

Efficient Coupling Methods for the Dynamic Modelling of Heterogeneous Systems

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Abstract

The ability to predict the behaviour of systems, subject to time-dependent loads, is crucial for a wide variety of engineering applications. Employed from the nano to the macro-scale, the Finite Element Method (FEM) has proven to be a versatile computational approach for dynamic modelling. However, current implementations of the method struggle to balance the competing demands of computational efficiency versus accurate and stable simulations. Coupling methods appear to be a solution to this problem. This research focuses on the formulation and application of novel coupling methods with explicit FEM. It enhances the current state-of-the-art methods, particularly for those applied to heterogeneous systems. This thesis investigates concurrent coupling methods; leveraging multi-time step integration temporally, and non-matching mesh algorithms spatially. Enabling the use of different time steps across subdomains, whilst circumventing their requirement to spatially conform, produces a framework to handle heterogeneous discretisations effectively.

The proposed method utilises a partitioning of a computational domain, to solve the dynamic equilibrium in each subdomain independently. Kinematic and kinetic continuity of these subdomain interfaces are enforced, to ensure a precise solution without the generation of numerical artifacts. This optimisation not only expedites the simulation runtime, but also enables more flexible geometric modelling. The algorithms are benchmarked against traditional monolithic methods, including special limit cases, with highly heterogeneous configurations. The tolerance to which conservative laws are obeyed are quantified, with particular attention given to the behaviour at the coupled interfaces.

The results show a combined coupling of multi-time stepping and non-matching meshes produce a computational speedup of over $12\times$ uncoupled methods. To assess the speedup and stability in complex heterogeneous systems, the stress wave propagation in metamaterials and the dynamic loading of a compact-tension specimen are demonstrated. These depict the ability of the framework to resolve deformation in real world systems. The proposed algorithms implicate the inefficient implementations of current solvers, by providing the tools for resolving short term phenomena.

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Dedicated to Nik
Your spirit will forever inspire

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Personal

A place I have frequented during my time in Oxford is a small restaurant on the corner of Gloucester Green, namely BBuona. Known for its pinsa, not pizza, I have enjoyed many a slice at this fine establishment with colleagues, friends, and family. In true BBuona fashion, I hope to express my deepest gratitude to all those that have supported me during my DPhil through the power of pinsa. However, I am sure that I will have missed some ingredients. To those below, and to those I may have forgotten - I would like to share a slice with you.

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Abstract

The ability to predict the behaviour of systems, subject to time-dependent loads, is crucial for a wide variety of engineering applications. Employed from the nano to the macro-scale, the Finite Element Method (FEM) has proven to be a versatile computational approach for dynamic modelling. However, current implementations of the method struggle to balance the competing demands of computational efficiency versus accurate and stable simulations. Coupling methods appear to be a solution to this problem. This research focuses on the formulation and application of novel coupling methods with explicit FEM. It enhances the current state-of-the-art methods, particularly for those applied to heterogeneous systems. This thesis investigates concurrent coupling methods; leveraging multi-time step integration temporally, and non-matching mesh algorithms spatially. Enabling the use of different time steps across subdomains, whilst circumventing their requirement to spatially conform, produces a framework to handle heterogeneous discretisations effectively.

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Dissemination

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List of Abbreviations

1-D, 2-D, 3-D	One- or two or three-dimensional, referring in this thesis to spatial dimensions.
BV	Bulk viscosity.
CPFEM	Crystal plasticity finite element method.
DOF	Degree(s) of freedom.
EFG	Element-free Galerkin.
FEM	Finite element method.
FSI	Fluid structure interaction.
IGA	Isogeometric analysis.
LHS	Left hand side.
LLM	Localised Lagrange multipliers.
ML	Machine learning.
MM	Mortar methods.
mts	Multi-time stepping.
mono.	Monolithic single time step solution.
NURBS	Non-uniform rational B-splines.
NEFEM	NURBS-enhanced finite element methods.
PFPB	Push-forward pullback.
PINN	Physics-informed neural network.
PUM	Partition of unity methods.
QS	Quasi-static.
RBF	Radial basis function.
RHS	Right hand side.
RKPM	Reproducing kernel particle methods.
RMSE	Root mean squared error.

RVE		Representative volume element.
ref.		Reference solution.
SEM		Spectral element method.
SIF		Stress intensity factor.
SPH		Smoothed-particle hydrodynamics.
VEM		Virtual element method.
XFEM		Extended Finite element method.

List of Symbols

A	area
$\mathcal{A}$	differential operator
α	weighting factor
$\mathcal{B}$	deformable body
$\mathbf{B}$	spatial derivatives of shape functions
$(\bar{\cdot})$	prescribed quantity
$\mathbf{C}$	incidence matrix (global to interface)
c	dilatational wave speed in medium
$\mathbf{D}$	rate of deformation
d	dimension
Δt	time step
Δt_C	critical time step
$\delta(\cdot)$	variational operator
E	Young's modulus
e	element
η	second component of the spatial coordinates in parent element domain
$\mathbf{F}$	deformation gradient
$\mathbf{f}^{ext}$	external force
$\mathbf{f}^{int}$	internal force
$(\cdot)_f$	frame quantity
G	shear modulus
g	mapping
Γ	interface
γ	hyperparameters

H	Heaviside function
h	characteristic length
$(\hat{\cdot})$	analytical quantity
$\mathbf{I}$	identity matrix
i	index
$ \mathbf{J} $	determinant of the Jacobian
$\mathbf{K}$	global stiffness matrix
K	stress intensity factor
k	step counter
$\mathbf{L}$	incidence matrix (interface to global)
$\mathbf{l}$	velocity gradient
λ	localised Lagrange multiplier
λ	Lamé's first constant
$\mathbf{M}$	mass matrix
m	time step ratio
μ	Lamé's second constant
$\mathcal{N}_{(\cdot)}$	number of quantity
$\mathbf{N}$	interpolation (or shape) functions
$\mathbf{n}$	unit normal
∇	divergence
Ω	subdomain
ω	frequency
P	power
$\mathbf{p}$	momentum
$\mathbf{R}$	restriction coupling operator
$\mathbb{R}$	set of real numbers
ρ	density
r	radius
$\mathcal{S}$	collection of subdomains
$\boldsymbol{\sigma}$	Cauchy stress tensor
$\mathbf{t}$	traction

T	final time
t	time
$(\cdot)_T$	trial quantity
τ	shear stress
θ	angle
$(\cdot)^{\mathbf{T}}$	transpose of a quantity
$(\tilde{\cdot})$	unconstrained kinematic quantity
$\mathbf{u}$	displacement
$\dot{\mathbf{u}}$	velocity
$\ddot{\mathbf{u}}$	acceleration
V	volume
$ \bar{\varepsilon} $	mean absolute error
φ	virtual basis functions
$\mathbf{W}$	spin tensor
W	work done
$\mathbf{X}$	Lagrangian (material) coordinates
$\mathbf{x}$	Eulerian (spatial) coordinates
ξ	first component of the spatial coordinates in parent element domain
$\mathbb{Z}$	integer set of numbers
z	thickness
ζ	third component of the spatial coordinates in parent element domain
$(\cdot)_0$	initial quantity

1

Introduction

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This chapter presents the motivation for this thesis, its key aims, and the objectives of the work. The research strategy to tackle these are provided, as well as the overall structure of the thesis.

1.1 Motivation

The demand for modelling the dynamic behaviour of complex engineering structures across multiple scales is following a rapidly increasing trend. Certification, design and optimisation are just some of the primary catalysts that drive this trend. From modelling the macroscopic response of entire systems, to the microscopic interactions of grains and molecules, the understanding of behaviour across multiple scales is critical to the performance of engineering structures. Creating computational approaches that bridge these analyses at different temporal and spatial scales are fundamental to today's models. Numerical methods allow engineers to capture the multi-scale behaviour of structures, whilst involving a variety of phenomena.

Spanning across multiple physical processes such as thermal, fluid dynamics, and mechanical, reliable numerical simulations are imperative to solving modern engineering challenges.

In the modern-era of scientific computing, challenges remain to fully resolve the behaviour of structures at all scales, and for all phenomena. Resolving such behaviour remains infeasible when considering the finest of scales in both space and time. In these cases, traditional numerical methods necessitate exceedingly small discretisations that lead to prohibitively high computational costs. To avoid such high computational costs coarser representations may be chosen, however such techniques may lead to approximate or incomplete solutions with severe error. This presents the trade-off between efficiency and accuracy, providing motivation for the development of methods that balance computational feasibility with the required fidelity.

To address these challenges of traditional methods, researchers have developed hierarchical and concurrent coupling methods. Hierarchical coupling methods focus on the up-scaling of the finer behaviour to coarser temporal or spatial scales. While significant progress has been made in hierarchical methods, concurrent coupling methods are still lacking. Concurrent coupling methods allow for real-time interactions between scales and phenomena to be resolved. Through the parallelism of these methods, both the localised phenomena and global system behaviour can be solved simultaneously. This highlights a potential benefit when compared to the prior, enabling rapid changes in behaviour to be captured accurately. Concurrency is therefore a clear necessity in the context of accuracy and efficiency, to allow for the parallel processing of a coupled structure.

Concurrent coupling methods have shown to be inherently versatile and applicable to a wide range of heterogeneous problems. In the context of solid mechanics, these problems are conventionally viewed as a structure with varying material properties throughout. However, more broadly heterogeneity comes in many forms, including the numerical choice of discretisation. Heterogeneous discretisations benefit from coupling methods through enabling larger time steps and mesh sizes in

less dynamic regions, whilst smaller in regions of high variability. This combination of coupling methods with heterogeneous discretisations is particularly compelling when considering the large-scale meshes of structures such as Figure 1.1. The finite element mesh of the gas turbine presented highlights the variation in discretisation that may be leveraged in real world structures. Subsequently, the work in this thesis is part of a wider research effort to drive new simulation technologies for ultra-high resolution at extreme scales. It forms a small piece of the Prosperity Partnership for Advanced Simulation and Modelling of Virtual Systems (ASiMoV), which looks to develop numerical methods that may one day be scaled to the next generation of Exascale supercomputers.

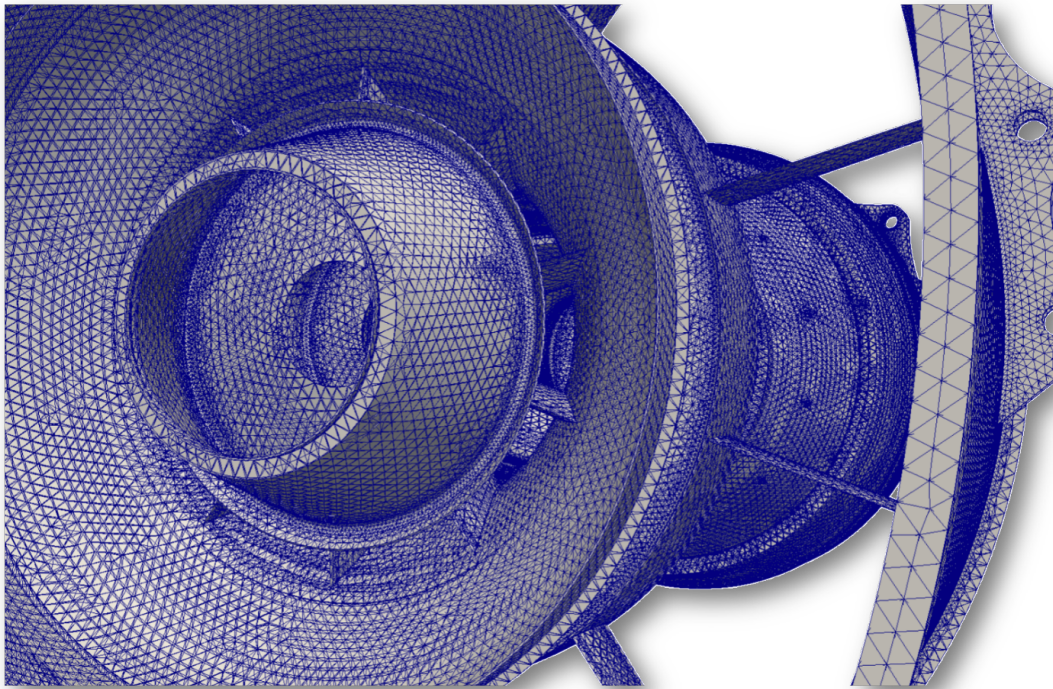


Figure 1.1: Finite element mesh of the gas turbine Crescendo mesh as presented by the ASiMoV consortium supported by Rolls Royce’s prosperity partnership with reference EP/S005072/1.

In summary, this thesis proposes the development of novel coupling algorithms that concurrently solve heterogeneously discretised structures both temporally and spatially. The need for accelerating simulations is clear, whilst also capturing accurately the physics of dynamic systems. Applying these coupling techniques

to short-term mechanical phenomena will therefore allow numerical methods to predict the deformation of materials subject to impact loading in a more efficient and precise manner. Consequently, by developing innovative algorithms and methodologies this work looks to advance the state-of-the-art coupling methods for robust implementation.

1.2 Aims and Objectives

The main aim of the conducted research is to significantly enhance the computational performance of numerical simulations involving heterogeneously discretised solid bodies subjected to dynamic loading. This is done by developing coupling techniques for multiple partitions of a structure within an explicit finite element method (FEM) framework. The algorithms must adhere to the laws of conservation, to preserve the accuracy and stability of conventional monolithic (uncoupled) approaches. Subsequently, the specific objectives of this thesis are:

- to develop novel numerical methods that enable the simulation of structures with multiple time steps,
- to develop numerical capability permitting discretisations in space that do not necessarily match throughout a structure,
- and to demonstrate the implementation of the coupling algorithms for mechanical phenomena, with comparison to traditional uncoupled solutions.

1.3 Research Strategy

To fulfil the aims and objectives the following strategy has been defined. Firstly, a comprehensive literature review guides the selection of the appropriate numerical methods required to model the dynamic behaviour of solid structures. This is followed by an assessment of those coupling methods that can be used in conjunction with the selected method. Methods that cover multiple numerically discretised scales, whilst modelling mechanical phenomena are the focus of this investigation.

The key limitations of each of the methods is explained, whilst foreshadowing the research gaps that the subsequent chapters aim to fulfil.

Algorithms that exploit multiple time steps are investigated, utilising a two-subdomain problem as the starting point of exploration. The partitioning of a solid structure with a large and small time step is proposed with the temporal coupling employed on the boundary of the two. Through the re-implementation of state-of-the-art methods that exercise the widely used Lagrange multiplier method, a comparison is made to assess the success of the novel algorithm, evaluating against the aims stated previously. The stability and continuity of kinematics over the interface between subdomains is assessed, even for very extreme configurations and loadings. At the interfaces between coupled domains, close attention is given to ensure the governing equations are obeyed and that the system is conservative. A new method in extending this two-domain algorithm to multiple domains is proposed, thereby enabling multiple time steps beyond the traditional two-time step coupling. Hence, the ingredients for integrating real world structures are provided with the evaluation of a stress wave propagation problem in metamaterials. Accuracy is shown to be maintained within a reasonable tolerance, whilst significantly speeding up the solution. Uncoupled simulations with a single time step are used as a baseline for the evaluation of the novel algorithms.

Coupling in space is presented with the prominent problem of non-matching meshes. It is subsequently addressed with the development of coupling algorithms that allow for the propagation of information from one subdomain to another. Starting similarly with two independently resolved regions, large and small mesh sizes are coupled on a non-matching interface in space. The coupling is achieved with conventional Lagrangian interpolation functions that ensure continuous interfacial quantities, regardless of spatial discretisation. The methodology is presented in its most basic form with 2-D spatial discretisations, defining each of the numerical operations required for a conservative coupling. Mixed element formulations and extensions to 3-D can then be extended to, allowing for greater flexibility when discretising a problem spatially. A common experimental problem is modelled with

varying spatial discretisations. The dynamic loading generates considerably high stress gradients in a localised region of a finely discretised domain. Once again, a quantitative comparison can be made for the coupled solution with an uncoupled reference that employs a single fine mesh discretisation. The final combination of both temporal and spatial coupling methods proves to be of great potential when accurately speeding up the solution of these dynamic models.

1.4 Thesis Outline

The thesis is organised as follows. Chapter 2 captures the state-of-the-art numerical techniques relevant to the dynamic modelling of heterogeneous solids and coupling methods. The literature review provides the foundation for this thesis, as well as identifying the open research questions that require addressing in the following chapters. Chapter 3 introduces the variational formulation of the governing equations, partitioning them to allow for the finite element discretisation of individual subdomains. A novel multi-time stepping algorithm is presented, with an assessment of its stability and comparison to the state-of-the-art. A practical extension to multiple subdomains is made and utilised within 3-D numerical examples. Chapter 4 formulates the coupling operators required to create an innovative spatial coupling algorithm for addressing the problem of non-matching meshes. The dynamic behaviour of numerical examples are captured with the method, and once combined with the temporal coupling a vast acceleration in simulation runtime is achieved. In Chapter 5, concluding remarks are made with recommendations for future work. Appendices include an additional highly heterogeneous benchmark, as well as description of an open source FEM code.

2

Literature Review

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The current state-of-the-art is assessed in this chapter, together with the building blocks of research that have preceded this thesis. The review initially describes the numerical methods used to conventionally capture the dynamic behaviour of solid structures, followed by those coupling techniques that define interfaces between meshes. Methods that couple subdomains with different time discretisations are

reported first, followed by those that vary spatial discretisations at the interface. Previous applications of coupling algorithms are mentioned, highlighting those opportunities for further investigation.

2.1 Dynamic Modelling of Heterogeneous Solids

Heterogeneous solids are materials composed of distinct regions or phases whose physical properties vary spatially throughout their volume [3]. These materials can exhibit non-uniformity in their structure with the presence of grains, fibres, inclusions or layers - just to name a few. Ubiquitous across engineering disciplines, heterogeneity is found in polycrystalline, polymeric and composite materials. The innate variance of properties in these materials create significant challenges in predicting the mechanical behaviour under a variety of loading conditions.

Capturing the dynamic response of heterogeneous solids is of prime importance when considering the design of impact-resistant structures. Multi-scale in their behaviour, short-term phenomena can require the knowledge of multiple temporal and spatial scales [4]. From micro- to macro-scale, the local deformation through time has been a topic of interest to evaluate the overall structural responses that emerge from the interplay of lower scales [5, 6]. At the continuum-level, heterogeneity is also vast throughout, where homogenised properties simply do not capture the behaviour of materials sufficiently [7]. The deformation of a solid domain Ω , at time $t \in [0, T]$, is governed by the following set of equations as:

$$\nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{b} = \rho \ddot{\mathbf{u}}, \text{ in } \Omega \times [0, T] \quad (2.1)$$

$$\dot{\mathbf{u}} = \bar{\dot{\mathbf{u}}}, \text{ on } \partial\Omega_v \times [0, T] \quad (2.2)$$

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \bar{\mathbf{t}}, \text{ on } \partial\Omega_t \times [0, T] \quad (2.3)$$

$$\mathbf{u}(\mathbf{X}, 0) = \mathbf{u}_0, \text{ in } \Omega \quad (2.4)$$

$$\dot{\mathbf{u}}(\mathbf{X}, 0) = \dot{\mathbf{u}}_0, \text{ in } \Omega \quad (2.5)$$

where in Equation 2.1 $\nabla \cdot \boldsymbol{\sigma}$ is the divergence of the Cauchy stress tensor, ρ the density, $\mathbf{b}$ the body force per unit mass and $\ddot{\mathbf{u}}$ the acceleration in the strong form of the linear momentum. The prescribed velocity $\bar{\dot{\mathbf{u}}}$ and prescribed traction $\bar{\mathbf{t}}$ act on

their own respective external boundaries $\partial\Omega$. Their definition is determined by $\mathbf{n}$ as the unit normal vector, and $\dot{\mathbf{u}}$ and $\boldsymbol{\sigma}$ called upon, as they are more conveniently determined in engineering problems [8]. Initial terms are denoted $(\cdot)_0$ with material $(\mathbf{X})$ coordinates. Within the solid domain, the interior continuity condition dictates:

$$\llbracket \mathbf{n} \cdot \boldsymbol{\sigma} \rrbracket = 0, \text{ on } \Gamma_{\text{int}} \quad (2.6)$$

$$\llbracket \mathbf{u} \rrbracket = 0, \text{ on } \Gamma_{\text{int}} \quad (2.7)$$

where the normal components of stress and the displacement field are continuous on internal interfaces Γ_{int} , also known as the interior continuity conditions. These conditions are key for the partitioning of a solid, where equilibrium across Γ is required through time. Numerous computational approaches have tackled this strong form, enabling the study of solid domains with dynamic effects. In the current section, these methods are broadly categorised to encompass the state-of-the-art techniques, consequently depicting which are optimal for the study of heterogeneous solids in the thesis.

2.1.1 Approximating the Strong Form

Various numerical methods can be employed to model the dynamic behaviour of solids. Starting with the foundational tool of the finite difference method (FDM), the derivatives of the partial differential equation (PDE) in Equation 2.1 are approximated in both space and time. The strong form of the momentum equation in 1D can be expressed as:

$$\frac{\partial \sigma}{\partial x} = \rho \frac{\partial^2 u}{\partial t^2} \quad (2.8)$$

where σ is the stress, u the displacement, ρ the density, x the position, and t the time. The body forces are omitted for simplicity in this preliminary introduction to methods. To solve Equation 2.8 with finite differences, a discretisation in space (Δx) and time (Δt) is required. The displacement at each grid point u_{i+1}^n is denoted with i as the spatial index, and n the time step. First and second-order finite differences are derived from the Taylor series by expanding a function about a point

and truncating higher-order terms [9]. Variations of FDM methods are plentiful, but the key ideas of approximating the derivatives are as follows:

$$\frac{\partial \sigma}{\partial x} \approx \frac{\sigma_{i+1}^n - \sigma_{i-1}^n}{2\Delta x}, \quad \frac{\partial^2 u}{\partial t^2} \approx \frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{(\Delta t)^2} \quad (2.9)$$

The finite difference approximations of the strong form are found at each grid point iterating for each time step. The method extends to higher dimensions in space through accounting for variation in Δy and Δz , whilst approximations in time remain the same. Figure 2.1 illustrates the standard templates of the 2-D and 3-D cases with spatial indexes i, j, k . For example, extending to 2-D in space requires the approximation with the additional index j and grid spacing Δy :

$$\nabla \cdot \boldsymbol{\sigma} \approx \left(\frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} \right) \approx \left(\frac{\frac{\sigma_{xx,i+1,j}^n - \sigma_{xx,i-1,j}^n}{2\Delta x} + \frac{\sigma_{xy,i,j+1}^n - \sigma_{xy,i,j-1}^n}{2\Delta y}}{\frac{\sigma_{yx,i+1,j}^n - \sigma_{yx,i-1,j}^n}{2\Delta x} + \frac{\sigma_{yy,i,j+1}^n - \sigma_{yy,i,j-1}^n}{2\Delta y}} \right) \quad (2.10)$$

These equations illustrate how finite difference methods are generally structured around regular grids. This limits their application when considering complex geometries or irregular domains. Managing these grid spacing aspects can become problematic when ensuring the accuracy and stability finite differences [10, 11]. Temporally, they have proven robust in the single dimension of time. As a result, numerical methods that replace these discrete points in space by subdomains or elements are further investigated. This starts with defining a mesh for the domain.

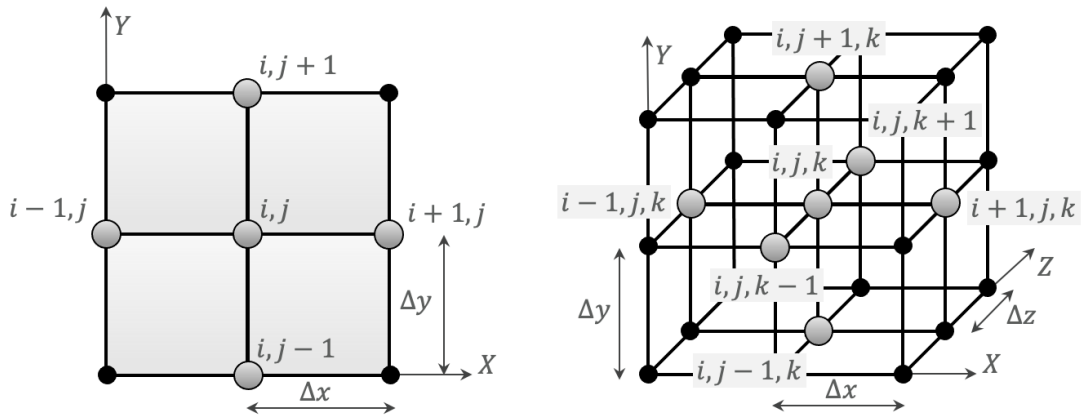


Figure 2.1: (a): 2-D finite difference grid with approximation between 5 grid points; (b): 3-D finite difference grid with approximation using 7 grid points.

2.1.2 Mesh-Based Methods with the Weak Form

This section examines various mesh-based numerical methods that approximate system variables, all of which are derived from the variational (weak) form of the governing PDE. While strong formulations directly enforce differential equations and require highly smooth solutions, their weak counterparts convert PDEs into integral forms that offer easier handling of complex boundary conditions, greater flexibility, and improved stability [12]. Firstly, an overview of these principles are given, as a common step to all proceeding mesh-based methods.

Through denoting a scalar quantity Π , the variation is presented as an integral for each point in a domain Ω with:

$$\delta\Pi = \int_{\Omega} \delta\dot{\mathbf{u}}^T \mathcal{A}(\dot{\mathbf{u}}) d\Omega = 0 \quad (2.11)$$

where $\dot{\mathbf{u}}$ is the unknown function, and $\mathcal{A}$ corresponds to the set of differential equations that govern a physical process. For arbitrary changes $\delta\dot{\mathbf{u}}$, the solution of the problem requires the variation to be $\delta\Pi = 0$. Considering the components of stress (σ, τ) in the strong form of Equation 2.1, this set of equations is represented as:

$$\mathcal{A} = \begin{Bmatrix} A_1 \\ A_2 \\ A_3 \end{Bmatrix} = - \begin{Bmatrix} \frac{\partial\sigma_x}{\partial x} + \frac{\partial\tau_{xy}}{\partial y} + \frac{\partial\tau_{xz}}{\partial z} + \rho b_x \\ \frac{\partial\tau_{xy}}{\partial x} + \frac{\partial\sigma_y}{\partial y} + \frac{\partial\tau_{yz}}{\partial z} + \rho b_y \\ \frac{\partial\tau_{xz}}{\partial x} + \frac{\partial\tau_{yz}}{\partial y} + \frac{\partial\sigma_z}{\partial z} + \rho b_z \end{Bmatrix} = 0 \quad (2.12)$$

Rate of deformation $\mathbf{D}$ is used as the strain measure for this thesis, where each component is defined as a function of velocities:

$$\dot{\mathbf{u}} = \begin{bmatrix} \dot{u}_x & \dot{u}_y & \dot{u}_z \end{bmatrix}^T \quad (2.13)$$

in three dimensions, storing each component in a vector defined with $(\cdot)^T$ denoting the transpose. A trial function is then defined, also referred to as an arbitrary weighting function. Notably, the interpolation functions of the different numerical methods can be interchanged here. Here this vector is introduced as:

$$\delta\dot{\mathbf{u}} = \begin{bmatrix} \delta\dot{u}_x & \delta\dot{u}_y & \delta\dot{u}_z \end{bmatrix}^T \quad (2.14)$$

Substituting Equations 2.12 - 2.14 into the integral of the variational form gives the following expression for the internal and external power of the system:

$$\delta\Pi = - \int_{\Omega} \left[\delta\dot{u}_x \left(\frac{\partial\sigma_x}{\partial x} + \frac{\partial\tau_{xy}}{\partial y} + \frac{\partial\tau_{xz}}{\partial z} + \rho b_x \right) + \delta\dot{u}_y (A_2) + \delta\dot{u}_z (A_3) \right] d\Omega = 0 \quad (2.15)$$

Through integration by parts, this expands to:

$$\begin{aligned} \int_{\Omega} \left[\frac{\partial\delta\dot{u}_x}{\partial x} \sigma_x + \left(\frac{\partial\delta\dot{u}_x}{\partial y} + \frac{\partial\delta\dot{u}_y}{\partial x} \right) \tau_{xy} + \cdots - \delta\dot{u}_x \rho b_x - \delta\dot{u}_y \rho b_y - \delta\dot{u}_z \rho b_z \right] d\Omega \\ - \int_{\Gamma} [\delta\dot{u}_x t_x + \delta\dot{u}_y t_y + \delta\dot{u}_z t_z] d\Gamma = 0 \end{aligned} \quad (2.16)$$

where the traction condition solely integrates over the boundary $d\Gamma$. Rewritten in a more succinct manner, the variational form for the internal and external components of a solid body in equilibrium can be written as:

$$\int_{\Omega} \delta\mathbf{D}^T \boldsymbol{\sigma} d\Omega - \int_{\Omega} \delta\dot{\mathbf{u}}^T \rho \mathbf{b} d\Omega - \int_{\Gamma} \delta\dot{\mathbf{u}}^T \mathbf{t} d\Gamma = 0 \quad (2.17)$$

From Equation 2.17, it is evident that methods employing the weak form of the physical process, seek the approximate forms of:

$$\dot{\mathbf{u}} \approx \sum_i \mathbf{N}_i \dot{\mathbf{u}}_i; \quad \delta\dot{\mathbf{u}} \approx \sum_i \mathbf{N}_i \delta\dot{\mathbf{u}}_i \quad (2.18)$$

where for now, $\mathbf{N}_i$ are introduced as arbitrary functions used in terms of independent variables. This introduction summarises some of the key concepts from mathematical pioneers such as Rayleigh and Ritz, demonstrating the variational process, used in many of today's numerical methods [13]. This literature review proceeds to investigate mesh-based methods and their approximation of system variables.

