multiplier rather than solved as part of the solution.

One option for pressure is to consider the nodal pressure constant. This would eliminate the pressure instability and the pressure would still vary as a function of the kernel. But how is this constant pressure defined? For the first test, constant pressure was defined this as the initial pressure of the system. This meant that there is still a link between pressure and strain as initial pressure is calculated from initial strain so there still is that link and as the interpolated pressure equals the kernel times the nodal pressure the pressure will vary i.e it will increase the closer it is to neighbour particles as the kernel will be higher the nearer the element is to a neighbour particle. This could have the secondary effect of acting as a repulsive force as if the particles begin to artificially clump, the increase in pressure between the particles could act as a repulsion. This does cure the tensile instability problem. The particles do not clump and energy of the system is conserved. The Lagrangian version of this problem is the expected baseline and the results are similar. The problem behaves as it should. The initial instability of the centre particle does not lead to particle clumping and the pressure values are not unphysical.

As described before, the Swegle box is not a real life physical problem and is a very simple problem which will not be sufficient to show whether there have been any undesirable side effects or verify whether the approach gives the correct physical response to a system.

The next step was to try this approach to a 2d bar test described by (De Vuyst 2003) as a scenario that exhibits zero energy nodes. This problem is described as two 2d bars initially in contact under tension and compression. The bars are steel with a Youngs modulus of $1.72\text{E}+09$ and follow a linear elastic stress-strain law. To simulate the bar under compression and tension, the top bar was acted up by positive 0.2 m/s and the second by negative 0.2m/s in the y direction. Contact between the bars is kernel contact which treats them as 1 material, thus the bars act as they are stuck together. The bar should in theory compress and contract and repeat this, with a pressure wave generated. The Lagrangian SPH approach describes correctly what should happen physically to the energy of the system, as the bars are compressed, the kinetic energy decreases as the internal energy of the system increases and then as the bars move away from the kinetic energy increases and the internal energy increases. Energy is conserved and particle clumping does not occur.

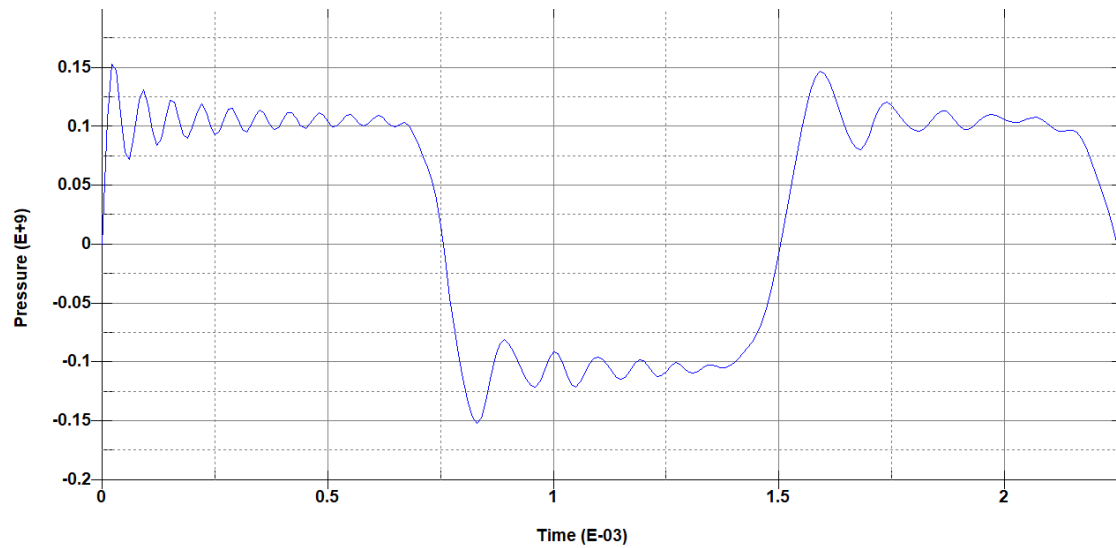


Figure 67: Pressure wave generated by compression and tension of 2D bar. Units are in seconds and Pascals.

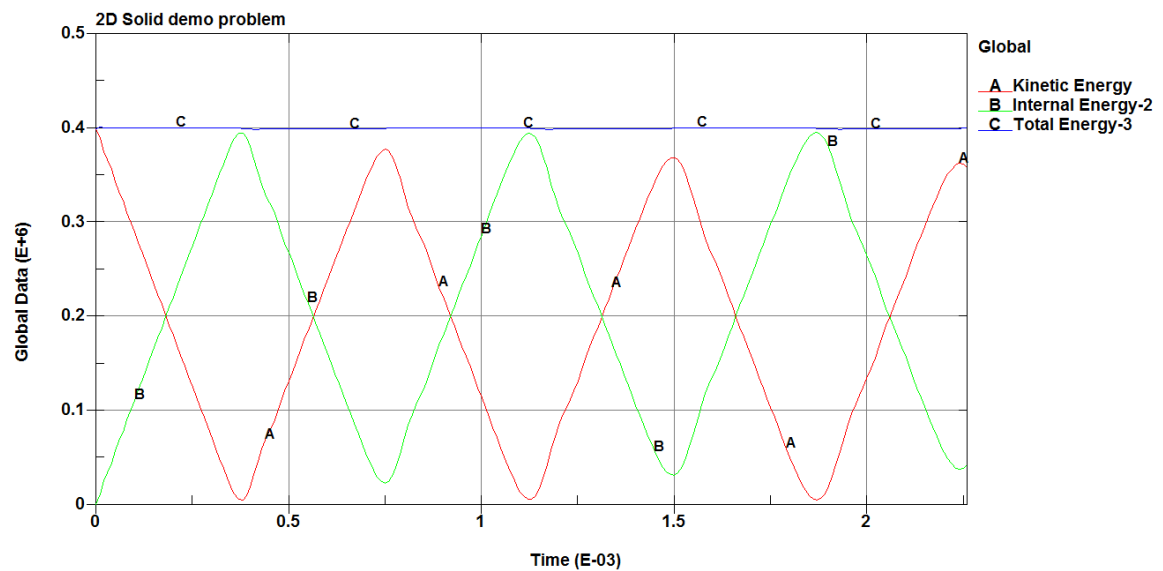


Figure 68: Global data for the Lagrangian 2D bar impact problem. This shows the variation of kinetic and internal energy as well as the conserved total energy. Energy is in J and time is seconds.