A foundational method that still lies at the forefront of mesh-based methods is the Finite Element Method (FEM). With widespread use in computational mechanics, the method has been thoroughly explored in literature, and employed across a broad spectrum of engineering industries [8, 14]. FEM discretises a geometry into elements and nodes, which are used to solve the mathematical equations necessary to determine the kinetic and kinematic quantities of a domain [12]. The velocity field $\dot{\mathbf{u}}(\mathbf{x})$ can be estimated through time t with:

$$\dot{\mathbf{u}}(\mathbf{x}, t) \approx \sum_{i=1}^{\mathcal{N}_n} \mathbf{N}_i(\mathbf{x}) \dot{\mathbf{u}}_i(t) \quad (2.19)$$

where the contribution over $\mathcal{N}_n$ nodes is summed with shape functions $N_i(\mathbf{x})$ for each node i . Traditional FEM solvers select one of two routes; implicit or explicit [8]. The prior is favoured for quasi-static or simulations with large time steps due to the property of unconditional stability [15]. At each time step, implicit methods solve a system of algebraic equations iteratively making them well suited for scenarios where convergence to equilibrium is critical. However, for problems involving short time scales, explicit FEM has dominated, due to its ability to handle higher strain rates, large deformation and nonlinear material behaviour [12]. Although explicit FEM requires much smaller time steps than implicit methods due to its conditional stability, it avoids solving global systems of equations at each time step, making it more favourable for modelling the highly dynamic behaviour of solids [8]. Its usage is widespread amongst multiple scales, as depicted in Figure 2.2, from the simulation of individual crystals to full structural systems. Several methods have also stemmed from traditional FEM.

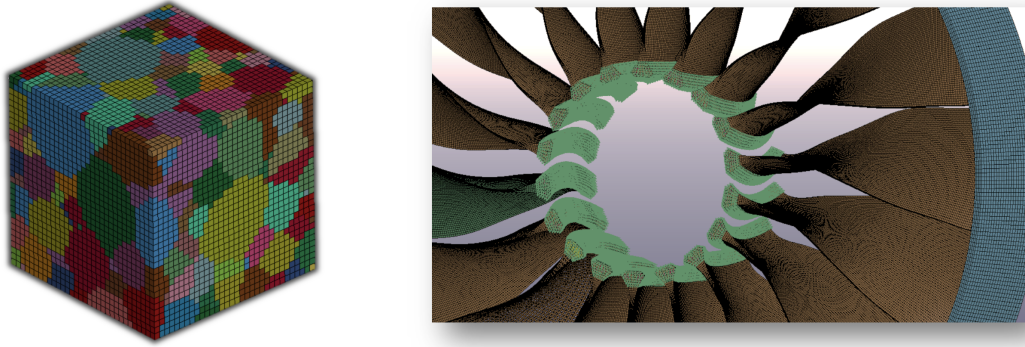


Figure 2.2: Applications of the FEM method across multiple length scales; (a): A representative volume element for modelling the grains of magnesium at the crystal plasticity [μm] scale [16]; (b): A fan blade system as part of a gas turbine engine at the component [m] scale.

Notably, Isogeometric Analysis (IGA) by Hughes et al. made use of spline-based functions to represent the geometry of models exactly [17]. Contrasting to Equation 2.19, IGA makes use of Non-Uniform Rational B-Spline (NURBS) functions R_i with:

$$\dot{\mathbf{u}}(\mathbf{x}, t) \approx \sum_{i=1}^{\mathcal{N}_{\text{cp}}} \mathbf{R}_i(\mathbf{x}) \dot{\mathbf{u}}_i(t) \quad (2.20)$$

summing over the number of control points $\mathcal{N}_{\text{cp}}$ to solve for the exact geometry and smooth representation of the solution field. Through using the same functions employed in computer-aided design (CAD) software, eliminating geometric approximation reduces the gap between design and analysis. Similarly to FEM, the governing PDE is transformed into its weak form, and conventionally solved with the Galerkin approach [17]. This approach is also used in the Spectral Element Method (SEM), which excels in smooth wave propagation problems, with the use of high-order basis functions. Originally developed for fluid dynamics, these methods have been more recently extended to solid mechanics [18]. To compute the integrals of the weak form, SEM tailors the Gaussian quadrature rules to the chosen basis functions, which are often Legendre or Chebyshev polynomials [19].

Last of the noteworthy element-based methods is the Virtual Element Method (VEM), which differs from FEM through the use of arbitrary polygonal and polyhedral meshes to capture geometries of heterogeneous structures more accurately [20]. Potentially, this allows for greater flexibility through requiring knowledge of certain degrees of freedom within each element. The approximation of the solution follows similarities to the aforementioned:

$$\dot{\mathbf{u}}(\mathbf{x}, t) \approx \sum_{i=1}^{\mathcal{N}_e} \boldsymbol{\varphi}_i(\mathbf{x}) \dot{\mathbf{u}}_i(t) \quad (2.21)$$

where $\mathcal{N}_e$ is the number of degrees of freedom of the virtual element, and $\boldsymbol{\varphi}$ are the virtual basis functions. This brief overview of initial methods depicts the foundational relationship of mesh-based methods to FEM. While more recent methods have evolved to more tailored variations, it has been shown how FEM ultimately remains the backbone of element-based methods with Equations 2.19 - 2.21, and how its development is still relevant today.

2.1.3 Meshfree / Meshless Methods

While modelling highly dynamic behaviour, meshfree and meshless methods emerged due to their ability to handle complex material behaviour and discontinuities in heterogeneous solids. Gingold and Monaghan's Smooth Particle Hydrodynamics

(SPH) method led the way for pioneering meshfree methods through approximating the strong form of the PDE [21, 22]. In SPH, strong formulations were initially proposed because the method enables direct interpretation of physical laws, without depending on a uniform distribution of interpolation points, unlike FDM. Modelling impact simulations, the continuum is represented with particles, containing physical properties such as mass, stress and velocity. These allow interactions between particles, which act as the interpolation points, to model extreme deformations without a predefined mesh [23]. The kinematic quantities are determined through a weighted summation of neighbouring particle properties. The contribution from neighbouring particles is determined through a smooth and compactly supported kernel function. Consequently, the method relies on this choice of a smooth kernel, $W(\mathbf{x}, h)$, where h is the smoothing length to localise the strong form of PDE. When considering the behaviour of solids, this localisation (averaging) operator can be written as:

$$\mathcal{A} \approx - \sum_{j=1}^N (\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_j) \cdot \nabla W(\mathbf{x}_i - \mathbf{x}_j, h) \Delta V_j \quad (2.22)$$

where $\boldsymbol{\sigma}$ remains the Cauchy stress, $\mathbf{x}$ are positions and ΔV_j the volume of particle j . A common kernel function, W , is the Gaussian function:

$$W(\mathbf{x}, h) = \frac{1}{(\pi h^2)^{d/2}} \exp \left[-\frac{\mathbf{x}^2}{h^2} \right], \quad 1 \leq d \leq 3 \quad (2.23)$$

where in general the kernel function is positive for a number of dimensions d . Difficulties with SPH include the accurate representation of material interfaces, with its lack of predefined structure leading to numerical issues relating instability and spurious pressure oscillations [24]. Careful consideration of these functions and smoothing lengths are possible limitations when comparing its capability to FEM.

Weak formulations of particle methods improved accuracy of predictions with the Reproducing Kernel Particle Method (RKPM) and Element-Free Galerkin (EFG) method of Liu et al. [25] and Belytschko et al. [26] being other prominent meshless approaches. The techniques share a common foundation of approximating field variables with the construction of flexible basis functions. RKPM extends the

aforementioned SPH approach by including correction functions into the kernel formulation. In doing so, RKPM ensures consistency conditions, hence avoiding some of the numerical artifacts observed in SPH, such as tensile instability [27]. EFG methods commonly approximate field variables with moving least squares shape functions offering high smoothness and flexibility. In the original paper by Belytschko et al. the variational form of Section 2.1.2 is altered to enforce the essential boundary condition of all meshfree interpolants [26]. Through incorporating the Lagrange multiplier method with a field $\boldsymbol{\lambda} \in H^0(\Omega)$:

$$\begin{aligned} \int_{\Omega} \delta (\nabla \dot{\mathbf{u}}^T) : \boldsymbol{\sigma} d\Omega - \int_{\Omega} \delta \dot{\mathbf{u}}^T \cdot \mathbf{b} d\Omega - \int_{\Gamma_t} \delta \dot{\mathbf{u}}^T \cdot \mathbf{t} d\Gamma \\ - \int_{\Gamma_u} \delta \boldsymbol{\lambda}^T \cdot (\mathbf{u} - \bar{\mathbf{u}}) d\Gamma - \int_{\Gamma_u} \delta \dot{\mathbf{u}}^T \cdot \boldsymbol{\lambda} d\Gamma = 0 \end{aligned} \quad (2.24)$$

where $\boldsymbol{\lambda}$ acts as reaction forces to ensure the approximated field $\bar{\mathbf{u}}$ (from the moving least squares functions) satisfy the boundary conditions of $\mathbf{u}$. Unlike the construction of basis functions on local elements in FEM, EFG handles deformation with a scattering of nodes that do not require explicit connectivity. A notable limitation for both RKPM and EFG methods is the complexity in enforcing boundary conditions, a obstacle shared by SPH [28]. In contrast, FEM imposes Dirichlet and Neumann boundary conditions in a much more straightforward manner due to their structured basis functions. Whilst meshfree methods offer superior flexibility and accuracy in select cases, their computational complexity remain significant challenges in comparison to mesh-based methods.

2.1.4 Physics-informed Machine Learning and Data-driven Methods

The explosion of machine learning techniques has spread to physics and mechanics in recent years. These techniques combine the power of machine learning models, such as neural networks, to approximate the solutions of PDEs. Integrating governing equations into the loss function of neural networks, has enabled Physics-Informed Neural Networks (PINNs) to solve partial differential equations, while respecting physics [29]. Relating specifically to dynamic solids, PINNs can be viewed as a

meshfree method that enables the use of smooth solutions, akin to basis functions, that minimise objective functions such as the strong form for 2-D linear elasticity:

$$\begin{aligned}
\mathcal{L} = & |u_x - u_x^*| + |u_y - u_y^*| + |\sigma_{xx} - \sigma_{xx}^*| + |\sigma_{yy} - \sigma_{yy}^*| \\
& + |\sigma_{xx,x} + \sigma_{xy,y} + b_x^*| + |\sigma_{xy,x} + \sigma_{yy,y} + b_y^*| \\
& + |(\lambda + 2\mu)\varepsilon_{xx} + \lambda\varepsilon_{yy} - \sigma_{xx}| + |(\lambda + 2\mu)\varepsilon_{yy} + \lambda\varepsilon_{xx} - \sigma_{yy}| \\
& + |2\mu\varepsilon_{xy} - \sigma_{xy}|
\end{aligned} \tag{2.25}$$

where $\mathcal{L}$ is also known as the loss of the system, u is the displacement, $(\cdot)^*$ asterisks represent given (analytical or high-fidelity simulation) data at collocation points, followed by conventional mechanics notation for σ , ϵ , b , λ , μ as stress, strain, body force, and Lamé's parameters, respectively [30, 31]. Methods based of this minimisation of physics loss have recently shown to be used in domain decomposition problems [32]. Flexible in nature, this approach shows potential with complex problems involving multi-physics phenomena and heterogeneous materials [33]. Within computational mechanics, data-driven techniques have been successfully utilised to bypass conventional constitutive models by using high-quality experimental data [34]. From a hybrid perspective, neural network-based approaches have been combined with adapted mesh refinement in the works of Capuano et al. [35]. Lu et al. also introduced DeepONet for learning operators that could be applied to mechanics problems [36]. Relating back to variational formulations, V-DeepONets that impose the weak form of the governing PDE have also been developed to improve solely data-driven techniques [37–39]:

$$\mathcal{L}(\boldsymbol{\theta}) = \gamma_1 \times \mathcal{L}_{\text{data}}(\boldsymbol{\theta}) + \gamma_2 \times \mathcal{L}_{\text{var}}(\boldsymbol{\theta}) \tag{2.26}$$

where $\boldsymbol{\theta}$ is the set of trainable parameters, γ_1 and γ_2 are hyperparameters (weights) pertaining to the data ($\mathcal{L}_{\text{data}}$) and variational ($\mathcal{L}_{\text{var}}$) loss. In the works of Goswami et al. [38] the latter minimises the fracture energy functional when applied to predicting crack propagation through ensuring that the network's predictions adhere to the variational principle.

Even with their potential, physics-informed and data-driven machine learning models face limitations that differ from the aforementioned numerical methods.

A large computational cost is associated to training these models, particularly in the case of forward simulation when evaluating higher order derivatives [32]. The optimisation process often requires careful hyperparameter tuning, along with concerns of generalisability of the models. Even with these limitations, deep learning research is rapidly advancing, and an increasing availability in physics-informed methods will play a prominent role in the modelling of heterogeneous media in the future. Computational tools that leverage both traditional methods and those cutting edge technologies shall be key, but for now, the focus on raising the benchmark of finite elements shall provide motivation for these future techniques to better.

2.2 Asynchronous Methods for Coupling in Time

The heterogeneous nature of solids plays a pivotal role in the temporal variability when computationally solving the dynamic behaviour of solids. Fundamentally, the Courant-Friedrichs-Lewy (CFL) condition governs the maximum stable time step an explicit finite element can integrate over [40]. The computational time step is directly proportional to the characteristic length, h_e , of a finite element e , and inversely to its dilatational wave speed, c_e . Most simply put, the critical time step Δt_C , in 1-D, becomes:

$$\Delta t_C \leq \min_e \left(\frac{h_e}{c_e} \right) \quad (2.27)$$

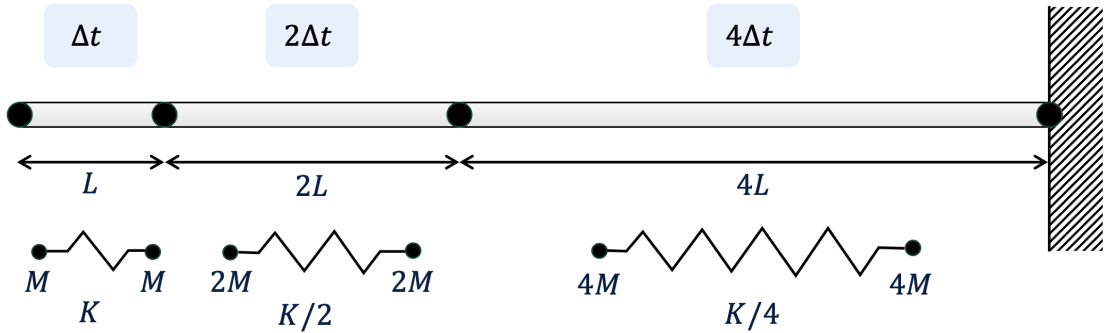
where h_e is taken as the characteristic length of the element, and dilatational wave speed, $c_e = \sqrt{E/\rho}$ a function of Young's modulus, E and density ρ . Equation 2.27 indicates how the use of a single time step is computationally inefficient granted both element size and material properties can vary drastically throughout a structure. Table 2.1 showcases the difference in wave speeds across some well-known engineering materials. Prominent in impact engineering, very small portions of a domain might require a fine discretisation, however with use of a monolithic (single time step) solver, the rest of the domain is limited by the smallest time step. This clear disadvantage, together with the desire to couple implicit and explicit schemes,

Table 2.1: Longitudinal Wave Speeds for a Selection of Engineering Materials [41, 42].

Material Property	Rubber	Concrete	Titanium	Diamond
Dilatational Wave Speed [m/s]	1,600	3,070	6,070	12,000

is what drove the pioneering ideas of Belytschko and Mullen [43] [44], and Hughes et al. [45] [46] to partition domains into subdomains that integrate with their own respective time step. Initially introduced as subcycling, these methods are also referred to as multi-time stepping, multi-step or asynchronous integration methods. These are used interchangeably in literature in the context numerical methods, particularly when solving differential equations. For the purpose of this thesis, they all describe the integration of different subdomains with different time steps. The definition of clocks were common amongst these methods of the last century, where nodal or element clocks determined the advancement of subdomains.

In Figure 2.3, a simple 1-D example depicts how elements were integrated with their own time step for the same material properties, but different element lengths. These methods directly partitioned the equations of motion, unlike asynchronous variational integrators, which looked to discretise the functional [47]. Through permitting independent time steps in each element, and operating with the integral of the Lagrangian directly, Lew et al. provided a very robust approach, however its implementation is highly complex, requiring the calculation of discrete variations [48]. For this reason, subcycling schemes, that use the direct solution of the partitioned equations of motion, are focused upon for temporal coupling.

**Figure 2.3:** A representation of 1-D configurations where initial subcycling investigations coupled bar elements with a different Δt and integer time step ratios, as recreated from the works of [49]. The mass, M , and stiffness, K , vary throughout the bar domain.

2.2.1 Time Step Ratios between Subdomains

Shortly later in time, Neal and Belytschko employed a more effective approach of subcycling, through developing methods that allowed for non-integer time step ratios [50]. These time step ratios m , crucially allowed for:

$$m = \frac{\Delta t_L}{\Delta t_s} \quad \text{where} \quad t_L, t_s \in \mathbb{R}^+ \quad \text{and} \quad m \in \mathbb{R} \setminus \mathbb{Z} \quad (2.28)$$

where $\mathbb{R}^+$ is a positive real number, and m does not necessarily belong to an integer set of numbers $\mathbb{Z}$. Here, notation is introduced for a two subdomain problem, m is a large time step Δt_L divided by a comparatively smaller time step Δt_s . Although this seems an obvious requirement for multi-time stepping methods, granted heterogeneity does not guarantee integer ratios, the majority of approaches still operate with $m \in \mathbb{Z}$. These include many of those methods based on the FETI [51] and mortar methods [52]. When modelling highly dynamic problems in an updated Lagrangian formulation, the critical time step of elements can change, as they are distorted or their material properties change as the simulation progresses. Considering this change in Δt_L and Δt_s , the expectation that m remains constant is also a limitation. Recent methods, such as the Schwarz alternating method in the works of Mota et al. [53], still adhere to this assumption, potentially integrating with time steps much smaller than required. Gravouil and Combescure developed methods that allowed for large time step ratios, through coupling implicit and explicit schemes, they stepped with m of the order of 100. This highlights the robustness of the multi-time stepping schemes to date, as well as the potential for computational savings. For now, this thesis focuses on couplings between explicit subdomains.

2.2.2 Interface Continuity and Ordering of Updates

Including the efforts of others, Gravouil and Combescure extended multi-time stepping to more than two subdomains, as well as using different time integration schemes with the heterogeneous asynchronous time integrators (HATI) [54, 55]. Integrating more than two subdomains is particularly pertinent, for the practical application of temporal coupling of real world materials and structures. Recently, it

has been shown that those methods based on the works of Gravouil and Combescure, do not necessarily ensure the continuity of all three kinematic quantities [56]. Cho et al. depicted these methods that enforce continuity of acceleration or velocity, do not lead to a displacement field that is continuous across subdomains under extreme conditions, namely drifting [57]. The topic of interface constraints, in the context of subcycling, has been explored thoroughly, but the a single preferred method is yet to be found. From the computation of a mid-point velocity [44], to a constant acceleration [58], and then to partial approaches [49], research has looked into which of the kinematic quantities should be enforced on the interface with multi-time stepping. More recent methods such as those by Mahjoubi, Krenk and Dhia favour displacements [59–62], leading to the conclusion that all three kinematic quantities have been explored. Constant acceleration has proven robust and more accurate than constant velocity [58], whilst also simple, without the need to interpolate subdomain interfaces at different times.

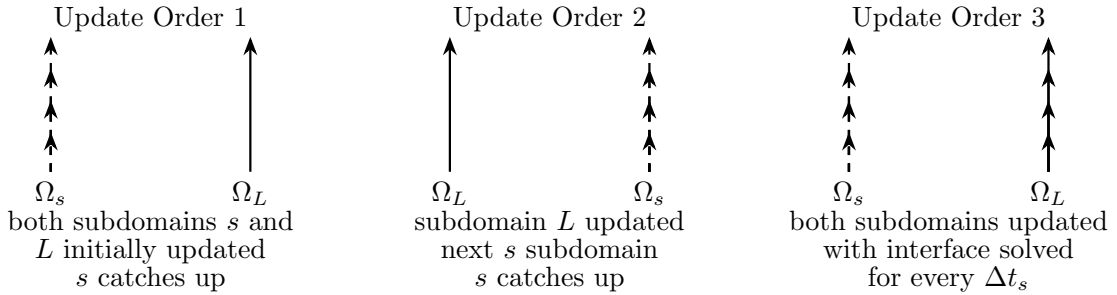


Figure 2.4: Ordering of subdomain advancement vary across literature, as depicted with a two-subdomain case with Δt_L and Δt_s representing large and small time steps. The magnitude of the arrow indicates the size of the time step, with adaptation of [58].

The choice of update strategy of subdomains is inherently problem-dependent, and several variations of the ordering of updates can be found in literature. Figure 2.4 depicts some of the most common interpretations of these update strategies in multi-time stepping algorithms. Smolinski, and works similar to that of his [63], elected for a common update of Ω_s and Ω_L , followed by subcycle updates of Ω_s that catch up to Ω_L . In Update Order 2, an integration step of Ω_L initially takes place, followed by a series of updates on Ω_s that catch up to Ω_L [64]. Those

methods that employ Lagrange Multipliers look to solve the interface conditions of both subdomains over Δt_s . This is equivalent to Update Order 3, where Ω_L is often held at constant acceleration or velocity. From this, it is clear that Update Order 3 is the most computationally expensive, despite being the most accurate option. Moreover, the choice of update order is influenced by the separation in time scales. In the case of Update Order 1 or 2, a delayed update of Ω_s relative to Ω_L may cause inaccuracies. A universal solution for updates does not fit all problems, moreover, the constraints of the interface are also key to ensuring the stability of the solution when using multi-time stepping methods.

2.2.3 Stability of Multi-Time Stepping Methods

The stability of asynchronous methods has undergone much scrutiny in the past. Notable works, that add to the aforementioned, include those pioneered by Daniel [65]. These methods analysed stability with use of amplification matrices and eigenvalue decomposition. Predominantly assessing linear problems, they assessed the state of the kinematics over each time step. Smolinski used the approach of pseudo-energy norms to depict the bounds of stability at each time step [63, 66, 67]. For nonlinear problems, where large deformations or plasticity may be invoked, assessment of the energy balance was recommended, as the system can regain stability after being unstable [50]. Consequently, the development of asynchronous integrators must go hand-in-hand with a stability analysis. Foundational to the stability, energy conserving methods, developed by Dvořák et al. capture the state-of-the-art where Lagrange multipliers are used at each Δt_s , whilst ensuring the energy at the interface is zero [56]. However, the limitations of the likes of these methods, cycle back to issue of integrating elements far from the critical time step. The balance between methods that do not infringe on the stability limits of the CFL condition, whilst ensuring they are computationally efficient portrays the exact trade-off with multi-time stepping methods. Figure 2.5 summarises the key works discussed through time, from pioneering works to the most recent developments.

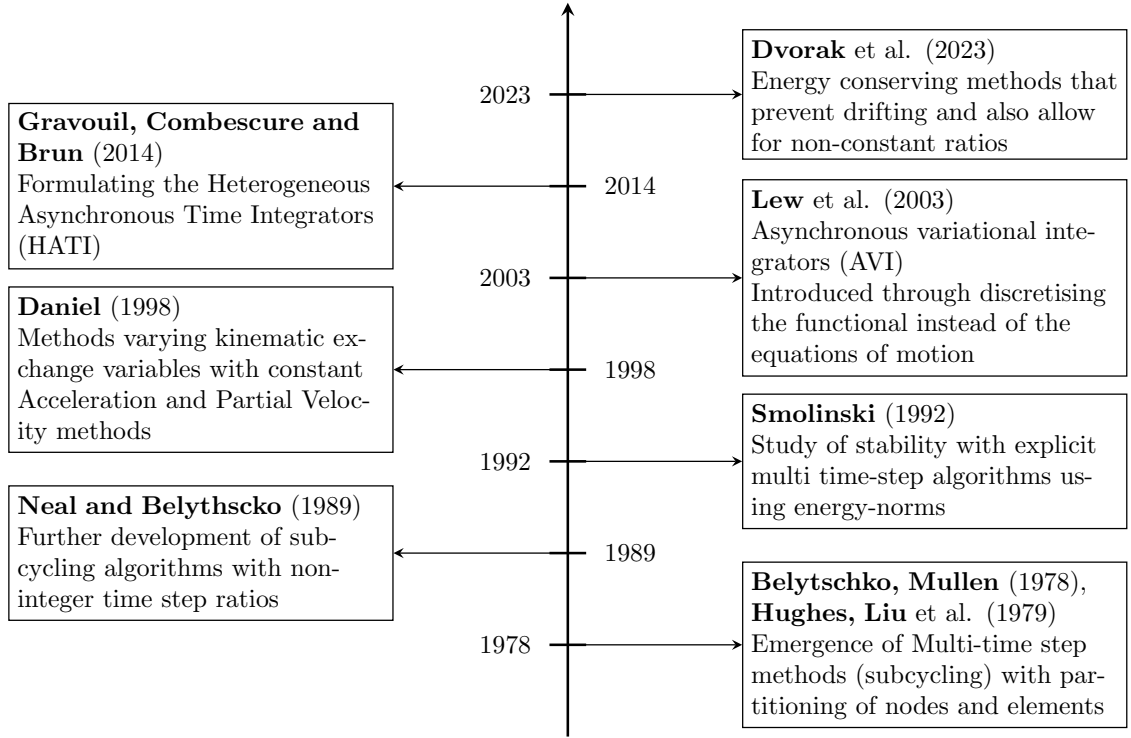


Figure 2.5: A timeline of key works from literature to summarise the development of multi-time stepping (MTS) methods.

2.3 Non-matching Mesh Coupling in Space

The heterogeneity of real physical systems, require complex discretisation spatially. The finite element description of domains is often decomposed into individual subdomain meshes that may not necessarily match at their interfaces. Referred to as non-matching meshes, non-conforming or non-contiguous, the problem is prevalent across a wide range of applications; including contact mechanics, domain decomposition, fluid-structure interaction, and multi-physics problems [68]. Although subdomain deformation can advantageously be resolved in parallel, an additional set of techniques are required to ensure the dynamic behaviour of the overall domain is captured accurately. In Table 2.2, a selection of the key limitations commonly found in literature have been highlighted. These outline the following sections that proceed to describe the disadvantages of parameter sensitivity, preserving conservation laws like mass and energy, the solving of additional degrees of freedom (DOF), as well as the computational expensive task of constructing an additional interface mesh.

2.3.1 Accuracy and Sensitivity to Parameters

The early development of methods applied to non-matching meshes date back to Nitsche in the early seventies [69]. The method introduced a variational approach that weakly imposed Dirichlet boundary conditions to handle constraints on interfaces. The method is well described in literature, as found in the book of Zienkiewicz et al. [12]. The method is flexible in coupling subdomains, as extended by Hansbo et al. for FSI problems [70, 71]. While maintaining high accuracy, the performance is sensitive to penalty parameters to balance the stability [72]. Following Nitsche’s method, Babuška similarly imposed conditions on the weak form of the problem, through introducing a penalty term [73]. A well-chosen parameter is key to stability and performance. With heavy reliance on the penalty’s parameter value, too small a penalty may fail in enforcing a desired level of continuity and a less accurate solution. Conversely, the method suffers from ill-conditioning of the system of equations when excessively large penalty parameters are chosen [74]. To choose an optimal penalty parameter empirical bounds and adaptive approaches have been researched, however this fine-tuning increases computational cost. Despite this, penalty methods are still widely used across solid mechanics due to their robustness [75], along with mortar methods to resolve contact problems [76, 77].

FETI-based methods are also relevant in a spatial setting, using Lagrange multipliers in a dual-schur formulation [78]. Recent works show a key disadvantage with results significantly impacted by blending parameters [79]. Towards the end of the 20th century, discontinuous Galerkin (DG) finite element methods were developed by allowing discontinuities in the solution across element interfaces [80, 81]. DG-based methods are advantageous in providing local conservation when handling discontinuities, however similarly to Nitsche’s and penalty-based methods, are highly parameter-sensitive [82]. These parameters regulate stability by minimising numerical dissipation [83]. Once more, careful tuning of parameters is key so that penalties or blending functions do not artificially dampen physical features, while sufficient enough to maintain stability.

Table 2.2: Comparison of methods in literature for algorithms that solve for non-matching interfaces, Γ . Specifically limitations, denoted ■, for methods associated to coupling with FEM.

Method	Parameter -sensitive	Additional DOFs	Conservation preserving	Costly Γ construction
Nitsche-based [71, 72, 82]	■	□	□	□
Mortar-based [76, 77, 84–86]	□	■	□	■
Arlequin [60, 61]	■	■	■	N/a
XFEM[87, 88]	□	■	■	□
IEM/CFE [89–91]	■	■	■	■
LLM-based [92–94]	□	■	□	■

2.3.2 Handling Complex Geometries and Boundary Conditions

The problem of non-matching meshes are conjointly found with challenges related to complex geometries and boundary conditions, particularly those in dynamic environments. With these meshing constraints, radial basis functions (RBFs) emerged to allow for meshfree interpolations and approximations [95, 96]. In the review of de Boer et al. RBFs were shown to approximate the displacements of interfaces through using the sum of different spline functions [68]. The flexibility allows for irregular data distributions along the interface, however can often lead to dense matrices that scale poorly for large scale problems. Enriching standard FEM approximation spaces with additional basis functions, was the idea of Mões et al. with the extended finite element method (XFEM) [87]. Essentially, part of the weighted residual methods, XFEM is based on the partition of unity (PUM) concept that allows for non-matching meshes in crack propagation problems. While effective XFEM faces challenges in integration for complex geometries [88]. Duarte’s generalised finite element method, clustered groups of nodes and elements to define a PUM to enrich finite elements as well [97]. Other weighted residual methods, include Jaiman et al. [98] and Li et al. [99], where standard shape functions can be used alongside different projection schemes or elements respectively to transfer the loads conservatively from one subdomain to another.

When subdomains are modelled with multiple scales, Dhia’s Arlequin method has proven effective not only for solids with non-matching discretisations but also for various multi-physics models [60]. The coupling zone defined between subdomains allows for overlapping regions where the different models can interact [61]. However, it is this same coupling zone, that can produce instabilities in the solution. The choice of coupling operators and treatment of boundary conditions particularly influence performance [100].

2.3.3 Computational Overhead and Implementation Complexity

In keeping with FEM, coupling finite elements or interface elements have also been called upon to facilitate the connection between subdomains [89, 90]. There are many adaptations of special elements that solve the issues of hanging nodes, and accommodate this change in discretisation. Consequently, their range of applications is wide and multi-scale [101–103]. However, they also introduce a significant computational overhead due to the increased degrees of freedom and complex element formulations that are required. Similar problems are faced with methods that adopt Lagrange multipliers. Pioneered by the works of Bernardi, the mortar method is one of the most used methods in literature, where Lagrange multipliers weakly enforce continuity across an interface [104]. Faucher et al. extended the use of these types of methods with the coupling in time as well [84]. The current state-of-the-art still utilises the method to enforce the continuity of the three kinematic fields [85, 86], however satisfying the inf-sup stability condition can be challenging, essential for a well-posed problem [105]. Such methods condense degrees of freedom, and require the adaptation of the stiffness matrix [106]. To reduce the computational effort of the mortar method, the enforcement of the constraints through localising the multipliers to a frame allowed the Localised Lagrange Multiplier method to be developed by Park et al [92]. The method is particularly useful in solid mechanics, especially for those problems where the mortar method may not perform well [93, 107, 108].

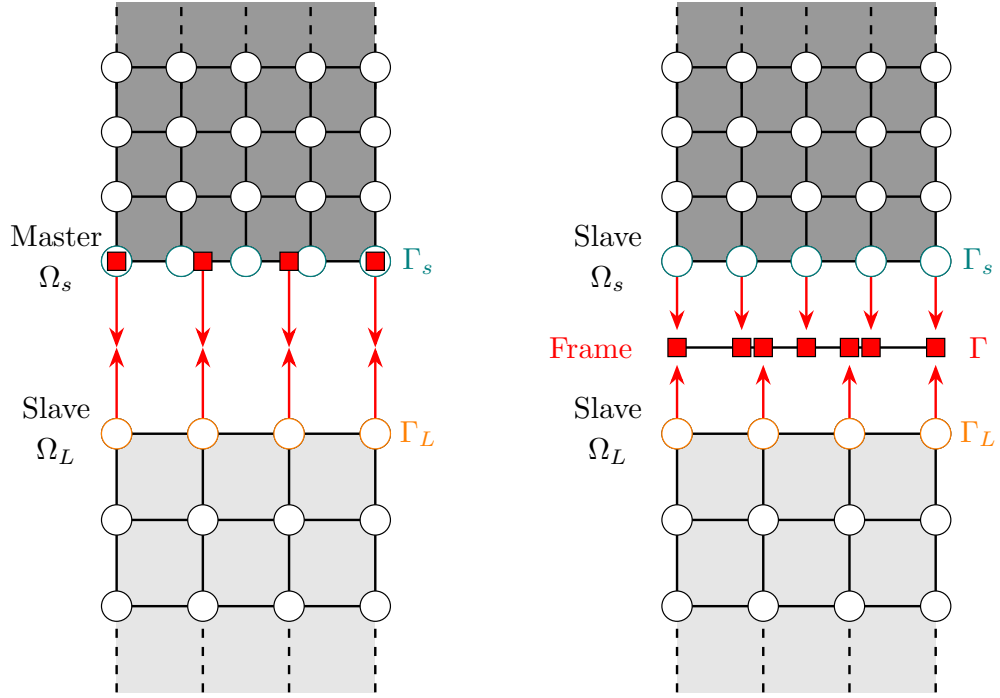


Figure 2.6: A comparison between the solution of non-matching interfaces with popular methods in literature; (a): Mortar methods solve the kinematic continuity at the red squares at the intersection between master and slave nodes, (b): the classical Localised Lagrange Multiplier method where the solution of Γ is solved on an external frame.

The difference between these two methods is visualised in Figure 2.6, where the kinematic continuity is enforced at the red squares. In essence, the aforementioned methods with Lagrange multipliers and interface elements introduce additional degrees of freedom. Together with the increased computational cost, the implementation of such methods could still be made more efficient.

2.4 Applications for Coupling Algorithms

In the following section the applications of methods that couple both in time and space are given, with emphasis on those coupling explicitly solved FEM subdomains.

2.4.1 Applications of Temporal Coupling Algorithms

Explicit asynchronous time integration methods have proven to efficiently model the dynamic behaviour of heterogeneous solids. These methods are particularly effective in impact analysis and wave propagation problems, where regions require vastly

different time steps [109]. Grunwald et al. have demonstrated how Belytschko's original subcycling algorithms are still effective to date across multiple scales with the blast loading of concrete [110]. Discontinuous wave propagation problems have also employed asynchronous methods to experimental setups with different materials throughout [111]. Localised failure in composite materials have been modelled by Selvaraj et al. with very small time steps used around those regions where fracture occurs [112]. Even at lower scales, Ghosh et al. have shown how multi-time stepping can be employed with conventional crystal plasticity finite element method (CPFEM) solutions, maintaining accuracy to a high level in representative volume elements (RVEs) [113].

2.4.2 Applications of Spatial Coupling Algorithms

Non-matching mesh methods, that utilise techniques such as mortar methods, LLMs and coupling interface elements, have also proven invaluable in modelling complex solids dynamically. Damage and fracture are common themes associated to the applications of coupling methods in space. Employing coupling interface elements has allowed capturing of crack surfaces more efficient [91, 114]. Puso et al. demonstrate just one of many works that resolve the non-matching mesh problem, applied to contact mechanics [76]. The complex dynamic behaviour of contact remains a hot topic, with spatial coupling algorithms a key piece in solving broader problems. The elasto-plastic response of RVEs is captured with overlapping and non-overlapping couplings by Yang and Soghrati [115]. This work looks at how spatial algorithms can be far extended past just two subdomains with cutting lines that also belong to different subdomains as also seen in the recent work of Zhou et al. [85]. This review shows there is no universal non-matching algorithm that can be applied to all dynamic problems, with each method having its own advantages and disadvantages. However, as captured in Table 2.2, the limitations frequently discussed in the burgeoning literature clearly need to be addressed.

2.5 Summary

The literature review has provided an insight into the computational techniques used for dynamically modelling heterogeneity. Explicit FEM still remains at the forefront of simulations that capture a material's dynamic behaviour. Multi-time stepping has not been fully leveraged to date, with algorithms still balancing stability and computational efficiency. Discretising with varying element sizes, with meshes that do not necessarily match has been investigated through use of mortar methods, coupling finite elements, and Localised Lagrange multipliers. However, serious computational costs are associated to each. The variety in applications of temporal and spatial coupling algorithms, provides motivation for continued research in the field. In particular, for those methods that leverage both types of algorithm, as shown in more recent literature [116–118]. The current state-of-the-art reveals a necessity to solve the following problems:

- Coupling algorithms that utilise explicit FEM for modelling the dynamic behaviour of solids;
- Multi-time stepping methods that allow all elements to integrate in time close to the CFL condition, thus reducing the computational effort required;
- Ensuring asynchronous methods are stable, energy-conserving and do not lead to the phenomena of drifting;
- Circumvent any limitations on temporal coupling that requires constant or integer time step ratios;
- Maintaining a low computational overhead when resolving the behaviour of non-matching meshes without unnecessarily adding degrees of freedom to solve;
- Allowance for interface operators to be adapted as interface conditions change;
- A combination of temporal and spatial algorithms that vastly speed up simulations.

3

Temporal Coupling Methods

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In this chapter, the equations that govern the motion of solids are introduced. Heterogeneously discretised solids are formulated with partitioned equations, to allow subdomains to be solved with their own respective time step.

3.1 Governing Equations for the Dynamical Behaviour of Solids

This section describes the governing equations for dynamic solids in an updated Lagrangian formulation. Starting from the strong form of a single solid body, the variational form is depicted to describe the discretised and partitioned equations for multiple solids.

3.1.1 Variational Formulation of a Single Solid Body

The momentum balance for a solid body $\mathcal{B}$ in an open region $\Omega \subset \mathbb{R}^3$ reads:

$$\rho \ddot{\mathbf{u}} = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{b}, \text{ in } \Omega \times [0, T] \quad (3.1)$$

where $\ddot{\mathbf{u}}$, $\boldsymbol{\sigma}$, ρ and $\mathbf{b}$ denote the acceleration field, the Cauchy stress tensor, the density of the solid, and the body force per unit mass, respectively. The variational (weak) form for an updated Lagrangian formulation is presented. Suppose $\delta \dot{\mathbf{u}}$ denotes a variational velocity function where $\forall \delta \dot{\mathbf{u}} \in H^1(\Omega)$. Here these trial velocities belong to a Sobolev space of order 1, giving the variational form for Ω as:

$$\int_{\Omega} \rho \ddot{\mathbf{u}} \cdot \delta \dot{\mathbf{u}} \, d\Omega = \int_{\Omega} \nabla \cdot \boldsymbol{\sigma} \cdot \delta \dot{\mathbf{u}} \, d\Omega + \int_{\Omega} \rho \mathbf{b} \cdot \delta \dot{\mathbf{u}} \, d\Omega \quad (3.2)$$

$$\int_{\Omega} \rho \ddot{\mathbf{u}} \cdot \delta \dot{\mathbf{u}} \, d\Omega = \int_{\Omega} \boldsymbol{\sigma} \cdot \mathbf{n} \cdot \delta \dot{\mathbf{u}} \, d\Omega - \int_{\Omega} \boldsymbol{\sigma} : \delta \mathbf{D} \, d\Omega + \int_{\Omega} \rho \mathbf{b} \cdot \delta \dot{\mathbf{u}} \, d\Omega \quad (3.3)$$

where velocity and displacement field are denoted $\dot{\mathbf{u}}$ and $\mathbf{u}$ respectively, $\mathbf{n}$ is normal to the domain, $\mathbf{D}$ is the rate of deformation. From the traction continuity in

Equation 2.6, the weak form becomes:

$$\underbrace{\int_{\Omega} \rho \ddot{\mathbf{u}} \cdot \delta \dot{\mathbf{u}} \, d\Omega}_{\text{Inertial Power}} = \underbrace{\int_{\Gamma} \mathbf{t} \cdot \delta \dot{\mathbf{u}} \, d\Gamma + \int_{\Omega} \rho \mathbf{b} \cdot \delta \dot{\mathbf{u}} \, d\Omega}_{\text{External Power}} - \underbrace{\int_{\Omega} \boldsymbol{\sigma} : \delta \mathbf{D} \, d\Omega}_{\text{Internal Power}} \quad (3.4)$$

where $\mathbf{t}$ are the surface tractions on Γ . Physically, these terms represent the virtual inertial (kinetic), external and internal power terms. In the following section, these integrals are split into the summation of individual elements to approximate the weak form.

3.1.2 Updated Lagrangian Finite Element Discretisation

Domain Ω is discretised into finite elements Ω_e , such that $\Omega \cup \Omega_e$. Each finite element approximates the velocity field with Lagrangian shape functions, denoted $\mathbf{N}_i$ for the number of nodes $\mathcal{N}_n$ in an element, giving:

$$\dot{\mathbf{u}}(\mathbf{X}, t) \approx \sum_{i=1}^{\mathcal{N}_n} \mathbf{N}_i(\mathbf{X}) \dot{\mathbf{u}}_i(t) = \mathbf{N}_i(\mathbf{X}) \dot{\mathbf{u}}_i(t) \quad (3.5)$$

where $\mathbf{X}$ is position vector of each node i . The velocity nodal components $\dot{\mathbf{u}} \in \mathbb{R}^{3\mathcal{N}_n \times 1}$, where in the 3-D case of a hexahedral element $\mathcal{N}_n = 8$. An isoparametric mapping is used to express the shape functions in terms of a parent domain. The displacement field is approximated in similar fashion with nodal displacements:

$$\mathbf{u}(\mathbf{X}, t) = \mathbf{N}_i(\mathbf{X}) \mathbf{u}_i(t) \quad (3.6)$$

All three kinematic quantities share the same dimensions. To capture the time dependence in the nodal variables with the finite element approximation the velocity gradient is approximated with derivatives of the shape functions:

$$\nabla \mathbf{v} = \dot{\mathbf{u}}_i \nabla \mathbf{N}_i(\mathbf{X}) \quad (3.7)$$

where for each element $\nabla \mathbf{v} \in \mathbb{R}^{3 \times 3}$. The global description of the domain results in the second-order hyperbolic ordinary differential equation.

The discretised form for an undamped structural dynamic system results in the following equation of motion:

$$\delta \dot{\mathbf{u}}^T (\mathbf{M} \ddot{\mathbf{u}} - \mathbf{f}^{\text{ext}} + \mathbf{f}^{\text{int}}) = 0 \quad (3.8)$$

At the level of the element e , the variational formulation is represented for each term. The element mass matrix is given by:

$$\mathbf{M}_e = \sum_{e=1}^{\mathcal{N}_e} \int_{\Omega_e} \rho \mathbf{N}_i^T \mathbf{N}_i d\Omega_e \quad (3.9)$$

where the integral is evaluated over the element Ω_e for a total number of elements $\mathcal{N}_e$. The mass is represented as a diagonal matrix of dimensions $3\mathcal{N}_n \times 3\mathcal{N}_n$. Here the current configuration and the parent domain are related by the determinants of the Jacobians. Next, body forces are omitted to result in the external forces being approximated by:

$$\mathbf{f}_e^{\text{ext}} = \sum_{e=1}^{\mathcal{N}_e} \int_{\Omega_e} \mathbf{N}_i^T \mathbf{t} d\Gamma_e \quad (3.10)$$

where element nodal external forces have dimensions $\mathbf{f}_e^{\text{ext}} \in \mathbb{R}^{3\mathcal{N}_n \times 1}$. The element internal forces are discretised as:

$$\mathbf{f}_e^{\text{int}} = \sum_{e=1}^{\mathcal{N}_e} \int_{\Omega_e} \mathbf{B}_e^T \boldsymbol{\sigma}_e d\Omega_e \quad (3.11)$$

with $\mathbf{f}_e^{\text{int}}$ and $\mathbf{f}_e^{\text{ext}}$ sharing similar dimensions, whereas strain-displacement matrix $\mathbf{B}_e^T \in \mathbb{R}^{3 \times 6}$ and Cauchy stress (in Voigt notation for computational efficiency) $\boldsymbol{\sigma}_e \in \mathbb{R}^{6 \times 1}$ for the 3-D case. Symmetry of stress and strain tensors is use to obtain the preceding notation, thus enabling representation of a second order tensor as a 1-D array. Each of the nodal forces ($\mathbf{f}_e^{\text{ext}}$ and $\mathbf{f}_e^{\text{int}}$) can be further assembled into global vectors ($\mathbf{f}^{\text{ext}}$ and $\mathbf{f}^{\text{int}}$) as column matrices.

Fundamental to solution of the system, an explicit time integration scheme is described. To solve the kinematics of the system, Equation 3.8 is solved first with the acceleration calculated at time step n :

$$\ddot{\mathbf{u}}^n = \mathbf{M}^{-1}(\mathbf{f}^{\text{ext}} - \mathbf{f}^{\text{int}}) \quad (3.12)$$

where $\mathbf{f}^{\text{ext}}$ and $\mathbf{f}^{\text{int}}$ are also vectors, even in 3-D, and $\mathbf{M}$ diagonal, should the masses be lumped. The leapfrog scheme is used, where the kinematic quantities are staggered in their solution leading to the computation of velocity at the half-time step as:

$$\dot{\mathbf{u}}^{n+1/2} = \dot{\mathbf{u}}^{n-1/2} + \ddot{\mathbf{u}}^n \cdot \Delta t^n \quad (3.13)$$

where Δt^n is the average of current and previous time steps. The final quantity, finds displacement at the full-time step:

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \dot{\mathbf{u}}^{n+1/2} \cdot \Delta t^{n+1/2} \quad (3.14)$$

with the current time step $\Delta t^{n+1/2}$. The advantageous characteristic of this procedure is that the time integration does not require the solution of any equations. This method is conditionally stable, meaning the use of a time step greater than Δt_C will lead to an unstable solution that grows unbounded. The critical time step Δt_C , governed by the Courant-Friedrichs-Lewy (CFL) condition [40], for a constant strain element is given by:

$$\Delta t_C \leq \frac{2}{\omega_C} \quad (3.15)$$

where ω_C is the maximum eigenfrequency of the problem. This stability condition can be approximated by solving the solution of a single degree of freedom system with a central difference-based time integration scheme:

$$\ddot{u}^n = \frac{u^{n+1} - u^{2n} + u^{n-1}}{(\Delta t)^2} = -\omega^2 u^n \quad (3.16)$$

to give the equation:

$$u^{n+1} - (2 - \omega^2(\Delta t)^2)u^n + u^{n-1} = 0 \quad (3.17)$$

where roots of this polynomial give the conditions of stability as presented in Equation 3.15. Furthermore, a conservative estimate of the critical time increment is given as the minimum over all elements in a domain:

$$\Delta t_C \leq \min_e \left(\frac{h_e}{c_e} \right) \quad (3.18)$$

where h_e is the characteristic length of the element, and c_e is the dilatational (longitudinal) wave speed. Equation 3.18 unveils how the computational speed of the solution is determined by both the spatial discretisation (h_e) and material properties (c_e) of a finite element.

3.1.3 Continuum Mechanics and Constitutive Equations

Next, the description of motion in the current configuration is given and the relationship between stress and strain, to depict the constitutive model used for this thesis.

The deformation of $\mathcal{B}$ is described at time $t \in [0, T]$ for a specified constant $T > 0$ by a smooth, invertible function $\phi(\mathbf{X}, t) : \Omega^0 \rightarrow \Omega^t$ where Ω^0 denotes the initial state of Ω and Ω^t denotes the (deformed) state of Ω at time t , as depicted in Figure 3.1. The spatial coordinates are expressed in terms of the material point $\mathbf{X}$ and time t . The deformation gradient $\mathbf{F} \in \mathbb{R}^{3 \times 3}$ of the motion ϕ is defined by:

$$\mathbf{F}(\mathbf{X}, t) = \nabla \phi(\mathbf{X}, t) = \frac{\partial \mathbf{x}^t}{\partial \mathbf{X}} \quad (3.19)$$

Rate of deformation $\mathbf{D}$ is the symmetric part of the deformation gradient, whereas the anti-symmetric part corresponds to the continuum spin, $\mathbf{W}$ as follows:

$$\mathbf{D} = \text{sym} \left(\frac{\partial \mathbf{v}}{\partial \mathbf{x}} \right) = \frac{1}{2} \left(\frac{\partial \mathbf{v}}{\partial \mathbf{x}} + \frac{\partial \mathbf{v}^T}{\partial \mathbf{x}} \right); \quad \mathbf{W} = \text{skew} \left(\frac{\partial \mathbf{v}}{\partial \mathbf{x}} \right) = \frac{1}{2} \left(\frac{\partial \mathbf{v}}{\partial \mathbf{x}} - \frac{\partial \mathbf{v}^T}{\partial \mathbf{x}} \right) \quad (3.20)$$

Here the definition of $\mathbf{D} \in \mathbb{R}^{3 \times 3}$ and $\mathbf{W} \in \mathbb{R}^{3 \times 3}$ are in terms of the spatial field velocity gradient, $(\nabla \mathbf{v})^T$, with:

$$\frac{\partial \mathbf{v}}{\partial \mathbf{x}} = (\nabla \mathbf{v})^T = \dot{\mathbf{F}} \mathbf{F}^{-1} \quad (3.21)$$

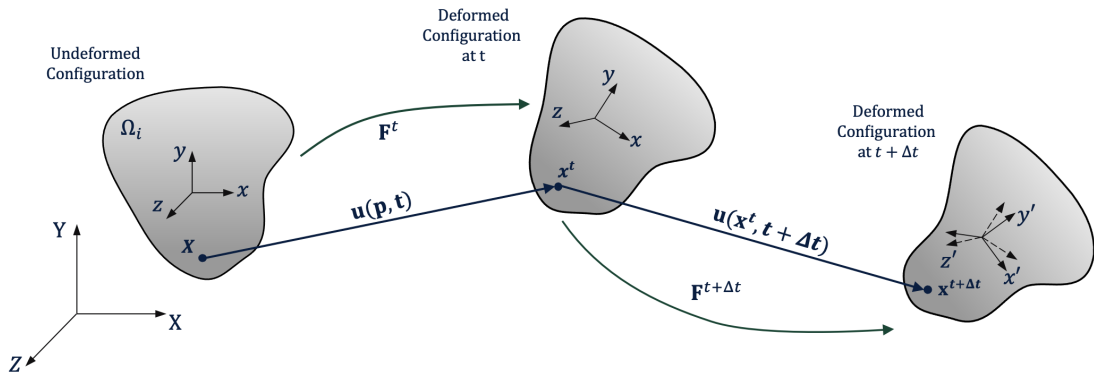


Figure 3.1: Motion of a solid subdomain Ω_i in its original configuration and deformed configurations at times t and $t + \Delta t$.

In this thesis, hypoelastic-plastic material behaviour is considered, where the elastic strains are considered small compared to the plastic strains. Although energy is not completely conserved for these descriptions, due to the small elastic strains this error is insignificant. For these models the additive decomposition of the rate-of-deformation is assumed such that:

$$\mathbf{D} = \mathbf{D}^e + \mathbf{D}^p; \quad \mathbf{W} = \mathbf{W}^e + \mathbf{W}^p \quad (3.22)$$

where terms are decomposed into elastic $(\cdot)^e$ and plastic $(\cdot)^p$ parts and $\mathbf{D}^p$ is determined by the chosen plastic flow rule. Definition of the algorithm that determines the plastic rate of deformation are explained in further detail later. $\mathbf{D}^e = \mathbf{D} - \mathbf{D}^p$ is key to obtaining the material stress rate $\dot{\boldsymbol{\sigma}}$:

$$\dot{\boldsymbol{\sigma}} = \mathbf{W}\boldsymbol{\sigma} + \boldsymbol{\sigma}\mathbf{W}^T + 2G\mathbf{D}^e + \lambda\text{Tr}(\mathbf{D}^e)\mathbf{I} \quad (3.23)$$

with G as the shear modulus and λ as Lamé's first constant. Here, it is convenient to state that the objective Jaumann stress rate $\overset{\nabla}{\boldsymbol{\sigma}}$ is:

$$\overset{\nabla}{\boldsymbol{\sigma}} = 2G\mathbf{D}^e + \lambda\text{Tr}(\mathbf{D}^e)\mathbf{I} \quad (3.24)$$

to give the final material rate of Cauchy stress tensor as:

$$\dot{\boldsymbol{\sigma}} = \overset{\nabla}{\boldsymbol{\sigma}} + \mathbf{W}\boldsymbol{\sigma} + \boldsymbol{\sigma}\mathbf{W}^T \quad (3.25)$$

Thus, stress can be computed from the material's constitutive response, reflected in the Jaumann stress rate in Equation 3.24, and the rotation by the spin tensors.

A brief description of the constitutive integration method required to iterate the state in stress space back to the von Mises yield criterion is described. An in-depth explanation of such derivations can be found in the works of de Souza et al. [119] and Dunne et al. [120]. A return mapping scheme is used to model the plasticity, specifically the backward Euler radial return method. The integration for k iterations can be succinctly described in four steps. At $k = 0$:

$$\boldsymbol{\varepsilon}^{p(0)} = \boldsymbol{\varepsilon}_n^p; \quad \bar{\boldsymbol{\varepsilon}}^{(0)} = \bar{\boldsymbol{\varepsilon}}_n; \quad \Delta p^{(0)} = 0; \quad \boldsymbol{\sigma}^{(0)} = \mathbf{C}^e : (\boldsymbol{\varepsilon}_{n+1} - \boldsymbol{\varepsilon}^{p(0)}) \quad (3.26)$$

where initial values of plastic strain, $\boldsymbol{\varepsilon}^{p(0)}$, and effective strain $\bar{\varepsilon}^{(0)}$, increment of plasticity parameter $\Delta p^{(0)}$ and elastic trial stress $\boldsymbol{\sigma}^{(0)}$ are initiated along with elasticity tensor $\mathbf{C}^e$. Whilst effective strain is a measure of accumulated plastic deformation, the plasticity parameter aids the definition of the conditions under which yielding occurs and how materials respond thereafter. With this information, let f be the yield function such that if $f^{(k)} < TOL$ convergence has been reached:

$$f = \bar{\sigma}^{(k)} - \sigma_y(\bar{\varepsilon}^{(k)}) = (\bar{\sigma}^{(0)} - 3G\Delta p^{(k)}) - \sigma_y(\bar{\varepsilon}^{(k)}) \quad (3.27)$$

where G is used for shear modulus, $\bar{\sigma}^{(k)}$ denotes the effective stress, as determined from the deviatoric stress tensor. The increment in plasticity parameter can be deduced through the substitution of the yield function into $\delta p = \frac{f^{(k)}}{3G+H^{(k)}}$ to give:

$$\delta p = \frac{(\bar{\sigma}^{(0)} - 3G\Delta p^{(k)} - \sigma_y(\bar{\varepsilon}^{(k)}))}{3G + H^{(k)}} \quad (3.28)$$

where the hardening modulus is $H = d\sigma_y/d\bar{\varepsilon}$. To complete an iteration of the backward Euler radial return method, the plastic strain tensor, equivalent plastic strain, increment in plasticity parameter and finally stress tensor are updated with the following:

$$\boldsymbol{\varepsilon}^{p(k+1)} = \boldsymbol{\varepsilon}^{p(k)} + \Delta \boldsymbol{\varepsilon}^{p(k)} \quad (3.29)$$

$$\bar{\varepsilon}^{(k+1)} = \bar{\varepsilon}^{(k)} + \delta p^{(k)} \quad (3.30)$$

$$\Delta p^{(k+1)} = \Delta p^{(k)} + \delta p^{(k)} \quad (3.31)$$

$$\boldsymbol{\sigma}^{(k+1)} = \mathbf{C}^e : (\boldsymbol{\varepsilon}_{n+1} - \boldsymbol{\varepsilon}^{p(k+1)}) = \boldsymbol{\sigma}^{(k)} + \Delta \boldsymbol{\sigma}^{(k)} \quad (3.32)$$

The procedure then returns to check the yield criterion $f^{(k)}$ for when $k \leftarrow k + 1$ and repeats the process of solving for increment in plasticity. Following the definition of the methodology for resolving the deformation of a single body with finite elements, attention can now be turned to multiple bodies.