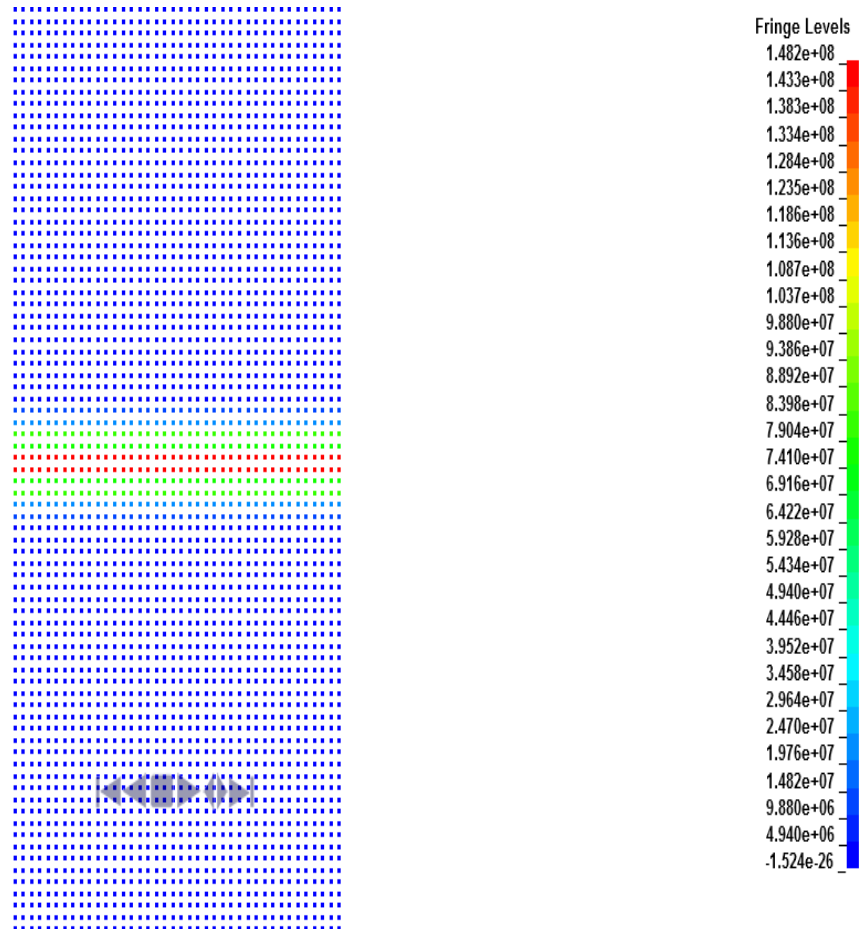


Figure 69: Pressure distribution at 0.00003s for Total Lagrange approach in Pa

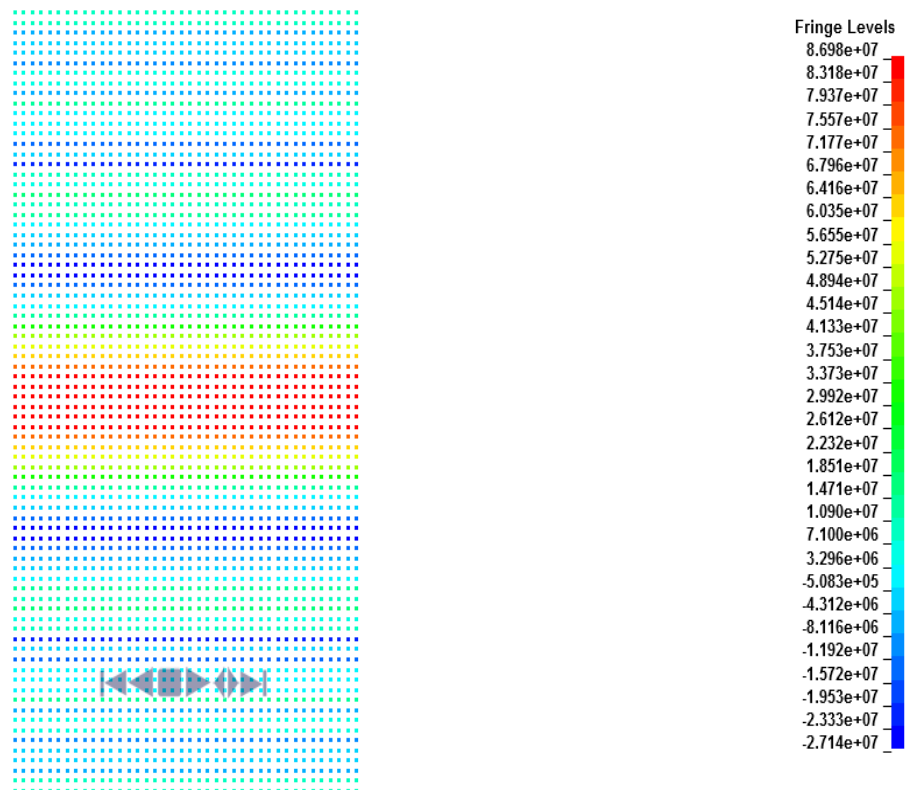


Figure 70: Pressure distribution of the 2D bar at 0.0007s in Pa

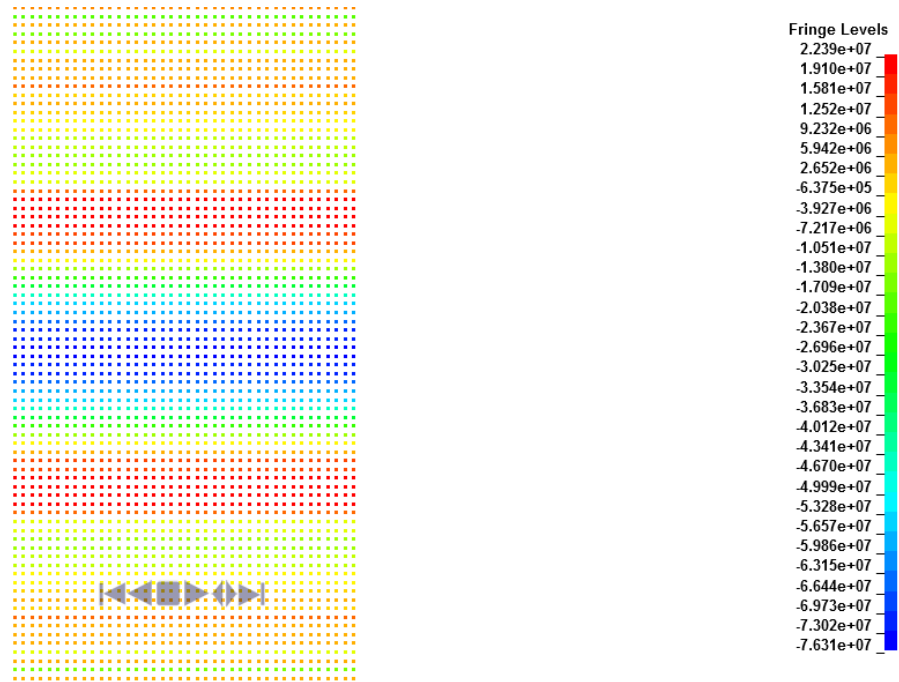


Figure 71: Pressure distribution of the 2d bar at 0.001s in Pa.

The Eulerian approach to this problem is not correct physically. The particle clumping occurs, leading to instability. The clumping leads to the zero-energy mode problem and hence the energy of the system is not correct. This is illustrated by Figure 72

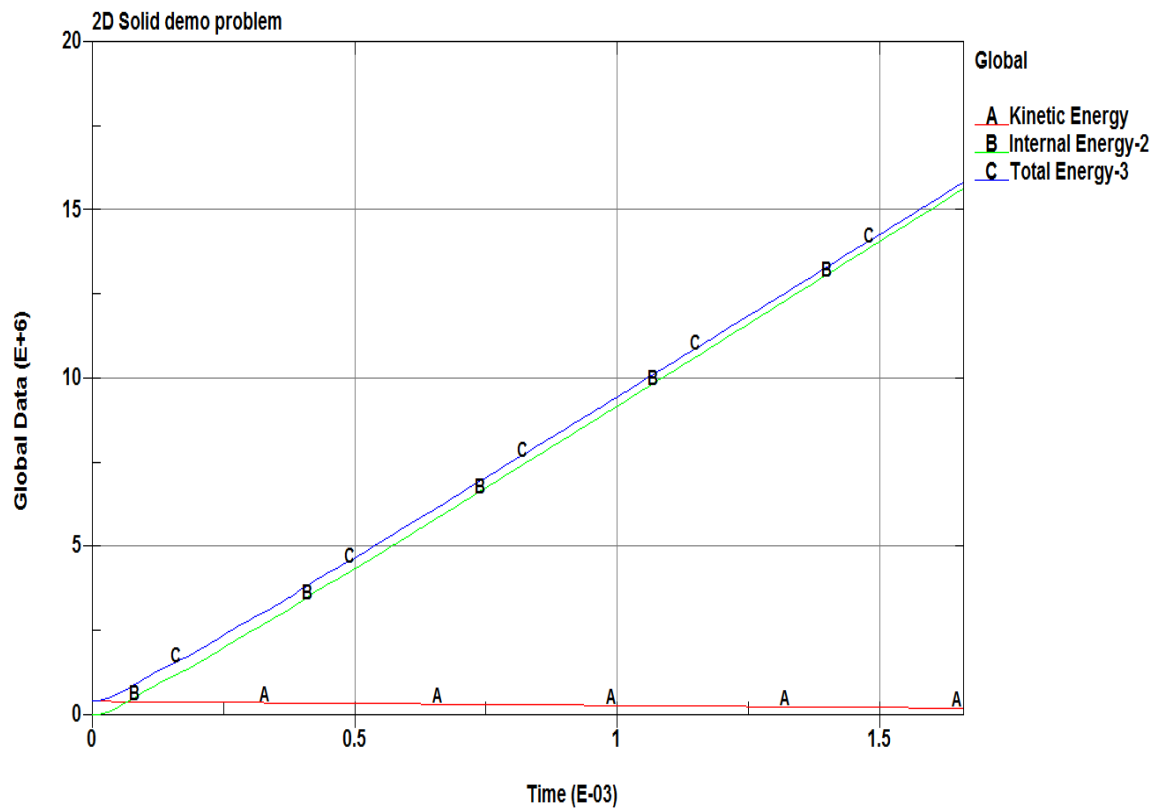


Figure 72 : Global data for the Eulerian 2d bar impact problem. This shows the variation of kinetic and internal energy as well as the conserved total energy. Energy is in J and time is seconds.

Clearly the internal energy should not continue to grow while the kinetic energy remains constant. Figure 72 does highlight the shortcoming of the Eulerian method.

The encouraging results from the Swegle box shows that the nodal interpolation approach is the way to go, however for this problem a constant pressure for the nodal pressure based upon the initial pressure of the system is not applicable in this case as the initial pressure of the system is 0. This makes using a constant pressure as the assumed pressure infeasible.

Another method of finding an 'assumed' pressure is to consider a nodal pressure average. This approach is simply to find an average pressure for a given node by adding up all the pressure values for the neighbour nodes and then dividing it by the number of neighbours. This in theory will eliminate the 'unstable' part of pressure and allow independent interpolation of pressure. For the particle clumping issue this work is trying to address, this would be a suitable nodal pressure as there is still a link between pressure and the other variables and the averaging aspect means that any spurious 0 strain nodes which will lead to 0 pressure nodes will be averaged out of the solution.

$$\hat{p} = p_j = \frac{\sum_1^n p_k}{n} \quad (192)$$

Hence:

$$p = H_j \frac{\sum_1^n p_k}{n} \quad (193)$$

It is this pressure that is used in the momentum equation (112). Using this new averaged pressure instead of constant pressure, it can be seen below there are some encouraging results.

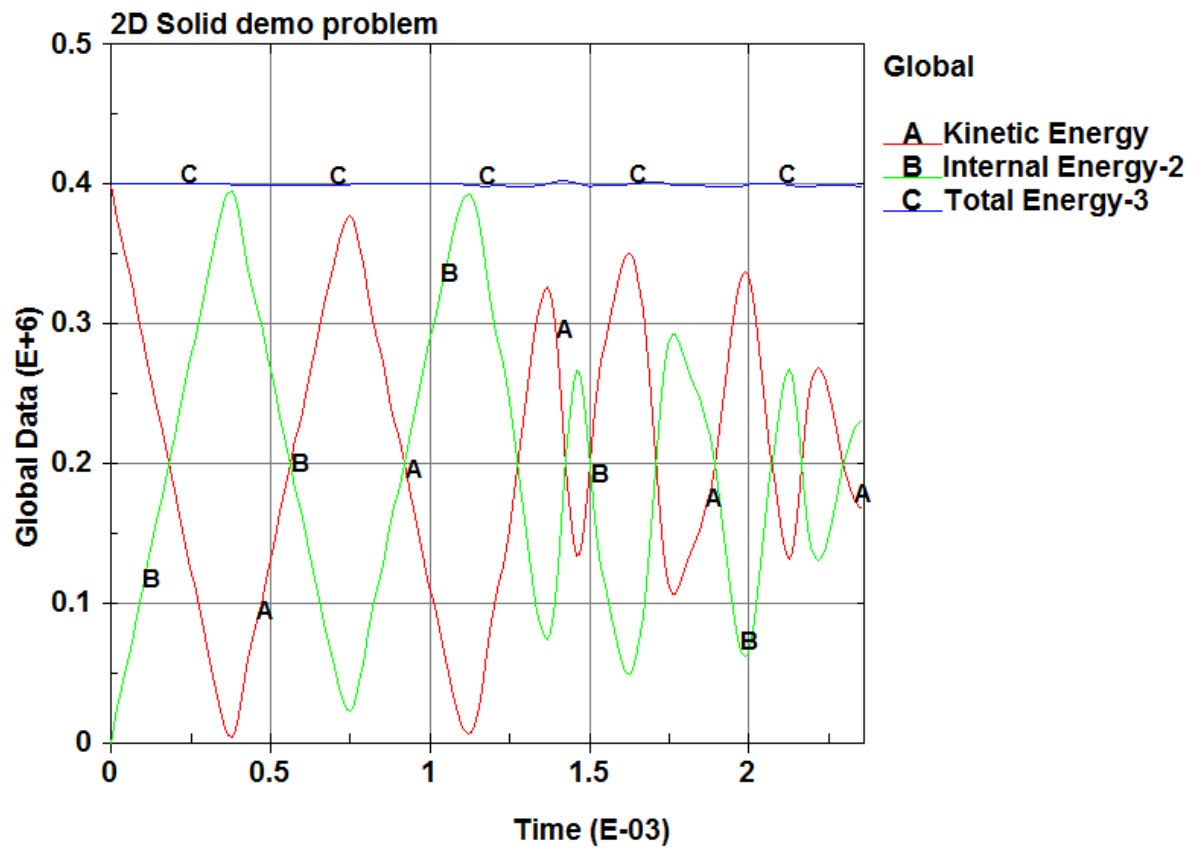


Figure 73: Energy distribution for the 2D bar using mixed formulation pressure averaged approach. Energy is in J and time is seconds.