3.1.4 Partitioned Formulation for Multiple Solid Bodies

Now, let $\mathcal{B}$ be a solid body in an open region $\Omega \subset \mathbb{R}^3$ subjected to an external force, and denote by $\partial\Omega$ its boundary. The domain Ω is divided into $\mathcal{S}$ non-overlapping subdomains:

$$\Omega = \bigcup_{i=1}^S \Omega_i \text{ and } \Omega_i \cap \Omega_j = \emptyset \text{ for } i \neq j \quad (3.33)$$

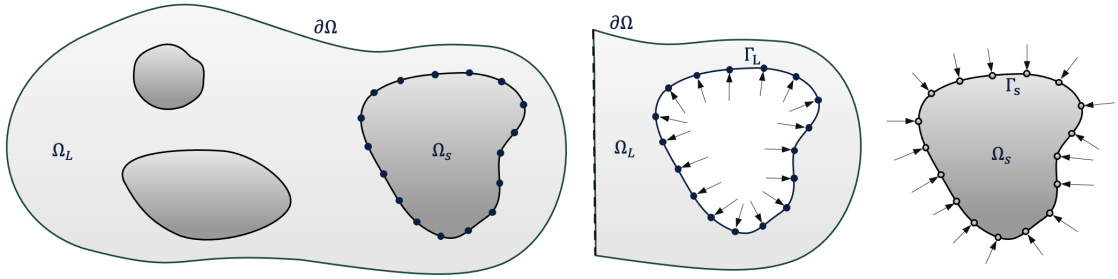


Figure 3.2: Decomposition of a Domain Ω into $\mathcal{S}$ subdomains, where Ω_L and Ω_s denote large and small subdomain respectively. Dots on Γ_i represent the nodes at which kinetic and kinematic quantities are coupled.

Two subdomains, as depicted in Figure 3.2, are described initially with Ω_L and Ω_s denoting large and small subdomains respectively. These represent subdomains with a large and comparatively small time step $\Delta t_L > \Delta t_s$. For each subdomain Ω_i the momentum balance equation is formulated with the boundary Γ_i between Ω_L and Ω_s as:

$$\rho_L \ddot{\mathbf{u}}_L = \nabla \cdot \boldsymbol{\sigma}_L + \rho_L \mathbf{b}_L, \text{ in } \Omega_L \times [0, T] \quad (3.34)$$

$$\rho_s \ddot{\mathbf{u}}_s = \nabla \cdot \boldsymbol{\sigma}_s + \rho_s \mathbf{b}_s, \text{ in } \Omega_s \times [0, T] \quad (3.35)$$

$$\ddot{\mathbf{u}}_L = \ddot{\mathbf{u}}_s, \text{ on } \Gamma \quad (3.36)$$

$$\mathbf{t}_L = \mathbf{t}_s, \text{ on } \Gamma \quad (3.37)$$

where both Dirichlet and Neumann boundary conditions are enforced, with matching conditions at the subdomain interfaces Γ_i with continuity of acceleration $\ddot{\mathbf{u}}$ and

tractions $\mathbf{t}$. Similar to the single body, Equations 3.2 can be represented as:

$$\int_{\Omega_L} \rho_L \ddot{\mathbf{u}}_L \cdot \delta \dot{\mathbf{u}} \, d\Omega = \int_{\partial\Omega_L} \mathbf{t}_L \cdot \delta \dot{\mathbf{u}} \, d\Gamma - \int_{\Omega_L} \boldsymbol{\sigma}_L : \delta \mathbf{D}_L \, d\Omega + \int_{\Omega_L} \rho_L \mathbf{b}_L \cdot \delta \dot{\mathbf{u}} \, d\Omega \quad (3.38)$$

$$\int_{\Omega_s} \rho_s \ddot{\mathbf{u}}_s \cdot \delta \dot{\mathbf{u}} \, d\Omega = \int_{\partial\Omega_s} \mathbf{t}_s \cdot \delta \dot{\mathbf{u}} \, d\Gamma - \int_{\Omega_s} \boldsymbol{\sigma}_s : \delta \mathbf{D}_s \, d\Omega + \int_{\Omega_s} \rho_s \mathbf{b}_s \cdot \delta \dot{\mathbf{u}} \, d\Omega \quad (3.39)$$

The partitioned equations are discretised with finite elements Ω^e , with the following equations summing the contributions from each element e :

$$\mathbf{M}_L = \sum_{e=1}^{\mathcal{N}_e} \int_{\Omega_L^e} \rho \mathbf{N}^T \mathbf{N} \, d\Omega_e; \quad \mathbf{f}_L^{\text{ext}} = \sum_{e=1}^{\mathcal{N}_e} \int_{\Omega_L^e} \mathbf{N}^T \mathbf{t} \, d\Omega_e; \quad \mathbf{f}_L^{\text{int}} = \sum_{e=1}^{\mathcal{N}_e} \int_{\Omega_L^e} \mathbf{B}^T \boldsymbol{\sigma} \, d\Omega_e \quad (3.40)$$

$$\mathbf{M}_s = \sum_{e=1}^{\mathcal{N}_e} \int_{\Omega_s^e} \rho \mathbf{N}^T \mathbf{N} \, d\Omega_e; \quad \mathbf{f}_s^{\text{ext}} = \sum_{e=1}^{\mathcal{N}_e} \int_{\Omega_s^e} \mathbf{N}^T \mathbf{t} \, d\Omega_e; \quad \mathbf{f}_s^{\text{int}} = \sum_{e=1}^{\mathcal{N}_e} \int_{\Omega_s^e} \mathbf{B}^T \boldsymbol{\sigma} \, d\Omega_e \quad (3.41)$$

With the discrete equilibrium equations partitioned, each subdomain, Ω_L and Ω_s , can integrate over time with their own respective time step.

3.2 A Novel Algorithm for Multi-Time Step Integration with Two Subdomains

The coupling of two subdomains with separate time steps is described through the development of a novel multi-time stepping algorithm. The method comprises of three salient features; the explicit solution of the interface problem, controlling the ordering of integration, and comparison of the time step reduction factor.

3.2.1 The Explicit Solution of Temporally Coupled Subdomain Interfaces

To couple two subdomains that share an interface, denoted by Γ , the equation of motion must be solved. As shown in Equation 3.12, acceleration is explicitly solved at each time step. When solely isolating, the interface problem the equation becomes:

$$\ddot{\mathbf{u}}_\Gamma = \mathbf{M}_\Gamma^{-1} (\mathbf{f}_\Gamma^{\text{ext}} - \mathbf{f}_\Gamma^{\text{int}}) \quad (3.42)$$

with dimensions $\mathbf{M}_\Gamma \in \mathbb{R}^{\mathcal{N}_\Gamma \times \mathcal{N}_\Gamma}$, $\mathbf{f}_\Gamma^{\text{ext}} \in \mathbb{R}^{\mathcal{N}_\Gamma \times 1}$ and $\mathbf{f}_\Gamma^{\text{int}} \in \mathbb{R}^{\mathcal{N}_\Gamma \times 1}$. Here $\mathcal{N}_\Gamma$ is equal to the number of nodes on the interface of the two subdomains. With $\mathbf{M}_\Gamma$ a diagonal

mass matrix, $\mathbf{f}_\Gamma^{\text{ext}}$ and $\mathbf{f}_\Gamma^{\text{int}}$ the force vectors of the interface nodes, a direct solution of the acceleration field on the interface can be achieved. Let these vector shapes be extended for additional spatial dimensions as with Equations 3.9 - 3.11. The mass on the interface is assembled as:

$$\mathbf{M}_\Gamma = (\mathbf{C}_s^T \mathbf{M}_s \mathbf{C}_s) + (\mathbf{C}_L^T \mathbf{M}_L \mathbf{C}_L) \quad (3.43)$$

where $\mathbf{C}_s$ and $\mathbf{C}_L$ are indicator vectors in 1-D, and matrices in 2-D and 3-D, for the purpose of identifying degrees of freedom on the interfaces of Ω_s and Ω_L , respectively. The entries of these are 1 for nodes that reside on the interface, or 0 if not. Their dimensions are $\mathbf{C}_s \in \mathbb{R}^{\mathcal{N}_{n_s} \times \mathcal{N}_\Gamma}$ and $\mathbf{C}_L \in \mathbb{R}^{\mathcal{N}_{n_L} \times \mathcal{N}_\Gamma}$, where $\mathcal{N}_{n_s}$ and $\mathcal{N}_{n_L}$ are simply the total number of nodes in the small and large subdomain. This technique follows a similar operation in the works of Banks et al. [121] with use of an added-mass. The external and internal forces are summed in similar fashion with:

$$\mathbf{f}_\Gamma^{\text{int}} = \mathbf{C}_s^T \mathbf{f}_s^{\text{int}} + \mathbf{C}_L^T \mathbf{f}_L^{\text{int}}; \quad \mathbf{f}_\Gamma^{\text{ext}} = \mathbf{C}_s^T \mathbf{f}_s^{\text{ext}} + \mathbf{C}_L^T \mathbf{f}_L^{\text{ext}} \quad (3.44)$$

With all the components of Equation 3.42, the interface acceleration can be computed. The interface is explicitly solved at each large time step. Thus, the following condition is imposed:

$$\ddot{\mathbf{u}}_\Gamma = \ddot{\mathbf{u}}_{\Gamma s} = \ddot{\mathbf{u}}_{\Gamma L} \quad (3.45)$$

Through prescribing the condition, adjoining subdomains fulfil the continuity of acceleration and tractions. Equation 3.43 need only be computed at $t = 0$ under the assumption that nodal masses do not vary throughout the simulation. Given Equation 3.42 is computed at a full integration step, the method employs the same acceleration across the interface for each Δt_L . Next, techniques that allow the two subdomains to integrate over their own respective time steps are explained.

3.2.2 Ordering of Integration Steps with Time Step Ratios

Multi-time stepping allows for the integration of subdomains with their own respective time step, however as depicted in Figure 2.4, the ordering in which

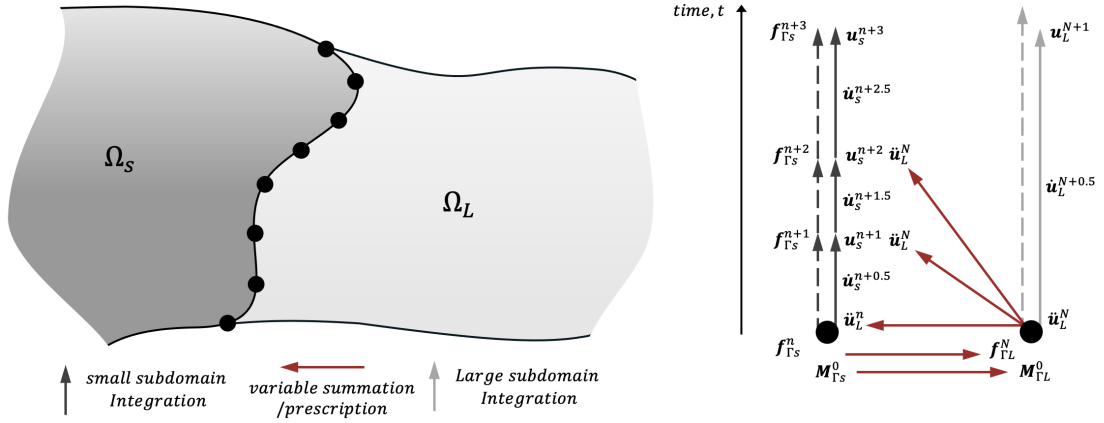


Figure 3.3: Visualisation of a full multi-time integration step for a coupling node on Γ solved with three time steps on the small subdomain to one large step with $t_s^{n+3} = t_L^{N+1}$. The dashed lines represent the computed trial time T_{Ti} , whereas the solid lines representing the time step used for the integration. Summation of forces $\mathbf{f}_\Gamma$ and masses $\mathbf{M}_\Gamma^0$ take place on the interface.

they do so varies vastly across literature. Starting from a common point in time, where $t_s^n = t_L^N$, the time steps of Ω_s and Ω_L are denoted by n and N respectively. Figure 3.3 shows the summation and prescription on the interface of two subdomains at this common time. To determine which subdomain to advance, the critical time step for each subdomain, defined as the *trial time* T_T is computed as:

$$t_{Ts}^{n+k} = t_s + \Delta t_{Cs}; \quad t_{TL}^{N+1} = t_L + \Delta t_{CL} \quad (3.46)$$

where k denotes the number of small time steps that have elapsed since the last common time step $t_s^n = t_L^N$ and $N + 1$ is the next large time step. The small subdomain is simply determined by the lesser of the two trial times. Two ratios are defined; the *current time step ratio*, t_{ratio}^{n+k} , and *next time step ratio*, t_{ratio}^{n+k+1} , with the following:

$$t_{ratio}^{n+k} = \frac{t_s^{n+k} - t_L^N}{t_{TL}^{N+1} - t_L^N}; \quad t_{ratio}^{n+k+1} = \frac{(t_s^{n+k} + \Delta t_s^{n+k}) - t_L^N}{t_{TL}^{N+1} - t_L^N} \quad (3.47)$$

The two ratios represent the advancement in time of the small subdomain, in relation to the large subdomain. The condition of $t_{ratio}^{n+k+1} \leq 1$ or ($t_{ratio}^{n+k} \leq 1$ and $t_{ratio}^{n+k+1} \leq 1$) determines if more integration steps on the small subdomain Ω_s , at its critical time step Δt_{Cs} , can be performed. For this a new trial time t_{Ts} is also required at each Δt_s to allow for the re-evaluation of Equations 3.47.

With this order, a small integration step can be described now. In the proposed approach, Ω_s is integrated first, where the acceleration field of the entire small subdomain at time step n is computed as:

$$\ddot{\mathbf{u}}_s^n = (\mathbf{I} - \mathbf{C}_s \mathbf{C}_s^T) \tilde{\mathbf{u}}_s^n + (\mathbf{C}_s \mathbf{L}_s) \ddot{\mathbf{u}}_\Gamma^N \quad (3.48)$$

where the unconstrained acceleration is defined as $\tilde{\mathbf{u}}_s^n = \mathbf{M}_s^{-1}(\mathbf{f}_s^{\text{ext}} - \mathbf{f}_s^{\text{int}})$ for those nodes that are not found on the interface and hence not prescribed an acceleration. Here, it is useful to define an identity matrix as $\mathbf{I} \in \mathbb{R}^{\mathcal{N}_{n_s} \times \mathcal{N}_{n_s}}$, and a square incidence matrix used to relate the interface degrees of freedom to the small global vectors, defined as $\mathbf{L}_s \in \mathbb{R}^{\mathcal{N}_\Gamma \times \mathcal{N}_s}$. The staggered integration scheme gives the kinematic quantities at time steps $t_s^{n+k+\frac{1}{2}}$ and t_s^{n+k+1} as:

$$\dot{\mathbf{u}}_s^{n+k+\frac{1}{2}} = \dot{\mathbf{u}}_s^{n+k-\frac{1}{2}} + \ddot{\mathbf{u}}_s^n \cdot \Delta t_s^n \quad (3.49)$$

$$\mathbf{u}_s^{n+k+1} = \mathbf{u}_s^{n+k} + \dot{\mathbf{u}}_s^{n+k+\frac{1}{2}} \cdot \Delta t_s^{n+k+\frac{1}{2}} \quad (3.50)$$

Here, the interface kinematics are updated with the rest of the subdomain. This differs from the works of Dvorak et al. [56] and Cho et al. [57], where separate regions are defined to enforce the coupling. It is crucial to mention at this point, that despite only the continuity of acceleration being enforced, the algorithm also enforces velocity and displacement. This is further elaborated upon in the coming sections of the thesis. Proceeding the integration of a single step on Ω_s to $n+1$, the time step ratios are computed. The re-computation of t_{Ts} at each Δt_s is particularly advantageous for highly dynamic problems where time steps may vary suddenly. The current time step ratio t_{ratio}^{n+k} is principal ensuring the correct ordering when $\Delta t_s \approx \Delta t_L$. Now that the ordering of updates have been determined, a method must be developed to ensure subdomains meet at the same point in time.

3.2.3 Controlling Subdomain Time Steps for Synchronisation with Reduction Factors

To ensure the synchronisation of subdomains in time, the proposed algorithm selects a time step that minimises the deviation from the trial times of t_{TL} and

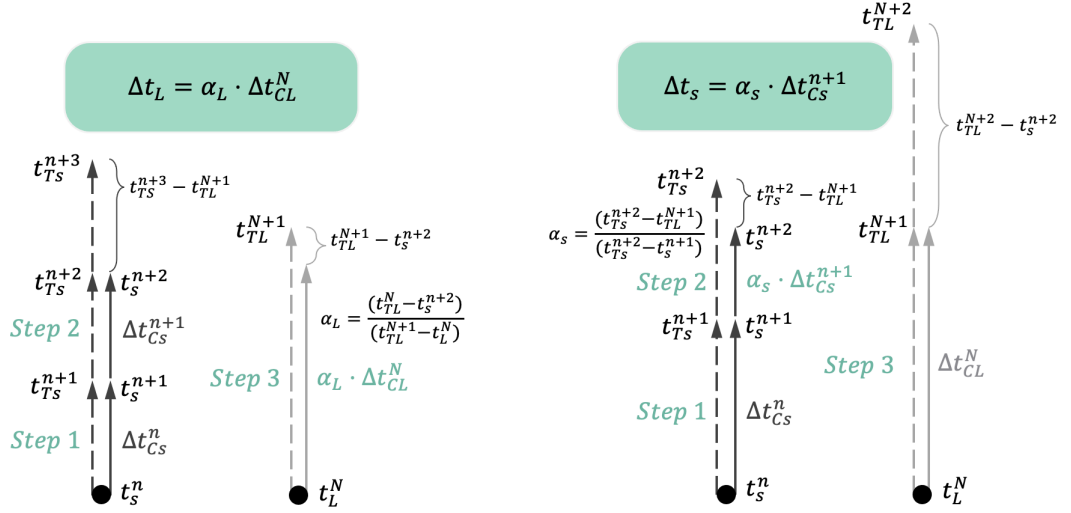


Figure 3.4: (a): Case where $\alpha_L > \alpha_s$ - Time Step Reduction Factor applied on the large subdomain for $m \approx 2.4$. The large subdomain time step is reduced to synchronise with the small time step; (b): Case where $\alpha_s \geq \alpha_L$ - Reduction Factor applied on the small subdomain for $m \approx 1.6$. The small subdomain's second time step is reduced to synchronise with the large time step.

t_{Ts} , as per the CFL condition. In an updated Lagrangian formulation, the time steps can change, resulting in an unknown synchronisation time a priori. Once the trial time of Ω_s exceeds that of Ω_L , two *reduction factors* are computed, denoted α_s and α_L . These reduction factors are computed with four quantities in time, where $0 < \alpha \leq 1$, as the following:

$$\alpha_L = 1 - \frac{(t_{TL}^N - t_s^{n+k})}{(t_{TL}^{N+1} - t_L^N)}; \quad \alpha_s = 1 - \frac{(t_{Ts}^{n+k} - t_{TL}^{N+1})}{(t_{Ts}^{n+k+1} - t_s^{n+k})} \quad (3.51)$$

Both factors utilise the aforementioned trial times to determine which subdomain is closest to the CFL condition. The reduction factor is only applied to one subdomain, allowing the other to step with its critical time step. Figure 3.4 accompanies the following definition of these factors. The two cases of time step reduction are found to be:

Case 1: $\alpha_s \geq \alpha_L$

$$\ddot{\mathbf{u}}_s^{n+1} = (\mathbf{I} - \mathbf{C}_s \mathbf{C}_s^T) \tilde{\mathbf{u}}_s^{n+1} + (\mathbf{C}_s \mathbf{L}_s) \ddot{\mathbf{u}}_L^N \quad (3.52)$$

$$\dot{\mathbf{u}}_s^{n+3/2} = \dot{\mathbf{u}}_s^{n+1/2} + \ddot{\mathbf{u}}_s^{n+1} \cdot \alpha_s \Delta t_s \quad (3.53)$$

$$\mathbf{u}_s^{n+2} = \mathbf{u}_s^{n+1} + \dot{\mathbf{u}}_s^{n+3/2} \cdot \alpha_s \Delta t_s \quad (3.54)$$

where the first case reduces the Δt_s and integrates one further step. The quantities over Ω_L can be computed via the following Equations 3.48, 3.49 and 3.50, effectively integrating the same equations, but for Ω_L . The application of the reduction factor on the large subdomain gives:

Case 2: $\alpha_L > \alpha_s$

$$\ddot{\mathbf{u}}_L^N = (\mathbf{I} - \mathbf{C}_L \mathbf{C}_L^T) \tilde{\ddot{\mathbf{u}}}_L^N + (\mathbf{C}_L \mathbf{L}_L) \ddot{\mathbf{u}}_\Gamma^N \quad (3.55)$$

$$\tilde{\ddot{\mathbf{u}}}_L^N = \mathbf{M}_\Gamma^{-1} (\mathbf{f}_L^{\text{ext}} - \mathbf{f}_L^{\text{int}}) \quad (3.56)$$

$$\dot{\mathbf{u}}_L^{N+1/2} = \dot{\mathbf{u}}_s^{N-1/2} + \ddot{\mathbf{u}}_L^N \cdot \alpha_L \Delta t_L \quad (3.57)$$

$$\mathbf{u}_L^{N+1} = \mathbf{u}_L^N + \dot{\mathbf{u}}_L^{N+1/2} \cdot \alpha_L \Delta t_L \quad (3.58)$$

Both cases ensure that the two subdomains will always find a common time. This is represented by the following:

$$t_L^{N+1} = t_s^{n+k} = \begin{cases} t_s^n + \sum_{k=0}^{k-1} \Delta t_{Cs}^{n+k} + \alpha_s \cdot \Delta t_{Cs}^{n+k}, & \alpha_s > \alpha_L \\ t_s^n + \alpha_L \cdot \Delta t_{CL}^N, & \alpha_L \geq \alpha_s \end{cases} \quad (3.59)$$

Through ensuring a common time is found, operations in Section 3.2.1 can be performed to solve the interface problem once more. A summary of the algorithm is provided to reiterate the steps of the method for a full integration step.

Algorithm 1 Summary of Algorithm for a Large step from N to $N + 1$

- 1: **procedure** A TWO-DOMAIN MULTI TIME INTEGRATION STEP
 - 2: **while** $t_{ratio}^{n+k+1} \leq 1$ or $(t_{ratio}^{n+k} \leq 1$ and $t_{ratio}^{n+k+1} \leq 1 + TOL)$ **do**
 - 3: Integrate small domain Ω_s with $\ddot{\mathbf{u}}_\Gamma$ and compute force vectors $\mathbf{f}_s^{\text{int}}, \mathbf{f}_s^{\text{ext}}$
 - 4: Compute trial times $t_{Ts}^{n+k}, t_{TL}^{N+1}$ and time step ratios $t_{ratio}^{n+k}, t_{ratio}^{n+k+1}$
 - 5: Compute time step reduction factors α_L, α_s
 - 6: **if** $\alpha_L \geq \alpha_s$ **then**
 - 7: $\Delta t_L = \alpha_L \cdot \Delta t_L$
 - 8: **else**
 - 9: $\Delta t_s = \alpha_s \cdot \Delta t_s$
 - 10: Integrate small domain Ω_s with $\ddot{\mathbf{u}}_\Gamma$ and recompute force vectors $\mathbf{f}_s^{\text{int}}, \mathbf{f}_s^{\text{ext}}$
 - 11: Recompute trial times $t_{Ts}^{n+k}, t_{TL}^{N+1}$ and time step ratios $t_{ratio}^{n+k}, t_{ratio}^{n+k+1}$
 - 12: Integrate Large domain Ω_L with $\ddot{\mathbf{u}}_\Gamma$ and compute force vectors $\mathbf{f}_L^{\text{int}}, \mathbf{f}_L^{\text{ext}}$
 - 13: Compute interface acceleration $\ddot{\mathbf{u}}_\Gamma$ with Eq. 3.42 for next time step
 - 14: Recompute trial times $t_{Ts}^{n+k}, t_{TL}^{N+1}$ and time step ratios $t_{ratio}^{n+k}, t_{ratio}^{n+k+1}$
-

3.3 Assessment of Stability and Drifting

The literature review in Section 2.2 identified the importance of evaluating the stability of subcycling algorithms. Cho et al. [57] also discussed the phenomena of drifting, in which, not all kinematic field variables are satisfied on the interface. For these reasons, the proposed method is verified to ensure stable and accurate in comparison to conventional methods and the state-of-the-art. Lagrange multipliers are examples of such methods, particularly effective for coupled solutions due to their ability to manage constraints across scales. Their introduction into the coupling of systems maintains optimal accuracy, without compromising overall stability. Therefore, this section gives an overview of the theory followed by a comparison of temporal coupling techniques to assess stability and drifting.

3.3.1 Comparison to Lagrange Multiplier Methods

Several of the aforementioned coupling methods utilise Lagrange multipliers to resolve the behaviour at the interfaces of subdomains [51, 55, 59, 122, 123]. The continuity of acceleration is enforced with those methods in the works of [56, 57]. In essence, Lagrange multiplier methods require the solution of additional fields $\boldsymbol{\lambda}$, to give the following equations of motion for the two subdomain problem:

$$\mathbf{M}_L \ddot{\mathbf{u}}_L + \mathbf{C}_L \boldsymbol{\lambda}_L = \mathbf{f}_L^{\text{ext}} - \mathbf{K}_L \mathbf{u}_L \quad (3.60)$$

$$\mathbf{M}_s \ddot{\mathbf{u}}_s + \mathbf{C}_s \boldsymbol{\lambda}_s = \mathbf{f}_s^{\text{ext}} - \mathbf{K}_s \mathbf{u}_s \quad (3.61)$$

Both large $\boldsymbol{\lambda}_L$ and small $\boldsymbol{\lambda}_s$ Lagrange multipliers require their corresponding incidence matrix $\mathbf{C}_L$ and $\mathbf{C}_s$. Aforementioned works, also utilise the global stiffness matrices $\mathbf{K}_L$ and $\mathbf{K}_s$, effectively denoting the internal force $\mathbf{f}^{\text{int}}$ when multiplied by the displacement field $\mathbf{u}$, of their respective subdomain. The Localised Lagrange Multiplier method (LLM) requires introducing the frame, denoted f , to enforce the continuity across subdomains.

$$\mathbf{C}_L^T \ddot{\mathbf{u}}_L - \mathbf{L}_L \ddot{\mathbf{u}}_f = 0; \quad \mathbf{C}_s^T \ddot{\mathbf{u}}_s - \mathbf{L}_s \ddot{\mathbf{u}}_f = 0 \quad (3.62)$$

The equilibrium over the interface is ensured by these reaction loads to give:

$$\mathbf{L}_L^T \boldsymbol{\lambda}_L + \mathbf{L}_s^T \boldsymbol{\lambda}_s = 0 \quad (3.63)$$

The system of equations on the interface can be formed as:

$$\begin{bmatrix} \mathbf{C}_L^T \mathbf{M}_L^{-1} \mathbf{C}_L & 0 & \mathbf{L}_L \\ 0 & \mathbf{C}_s^T \mathbf{M}_s^{-1} \mathbf{C}_s & \mathbf{L}_s \\ \mathbf{L}_L^T & \mathbf{L}_s^T & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda}_L^{n+k} \\ \boldsymbol{\lambda}_s^{n+k} \\ \ddot{\mathbf{u}}_f^{n+k} \end{bmatrix} = \begin{bmatrix} \mathbf{C}_L^T \tilde{\mathbf{u}}_L^{n+k} \\ \mathbf{C}_s^T \tilde{\mathbf{u}}_s^{n+k} \\ 0 \end{bmatrix} \quad (3.64)$$

where the system is solved at each small time step Δt_s , hence at each step k . The vector of unknowns can be evaluated to obtain:

$$\boldsymbol{\lambda}_L^{n+k} = (\mathbf{C}_L^T \mathbf{M}_L^{-1} \mathbf{C}_L)^{-1} (\mathbf{C}_L^T \tilde{\mathbf{u}}_L^{n+k} - \mathbf{L}_L \ddot{\mathbf{u}}_f^{n+k}) \quad (3.65)$$

$$\boldsymbol{\lambda}_s^{n+k} = (\mathbf{C}_s^T \mathbf{M}_s^{-1} \mathbf{C}_s)^{-1} (\mathbf{C}_s^T \tilde{\mathbf{u}}_s^{n+k} - \mathbf{L}_s \ddot{\mathbf{u}}_f^{n+k}) \quad (3.66)$$

$$\ddot{\mathbf{u}}_f^{n+k} = \left[\sum_{i=1}^2 \left(\mathbf{L}_i^T (\mathbf{C}_i^T \mathbf{M}_i^{-1} \mathbf{C}_i)^{-1} \mathbf{L}_i \right) \right]^{-1} \sum_{i=1}^2 \left(\mathbf{L}_i^T (\mathbf{C}_i^T \mathbf{M}_i^{-1} \mathbf{C}_i)^{-1} \mathbf{C}_i^T \tilde{\mathbf{u}}_i^{n+k} \right) \quad (3.67)$$

Equation 3.67 is of particular interest, as this represents the resolved acceleration to be coupled across both subdomains. The following sections look to compare $\ddot{\mathbf{u}}_f$ to the proposed $\ddot{\mathbf{u}}_f$, and its equivalence. The substitution of the unconstrained acceleration $\tilde{\mathbf{u}}_i^{n+k}$ for each subdomain gives the constrained acceleration to complete the solution of the interface at $n + k$ as:

$$\ddot{\mathbf{u}}_s^{n+k} = \mathbf{M}_s^{-1} (\mathbf{f}_L^{\text{ext}} - \mathbf{K}_s \mathbf{u}_s) - \mathbf{M}_s^{-1} \mathbf{C}_s \boldsymbol{\lambda}_s^{n+k} = \tilde{\mathbf{u}}_s^{n+k} - \mathbf{M}_s^{-1} \mathbf{C}_s \boldsymbol{\lambda}_s^{n+k} \quad (3.68)$$

Through comparing the methods of evaluating the interface with LLMs, the proposed novel coupling can now be tested for its stability. The two-domain algorithm shall now be compared under the severe conditions of a square pulse propagation.