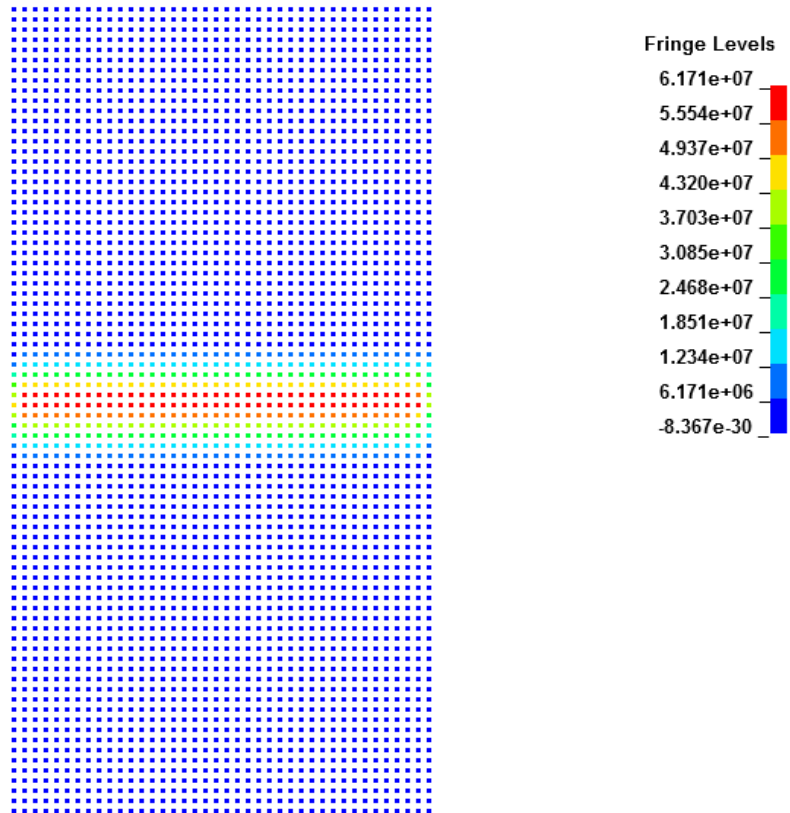


Figure 74: Pressure distributed of 0.00003s for mixed formulation pressure averaged approach. Pressure is in Pa

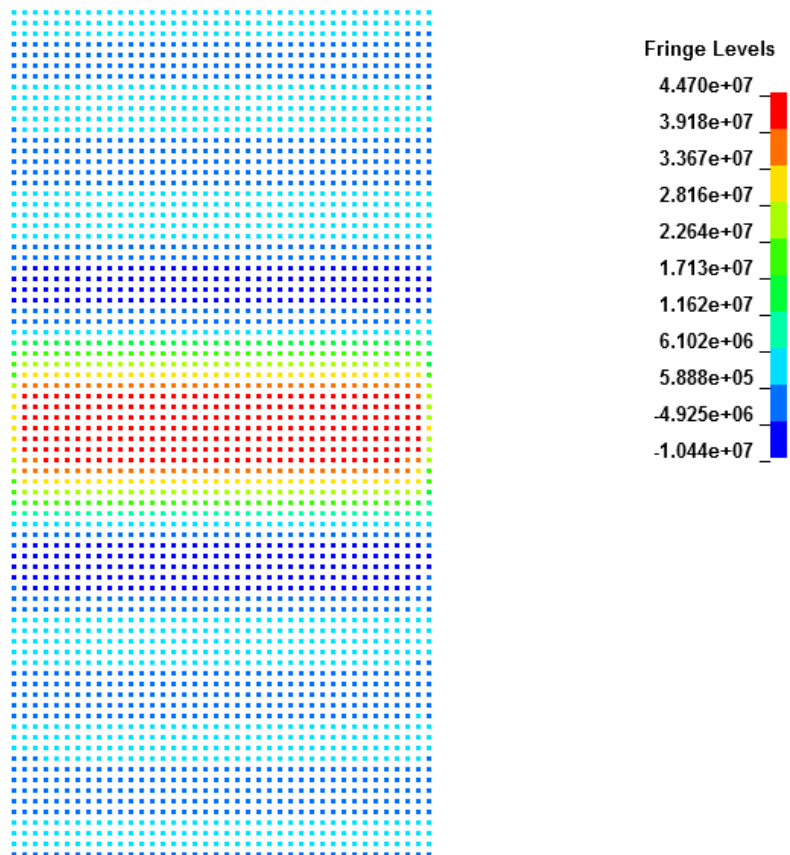


Figure 75: Pressure distribution of the 2D bar using mixed formulation pressure averaging at 0.0007s. Pressure is in Pa

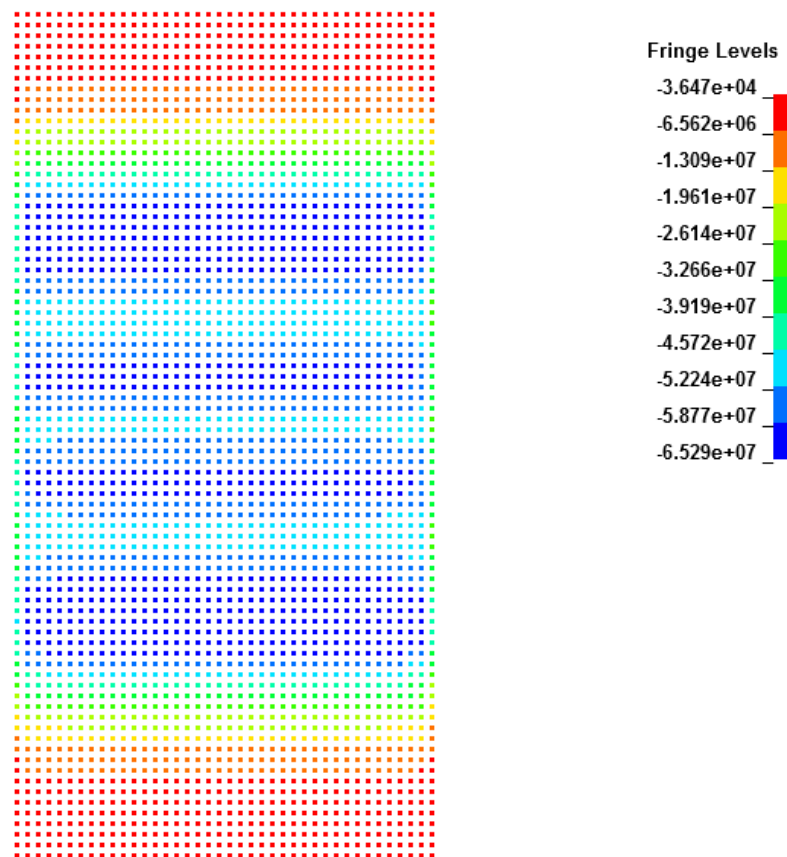


Figure 76: Pressure distribution of the 2d bar using mixed formulation pressure averaged approach at 0.001s. Pressure is in Pa

The above figures show that the mixed element displacement-pressured averaged approach does go some way to addressing the zero-energy mode issue as the energy pattern follows the same oscillating nature as the Lagrangian approach. Clearly the displacement-pressured averaged approach performs better than the Eulerian approach (Figure 72). However after 0.001s the amplitude dies down and continues to reduce even though the oscillating pattern remains the same. This would suggest some form of artificial energy loss. It would also seem that the mixed element approach gives marginally better profiles.

Extending the test to 3D it can be seen below for a Lagrangian approach the expected energy profile is shown.

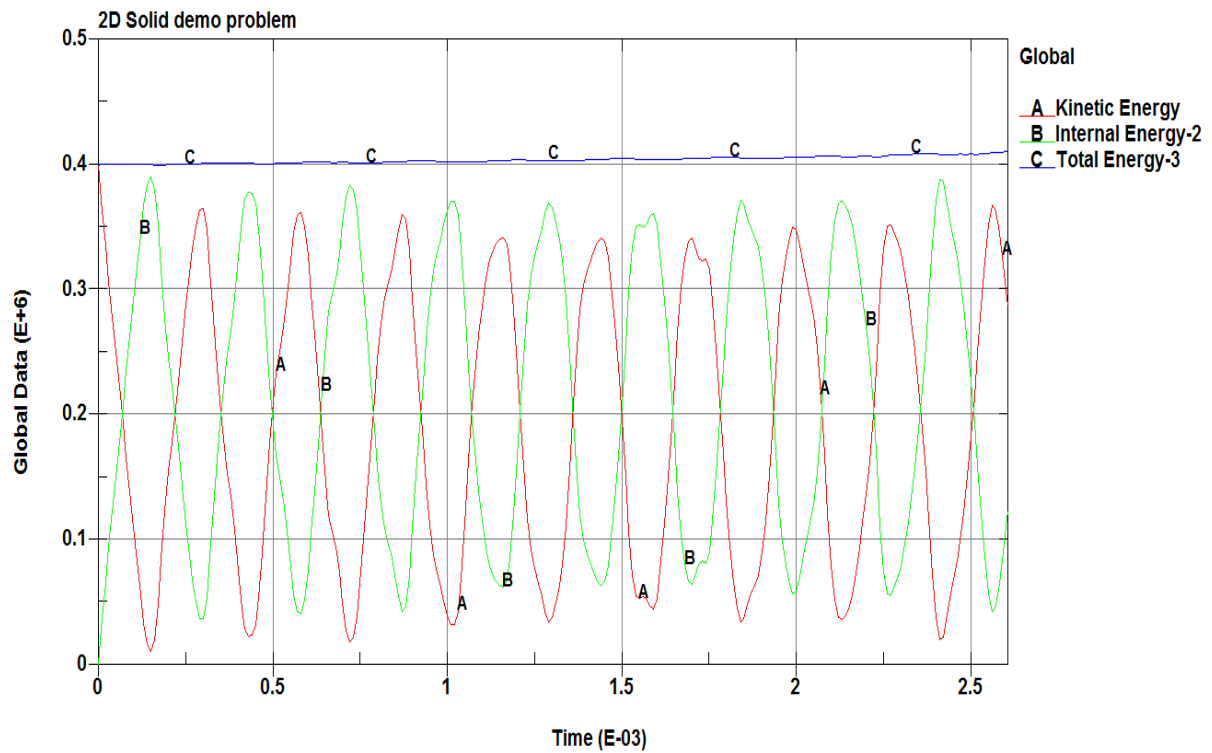


Figure 77: Energy profile for 3D bar using Total Lagrange approach. Energy is in J and time is seconds.

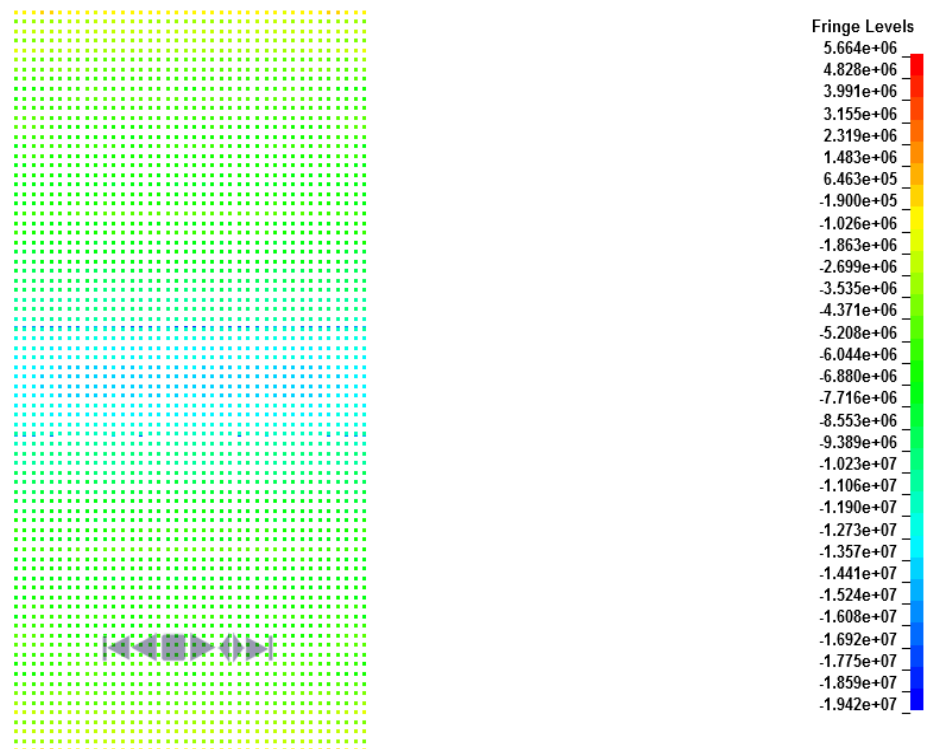


Figure 78: Pressure distribution at 0.004 seconds for the 3D bar using the Total-Lagrangian approach. At this point the beam is in tension as shown by the pressure profile. Pressure is in Pa

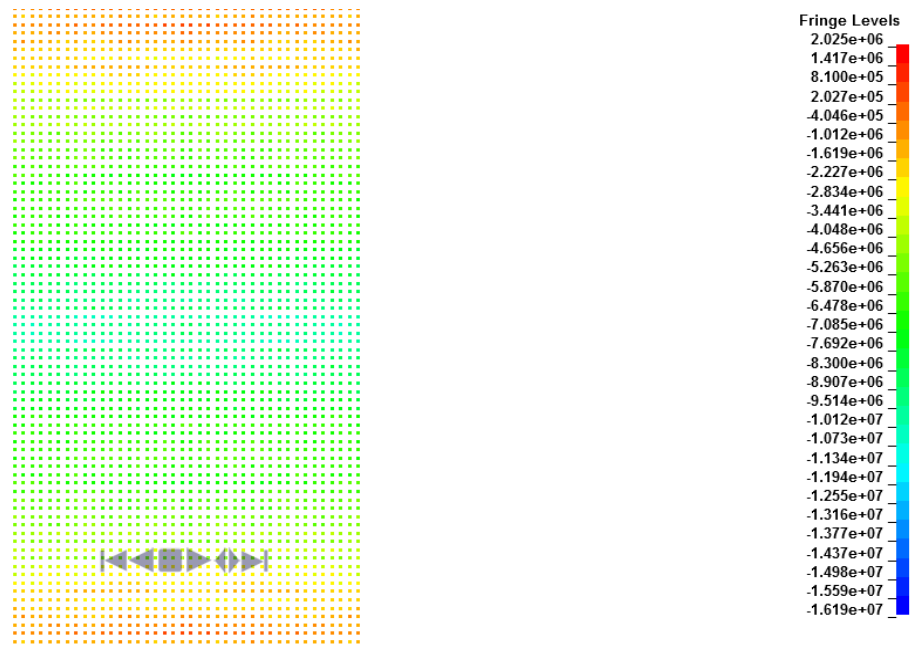


Figure 79: Pressure distribution of the 3D bar at 0.008s. At this point the bar is in tension as shown by the pressure distribution. Pressure is in Pa.

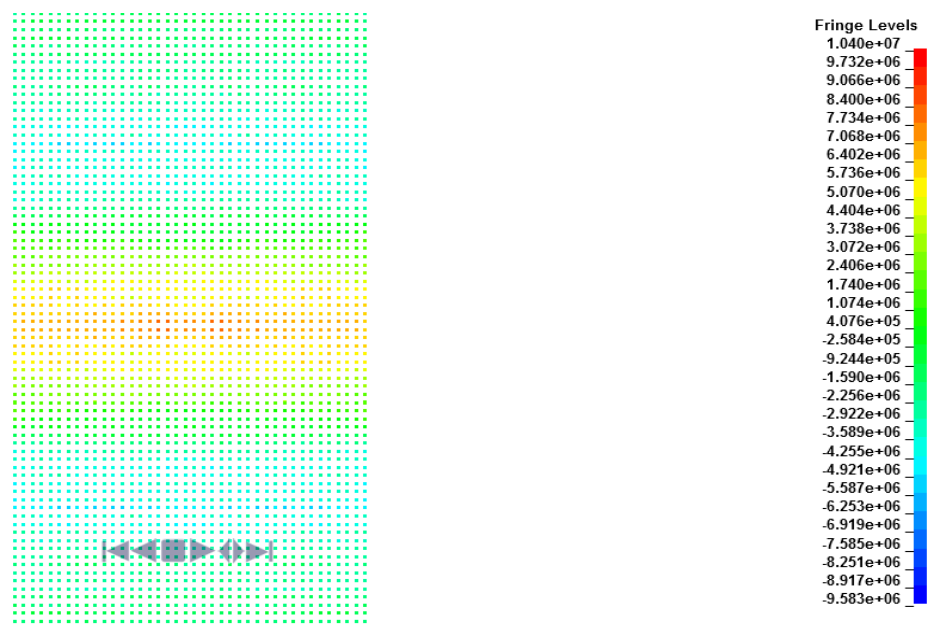


Figure 80: Pressure distribution of the 3D bar at 0.012s. At this point the bar is in compression as shown by the pressure distribution. Pressure is in Pa.

The mixed approach gives us:

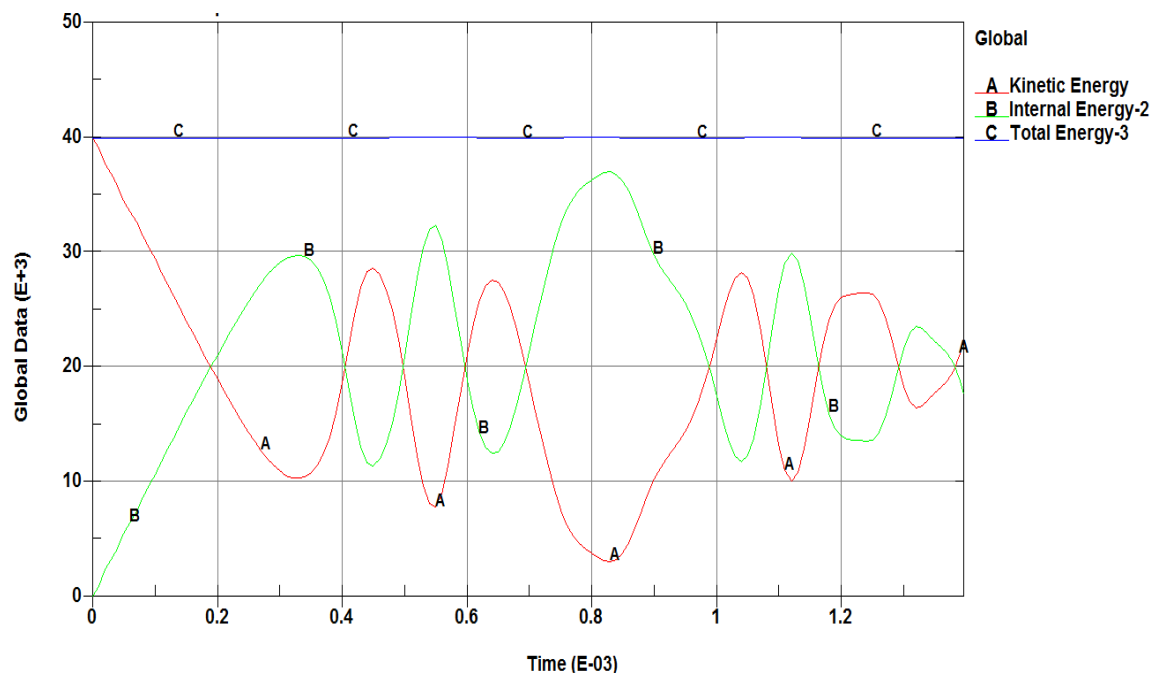


Figure 81: Energy distribution of the 3D bar for the mixed displacement-pressure approach. Energy is in J and time is seconds

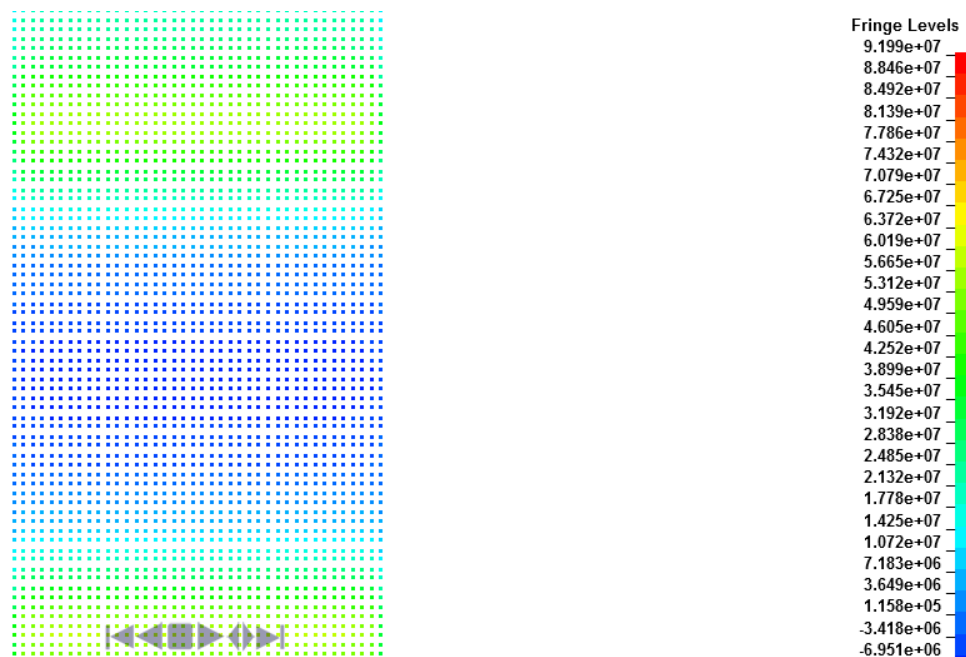


Figure 82: 3D bar at time 0.008s seconds. At this point the bar is in tension. Pressure is in Pa.