3.3.2 Propagation of a Square Pulse through a Bi-material Interface

To demonstrate the stability of the two-domain algorithm, an extreme loading case is considered with a discontinuous wave propagation problem (i.e. Heaviside function loading) in a bi-material bar configuration. This is preferred over the smooth pulse, where higher frequencies of the wave are not activated. Suppose

the domain Ω is split into two subdomains with the elastic properties tabulated in Table 3.1. The bar is consecutive in its subdomains, with a time step ratio $m = \pi$ calculated as a result of the difference in dilatational wave speed. The same spatial

Table 3.1: Summary of material properties for elastic square wave propagation problem.

Material Property	Large Subdomain Ω_L	Small Subdomain Ω_s
Young's Modulus, E	0.02 GPa	$8000(\frac{\pi}{0.02})^2$ GPa
Density, ρ	8000 kgm^{-3}	8000 kgm^{-3}
Length, L	$50 \times 10^{-3} \text{ m}$	$100 \times 10^{-3} \text{ m}$
Area, A	1.0 m^2	1.0 m^2
Dilatational Wave Speed, c	50 ms^{-1}	157.08 ms^{-1}

discretisation is used with 1-D linear finite elements, counting 300 in Ω_L and 600 in Ω_s . The square wave is applied as a prescribed velocity boundary condition at the position $x = 0$, where an equivalent sine period is $L_L/2 \cdot \sqrt{\rho/E_L}$. This therefore leads to a forward travelling wave that covers half of Ω_L by the time the pulse has been fully applied. Figure 3.5 depicts the heterogeneous bar to fully define the problem, hence the conditions on the interface Γ can now be assessed.

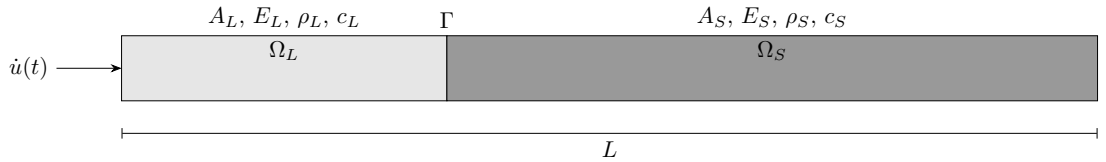


Figure 3.5: A one-dimensional heterogeneous domain Ω split into large time step subdomain Ω_L and small time step subdomain Ω_s of length $L_L = 50 \text{ mm}$ and $L_s = 100 \text{ mm}$. The problem assuming uniaxial motion with Poisson's ratio $\nu = 0$. A square wave velocity boundary condition is applied from Ω_L .

3.3.3 Stability Check via Energy Conservation and Continuity of Interface Kinematics

As Section 2.2.3 identified, the stability of multi-time stepping methods have been scrutinised in literature. In the following analysis, a comparisons of energies is made to the aforementioned Localised Lagrange Multipliers, due to the claims of the method being energy-conserving [56]. Consequently, should a similar tolerance

of energy conservation be made with the proposed method, a statement for its stability can be made. The square wave benchmark is adopted to present the solution of the interface system of equations with Lagrange multipliers and the proposed method. The frame acceleration is computed via the LLMs with Equation 3.67, then it can be proved that:

$$\ddot{\mathbf{u}}_\Gamma^{N+1} = \ddot{\mathbf{u}}_f^{N+1} \quad (3.69)$$

In 1-D, Equation 3.42 and 3.67 can be shown to produce an identical acceleration with the incidence vectors and matrices reducing to:

$$\mathbf{C}_L = \begin{bmatrix} 0 \\ \vdots \\ 1 \end{bmatrix}; \quad \mathbf{C}_s = \begin{bmatrix} 1 \\ \vdots \\ 0 \end{bmatrix}; \quad \mathbf{L}_L = [1]; \quad \mathbf{L}_s = [1] \quad (3.70)$$

Assuming the coupling corresponds solely to the stresses in the material, the external term in Equation 3.42 is assumed negligible. From this, the frame acceleration is split into the product of two summations to give:

$$\mathbf{M}_\Gamma^{-1} = \left[(\mathbf{C}_s^T \mathbf{M}_s \mathbf{C}_s) + (\mathbf{C}_L^T \mathbf{M}_L \mathbf{C}_L) \right]^{-1} = \left[\sum_{i=1}^2 \left(\mathbf{L}_i^T (\mathbf{C}_i^T \mathbf{M}_i^{-1} \mathbf{C}_i)^{-1} \mathbf{L}_i \right) \right]^{-1} \quad (3.71)$$

$$-\mathbf{f}_\Gamma^{\text{int}} = -(\mathbf{C}_s^T \mathbf{f}_s^{\text{int}} + \mathbf{C}_L^T \mathbf{f}_L^{\text{int}}) = \sum_{i=1}^2 \left(\mathbf{L}_i^T (\mathbf{C}_i^T \mathbf{M}_i^{-1} \mathbf{C}_i)^{-1} \mathbf{C}_i^T \tilde{\mathbf{u}}_i^{n+k} \right) \quad (3.72)$$

where the inverse of Equation 3.43 gives the same result as the LHS summation. The internal forces in Equation 3.44 correspond to the RHS summation with the unconstrained acceleration at the large time step $\tilde{\mathbf{u}}_i^{N+1}$ from each subdomain Ω_i .

The Lagrange multipliers are the coupling forces of each subdomain, also referred to as the linking forces in the works of Gravouil and Combescure [122, 124]. The system of Equations 3.64, shows that these forces much satisfy:

$$\mathbf{L}_L^T \boldsymbol{\lambda}_L^{N+1} = -\mathbf{L}_s^T \boldsymbol{\lambda}_s^{N+1} \quad (3.73)$$

The proposed method assumes a constant acceleration across a Δt_L . In the first part of the stability check, the interface equations of motion in Equations 3.64 are solved every large time step too. In Figure 3.6 coupling forces, $\boldsymbol{\lambda}$, are plotted, as well as the equivalence of the accelerations recovered from the frame $\ddot{\mathbf{u}}_f$ and the

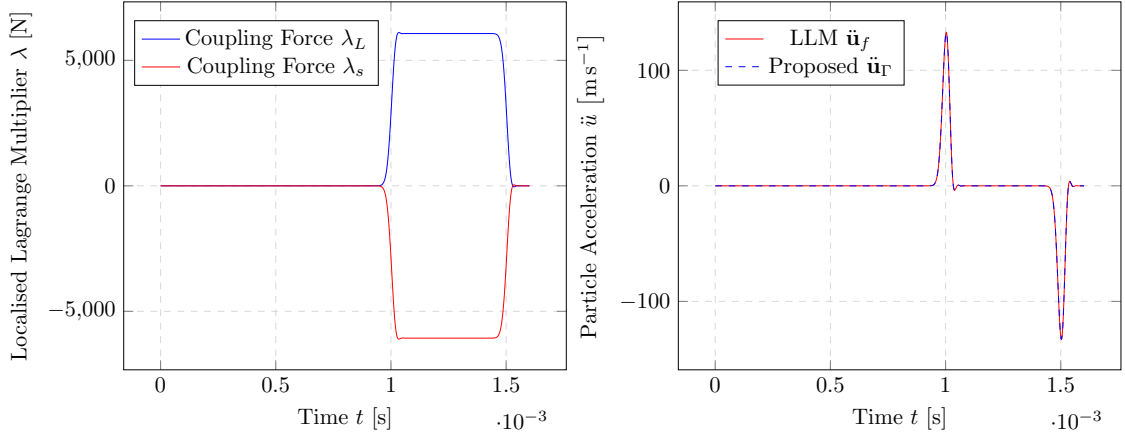


Figure 3.6: Comparison to Localised Lagrange Multiplier methods; (a): Computed coupling forces from equivalent interface equations of motion; (b): Acceleration computed from LLMs [56] compared to the proposed method in Equations 3.67 and 3.42.

proposed method $\ddot{\mathbf{u}}_\Gamma$. Hughes and Liu's energy method [125] is a common method for evaluating the stability of the system, as adopted also in the works of [45, 124]. To assess the energy for two subdomains, the method writes:

$$W_{\text{ext},L} - W_{\text{int},L} + W_{\text{kin},L} + W_{\text{ext},s} - W_{\text{int},s} + W_{\text{kin},s} = W_{\text{Link},L} + W_{\text{Link},s} \quad (3.74)$$

where each energy term can be generally expanded for a subdomain Ω_i as:

$$W_{\text{int},i} = \frac{1}{2} \mathbf{u}_i^T (\mathbf{f}_{\text{int},i}); \quad W_{\text{ext},i} = \frac{1}{2} \mathbf{u}_i^T (\mathbf{f}_{\text{ext},i}); \quad W_{\text{kin},i} = \frac{1}{2} (\dot{\mathbf{u}}_i)^T \mathbf{M} \dot{\mathbf{u}}_i \quad (3.75)$$

and the energy associated to the coupling of the two subdomains is named the link energy to be consistent with literature [122], thus:

$$W_{\text{Link},i} = \frac{1}{2} (\mathbf{C}_i^T \mathbf{u}_i) \boldsymbol{\lambda}_i \quad (3.76)$$

At a time step t^{N+1} , it is shown that the force equilibrium at the interface nodes can be used to evaluate the energy on Γ . The balance of forces on Γ_L and Γ_s reads:

$$\begin{aligned} \mathbf{f}_{\Gamma_L}^{N+1} &= \mathbf{C}_L \boldsymbol{\lambda}_L^{N+1} + (\mathbf{C}_L^T \mathbf{M}_L^{-1} \mathbf{C}_L)^{-1} \ddot{\mathbf{u}}_\Gamma^{N+1} + \mathbf{C}_L \mathbf{f}_{\text{int},L}^{N+1} \\ &= \mathbf{f}_{\Gamma_s}^{N+1} = \mathbf{C}_s \boldsymbol{\lambda}_s^{N+1} + (\mathbf{C}_s^T \mathbf{M}_s^{-1} \mathbf{C}_s)^{-1} \ddot{\mathbf{u}}_\Gamma^{N+1} + \mathbf{C}_s \mathbf{f}_{\text{int},s}^{N+1} \\ &= 0 \end{aligned} \quad (3.77)$$

Here $\mathbf{f}_{\Gamma_L}^{N+1}$ and $\mathbf{f}_{\Gamma_s}^{N+1}$ represent the sum of all forces on Γ_L and Γ_s respectively. The proposed method does not require the solution of Γ_L and Γ_s at each Δt_s ,

rather it solves each Δt_L . The energy across Γ , over each Δt_L , is computed with Equation 3.77 as:

$$\begin{aligned}
 W_{\Gamma}^{N+1} &= W_{\Gamma L}^N + \delta W_{\Gamma L} + W_{\Gamma s}^N + \delta W_{\Gamma s} \\
 &= W_{\Gamma L}^N + \frac{1}{2}(\mathbf{C}_L^T \mathbf{u}_L^{N+1} - \mathbf{C}_L^T \mathbf{u}_L^N)^T (\mathbf{f}_{\Gamma L}^{N+1}) + W_{\Gamma s}^N + \frac{1}{2}(\mathbf{C}_s^T \mathbf{u}_s^{N+1} - \mathbf{C}_s^T \mathbf{u}_s^N)^T (\mathbf{f}_{\Gamma s}^{N+1}) \\
 &= 0
 \end{aligned} \tag{3.78}$$

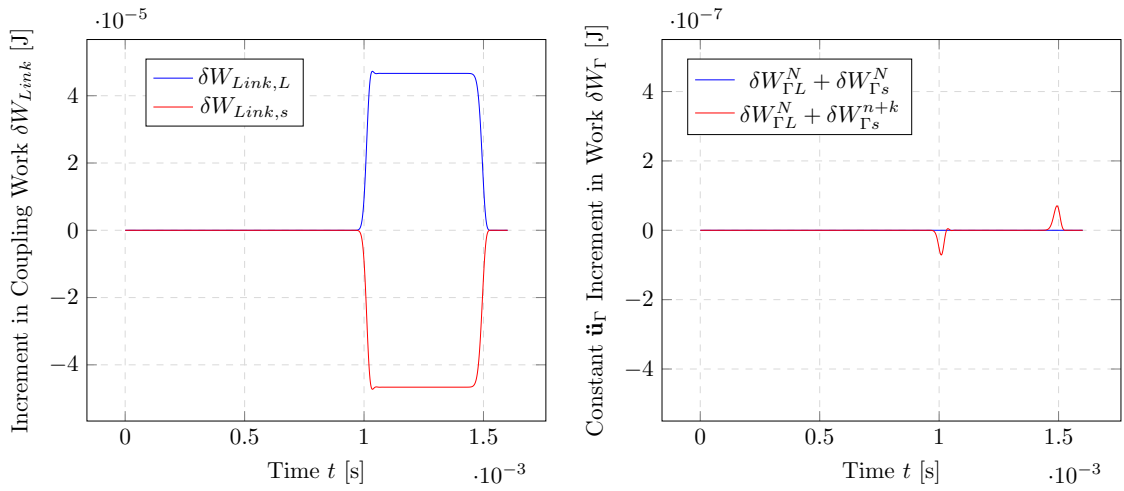


Figure 3.7: Increments in work with Energy Methods; (a): Increment in work associated to the coupling of the subdomains recovered at each Δt_s ; (b): Increment in work done to maintain constant $\ddot{\mathbf{u}}_{\Gamma}$.

Part (a) of Figure 3.7 plots the increments in work done over Δt_L and Δt_s for respective subdomains. The energy associated to the coupling of subdomains, from Equation 3.76, can be isolated from the energy equation to give just the increments in W_{Link} as:

$$\begin{aligned}
 W_{\text{Link}}^{N+1} &= W_{\text{Link},L}^N + \delta W_{\text{Link},L} + W_{\text{Link},s}^N + \delta W_{\text{Link},s} \\
 &= W_{\text{Link},L}^N + \frac{1}{2}(\mathbf{C}_L^T \mathbf{u}_L^{N+1} - \mathbf{C}_L^T \mathbf{u}_L^N)^T (\boldsymbol{\lambda}_L^N + \boldsymbol{\lambda}_L^{N+1}) \\
 &\quad + W_{\text{Link},s}^N + \frac{1}{2}(\mathbf{C}_s^T \mathbf{u}_s^{N+1} - \mathbf{C}_s^T \mathbf{u}_s^N)^T (\boldsymbol{\lambda}_s^N + \boldsymbol{\lambda}_s^{N+1})
 \end{aligned} \tag{3.79}$$

Proper evaluation of stability, requires accounting for the changes of a small time step too. This becomes more challenging granted the interface Equations 3.64 need the coupling forces $\boldsymbol{\lambda}_L^{n+k}$ at Δt_s to be recovered. At small steps k , the internal force

$\mathbf{f}_{\text{int},L}^{n+k}$ becomes an unknown of the system. This variation in kinematic quantities over Δt_s can be computed with the small increments:

$$\begin{aligned} W_{\text{Link}}^{n+1} &= W_{\text{Link},L}^N + \delta W_{\text{Link},L} + W_{\text{Link},s}^n + \delta W_{\text{Link},s} \\ &= W_{\text{Link},L}^n + \frac{1}{2}(\mathbf{C}_L^T \mathbf{u}_L^{N+1} - \mathbf{C}_L^T \mathbf{u}_L^N)^T (\boldsymbol{\lambda}_L^N + \boldsymbol{\lambda}_L^{N+1}) + W_{\text{Link},s}^n \\ &\quad + \sum_{k=0}^m \frac{1}{2}(\mathbf{C}_s^T \mathbf{u}_s^{n+k} - \mathbf{C}_s^T \mathbf{u}_s^{n+k+1})^T (\boldsymbol{\lambda}_s^{n+k} + \boldsymbol{\lambda}_s^{n+k+1}) \end{aligned} \quad (3.80)$$

The summation over the small time steps shows the variation in displacements and coupling forces on Γ_s . Once again, it is noted that the summation is computed at each common time step, where $t_L = t_s$ at steps N and n respectively. To clarify, for the preceding benchmark where time step ratio $m = \pi$, the Lagrange multipliers at each Δt_L so the same problem on either side of the interface so that:

$$\mathbf{L}_L^T \boldsymbol{\lambda}_L^{N+1} + \mathbf{L}_s^T \boldsymbol{\lambda}_s^{N+1} = \mathbf{L}_L^T \boldsymbol{\lambda}_L^{n+3} + \mathbf{L}_s^T \boldsymbol{\lambda}_s^{n+3} = 0 \quad (3.81)$$

where three small time steps correspond to a single large time step (with a reduction factor α_L applied). Part (b) of Figure 3.7 plots increment in interface energy δW_Γ for each of the subdomains, accounting for the variation across Δt_s as well. This non-zero energy production leads investigation into the implications of this assumption over Δt_L of a constant acceleration.

3.3.4 The Assumption of Constant Acceleration over a Large Time Step

A potential limitation of the algorithm is the computation of $\ddot{\mathbf{u}}_\Gamma$ only at each Δt_L . For the square wave benchmark the interface acceleration on both subdomains can be visualised in Figure 3.8. Focusing on the time period where Γ first sees the pulse, a magnified view of the acceleration is plotted in Figure 3.9. The application of $\ddot{\mathbf{u}}_\Gamma$ for three Δt_s is observed to give the stepping nature of of Figure 3.9. The imposed inertial force on Γ over a large Δt_L gives the following:

$$\mathbf{M}_\Gamma^N \ddot{\mathbf{u}}_\Gamma^N = \mathbf{C}_L^T \boldsymbol{\lambda}_L^N + \mathbf{C}_s^T \boldsymbol{\lambda}_s^n + \mathbf{C}_L^T \mathbf{f}_{\text{int},L}^N - \mathbf{C}_s^T \mathbf{f}_{\text{int},s}^n = 0 \quad (3.82)$$

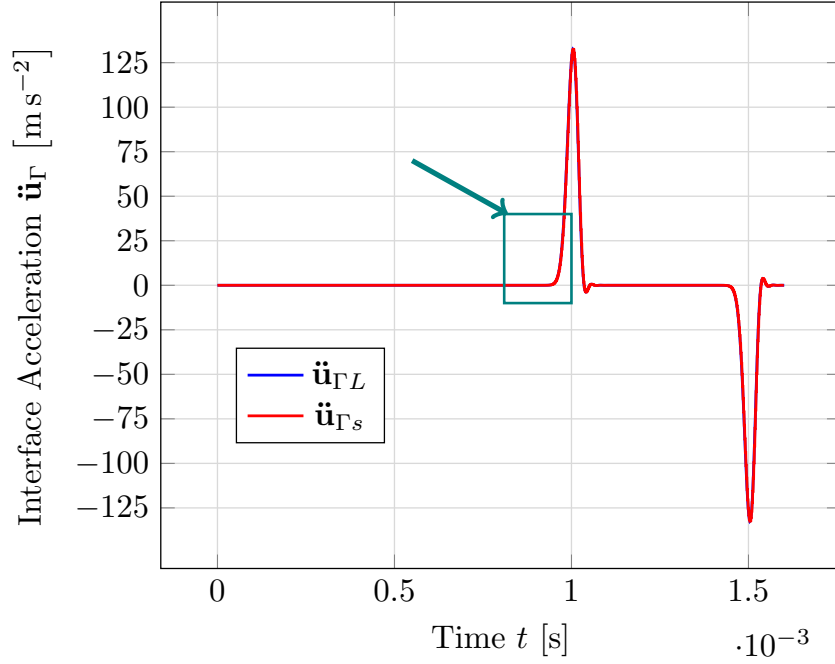


Figure 3.8: Large and Small Interface accelerations $\ddot{\mathbf{u}}_{\Gamma}$ through time for the 1-D benchmark with multi-time stepping.

where $N = n$, whereas over a small Δt_s , the imposed acceleration creates a small contribution:

$$\mathbf{M}_{\Gamma}^N \ddot{\mathbf{u}}_{\Gamma}^N = \mathbf{C}_L^T \boldsymbol{\lambda}_L^N + \mathbf{C}_L^T \mathbf{f}_{\text{int},L}^N + \mathbf{C}_s^T \boldsymbol{\lambda}_s^{n+k} - \mathbf{C}_s^T \mathbf{f}_{\text{int},s}^{n+k} + \delta \mathbf{f}_{\Gamma_s}^{n+k} = 0 \quad (3.83)$$

where an additional inertial term is found in $\delta \mathbf{f}_{\Gamma_s}^{n+k}$ for each Δt_s . The associated energy can be seen as the contribution from Equation 3.83, where $\delta W_{\Gamma_s}^{n+k} = 0$, only if the motion of Γ_s follows a constant acceleration. In the case of $m = \pi$, the observed energy difference is $< 0.25\%$ of the increment in coupling energies δW_{Link} , and $< 0.001\%$ of the internal and kinetic energy of system. Therefore the use of $\ddot{\mathbf{u}}_{\Gamma}$ can be deemed reasonable over Δt_L . Despite this, special limit cases exist; in the case of highly heterogeneous configurations. Appendix section A.2 simulates a large difference in impedance, resulting in $m = 100$ between subdomain time steps. Where large values of m are used, instability may occur when using the constant $\ddot{\mathbf{u}}_{\Gamma}$. For these limit cases, one of two simple methods could be adopted:

- Reducing the Courant number Co_L for integration on Ω_L ;
- Integrating the element on Ω_L closest to the material interface with Δt_s .

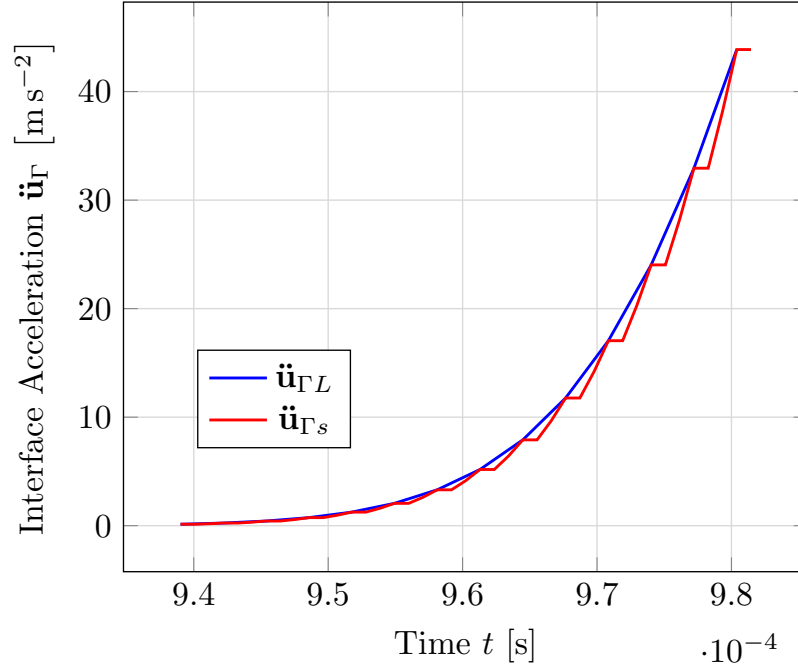


Figure 3.9: Magnifying the green box in Figure 3.8 to depict the constant $\ddot{\mathbf{u}}_{\Gamma}$ assumption of N to $N + 1$ shows the "stepping" nature of the acceleration on the small interface.

Both methods increase the number of element integration steps, and therefore the computational effort. However, the algorithm does not require adaptation for these scenarios. Ultimately, this highlights the trade-off between computational efficiency and the accuracy of multi-time stepping methods.

3.3.5 A Three-field Kinematic Continuity Study for Drifting on the Interface

The phenomena of drifting is a key issue, as highlighted by Cho et al. [57], where interface subdomains do not preserve continuity across all three kinematic quantities - acceleration, velocity and displacement. For this reason, an assessment of all three is made, given the constant acceleration imposed on the two subdomains. Leapfrog time integration, derived from the central difference method, imposes the same motion of externally assembled Γ between two time steps. Through imposing $\ddot{\mathbf{u}}_{\Gamma}$ as a boundary condition, Γ_L and Γ_s follow the same motion, thus avoiding the concept of drifting.

To measure the continuity of kinematics on the interface, a relative squared error is defined for each:

$$\mathbf{A}_{\Gamma, RSE} = \left(\frac{|\mathbf{A}_{\Gamma L} - \mathbf{A}_{\Gamma s}|}{\mathbf{A}_{\Gamma L}} \right)^2 \quad (3.84)$$

where the $\mathbf{A}$ denotes the kinematic quantity. The absolute difference is taken between subdomains, with the value on Γ_L used as the reference. The absolute differences found were the following $\ddot{u}_\Gamma < 1 \times 10^{-32}$, $\dot{u}_\Gamma < 5 \times 10^{-16}$, $u_\Gamma < 5 \times 10^{-9}$ for interface acceleration, velocity and displacement respectively. Figure 3.10 plots each of the three kinematics. To avoid round-off errors on the interface, one could enforce the following:

$$\mathbf{C}_i^T \dot{\mathbf{u}}_i^{n+1} - \mathbf{L}_i \dot{\mathbf{u}}_\Gamma^{n+1} = 0 \quad (3.85)$$

$$\mathbf{C}_i^T \mathbf{u}_i^{n+1} - \mathbf{L}_i \mathbf{u}_\Gamma^{n+1} = 0 \quad (3.86)$$

however this effectively introduces very small amounts of external work into the system. With the use of consistent integration schemes in subdomains, the violation of continuity on the interface is not expected when using the proposed multi-time stepping algorithm.

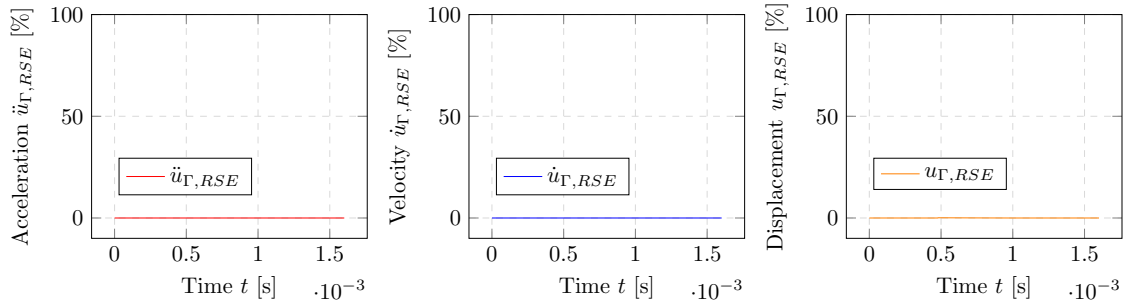


Figure 3.10: Continuity of kinematic quantities; (a): Error of interface accelerations; (b): Error of interface velocities; (c): Error of interface displacements.

3.3.6 Comparison to the State-of-the-Art

The following section highlights some of the key novelties of the proposed algorithm and advantageous properties over the methods in literature. The propagation of a square pulse through a heterogeneous bar, in Section 3.3.2 is used to study

the time steps taken by subdomain. The difference in dilatational wave speed results in a time step ratio $m = \pi$. To reduce the computational cost of the simulation, the largest time step should be used to integrate subdomains, ideally at the CFL condition with Δt_C .

Table 3.2: A comparison of the minimum time step $\min\{\Delta t\}$ from proposed method with Cho et al. [57] and Dvorak et al. [56] for the first nine time steps in corresponding Figure 3.11.

Critical Time Step and subdomain		$\min\{\Delta t\}$ [s]
Largest	$\Delta t_L^{CFL} = \Omega_L^{Dvo} = \Omega_L^{Cho}$	1.667×10^{-6}
	$\Omega_L^{Prop.}$	1.592×10^{-6}
	$\Delta t_s^{CFL} = \Omega_s^{Dvo} = \Omega_s^{Prop.}$	5.305×10^{-7}
	$\Omega_s^{Cho} = \Omega_s^{2El}$	4.167×10^{-7}
Smallest	$\Omega_f^{Dvo.} = \Omega_{rL}^{Dvo.} = \Omega_{rS}^{Dvo.}$	7.512×10^{-8}

The recent methods of Dvorak et al. [56] and Cho et al. [57] are re-implemented for this comparison. Both are solved with respect to the total Lagrangian formulation, where the state at $t = 0$ is used as reference for computation of critical time steps. Firstly, Dvorak prepares the solution of the interface through introducing sub-regions, defined $\Omega_{rL}^{Dvo.}$ and $\Omega_{rL}^{Dvo.}$, one for each connected to each subdomain and a frame $\Omega_f^{Dvo.}$. These interface regions include the area in the subdomain $\Omega_i^{Dvo.}$ that is affected by the wave propagating from the frame. Similarly, Cho computed two elements next to the interface on the large domain for each Δt_s , here this region is denoted Ω_{2EL}^{Cho} . In the proposed method, the definition of sub-regions or additional subdomains is not required.

Table 3.3: Comparison of methods for minimum time step throughout entire simulation and integration steps for a square wave benchmark with $m = \pi$.

Method	Time Step Ratio	Minimum Δt [s]	Element Steps
Single Time Step	1 (CFL of Ω_s)	5.3052×10^{-7}	2,714,400
Cho (2019)	4	4.1666×10^{-7}	2,599,680
Dvorak (2023)	π	1.5992×10^{-11}	2,112,900
Proposed (2024)	π	5.3052×10^{-7}	2,112,600

In Table 3.2, and corresponding Figure 3.11, the first 9 integration steps are tabulated and plotted, where the length of the bar indicates the size of the time step used to integrate the subdomain. The subdomains $\Omega^{Dvo.}$ indicate the different additional regions and frame defined by the Dvorak et al. The frame $\Omega_f^{Dvo.}$ and sub-regions $\Omega_{ri}^{Dvo.}$ integrate with identical time steps to ensure the nearest desired subdomain time level. The large $\Omega_L^{Dvo.}$ and small $\Omega_s^{Dvo.}$ subdomain step at the CFL condition, the maximum time step possible. The large subdomain of Cho also integrates at the maximum step possible, however the requirement of integer time step ratios hinders the solution of those subdomains integrated with Δt_s . Even for a ratio of $m = \pi$, the Cho et al. method is forced to integrate at larger ratio of $m = 4$.

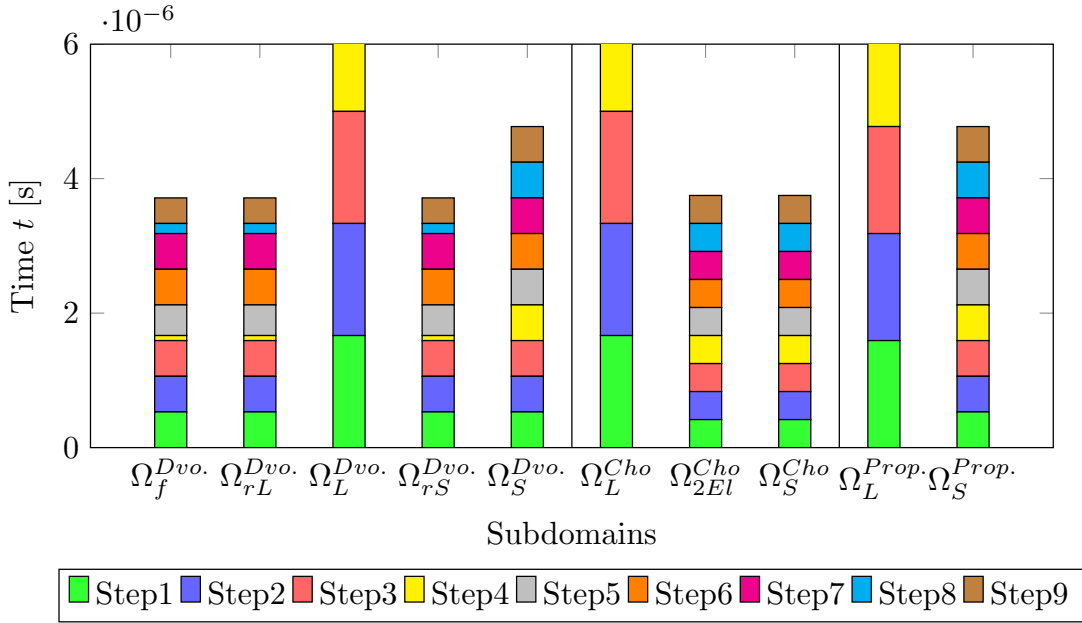


Figure 3.11: Comparison of subdomain integration steps for recent Multi-Time Stepping algorithms by Dvorak et al. [56], Cho et al. [57] and the proposed method [1].

The final two bars represent the time steps taken by the proposed method. $\Omega_s^{Prop.}$ steps at Δt_C for the small subdomain, with $\Omega_L^{Prop.}$ just below that of its critical time step. The use of α_L gives this slight decrease in time step, however without the use of reduction factors, subdomains would be out of synchronisation. In Table 3.3, the time step ratio (m), minimum time step ($\min\{\Delta t\}$) and the number of element integration steps are tabulated. The time step ratios reiterate the shortcoming of

Cho, with integer time step ratios. Next, the minimum time step reveals that both methods in literature step much smaller than the Δt_C increasing the computational cost of the solution. This is also evident in the total number of element integration steps performed by the entire domain of each method. This simple benchmark shows the advantageous properties of the proposed method, with the computational savings potentially even larger with increasing numbers of interfaces.

The propagation of the square wave is plotted at three distinct time steps to compare the velocity distribution along the bar. With a $\Delta t = 0.5h_e/c_e$ the central difference based multi-time stepping methods produce significant spurious oscillations when modelling a square wave. For this reason, the pushforward-pullback method (PFPB) is also re-implemented, in its single time step form [126]. The method uses a weighted combination to filter out front-shock and post-shock oscillations with a computation of the kinematics at the Δt_C , as well as the actual time step taken. A fifth method is combined with the proposed multi-time stepping algorithm to alleviate the dispersion. The traditional implementation of bulk viscosity (BV), found in the works of Von Neumann and Richtmyer [127], has been added to the solution of each subdomain. Despite the method being proposed several decades ago, its robustness gives reason for its use still today. Other methods are available, such as those by Maheo [128], however the simplicity of BV is favoured for the proposed method without the need to invert or modify any global stiffness matrices. The application of BV requires additional stress term being added at each time step with:

$$\boldsymbol{\sigma}^{bv} = \rho_i h_e (C_0 \text{Tr } \mathbf{D})^2 - C_1 c_e (\text{Tr } \mathbf{D}) \quad (3.87)$$

where ρ_i , h_e , c_e and $\mathbf{D}$ maintain the aforementioned definitions. The constants of $C_0 = 0.0$ and $C_1 = 0.06$ correspond to the quadratic and linear terms of the equation. The following Figures 3.12 - 3.14 plot the distribution of velocity along the bar as the wave reaches the bi-material interface, as it partially propagates through and when both reflected and transmitted wave have been produced. At $t = 1.00$ ms, the applied boundary condition has been fully applied from Ω_L and

begins to interact with Γ_i . The spurious oscillations produced by the CDM-based methods are of similar magnitude for Cho, Dvorak and the proposed method. The proposed method with bulk viscosity is comparable to Park et al.'s monolithic PFPB method where a clear smoothing of the square wave is visible.

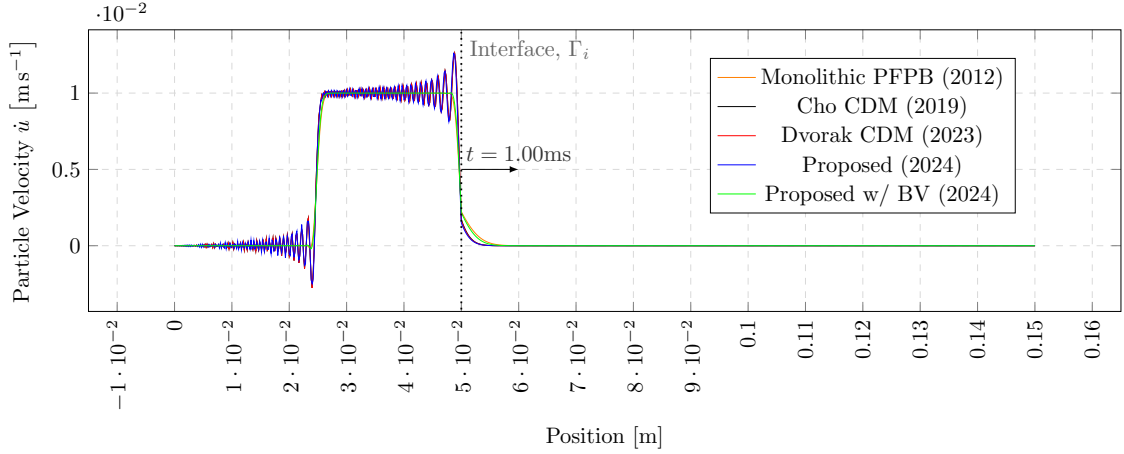


Figure 3.12: Square wave propagation through a 1-D heterogeneous bar at $t = 1.00$ ms with Monolithic PFPB [126], Cho [57], Dvorak [56] and the proposed method [1] with and without bulk viscosity.

At $t = 1.25$ ms, the wave is partially propagated through Γ . The wave reduces to half of its magnitude at this point, reading a value of $5 \times 10^{-3} \text{ ms}^{-1}$. Once again, the CDM-based multi-time stepping methods obtains results that are agreeable with each other. Similar evaluations are made to the previous time step with the PFPB and multi-time step solution with BV. Figure 3.14 depicts the distribution at 1.50 ms, where both transmitted and reflected waves are fully formed. This difference in impedance between materials is evident, as shown by the wave travelling much further in Ω_s , comparatively to the reflected wave back into Ω_L . The comparison of methods follows the same trend as the two previous time steps. The observations of the velocity distribution, give confidence for the correctness of implementation as well as the accuracy of the novel multi-time stepping algorithm.

3.4 Extension to Multiple Subdomains

For practical use of multi-time stepping algorithms, the coupling procedure must be extended to allow for more than two subdomains. Section 2.2 highlights how very few

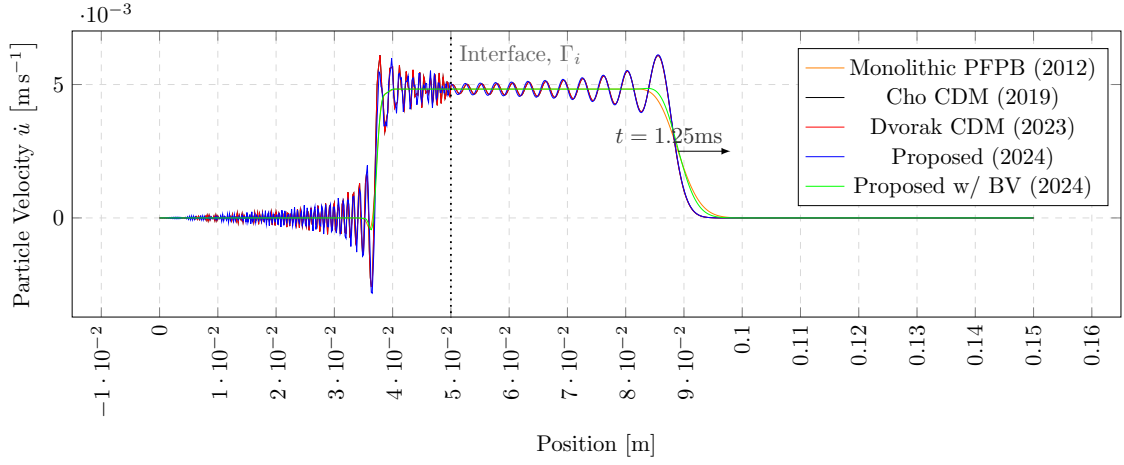


Figure 3.13: Square wave propagation through a 1-D heterogeneous bar at $t = 1.25$ ms with Monolithic PFPB [126], Cho [57], Dvorak [56] and the proposed method [1] with and without bulk viscosity.

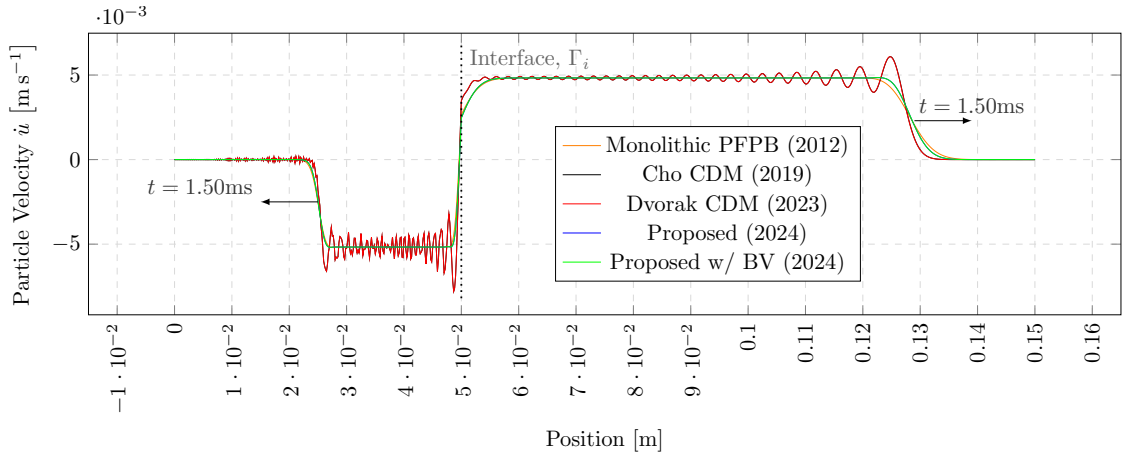


Figure 3.14: Square wave propagation through a 1-D heterogeneous bar at $t = 1.50$ ms with Monolithic PFPB [126], Cho [57], Dvorak [56] and the proposed method [1] with and without bulk viscosity.

methods in literature expand on the use of temporal coupling algorithms for multiple subdomains. Therefore, in the following section, Algorithm 1 is taken as a function of the following algorithm to allow for $\mathcal{N}_S > 2$. The method in Section 3.2 is referred to as `two-domain-algorithm` in the succeeding multiple subdomain algorithm.

3.4.1 Multi-Time Stepping Integration for Multiple Subdomains

Let the collection of subdomains $\mathcal{S} = \{\Omega_j, \Omega_k, \Omega_l, \Omega_m\}$ with their corresponding time steps $\{\Delta t_i | \Omega_i \in \mathcal{S}\}$. A sequence of subdomains is defined as $\Omega_{i1}, \Omega_{i2}, \Omega_{i3}, \Omega_{i4}$ such

that:

$$\begin{aligned}
 \Omega_{i1} &:= \operatorname{argmin}_{\Omega_i \in \mathcal{S}} \{\Delta t_i\} \\
 \Omega_{i2} &:= \operatorname{argmin}_{\Omega_i \in \mathcal{S} \setminus \{\Omega_{i1}\}} \{\Delta t_i\} \\
 \Omega_{i3} &:= \operatorname{argmin}_{\Omega_i \in \mathcal{S} \setminus \{\Omega_{i1}, \Omega_{i2}\}} \{\Delta t_i\} \\
 \Omega_{i4} &:= \operatorname{argmin}_{\Omega_i \in \mathcal{S} \setminus \{\Omega_{i1}, \Omega_{i2}, \Omega_{i3}\}} \{\Delta t_i\}
 \end{aligned} \tag{3.88}$$

where the sequence ascends in order, starting from the smallest Δt_i , and ending with the largest. $\mathcal{S} \setminus \{\Omega_{i1}, \Omega_{i2}, \dots\}$ removes the subdomains that have been assigned previously in the sequence. A serial merge sort algorithm is utilised to order the subdomains, doing so with a time complexity of $\mathcal{O}(\mathcal{N}_S \log \mathcal{N}_S)$. Following the sorting step, the first call of the **two-domain-algorithm** can be made. In Figure 3.15, a domain with partitioned with multiple subdomains is depicted. Subdomains with common colours can be thought of as regions of the domain with similar material properties. The subdomains are integrated in pairs so that the first couple are defined:

$$\Omega_s := \Omega_{i1}; \quad \Omega_L := \Omega_{i2} \tag{3.89}$$

with the corresponding time step $\Delta t_s := \Delta t_{i1}$ and $\Delta t_L := \Delta t_{i2}$.

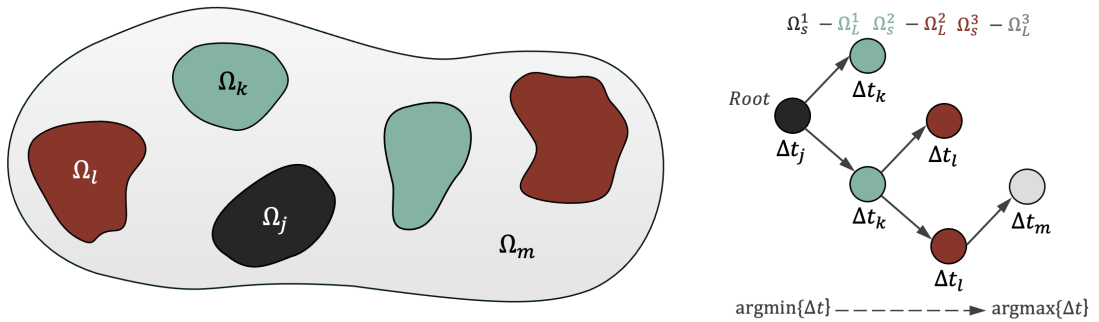


Figure 3.15: (a): Partitioning of a domain grouping regions with similar material properties, hence four distinct time steps where $\Delta t_i < \Delta t_j < \Delta t_k < \Delta t_l$; (b): Each subdomain is solved in pairs from the root of the tree diagram, following $\Omega_s - \Omega_L$ pairs. Integration increases from minimum Δt_i to the maximum.

After solving for the first two subdomains over the time step Δt_L , a re-evaluation of the sequence $\mathcal{S}$ is made. The sorting algorithm requires the computation of

the new Δt_s and Δt_L . At this point it is also convenient to update the trial time $t_{Ti} = t_i + \Delta t_i$ for each Ω_i . In the presence of more subdomains in the sorted collection, the current pair of Ω_s, Ω_L is checked to see if further steps can be taken, before moving up to the next pair of subdomains. This check can be written as the equality:

$$t_{Ts} < t_{TL+1} \quad (3.90)$$

where t_{Ts} is the small subdomain's trial time and t_{TL+1} is the trial time for the subdomain next in $\mathcal{S}$, hence the next $\Delta t_i > \Delta t_L$. If Equation 3.90 is valid, the current pair integrate once more, otherwise the large subdomain is assigned to be the small and the next largest Ω_i is assigned to be the large. Simply, this is written as $\Omega_s := \Omega_{i2}$ and $\Omega_L := \Omega_{i3}$ in the case above.

Once all subdomain pairs have been integrated for at least one single step, the subdomains should be all synchronised in time. At this point the system reaches t^N where $\forall t_i = t^N$. From there, the multi-domain algorithm starts again with the integration of the smallest time step pair. An advantageous property of the algorithm is noticed by the grouping of subdomains with similar time steps. The implementation of the algorithm allows for subdomains to be concurrently solved, favourable when subdomains are discretised with similar discretisations or material properties. A summary of the multi-domain procedure is made in Algorithm 2. The step to re-sort the subdomains, after the integration of a coupling pair, is

Algorithm 2 Summary of Algorithm for Multiple Domains

- 1: **procedure** A MULTI-DOMAIN ALGORITHM
 - 2: Sort subdomains Ω_i from $\text{argmin}\{\Delta t_i\}$ to $\text{argmax}\{\Delta t_i\}$;
 - 3: **while** All subdomains Ω_i have a $t_i < t_{max}$ and for $\mathcal{N}_S > 1$ **do**
 - 4: Integrate with the **two-domain-algorithm** (Ω_s, Ω_L)
 - 5: Re-sort subdomains Ω_i from $\text{argmin}\{\Delta t_i\}$ to $\text{argmax}\{\Delta t_i\}$;
 - 6: **if** Larger time step subdomains Ω_{L+1} exist **then**
 - 7: **if** $t_{Ts} < t_{TL+1}$ **then**
 - 8: Integrate current small-Large (Ω_s, Ω_L) pair;
 - 9: **else**
 - 10: Define next pair with subdomains $\Omega_s := \Omega_L$ then $\Omega_L := \Omega_{L+1}$;
 - 11: **else**
 - 12: Exit the Loop and Break;
-

imperative in the algorithms ability to adapt to changes in m between subdomains. As previously mentioned, several applications lead to sudden variation in time steps; this algorithm allows for Ω_s and Ω_L to interchange, should this also be the case. A slight modification is required from Algorithm 1 for those subdomain pairs that are temporally adjacent in $\mathcal{S}$, but not spatially. To reiterate once more, the subdomains still integrate with the subdomain it is temporally adjacent to, however the quantities at which they couple over change. For the mass, the modification:

$$\mathbf{M}_\Gamma = (\mathbf{C}_s^T \mathbf{M}_s \mathbf{C}_s) + (\mathbf{C}_{\bar{L}}^T \mathbf{M}_{\bar{L}} \mathbf{C}_L) \quad (3.91)$$

where $(\bar{L})$ denotes the spatially adjacent large subdomain. The internal and external forces similarly are modified to:

$$\mathbf{f}_\Gamma^{\text{int}} = \mathbf{C}_s^T \mathbf{f}_s^{\text{int}} + \mathbf{C}_{\bar{L}}^T \mathbf{f}_{\bar{L}}^{\text{int}}; \quad \mathbf{f}_\Gamma^{\text{ext}} = \mathbf{C}_s^T \mathbf{f}_s^{\text{ext}} + \mathbf{C}_{\bar{L}}^T \mathbf{f}_{\bar{L}}^{\text{ext}} \quad (3.92)$$

with the interface acceleration:

$$\ddot{\mathbf{u}}_\Gamma = \ddot{\mathbf{u}}_{\Gamma s} = \ddot{\mathbf{u}}_{\Gamma \bar{L}} \quad (3.93)$$

Regardless of temporal or spatial adjacency, the foundation of the coupling is the conservation of mass and tractions is obeyed, as well as the continuity of kinematic quantities. In the next section, the multi-domain algorithm is applied to a 3-D numerical example, requiring the concurrent simulation of multiple subdomains.

3.5 3-D Numerical Examples

This section presents the results of simulations that model the stress wave propagation in a metamaterial, named Metaconcrete. The kinematics and kinetics are solved with monolithic (single time step) integration, and multi-time stepping integration with the use of Algorithms 1 and 2. The accuracy is evaluated through the comparison of the two, with particular attention paid to the behaviour of nodes on the coupled interfaces. The stability of the system is computed through time, with the evaluation of the energy balance of each subdomain. Moreover, this work looks to demonstrate the speedup in solution when utilising multi-time step solutions. Significant gains are evidenced with the runtime of the simulations.

3.5.1 Accelerating the Simulation of Novel Metamaterials with Multi-Time Stepping

An area of active research is the study and design of novel metamaterials that exhibit enhanced properties that can be directly engineered into the material. Through artificially structuring these composite materials, wave propagation can be manipulated, with successful applications in acoustic, electromagnetic and stress waves demonstrated [129]. The design of *metaconcrete*, proposes a new metamaterial for the purpose of absorbing mechanical energy and reducing stress in the structure when subjected to dynamic loading [130]. Mitchell, Pandolfi and Ortiz engineered metaconcrete to replace conventional aggregates in concrete with a heavy metal inclusion, surrounded by a soft outer layer, both within a mortar matrix. Metaconcrete prevents the propagation of waves, especially those occurring near the natural frequency of the metal inclusion. The derivation of a mass-spring system, with each material, gives the natural frequency [130]:

$$\omega = \left(\frac{3E_c}{2R_I z \rho_I} \right)^{\frac{1}{2}} \quad (3.94)$$

where ω is given in $[\text{rads}^{-1}]$, E_c is the Young's modulus of the coating material, R_I is the radius of the inclusion, z is the thickness of the coating and ρ_I is the density of the inclusion. In Figure 3.16, a unit cell of the three-phase composite is depicted. Each material is denoted by its own subdomain, where Ω_m , Ω_c and Ω_I denote the matrix, coating and inclusion, respectively. The three phases have differing material properties, hence altering the time step in each subdomain. In part (b) of Figure 3.16, the points of interest are highlighted. These include the nodes where the boundary condition is applied, the interface between matrix and coating, the coating-inclusion interface and the centre of the inclusion. The focus of this study, is the comparison between the monolithic solution and the multi-time solutions for the propagation of stress waves in an elastic and plastic configuration of a bar made of metaconcrete. The bar geometry is defined with a repeating unit cell structure, where dimensions are defined similar to that of Mitchell et al. [131]. The inclusion radius takes a value of $r_I = 9$ mm, where as the coating encapsulates

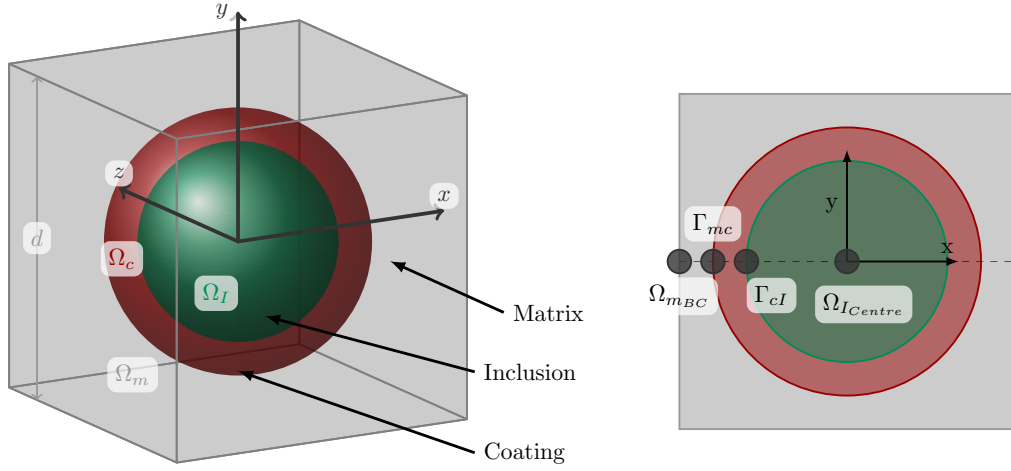


Figure 3.16: Constituents of a Metaconcrete Unit Cell and labelling convention; (a): Metaconcrete unit cell, partitioned with the matrix Ω_m , coating Ω_c and inclusion Ω_i . (b): Sampling points taken for elastic wave propagation simulation.

the inclusion with $r_c = 12$ mm. The heavy core and compliant coating are contained within a mortar matrix cube of diameter $d = 30$ mm. Interestingly, recent works also look to vary the configurations of these three materials, some of which have also included the experimental testing of metaconcrete [132–134]. For now, the aforementioned configuration is used to first examine the performance of multi-time stepping with a constant time step ratio m , between each of the composite phases, and then with a variable m , through invoking plasticity into the materials. The following simulations utilise the algorithm described in Section 3.4.