Total energy is conserved but the same variation in amplitude occurs as in the 2D model.

The pressure averaging mixed element approach does address and solve the zero-energy problem as energy is conserved and does give correct physical behaviour in the oscillations of kinetic and internal energy. The pressure profiles are also good as they show the correct behaviour of the pressure waves during tensions and compression.

The drawback is the dissipation of energy of the system. This is likely due to the pressure averaging process in that while any 0 energy nodes are averaged out and thus restores the full rank of the

system, if there are 0 valued neighbours in the averaging process, it will give a lower value of pressure and hence energy of the system. This is corroborated by the lower pressure values in the mixed element approach compared to the Lagrangian approach.

8.8 Further testing of mixed pressure averaging approach

To illustrate the uniformity of the mixed-displacement pressure-averaging approach to address particle clumping, it is necessary to test this theory on other tests. The first logical approach is to return to the Sweigle box case to see if this has any impact on tensile instability.

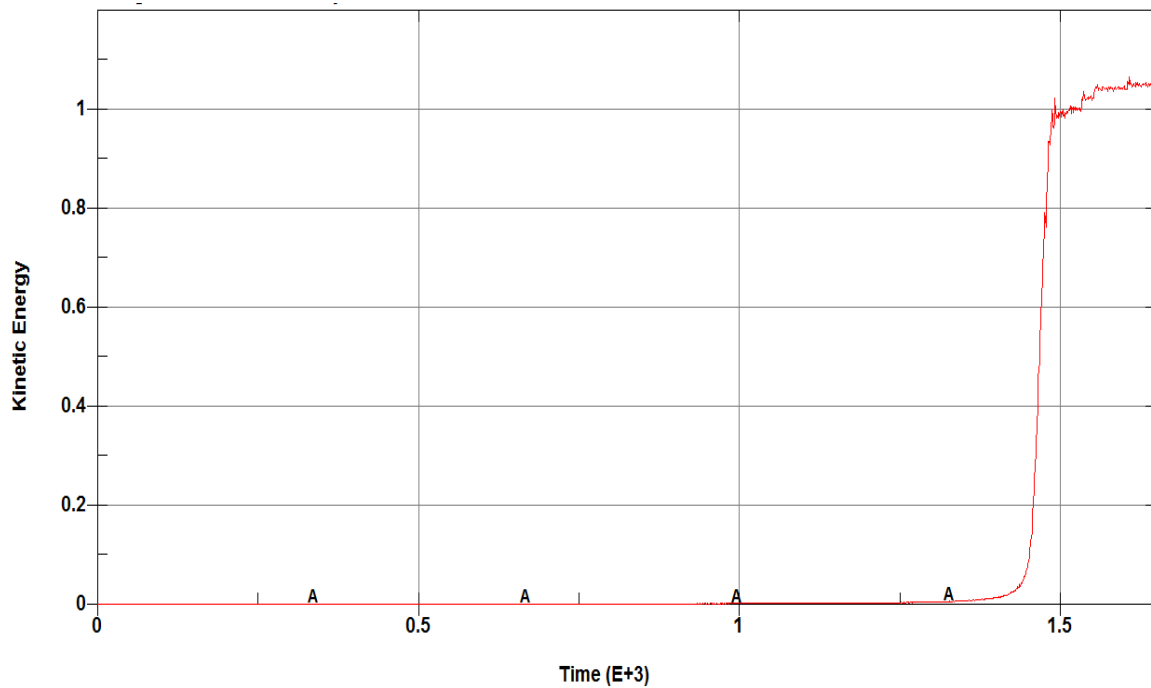


Figure 83: Kinetic energy profile of the Sweigle problem using pressure averaging displacement-pressure formulation. Kinetic energy is in J and time in s.

This has no influence on the tensile instability issue but does influence the pressure values. This was an interesting development and hence it can be concluded that the mixed approach with nodal pressure averaging addresses zero energy but not tensile instability. The rationale behind this lies in the different mechanisms that causes the particle clumping. For tensile instability, it is the kernel relationship between stress and strain which this approach makes no effort to change, there is still the explicit link between pressure and strain and there is no penalty force involved either. However, where it does influence is the pressure values and hence the energy of the system. It would further explain why changing the kernel has no influence on the zero-energy effectiveness.

Recreating the rubber pull test described in (Ganzenmuller 2015) for Eulerian, Lagrangian and mixed formulation displacement pressure averaging approach it can be seen below:

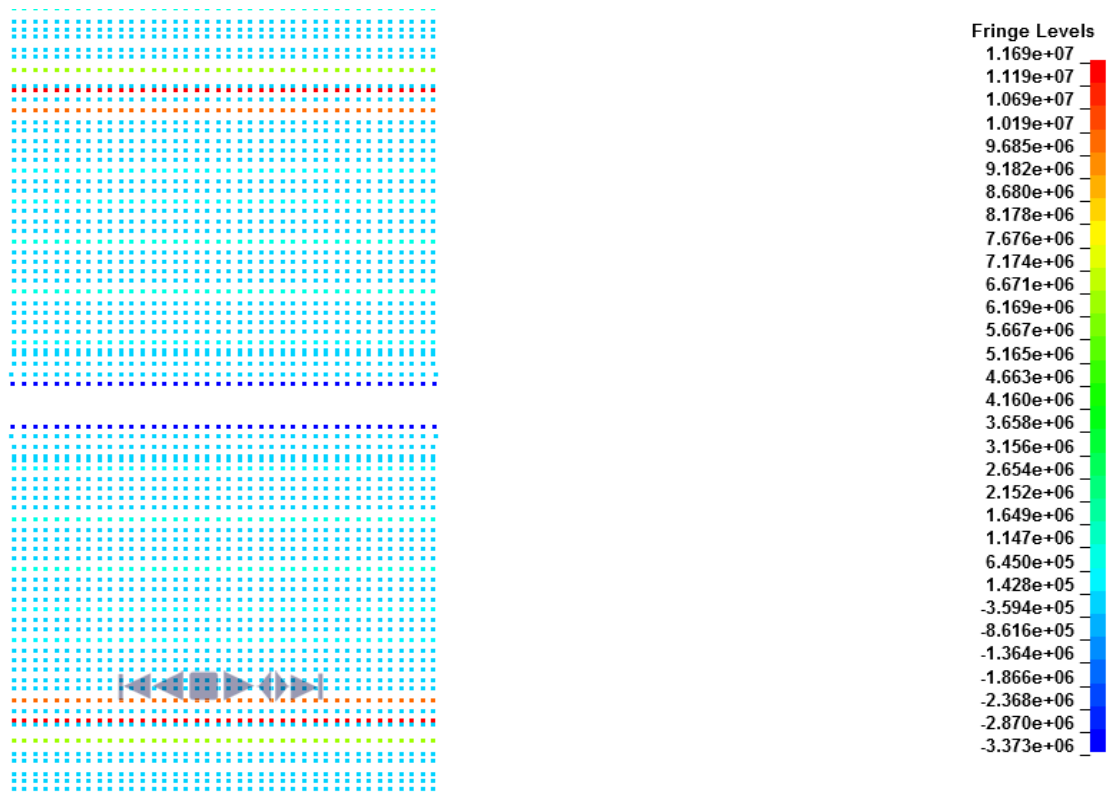


Figure 84 2D rubber pull test for Eulerian approach at time 0.01s Pressure is in Pa.

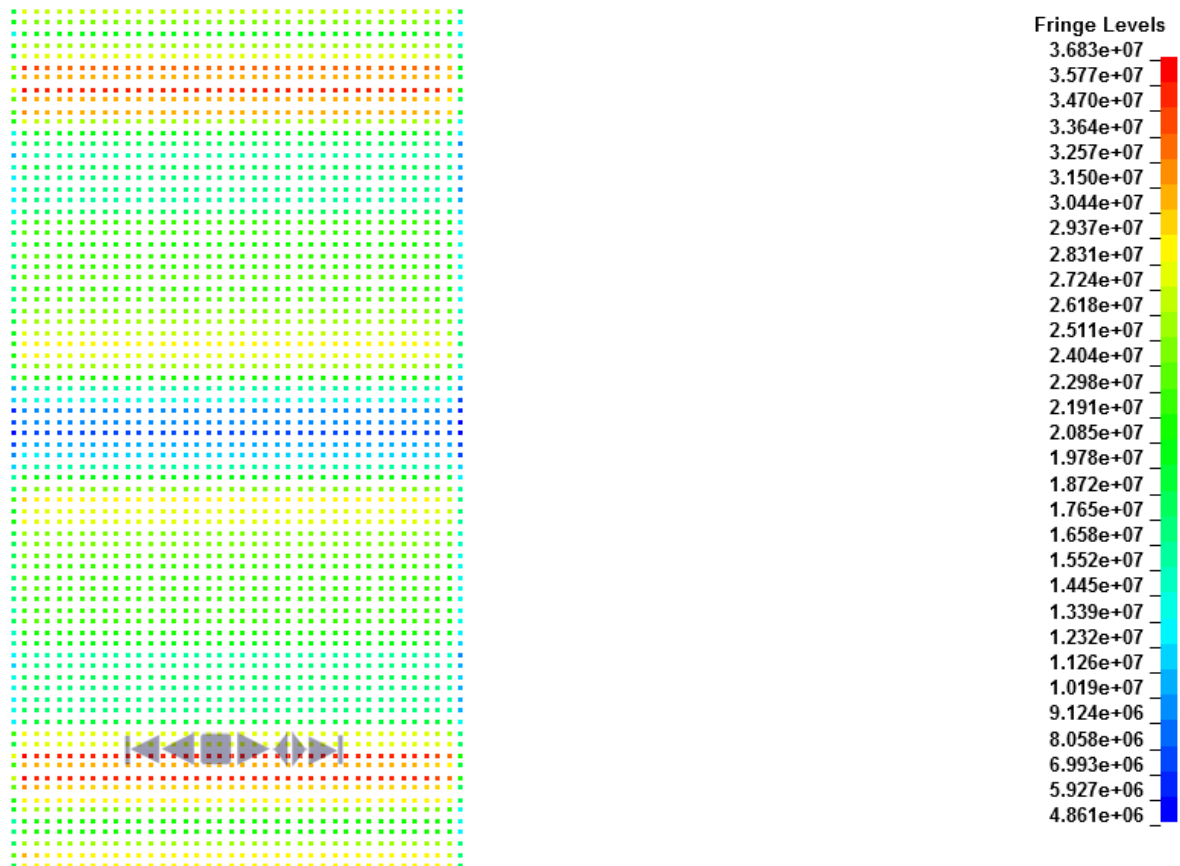


Figure 85: 2D rubber pull test for Mixed formulation approach at 0.01s. Pressure is in Pa.