3.5.2 Elastic Wave Propagation in Metaconcrete for Constant Time step ratios

The first 3-D simulation considers the propagation of elastic waves, with the dynamic excitation of a half sinusoidal wave from one end of the bar. A repeating structure of eight unit cells is created with the boundary condition applied to all the nodes on one face of the first unit cell, denoted Ω_0 . Figure 3.17 illustrates problem, where those nodes at $x = -15$ mm on the matrix of the first unit cell are prescribed a velocity of $\dot{u}(t) = 0.01\sin(2\pi\omega_m t)$ ms⁻¹, where $\omega_m = 18.35$ rads⁻¹. The equivalent wavelength of the boundary condition is 90 mm, the same as 3 unit cells. The velocity's amplitude is low, maintaining deformation well within the elastic region

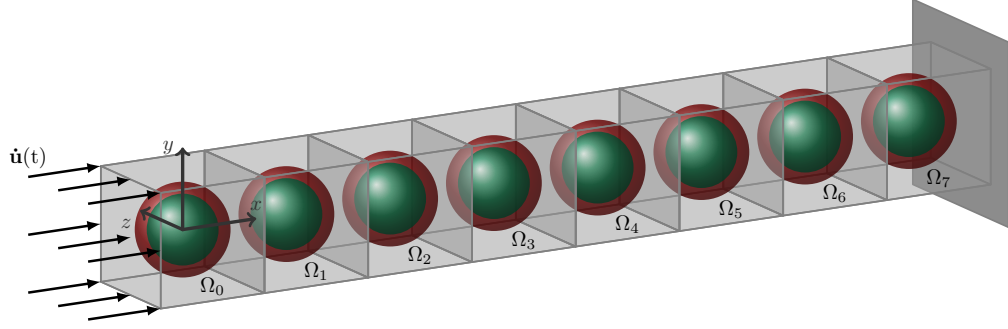


Figure 3.17: Diagram of Metaconcrete bar consisting of 8 unit cells prescribed velocity at $x = -15$ mm and support at $x = 225$ mm.

Table 3.4: Discretisation of structured Metaconcrete bar mesh data and dilatational wave speed.

Material	Nodes	Elements	Vol. Fr. $V_i(\%)$	Wave Speed c_{3-D} [m/s]
Matrix	447,065	403,840	73.19	2,200
Coating	194,784	162,240	15.50	3,780
Inclusion	189,928	173,056	11.31	6,110

of all three materials. To discretise the metaconcrete bar, a structured hexahedral mesh is created with a uniform mesh size of $h = 0.65$ mm, where a reduction is observed in volumes of interest. The number of nodes, elements and volume fraction of each material are tabulated in Table 3.4, with the meshes visualised in Figure 3.18.

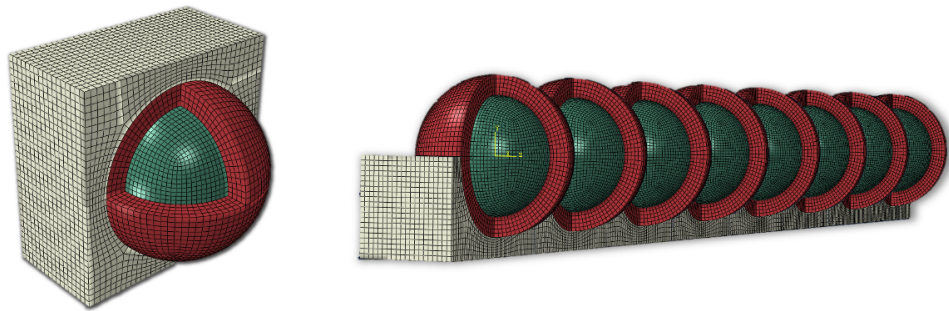


Figure 3.18: Mesh of a Metaconcrete unit cell and bar with section cuts made.

The isotropic elastic properties of the three materials give a Young's modulus, density and Poisson's ratio of $E_m = 3$ GPa, $\rho_m = 1.10 \times 10^{-6}$ kg/mm³, $\nu_m = 0.37$, $E_c = 10$ GPa, $\rho_c = 1.50 \times 10^{-6}$ kg/mm³, $\nu_c = 0.4$, $E_I = 210$ GPa, $\rho_I =$

$7.57 \times 10^{-6} \text{ kg/mm}^3$ and $\nu_I = 0.3$. Other combinations of the material properties are found in literature [130, 134–137]. The difference in material properties, leads to a dilatational wave speed that varies throughout the unit cell. For each subdomain Ω_i , the wave speed in 3-D is calculated as:

$$c_{3-D} = \sqrt{\frac{E_i(1 - \nu_i)}{(1 + \nu_i)(1 - 2\nu_i)\rho_i}} \quad (3.95)$$

This leads to the speeds calculated in the RHS of Table 3.4. For multi-time stepping a pre-processing step is needed to define those nodes that match on the interface, Γ , between phases. In the case of metaconcrete, the matrix-coating is defined by Γ_{mc} and coating-inclusion by Γ_{cI} . The knowledge of which subdomain shall proceed as Ω_L and Ω_s is not needed a priori, as this is computed by Algorithm 2. With the difference in dilatational wave speeds and spatial discretisation, the effectiveness of multi-time stepping becomes evident with the ability to run Δt_m , Δt_c and Δt_I concurrently. The periodic nature of composites, is what makes them so suited for running with partitioned equations of motion.

The results of the velocity distribution in the first unit cell Ω_0 are plotted along the X axis of the domain where coordinates $Y = Z = 0$. Figure 3.19 demonstrates the axial velocity $\dot{\mathbf{u}}_x$ for nodes on the Ω_{mBC} , Γ_{mc} , Γ_{cI} and $\Omega_{I_{Centre}}$. The first node plots the boundary condition (BC) applied to each of the nodes at one end of the metaconcrete bar. The behaviour of the following three nodes are chosen due to their position on the interface of each of the three subdomains. The purpose of this plot illustrates the accuracy of the temporally coupled method, relative to the uncoupled method, with nodes that use the computed interface acceleration. The solutions of the multi-time stepping, abbreviated to mts, and the monolithic (mono) are plotted for each n^{th} value. For example, on the boundary condition node, it is shown that for every mts solution point there are four monolithic points. Remarkably, despite solving on a much higher time step, the results of the mts solution agree well with the monolithic solution, even for those nodes on the interface.

The Cauchy stress field can be evaluated at each integration point within the domain. Figures 3.20 - 3.22 assess the stress at three points in time, where the

monolithic plot is depicted above the mts solution and each plot takes a slice in the $X - Y$ plane. The first time stamp in Figure 3.20 shows the initial application of the boundary condition, and the waves interaction with the coating and hard inclusion. The stress field plot further confirms the accuracy of the mts solution, with no visible difference with the single time step solution. In Figure 3.21 the difference in wave speed is evident, as the stress travels faster through the centre of the bar, where the hard inclusion constitutes a larger proportion of the unit cell volume. Once again the mts and monolithic solutions agree well with each other. In the final time stamp, some reflection of the wave is evident, as well as the difference in impedance showing further progression of the stress wave through the inclusion, in comparison to the "slow" coating and matrix. All three time stamps further confirm the accuracy of multi-time stepping, however questions arise to the stability of the results in comparison to monolithic solutions.

An evaluation of the stability is made numerically, with the energy balance of each subdomain Ω_i . For this analysis, the approach by Neal and Belytschko is called upon [50, 64]. A subdomain, Ω_i , computes its total energy satisfying:

$$|W_{\text{ext},i} - W_{\text{int},i} + W_{\text{kin},i}| \leq \delta ||W_i|| \quad (3.96)$$

where $W_{\text{ext},i}$ denotes the external work, $W_{\text{int},i}$ the internal and $W_{\text{kin},i}$ the kinetic energies of a subdomain, respectively, and δ is a tolerance value to be depicted. Aligning with the leapfrog integration method in Section 3.1.1, the energies are computed with velocities on the half time step. Each individual component of energy is therefore computed as:

$$\begin{aligned} W_{\text{int},i}^{n+1} &= W_{\text{int},i}^n + \frac{\Delta t_i^{n+1/2}}{2} (\dot{\mathbf{u}}_i^{n+1/2})^T (\mathbf{f}_{\text{int},i}^n + \mathbf{f}_{\text{int},i}^{n+1}) \\ &= W_{\text{int},i}^n + \frac{1}{2} \Delta \mathbf{u}_i^T (\mathbf{f}_{\text{int},i}^n + \mathbf{f}_{\text{int},i}^{n+1}) \end{aligned} \quad (3.97)$$

$$\begin{aligned} W_{\text{ext},i}^{n+1} &= W_{\text{ext},i}^n + \frac{\Delta t_i^{n+1/2}}{2} (\dot{\mathbf{u}}_i^{n+1/2})^T (\mathbf{f}_{\text{ext},i}^n + \mathbf{f}_{\text{ext},i}^{n+1}) \\ &= W_{\text{ext},i}^n + \frac{1}{2} \Delta \mathbf{u}_i^T (\mathbf{f}_{\text{ext},i}^n + \mathbf{f}_{\text{ext},i}^{n+1}) \end{aligned} \quad (3.98)$$

$$W_{\text{kin},i}^n = \frac{1}{2} (\dot{\mathbf{u}}_i^{n+1/2})^T \mathbf{M} \dot{\mathbf{u}}_i^{n+1/2} \quad (3.99)$$

Table 3.5: Monolithic and Multi-Time Step runtimes and minimum time steps of the matrix Ω_m , coating Ω_c and inclusion Ω_I .

Simulation	Runtime [s]	$\min\{\Delta t\}$ [ms]
Monolithic	14,400	2.4064×10^{-6}
Matrix, Ω_m (mts)	8,400	9.6256×10^{-6}
Coating, Ω_c (mts)	-	4.8128×10^{-6}
Inclusion, Ω_I (mts)	-	2.4064×10^{-6}

A similar evaluation is found in Belytschko's [8], where a similar expression for the internal force can also be found with quantities at the integration points:

$$\begin{aligned}
W_{\text{int},i}^{n+1} &= W_{\text{int},i}^n + \frac{1}{2} \sum_{e=1}^{\mathcal{N}_e} \Delta \mathbf{u}_e^T (\mathbf{f}_{\text{int},e}^n + \mathbf{f}_{\text{int},e}^{n+1}) \\
&= W_{\text{int},i}^n + \frac{\Delta t_i^{n+1/2}}{2} \sum_{e=1}^{\mathcal{N}_e} \sum_{q=1}^{N_Q} w_Q \mathbf{D}_Q^{n+1/2} : (\boldsymbol{\sigma}_Q^n + \boldsymbol{\sigma}_Q^{n+1}) J_{\xi Q}
\end{aligned} \tag{3.100}$$

where Q denotes the quadrature points element e , with local coordinates ξ , weights w , rate of deformation $\mathbf{D}$, Cauchy stress $\boldsymbol{\sigma}$ and the Jacobian J . In Figure 3.23 the energy balance from Equation 3.96 is plotted for each material in the mts, and the monolithic solution. Slight dissipation is observed, comparatively larger in magnitude for the Ω_m , however at 10^{-12} , the values are close to machine precision and several order of magnitude below the total energy. This leads to the conclusion that the solution is stable.

Figure 3.24 plots the four time steps used. The smallest time step, the inclusion, limits the time step at which the monolithic solution can proceed, hence all elements integrate at an identical time step. This graph highlights how the coating and matrix can run on time steps $2\times$ and $4\times$ the time step of the smallest time step respectively. This therefore leads to superior runtimes, as tabulated in Table 3.5, where the single time step solution runs for 14,400 seconds, in comparison to the multi-time step 8,400 seconds. Multi-time step integration yields a $1.71\times$ speedup with a reduction of 41.67% in total runtime. From this, it is clear that the solution of wave propagation in metaconcrete can be accelerated, without sacrificing stability for small amounts of deformation. Despite this, further improvement can be made on the speedup with more complex constitutive models invoked in the following section.

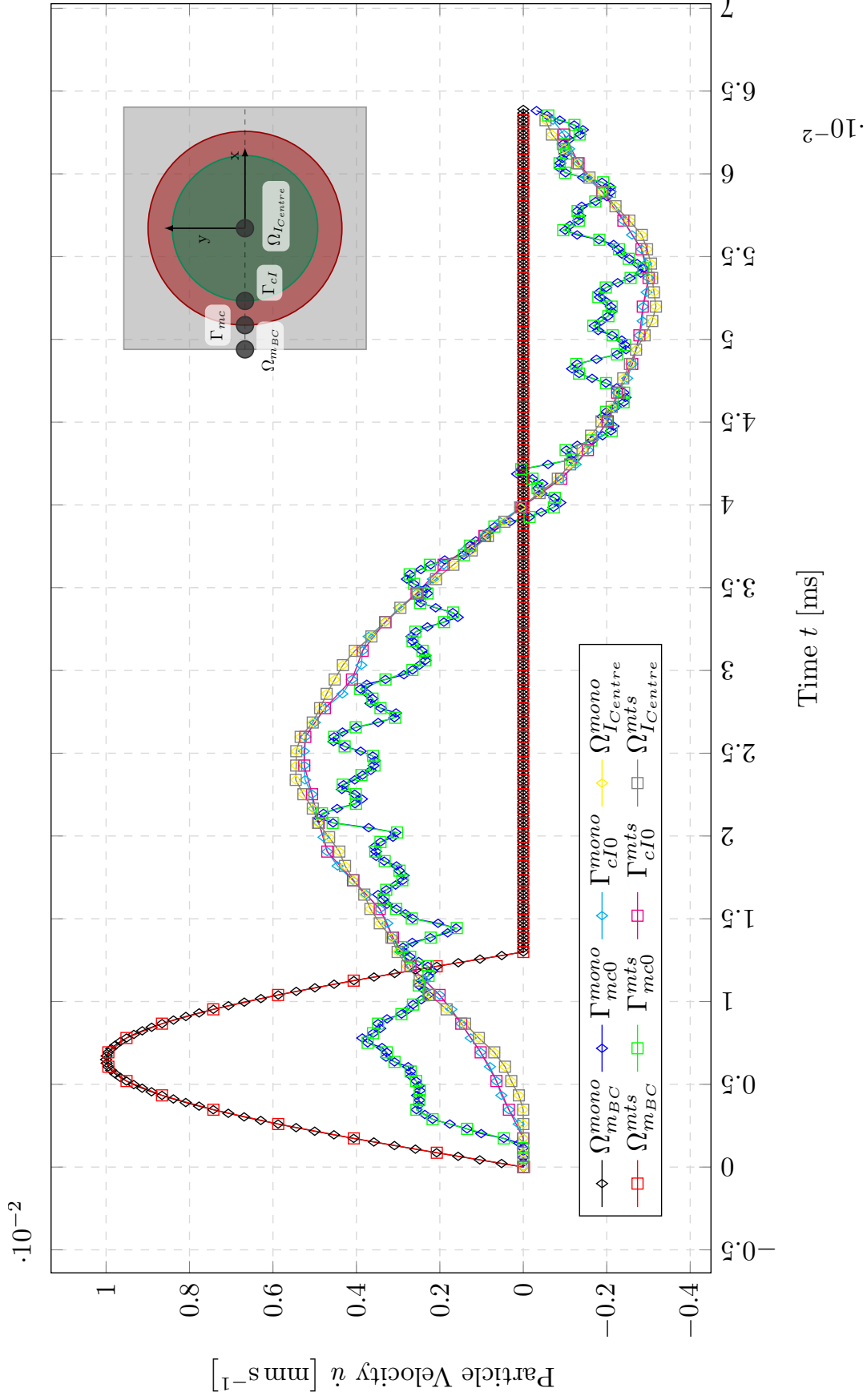


Figure 3.19: Elastic wave propagation through a Metaconcrete bar with monolithic *mono* and multi-time step *mts* solutions in the first Unit Cell at the coordinates $\{-15.0, 0.0, 0.0\}$, $\{-12.0, 0.0, 0.0\}$, $\{-9.0, 0.0, 0.0\}$ and $\{0.0, 0.0, 0.0\}$ mm where *BC*, *mc*, *cI* and I_{Centre} represent the boundary condition, matrix-coating, coating-inclusion and the centre of the inclusion respectively



Figure 3.20: Top: Monolithic solution $\Omega_{\sigma_{xx}}^{mono}$, **Bottom:** Multi-time step solution Ω_{σ}^{mts} ; Elastic wave propagation at $t = 0.0065$ ms.



Figure 3.21: Top: Monolithic solution $\Omega_{\sigma_{xx}}^{mono}$, **Bottom:** Multi-time step solution $\Omega_{\sigma_{xx}}^{mts}$; Elastic wave propagation $t = 0.0260$ ms.

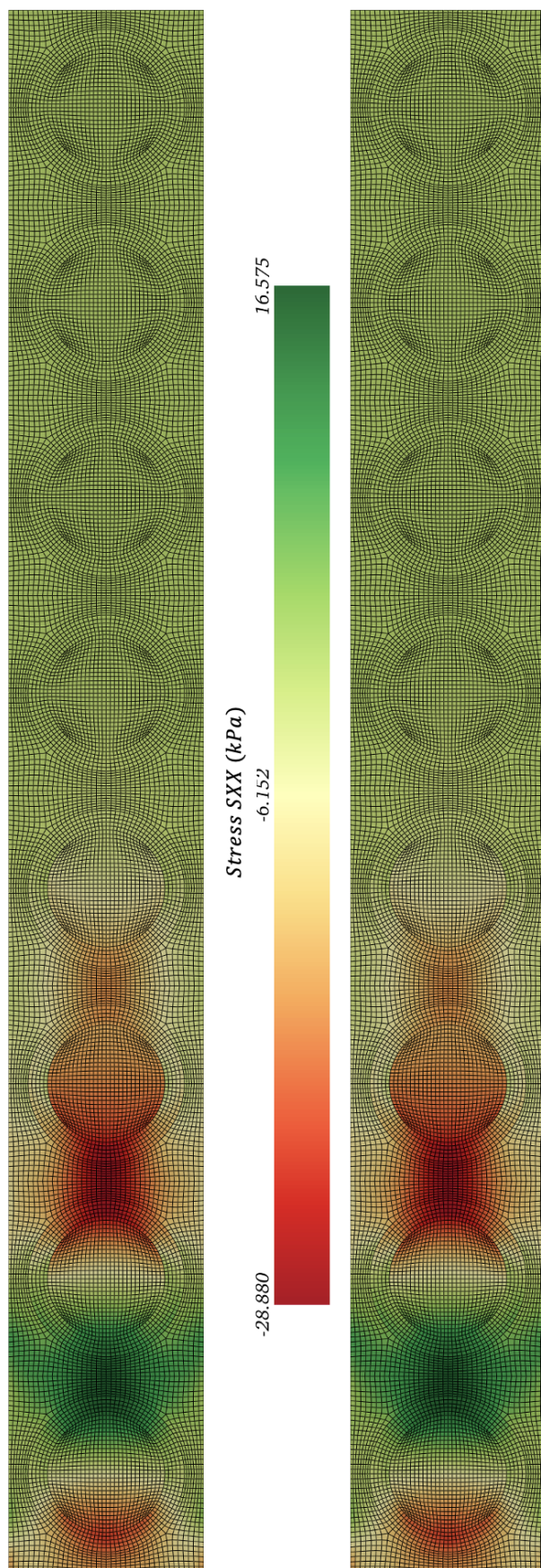


Figure 3.22: Top: Monolithic solution $\Omega_{\sigma_{xx}}^{mono}$, **Bottom:** Multi-time step solution $\Omega_{\sigma_{xx}}^{mts}$; Elastic wave propagation $t = 0.0520$ ms.

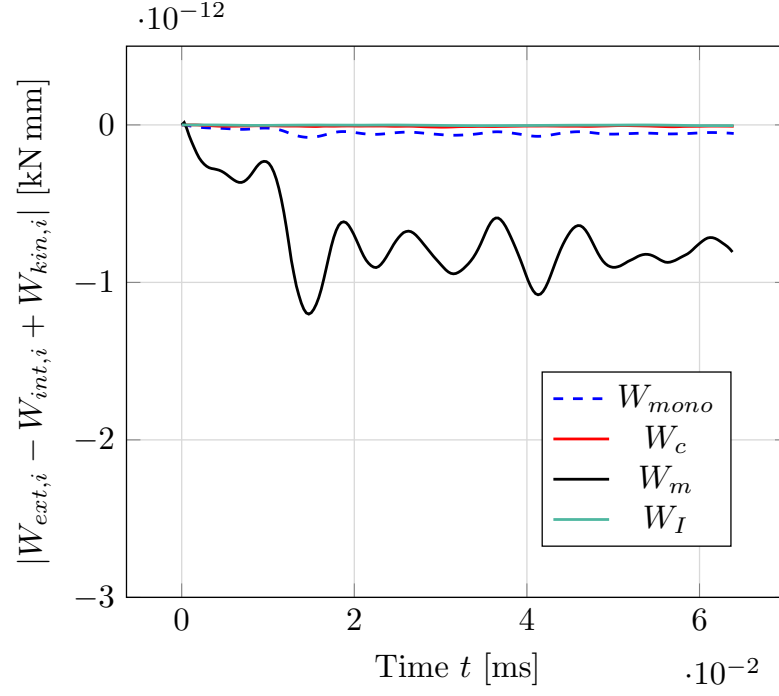


Figure 3.23: Energy balance check $|W_{ext,i} - W_{int,i} + W_{kin,i}| \approx 1 \times 10^{-12}$ of elastic wave propagation through a Metaconcrete bar with monolithic and multi-time step solution.

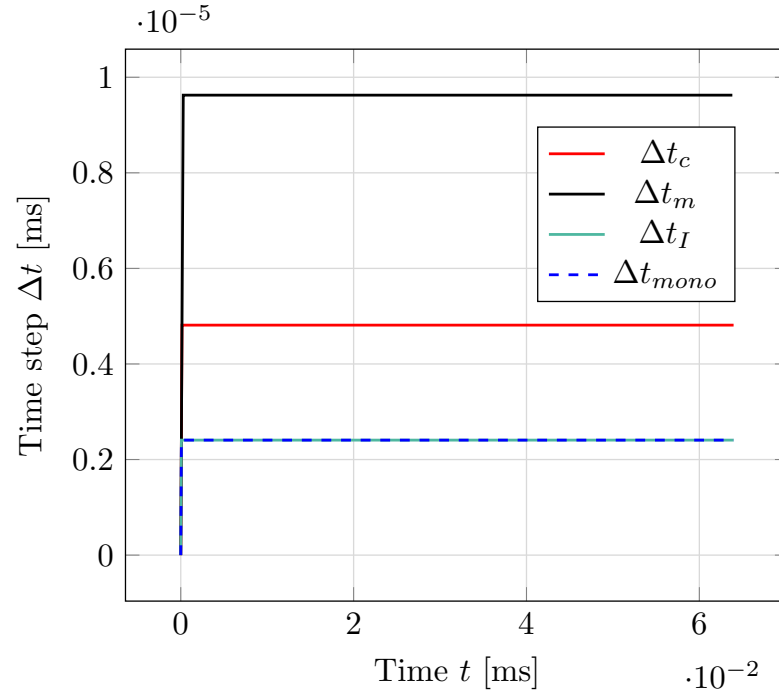


Figure 3.24: Time step history for each subdomain Ω_i in the elastic wave propagation example, where time steps maintain a constant time step ratio m when multi-time stepping.

3.5.3 Plastic Wave Propagation in Metaconcrete for Variable Time step ratios

Whilst, elastic wave propagation allowed for asynchronous integration with constant time step ratios, a key novelty of the proposed algorithm is that it allows for variable time step ratios. Plasticity allows for larger deformation, and hence a greater distortion of elements. Multi-time stepping is shown to be more computationally efficient, whilst accurate, as justified further with evaluations of runtime and energy balance in this additional numerical example. To ensure that the time step is solely determined by the materials properties of the metaconcrete constituent, and the change in characteristic length of the element, the bar is voxelised with a raster mesh.

The use of voxel meshes is widespread in literature due to the ease and speed at which they can be generated [138–141]. For the case of metaconcrete, the geometry of the elastic bar can be maintained, with a minimum element size h_e determined for the entire mesh. Through iterating about each of the elements e_i , and determining it's distance from the centre of a metaconcrete unit cell (j, k, l) , each element is assigned to a subdomain Ω_i . Algorithm 3 summarises the meshing algorithm for rasterising a metaconcrete unit cell. The radius' of each of inclusion and coating are denoted r_I and r_c respectively. The procedure in Algorithm 3 can be repeated for each of the eight unit cells in the bar. For the following example, a element length of $h_e = 0.326$ mm is defined, comparatively smaller to that of the previous section to allow for larger deformation. A quarter symmetry is used to model plasticity, so

Algorithm 3 A Simple Meshing algorithm for a Metaconcrete Unit Cell

```

1: procedure VOXELISE METACONCRETE CELL
2:   Input minimum element length  $h_e$ 
3:   for all elements  $e_i$  do
4:     compute element centre position  $(j, k, l)$ ;
5:     compute distance from unit cell centre  $d_i = (x - j)^2 + (y - k)^2 + (z - l)^2$ ;
6:     if  $d_i < r_I$  then
7:        $e_i \in \Omega_I$ ;
8:     else if  $d_i < r_c$  then
9:        $e_i \in \Omega_c$ ;
10:    else
11:       $e_i \in \Omega_m$ ;

```

Table 3.6: Discretisation of structured Metaconcrete bar mesh data and Elastic dilatational wave speed

Material	Nodes	Elements	Vol. Fr. $V_i(\%)$	Wave Speed c_{3-D} [m/s]
Matrix	1,219,057	1,139,872	73.19	2,020
Coating	290,424	241,808	15.53	4,200
Inclusion	200,520	175,696	11.28	11,200

to reduce the number of elements in the mesh. Those nodes on $\Omega_{m_{BC}}$ at $x = -15$ mm are externally loaded with a boundary condition $F(t) = 0.0025 \sin(2\pi\omega_m t)$ kN, where $\omega_m = 17.20 \text{ rads}^{-1}$. The use of a quarter domain, requires symmetrical boundary conditions, so that those nodes residing on the edges are forced with $0.5F(t)$, and corner nodes with $0.25F(t)$. Perpendicular to the symmetry planes, displacements are set to zero, where a similar wavelength of three unit cells is maintained for this simulation. Table 3.6 shows the data of the voxel mesh, as well as the elastic wave speeds that dictate the time step at the start of the simulation.

Hypoelastic-plasticity is invoked, as the constitutive model for the variable time step simulations. The description of Section 3.1.3 is recalled to relate stress and strain. Firstly, the elastic material properties are summarised as the following; $E_m = 3.5 \text{ GPa}$, $\rho_m = 1.46 \times 10^{-6} \text{ kg/mm}^3$, $\nu_m = 0.363$, $E_c = 4 \text{ GPa}$, $\rho_c = 1.05 \times 10^{-6} \text{ kg/mm}^3$, $\nu_c = 0.46$, $E_I = 240 \text{ GPa}$, $\rho_I = 2.74 \times 10^{-6} \text{ kg/mm}^3$ and $\nu_I = 0.32$, where a larger initial m is computed between subdomains. As the material exceeds the yield point, a nonlinear isotropic hardening constitutive model is called upon to model the plasticity in the matrix and the coating. A summary of the plastic properties is made in Table 3.7. Plasticity is invoked for the matrix Ω_m and the coating Ω_c , but not the inclusion granted the much large yield strength. It should be noted, to further improve the accuracy of the material response, fracture and damage models could also be incorporated, as demonstrated by Mitchell et al. [142]. This is of particular relevance when modelling the brittle behaviour of matrix materials such as mortar.

Table 3.7: Plastic material properties of metaconcrete model for Ω_m and Ω_c subdomains.

Matrix		Coating	
Plastic Strain, ϵ^p	Yield Stress, σ_y [GPa]	Plastic Strain, ϵ^p	Yield Stress, σ_y [GPa]
0.000	0.08	0.00	0.025
0.075	0.10	0.05	0.040
0.380	0.12	0.06	0.043
		0.08	0.048
		0.10	0.0505
		0.35	0.055

The results of the hypoelastic-plastic numerical example are presented with further comparison of monolithic and multi-time step solutions. The dynamic behaviour of the interfaces are highlighted with Γ_{mc} and Γ_{cI} analysed throughout the metaconcrete bar, as depicted by the sampling points the top corner of both Figure 3.25 and 3.26. Once again, the sample points are taken about the X -axis.

In contrast to Figure 3.19, the kinematic behaviour of interface nodes throughout the entire bar is depicted. The matrix-coating nodes are visualised in one plot, followed by the coating-inclusion nodes in another. Even when invoking plasticity, these plots show good accuracy between multi-time stepping and monolithic solution. The Γ_{mc} interfaces are plotted in Figure 3.25, through each of the eight unit cells. The comparison between *mono* and *mts* solutions reveal good alignment between the two, where peak amplitudes are matched, even with fewer time steps. Wave reflection is evident, most prominently with visual inspection of the first wave, where the difference in impedance between matrix and coating produces a transmitted and reflected wave from the incidence. Figure 3.26 plots the behaviour of interface nodes Γ_{cI} , where solutions are comparatively smoother to Figure 3.25, as the motion through the bar decreases in amplitude gradually and higher frequencies are filtered out. For every four uncoupled solutions, one monolithic solution can be observed. Complementary to previous results, an even closer match to the single time step results is achieved with multi-time stepping, depicting the accuracy of the method. Figures 3.27 - 3.29 view the stress distribution in the voxel mesh as plasticity is

Table 3.8: Monolithic and Multi-Time Step runtimes and minimum time steps of the matrix Ω_m , coating Ω_c and inclusion Ω_I .