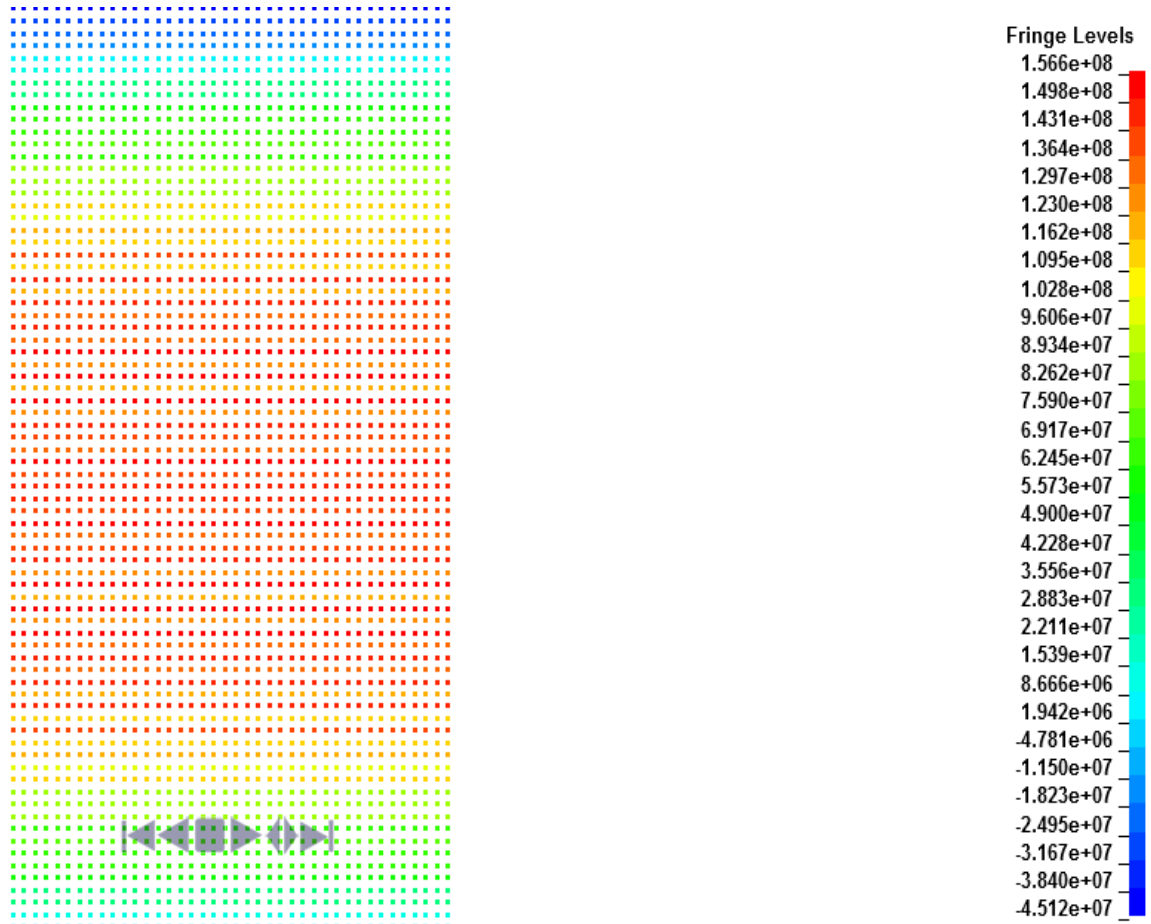


Figure 86: 2D rubber pull test for Total Lagrangian approach at 0.01s. Pressure is in Pa

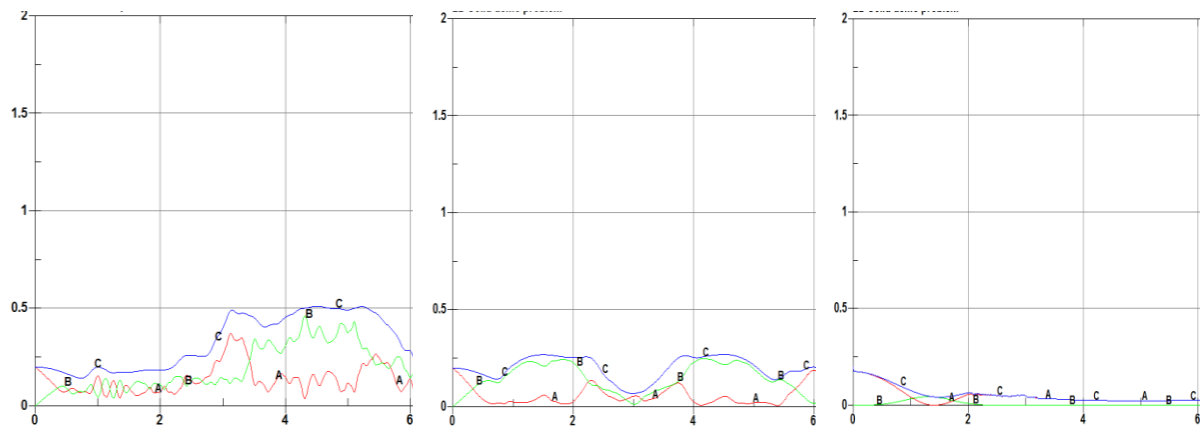


Figure 87: Energy profiles for the 2d rubber pull test. The far left is the Lagrangian, the middle the mixed formulation and the right the Eulerian. Blue is total energy, red kinetic, green internal. Time is in seconds in the x axis, energy in J on the y axis.

The profiles show that the mixed approach is closer to the Lagrangian in amplitude and phase. It also behaves correctly in that the kinetic and internal oscillate and there is no unphysical growth.

The Lagrangian pressure distribution is the most accurate with mixed formulation also following the correct pressure distribution as a whole, however there is a lot more noise. The Eulerian behaves very poorly.

8.9 Other solution procedures

Using static condensation to filter out pressure unknowns was not viable, however the development of another technique to get an exact solution for the pressure unknowns was developed that would eliminate the problem of degrees of freedom in the system.

For a n particle system we write it as:

$$K_{pu}\hat{u} = -K_{pp}\hat{p} \quad (194)$$

$$B_v\hat{u} = -\frac{H}{K}\hat{p} \quad (195)$$

In words, rate of deformation of a particle = interpolated pressure over the constitutive constant.

Or as an n particle system:

$$\begin{bmatrix} u'_1 \\ u'_2 \\ \vdots \\ u'_n \end{bmatrix} = \begin{bmatrix} \frac{h_1}{k} & \frac{h_1}{k} & \frac{h_n}{k} \\ \frac{h_1}{k} & \frac{h_1}{k} & \frac{h_1}{k} \\ \vdots & \vdots & \vdots \\ \frac{h_n}{k} & \frac{h_1}{k} & \frac{h_1}{k} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ \vdots \\ p_n \end{bmatrix} \quad (196)$$

This is in $Ax = b$ system. In this form, Gaussian elimination technique can be employed to solve for the vector x. By doing this exact values for pressure nodes can be obtained and not have to rely on the inversion of a matrix.

This approach differs from anything in literature. In employing the mixed element technique, the 2 approaches seems to be the direct solution which involves using static condensation to substitute the pressure unknown from the constraint equation into the momentum equation or coming up with enhanced or assumed variables that are stable due to the fact they satisfy the Brezzi condition (Bathe 1996) and designed so that they address the particular problem they wish to solve. The direct approach is more mathematically sound as there is no 'artificial' insertion of variables, but it is only feasible in a small number of cases. The second is less mathematically sound, lacks generality but does allow in theory more independence between interpolated quantities and faster computational time.

The Gaussian elimination procedure solves the issue of direct approach as it doesn't matter whether a particle has no neighbours or 20, this will be considered by the matrix of shape functions and any solution of p will take into account the neighbours.

8.9.1 Testing of alternate solution procedure

A smaller scale version of the 2d bar was tested. The bar is made of 90 particles and has dimension 0.125m x 0.45m. All other quantities are the same as the 2d bar depicted in Figure 68

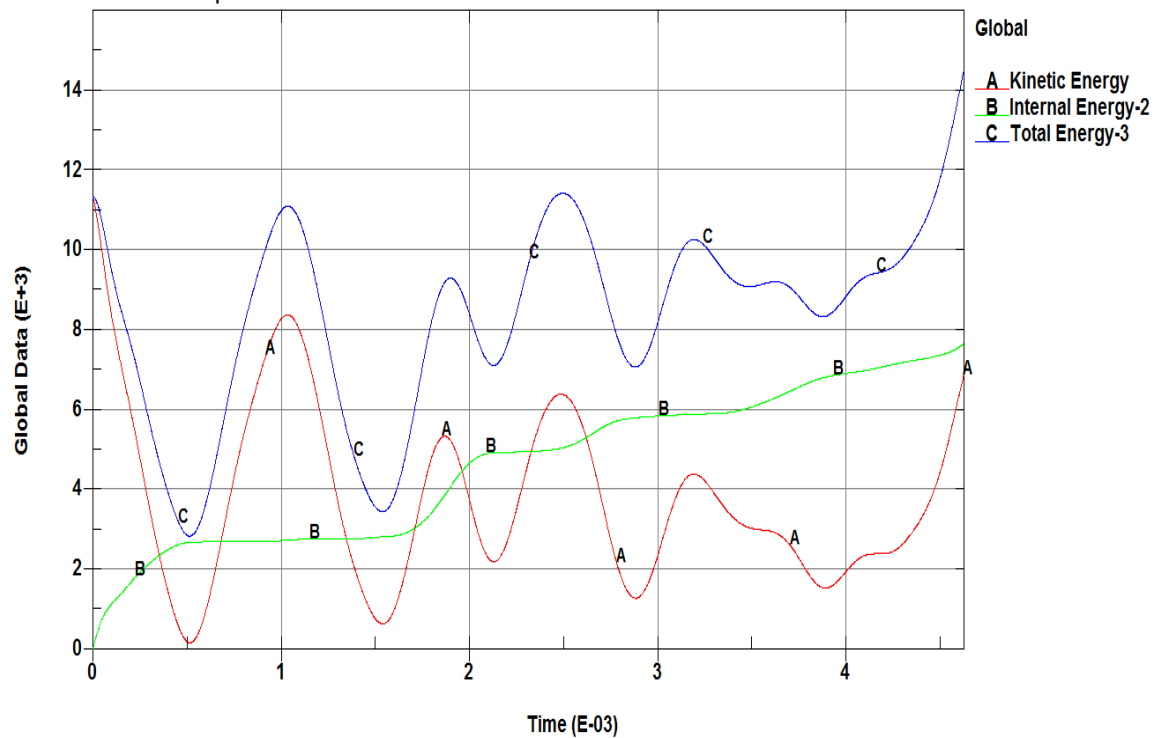


Figure 88: Energy profile for the 2d bar using the Gaussian elimination approach to solve for pressure unknowns in the mixed formulation approach. Time is in seconds, energy in J on the y-axis.

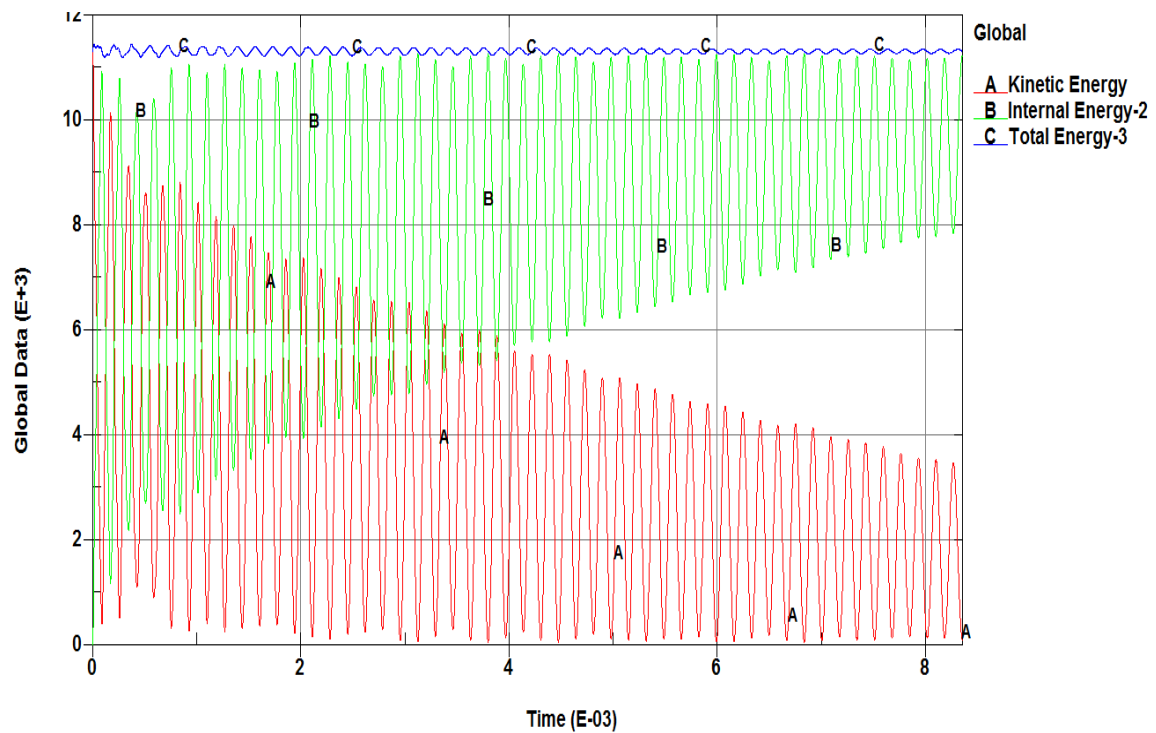


Figure 89: Energy distribution for the 2d bar using the Total Lagrange approach. Time in seconds, energy in the y axis in J.

The Gaussian approach has potential due to its capturing of the oscillations but accurate representation of the pressure and energy fields does need work. Furthermore, the huge computational cost makes it infeasible at this point.

8.10 Testing of different MEF approaches

Different field approaches were tested such as displacement-strain, velocity-rate of deformation and velocity-rate of deformation-stress. The other 2 field approaches had no effect on tensile instability, however the three-field approach had the effect of delaying the tensile instability of the Swegle box as shown.

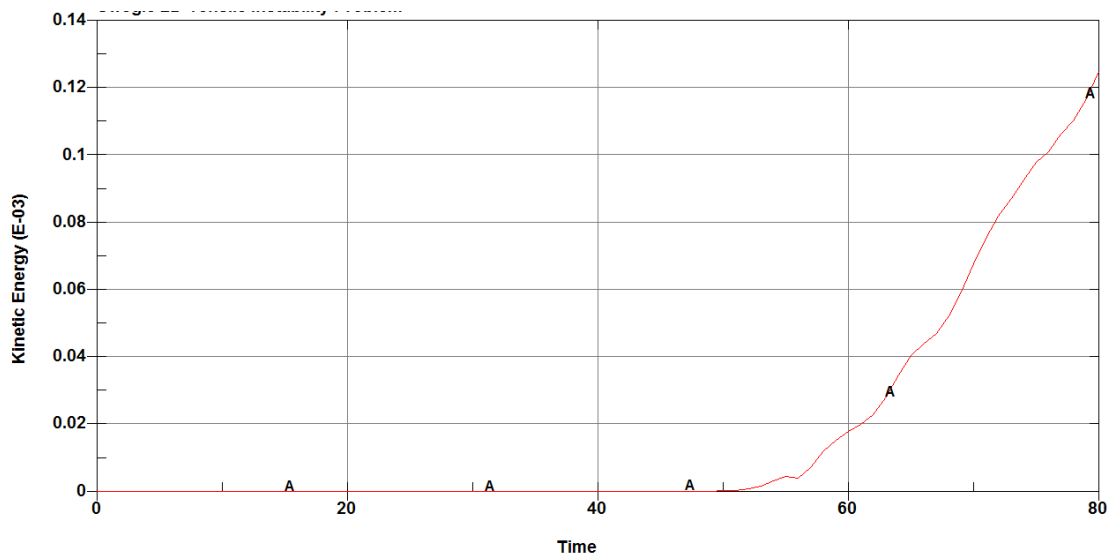


Figure 90: Energy profile of the Swegle box using the three-field velocity-Rate of deformation and stress approach. Time in seconds and energy in J.

The assumed fields were all averaged quantities and it is known that these fields have no effect on tensile instability, however the three-field approach means that the link between stress and strain as a function of displacement was weakened since so many other terms were between them. This implies that there is scope to this area of research for tensile instability.

8.11 Conclusions

This section shows the merit of using a mixed element approach to address particle clumping. A two-field approach using displacement- pressure with the assumed pressure being a pressure average was shown to address the issue and while there is the drawback of energy dissipation, that can be potentially addressed by investigation of multiplication factors that could increase in time or be sensitive to energy drops. This also acts as a good test to see if something that exhibits particle clumping is a tensile instability or zero energy problem. If it is zero energy, the mixed interpolation will suppress it, if it is tensile instability, it will not.

The work done also found that applying the difference between interpolated and approximated field quantities, no matter what scheme as a constraint on the momentum has no effect on the tensile instability problem. This approach doesn't address the cause of tensile instability. The biggest influence on the tensile instability was shown to be using a MLS kernel which emphasises that the kernel is the biggest factor in this issue and any work should look to address this or derive a force

factor that will have a realistic force profile and thus should counteract any spurious growth as if the growth goes beyond a certain point, the attractive forces shall pull it back.

Therefore, future work in applying this approach to SPH should focus on:

- Development of a factor that will stop the dissipation of energy for the displacement-averaged pressure approach.
- Further research into enhanced or assumed quantities including artificial quantities such as a repulsion or attractive force factor based on Leonard-Jones potential.
- Despite the potential of exact solution procedures, computational time and oversensitivity of matrices means that it is not feasible as a computational solution.

Chapter 9

This thesis has taken on the dual issue of addressing SPH shortcomings which are very theoretical in nature and the more practical side of extending the capability of the method to more complex fluid-structure interactions in the form of highly deformable structures and scenarios such as rotation and shaking.

The rationale for this dual approach is that any development of the SPH method needs to start from theory. As a growing numerical method which is still in its infancy, there is huge scope for research to expand the theories capability and address its shortcomings. Particle clumping is a huge issue that degrades any simulation and so by focussing on trying to reduce or eliminate this problem, we will output simulations with better results and furthermore have generality. Research that generally focuses on this issue tends to be as mentioned addressing the symptom and not the cause, or such as the case of the pressure smoothing focuses on reducing the pressure instability but not the overarching problem, which is the work of this thesis and other literature concludes from using pressure smoothing, tends to lead to further instabilities in other fields.

The work done in this thesis in the research into the use of mixed formulation in SPH as an attempt to cure SPH of the particle clumping issue indicates huge promise but practical concerns. A two-field approach using pressure nodal averaging as the pressure field gives some success in reducing the zero-energy mode problem but ultimately the solution still degrades. Making the node a pressure averaged field does make sense from a practical point of view as the nodal averaging will average out instabilities but does lack the conservation property of the 2nd mixed formulation governing equation. Attempts to use Gaussian elimination to achieve an exact solution for both pressure and displacement that satisfies the governing equations is probably too computationally expensive for a single processor computer but parallel processors could make this work.

The main thing I can conclude from the investigation is that further research into the nature of the fields is needed to make this work. Mathematically, the theory is robust and practically it does address the zero-energy node problem at its core as opposed to a heuristic addition of terms that lacks generality and rigour. It does make SPH a complete theory and adds to its development and I can conclude that mixed formulation is a viable area of research. This work has proven that it fits into the SPH framework, that it is robust mathematically, dealt with any unforeseen issues that come as a consequence to SPH application (such as singular matrices and the symmetry of the momentum equation), shown that some avenues research in the theory will not be practical in the

SPH method (such as static condensation and the 3-field approach in its pure mixed element form) and developed solution techniques not seen in literature (such as Gaussian elimination to find exact solution for the nodal fields). In addition, it has shown that unless there is research into a field that will counteract the tensile instability issue, the mixed formulation in its current form does not address tensile instability as it does nothing to break the kernel link between stress and strain. Future work in this field should now be focussed on finding fields that will a) Satisfy the Brezzi condition b) Satisfy both mixed formulations governing equations and c) Be problem specific.

In terms of the extension of the capability to complex fluid-structure interaction problems with highly deformable structures, the work has overall been a success and shown that SPH can be used to do this. The work shown shows that SPH is at least as good in terms of beam and free-surface profile as other numerical methods and is the most complex example of FSI simulation using pure SPH as opposed to coupled SPH-FE in SPH literature. Future work in this field should now be focused on extending the capability of our method in the form of a dynamic, deformable friction algorithm and cohesion that will better represent the physics of the problem and address what occurs when a deformable solid meet with a dynamic fluid more accurately as opposed to just repulsion contact. The work I have done is already developing this idea by extending the contact algorithm to include an attractive component derived on from the Leonard Jones potential and future work should focus on this. Like in the example of addressing particle clumping, by making our algorithms more robust, this will have the consequence of more accurate simulations.

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Appendix

Flowcharts for the MCM solver are detailed here. The original time integral solution loop before the additions detailed in this these is in this appendix. The additions made are in the following sub-appendices. The additions are divided into 3 sub-appendices. Appendix 1.1 details the addition of MLS density update and where that sits in within the main code. Appendix 1.2 details the addition of the boundary conditions and the repulsive force modifier and Appendix 1.3 details how the MCM solution loop looks now with the mixed element additions. Due to the complexity of the mixed element formulation, this has required creation of a new loop as opposed to the subroutine additions of MLS and boundary condition routines which can sit in within the original solution loop.

MCM central difference time integration loop

START OF STEP n

Know: $x^n, v^{n-1/2}, t^n, \Delta t^{n-1/2}, \sigma^{n-1}, \rho^{n-1}$

Calculate strain rate using positions at half step

$$x^{n-1/2} = x^n - 1/2 v^{n-1/2} \Delta t^{n-1/2}$$

$$L = (\nabla v)^T$$

$$\dot{\epsilon}^{n-1/2} = \frac{1}{2}(L + L^T) = [B]v$$

Update density

$$\rho^n = \rho^{n-1} + \rho^{n-1/2} \Delta t^{n-1/2} = \rho^{n-1} + \nabla \cdot v^{n-1/2} \Delta t^{n-1/2}$$

Calculate stress using relevent constitutive model

$$\dot{\sigma}^{n-1/2}_d = g\left(\dot{\epsilon}_d^{n-1/2}\right) = C[B]v$$

$$\sigma = \sigma^{n-1} + \dot{\sigma}^{n-1/2} \Delta t^{n-1/2}$$

Solve momentum equation

$$f_i^n = \int ([B_d]^T \sigma^n) = \int ([B_d]^T C[B] dV v)$$

M is lumped mass, so we get:

$$Ma + f_i^n = 0$$

Time, velocity and position are all updated then the loop repeats

This loop solves equation (152)

Appendix 1.1 MCM time integration loop with MLS code addition.

START OF STEP n

Know: $x^n, v^{n-1/2}, t^n, \Delta t^{n-1/2}, \sigma^{n-1}, \rho^{n-1}$

Calculate strain rate using positions at half step

$$x^{n-1/2} = x^n - 1/2 v^{n-1/2} \Delta t^{n-1/2}$$

$$L = (\nabla v)^T$$

$$\dot{\varepsilon}^{n-1/2} = \frac{1}{2}(L + L^T) = [B]v$$

Update density

$$\begin{aligned} \rho^n &= \rho^{n-1} + \rho^{n-1/2} \Delta t^{n-1/2} \\ &= \rho^{n-1} + \nabla \cdot v^{n-1/2} \Delta t^{n-1/2} \end{aligned}$$

MLS update

$$\begin{aligned} \rho^n &= \rho^{n-1} + \rho^{n-1/2} \Delta t^{n-1/2} \\ &= \rho^{n-1} + W_{MLS}^{n-1/2} \Delta t^{n-1/2} \end{aligned}$$

Calculate stress using relevant constitutive model

$$\dot{\sigma}^{n-1/2}_d = g\left(\dot{\varepsilon}_d^{n-1/2}\right) = C[B]v$$

$$\sigma = \sigma^{n-1} + \dot{\sigma}^{n-1/2}_d \Delta t^{n-1/2}$$

Solve momentum equation

$$f_i^n = \int ([B_d]^T \sigma^n) = \int ([B_d]^T C[B] dV v)$$

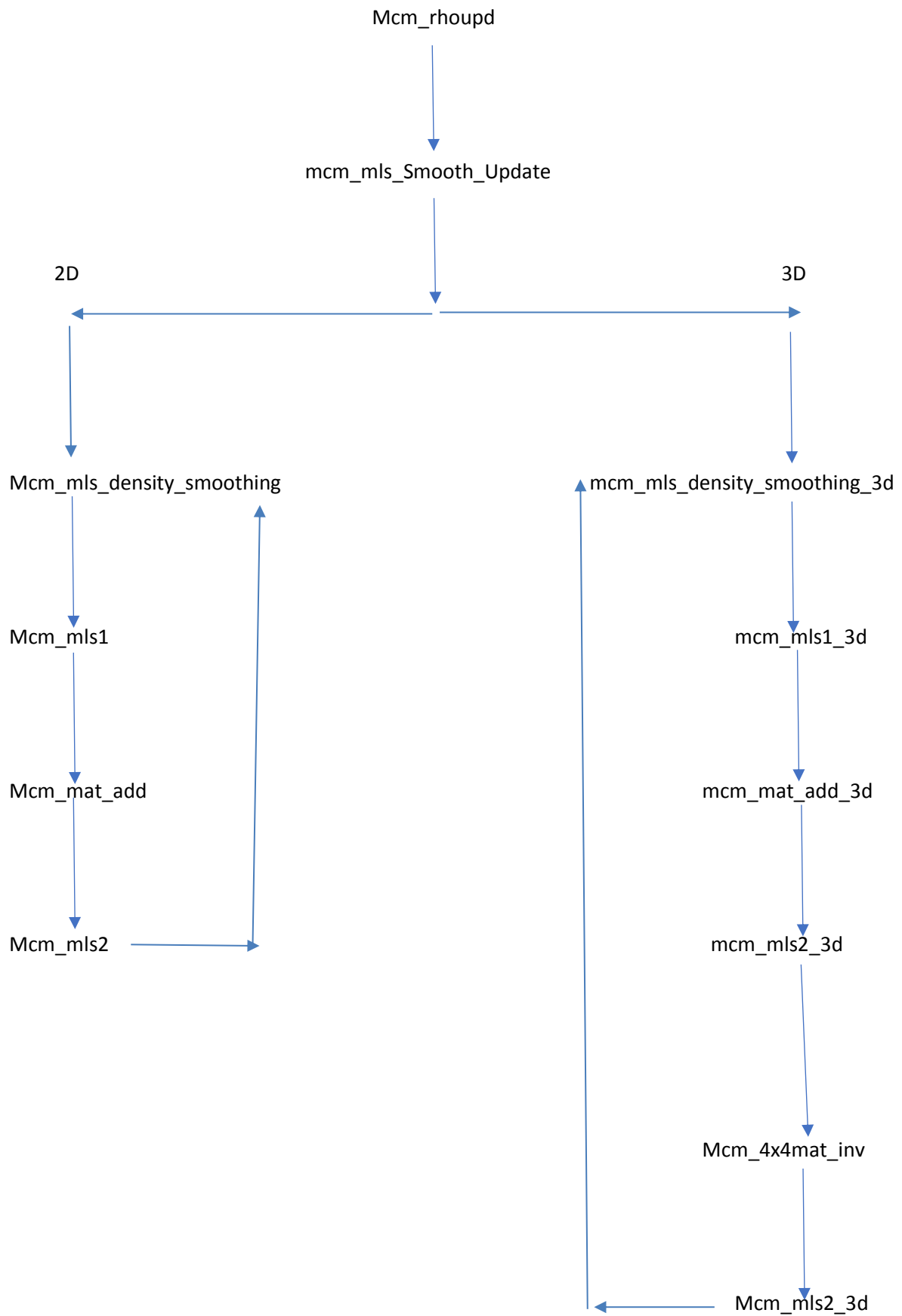
M is lumped mass, so we get:

$$Ma + f_i^n = 0$$

Time, velocity and position are all updated then the loop repeats

This loop solves equation (152)

Local MLS code structure



Appendix 1.2: Loop for rotational boundary conditions

START OF STEP n

Know: $x^n, v^{n-1/2}, t^n, \Delta t^{n-1/2}, \sigma^{n-1}, \rho^{n-1}$

Calculate strain rate using positions at half step

$$x^{n-1/2} = x^n - 1/2 v^{n-1/2} \Delta t^{n-1/2}$$

$$L = (\nabla v)^T$$

$$\dot{\epsilon}^{n-1/2} = \frac{1}{2}(L + L^T) = [B]v$$

Update density

$$\rho^n = \rho^{n-1} + \rho^{n-1/2} \Delta t^{n-1/2} = \rho^{n-1} + \nabla \cdot v^{n-1/2} \Delta t^{n-1/2}$$

Calculate stress using relevant constitutive model

$$\dot{\sigma}^{n-1/2}_d = g\left(\dot{\epsilon}_d^{n-1/2}\right) = C[B]v$$

$$\sigma = \sigma^{n-1} + \dot{\sigma}^{n-1/2} \Delta t^{n-1/2}$$

Solve momentum equation

$$f_i^n = \int ([B_d]^T \sigma^n) = \int ([B_d]^T C[B] dV v)$$

M is lumped mass, so we get:

$$Ma + f_i^n = 0$$

Apply boundary conditions

$$d = \bar{d}$$

$$v = \bar{v}$$

Time, velocity and position are all updated then the loop repeats

This loop solves equation (152) and the boundary conditions are applied as rotational prescribed displacements by equation (118) for 2D and (120)-(122) for 3D. The code also prescribes velocity boundary conditions by resolving velocity into parallel and perpendicular components. Both algorithms are in the following link.

Appendix 1.3: Mixed element solution loop

START OF STEP n

Know: $x^n, v^{n-1/2}, t^n, \Delta t^{n-1/2}, \sigma^{n-1}, \rho^{n-1}$

Calculate strain rate using positions at half step

$$x^{n-1/2} = x^n - 1/2 v^{n-1/2} \Delta t^{n-1/2}$$

$$L = (\nabla v)^T$$

$$\dot{\varepsilon}^{n-1/2} = \frac{1}{2}(L + L^T) = [B]v$$

For displacement-pressure formulation, B needs to be split, so that strain can be decomposed into volumetric and deviatoric strain rate.

Calculate deviatoric strain rate

$$\dot{\varepsilon}_d^{n-1/2} = [B_d]v$$

Calculate volumetric strain rate

$$\dot{\varepsilon}_v^{n-1/2} = [B_v]v$$

Update density

$$\rho^n = \rho^{n-1} + \rho^{n-1/2} \dot{\varepsilon}_v^{n-1/2} \Delta t^{n-1/2} = \rho^{n-1} + \nabla \cdot v^{n-1/2} \Delta t^{n-1/2}$$

Calculate pressure using relevant constitutive model/equation of state(f) and develop Kpp matrix using perturbed lagrangian if not invertable.

$$\dot{p}^{n-1/2} = K_{pp}^{-1} K_{pu} v = \frac{1}{f} H_p^T H_p B_v^T H_p \hat{u}$$

$$p^n = p^{n-1} + \dot{p}^{n-1/2} \Delta t^{n-1/2}$$

Calculate deviatoric stresses using relevant constitutive model/equation of state(g)

$$\dot{\sigma}_d^{n-1/2} = g \left(\dot{\varepsilon}_d^{n-1/2} \right) = C [B_d]v$$

$$\sigma_d^n = \sigma_d^{n-1} + \dot{\sigma}_d^{n-1/2} \Delta t^{n-1/2}$$

Solve mixed element momentum equation

$$f_i^n = \int ([B_v]^T P^n + [B_d]^T \sigma_d^n)$$

$$\mathbf{M}\hat{\mathbf{u}} + \mathbf{K}_{uu}\hat{\mathbf{u}} + \mathbf{K}_{up}\hat{\mathbf{p}} = 0$$

Update time, velocity and position in the same way as we normally do in the code.

The three key differences between this and the pure displacement approach used to derive our time integration loop are

- 1) The splitting of strain tensor into deviatoric and volumetric parts at the top level as opposed to at the constitutive level
- 2) Calculation of $\mathbf{K}_{pp}$ matrix when solving for pressure at the constitutive relation level and the smoothing of the rate of deformation by $\mathbf{H}_p$
- 3) The additional terms added to the momentum equation which come as a consequence of the mixed formulation