Simulation	Runtime [s]	$\min\{\Delta t\}$ [ms]
Monolithic	396,780	2.577599×10^{-7}
Matrix, Ω_m (mts)	122,151	1.491133×10^{-6}
Coating, Ω_c (mts)	-	7.455663×10^{-7}
Inclusion, Ω_I (mts)	-	2.297713×10^{-7}

activated. To better visualise the solution, a clipping from -20 GPa to 10 GPa is used, with the single time step solution visualised above the asynchronous solution. Likewise, the stress propagates through the centre of the bar quickest, the same can be deduced at $t = 0.045$ ms and $t = 0.060$ ms. Impressively, even for larger stresses, the solutions both align very well. The energy balance method in Equation 3.96 is recalled, whilst also accounting for plastic component of the internal energy. Figure 3.30 plots the energies, showing a similar order of magnitude for each subdomain. The matrix subdomain dissipates the most energy, following the trend of the elastic simulation, however this could be distorted by the number of elements in the matrix being much larger than the other constituents. The energy balance gives confidence in the algorithm, granted its magnitude relative to the total energy.

The variable time step ratio is evident in Figure 3.31, where the compressive boundary condition reduces the characteristic length of the elements. A drop in all three phases of metaconcrete is visible, with oscillation in Δt_I , where the reduction factor α_s is applied to synchronise subdomains. Finally, Table 3.8 summarises the speedup and the minimum time steps for each of the subdomains. The reduction in runtime is even more prominent with the hypoelastic-plastic simulation resulting in a 69.22% decrease. Remarkably, this corresponds to a $3.25\times$ speedup. Conversely, to the elastic simulation the $\min\{\Delta t\}$ of the inclusion phase is lower than the monolithic Δt , a small price to pay to ensure the subdomains synchronise in time. This section successfully demonstrates reduction in runtime for simulating both elastic and plastic 3-D wave propagation numerical examples. Simulations remain stable throughout, even when considering a variable time step ratio, where compression of the domain results in a time step that drops.

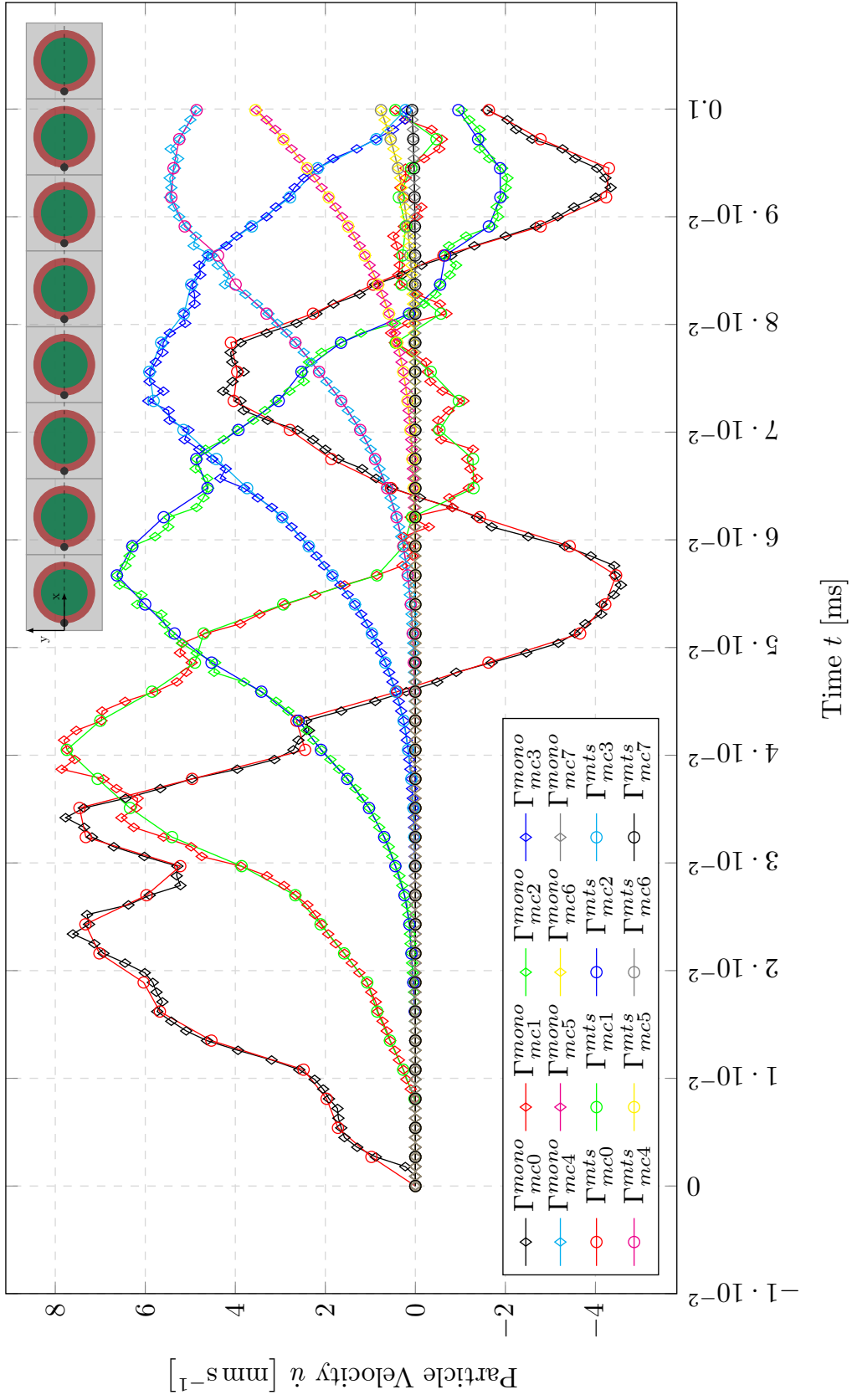


Figure 3.25: Elasto-plastic wave propagation; matrix-coating velocity history of coupling nodes on Γ_{mc} for *mono* and *mts* solutions taken at coordinates on the interfaces.

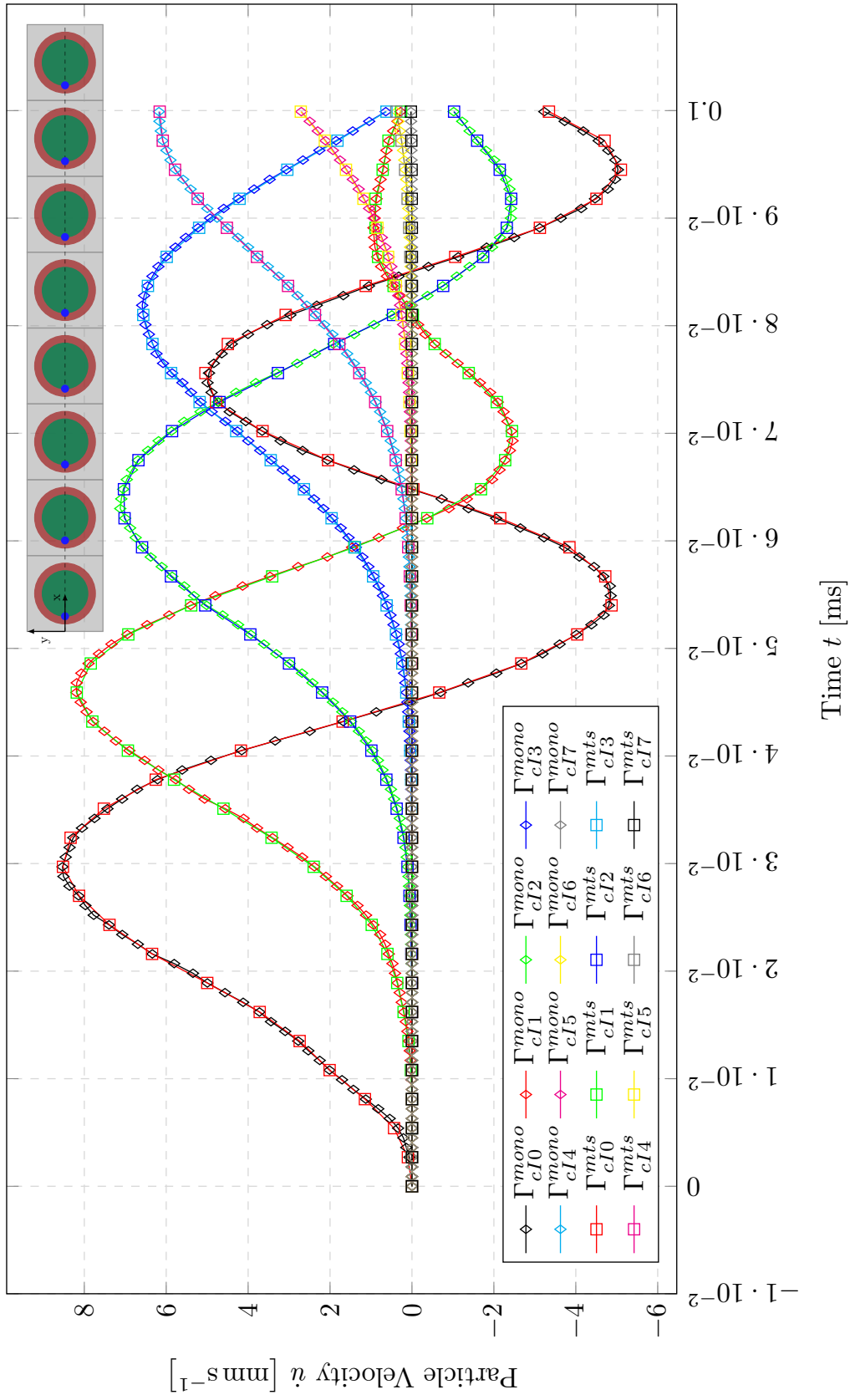


Figure 3.26: Elastoplastic wave propagation; coating-inclusion velocity history of coupling nodes on Γ_{cI} for *mono* and *mts* solutions taken at coordinates on the interfaces.

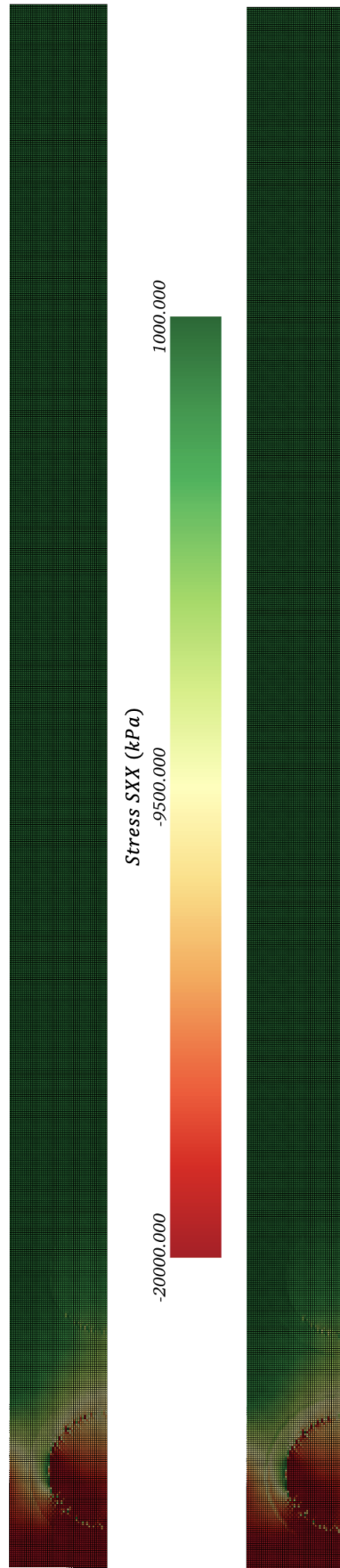


Figure 3.27: Top: Monolithic solution $\Omega_{\sigma_{xx}}^{mono}$, **Bottom:** Multi-time step solution $\Omega_{\sigma_{xx}}^{mts}$, Elasto-plastic wave propagation at $t = 0.015$ ms.



Figure 3.28: Top: Monolithic solution $\Omega_{\sigma_{xx}}^{mono}$, **Bottom:** Multi-time step solution $\Omega_{\sigma_{xx}}^{mts}$; Elasto-plastic wave propagation at $t = 0.0450$ ms.

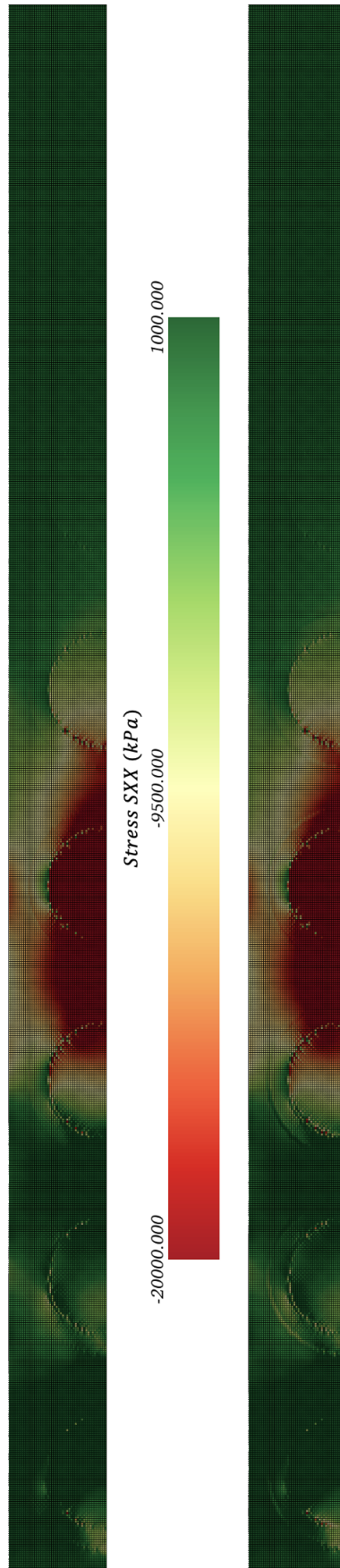


Figure 3.29: Top: Monolithic solution $\Omega_{\sigma_{xx}}^{mono}$, **Bottom:** Multi-time step solution $\Omega_{\sigma_{xx}}^{mts}$; Elasto-plastic wave propagation at $t = 0.0600$ ms.

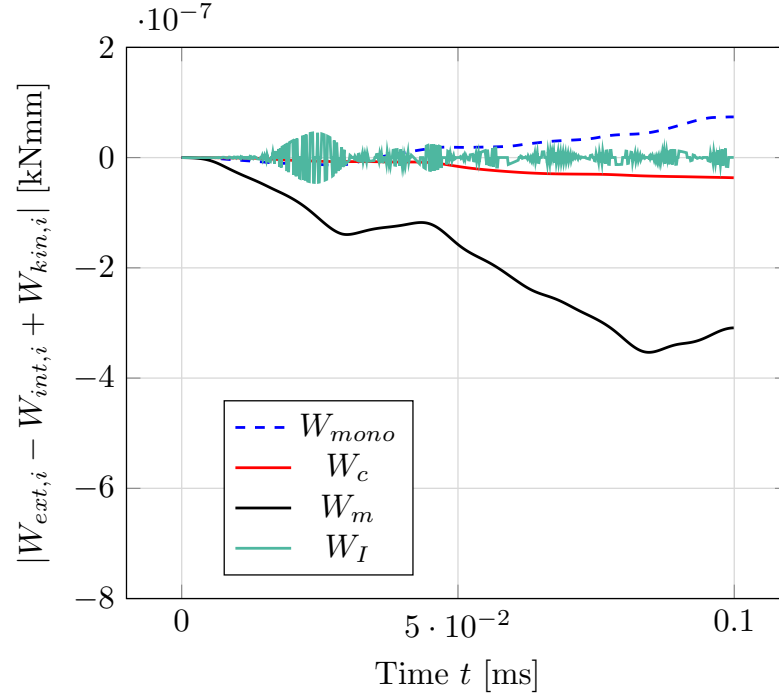


Figure 3.30: Energy balance check $|W_{ext,i} - W_{int,i} + W_{kin,i}| \approx 1 \times 10^{-7}$ of Elasto-plastic wave propagation numerical example with monolithic and multi-time step solution.

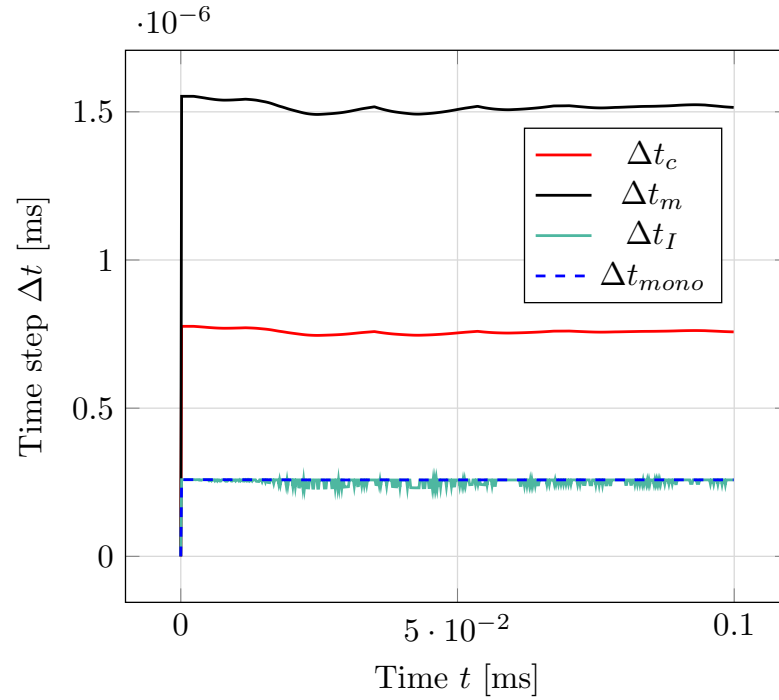


Figure 3.31: Time step history for each Ω_i of the Elasto-plastic wave propagation numerical example where time steps are no longer constant. The proposed multi-time stepping algorithm adapts to these changes in time steps between the subdomains.

4

Spatial Coupling Methods

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This chapter tackles another significant challenge in non-matching meshes. A novel algorithm is described, with the coupling operators defined on each of the two subdomains. These operators relax the constraint of conforming subdomain interfaces. Numerical examples are presented with an axial wave propagation benchmark and the modelling of a compact-tension test. The work of the preceding chapter is combined to demonstrate the potential for an even larger speedup in simulation.

4.1 A Novel Algorithm for Coupling Non-Matching Meshes

In the following section, the procedure for efficiently coupling non-matching meshes is presented. Starting from the the variational formulation with the virtual power of subdomains, special attention is now made for non-matching Γ_i . Through defining the operators on the interfaces between subdomains, the method abides by conservation laws to accurately capture the dynamic behaviour of solids.

4.1.1 Variational Formulation for Partitioned Non-Matching Domains

Recalling the principle of virtual power, variation in velocity is used to define the weak form of the governing momentum equation, producing the equations for Ω_L and Ω_s as:

$$\delta P_L(\delta \dot{\mathbf{u}}_L, \dot{\mathbf{u}}_L) = \delta P_L^{\text{int}} - \delta P_L^{\text{ext}} + \delta P_L^{\text{kin}} = 0 \quad (4.1)$$

$$\delta P_s(\delta \dot{\mathbf{u}}_s, \dot{\mathbf{u}}_s) = \delta P_s^{\text{int}} - \delta P_s^{\text{ext}} + \delta P_s^{\text{kin}} = 0 \quad (4.2)$$

where δP^{int} is the virtual internal power, δP^{ext} the external and δP^{kin} the kinetic. The momentum balance equation, multiplied by trial functions $\delta \dot{\mathbf{u}}_L$ and $\delta \dot{\mathbf{u}}_s$, allows the weak form to be written as:

$$\delta P_L = \int_{\Omega_L} \boldsymbol{\sigma}_L \cdot \delta \mathbf{D}_L \, d\Omega - \left(\int_{\Omega_L} \rho_L \mathbf{b}_L \cdot \delta \dot{\mathbf{u}}_L \, d\Omega + \int_{\Gamma_L} \mathbf{t}_L \cdot \delta \dot{\mathbf{u}}_L \, d\Gamma \right) + \int_{\Omega_L} \rho_L \ddot{\mathbf{u}}_L \cdot \delta \dot{\mathbf{u}}_L \, d\Omega \quad (4.3)$$

$$\delta P_s = \int_{\Omega_s} \boldsymbol{\sigma}_s \cdot \delta \mathbf{D}_s \, d\Omega - \left(\int_{\Omega_s} \rho_s \mathbf{b}_s \cdot \delta \dot{\mathbf{u}}_s \, d\Omega + \int_{\Gamma_s} \mathbf{t}_s \cdot \delta \dot{\mathbf{u}}_s \, d\Gamma \right) + \int_{\Omega_s} \rho_s \ddot{\mathbf{u}}_s \cdot \delta \dot{\mathbf{u}}_s \, d\Omega \quad (4.4)$$

The virtual power states $\forall \delta \dot{\mathbf{u}}(\mathbf{x}) \in \mathcal{V}_0$, where in an updated Lagrangian, the current configuration is integrated over. Similar to Section 3.1.1, a convenient starting point is the coupling of two subdomain Ω_L and Ω_s , as depicted in Figure 4.1. The nodal forces can be defined for each of the virtual power terms, thus:

$$\delta P_L \approx \sum_{n=1}^{\mathcal{N}_{n_L}} \delta \dot{\mathbf{u}}_L \cdot (\mathbf{f}_L^{\text{int}} - \mathbf{f}_L^{\text{ext}} + \mathbf{f}_L^{\text{kin}}) \quad (4.5)$$

$$\delta P_s \approx \sum_{n=1}^{\mathcal{N}_{n_s}} \delta \dot{\mathbf{u}}_s \cdot (\mathbf{f}_s^{\text{int}} - \mathbf{f}_s^{\text{ext}} + \mathbf{f}_s^{\text{kin}}) \quad (4.6)$$

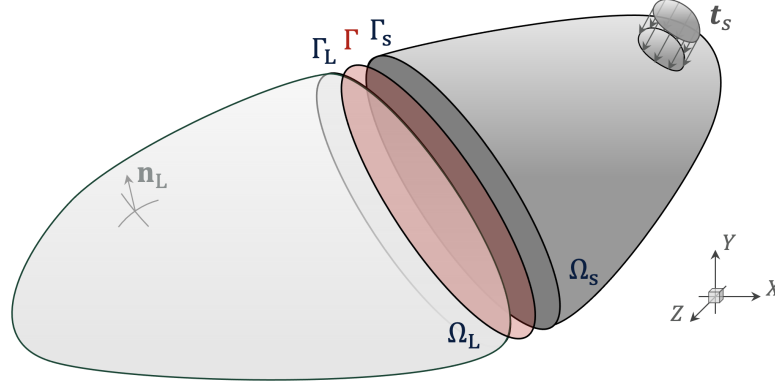


Figure 4.1: A 3-D domain Ω decomposed into Ω_L and Ω_s where Γ_L and Γ_s are non-matching interfaces to be externally resolved on Γ . Normal vector and tractions are visualised on Ω_L and Ω_s respectively.

Each of these nodal forces are written as:

$$\mathbf{f}_L^{\text{int}} = \int_{\Omega_L} \mathbf{B}_L^T \boldsymbol{\sigma}_L d\Omega; \quad \mathbf{f}_L^{\text{ext}} = \int_{\Omega_L} \rho_L \mathbf{b}_L d\Omega + \mathbf{N}^T \mathbf{t}_L|_{\Gamma}; \quad \mathbf{f}_L^{\text{kin}} = \int_{\Omega_L} \rho_L \mathbf{N}^T \mathbf{N} \ddot{\mathbf{u}}_L d\Omega \quad (4.7)$$

$$\mathbf{f}_s^{\text{int}} = \int_{\Omega_s} \mathbf{B}_s^T \boldsymbol{\sigma}_s d\Omega; \quad \mathbf{f}_s^{\text{ext}} = \int_{\Omega_s} \rho_s \mathbf{b}_s d\Omega + \mathbf{N}^T \mathbf{t}_s|_{\Gamma}; \quad \mathbf{f}_s^{\text{kin}} = \int_{\Omega_s} \rho_s \mathbf{N}^T \mathbf{N} \ddot{\mathbf{u}}_s d\Omega \quad (4.8)$$

where their discretised form follows similar Equations to 3.9 - 3.10. Subsequently, Ω_L and Ω_s are globally assembled to form the following vectors:

$$\mathbf{M}_L = \begin{bmatrix} \mathbf{M}_{L1} \\ \mathbf{M}_{L2} \\ \vdots \\ \mathbf{M}_{\mathcal{N}_{n_L}} \end{bmatrix}; \quad \mathbf{f}_L^{\text{ext}} = \begin{bmatrix} \mathbf{f}_{L1}^{\text{ext}} \\ \mathbf{f}_{L2}^{\text{ext}} \\ \vdots \\ \mathbf{f}_{\mathcal{N}_{n_L}}^{\text{ext}} \end{bmatrix}; \quad \mathbf{f}_L^{\text{int}} = \begin{bmatrix} \mathbf{f}_{L1}^{\text{int}} \\ \mathbf{f}_{L2}^{\text{int}} \\ \vdots \\ \mathbf{f}_{\mathcal{N}_{n_L}}^{\text{int}} \end{bmatrix} \quad (4.9)$$

$$\mathbf{M}_s = \begin{bmatrix} \mathbf{M}_{s1} \\ \mathbf{M}_{s2} \\ \vdots \\ \mathbf{M}_{\mathcal{N}_{n_s}} \end{bmatrix}; \quad \mathbf{f}_s^{\text{ext}} = \begin{bmatrix} \mathbf{f}_{s1}^{\text{ext}} \\ \mathbf{f}_{s2}^{\text{ext}} \\ \vdots \\ \mathbf{f}_{\mathcal{N}_{n_s}}^{\text{ext}} \end{bmatrix}; \quad \mathbf{f}_s^{\text{int}} = \begin{bmatrix} \mathbf{f}_{s1}^{\text{int}} \\ \mathbf{f}_{s2}^{\text{int}} \\ \vdots \\ \mathbf{f}_{\mathcal{N}_{n_s}}^{\text{int}} \end{bmatrix} \quad (4.10)$$

The non-overlapping interface between the two subdomains is $\Gamma = \Gamma_L \cap \Gamma_s$, where the compatibility for each subdomain Ω_i remains:

$$\ddot{\mathbf{u}}_{\Gamma_L}(\mathbf{C}_L \mathbf{x}_L) = \ddot{\mathbf{u}}_{\Gamma_s}(\mathbf{C}_s \mathbf{x}_s) = \ddot{\mathbf{u}}_{\Gamma}(\mathbf{x}_{\Gamma}) \quad (4.11)$$

$$\mathbf{t}_{\Gamma_L}(\mathbf{C}_L \mathbf{x}_L) = \mathbf{t}_{\Gamma_s}(\mathbf{C}_s \mathbf{x}_s) = \mathbf{t}_{\Gamma}(\mathbf{x}_{\Gamma}) \quad (4.12)$$

where on each subdomain $\mathbf{C}_L \mathbf{x}_L \in \Gamma_L$, $\mathbf{C}_s \mathbf{x}_s \in \Gamma_s$, and the external interface $\mathbf{x}_{\Gamma} \in \Gamma$, to describe a common boundary between subdomains. $\mathbf{C}_L$ and $\mathbf{C}_s$ remain the

indicator matrices identifying the interface degrees of freedom on large and small subdomain, respectively. Contrasting to the previous chapter, $\dim(\cdot)_{\Gamma_L} \neq \dim(\cdot)_{\Gamma_s}$, where discretisations of each interface do not match, hence the kinematic and kinetic quantities $(\cdot)$ are not consistent in dimensions. The shape functions used for coupling become functions of the interface node locations $\mathbf{x}_\Gamma$ and $\mathbf{x}_{\Gamma_i}$:

$$\mathbf{N}_{\Gamma_L}(\mathbf{x}) = \delta(\mathbf{x}_\Gamma - \mathbf{x}_{\Gamma_L}); \quad \mathbf{N}_{\Gamma_s}(\mathbf{x}) = \delta(\mathbf{x}_\Gamma - \mathbf{x}_{\Gamma_s}) \quad (4.13)$$

where shape functions are found for Ω_L and Ω_s separately, and variation δ can be viewed as a Dirac delta function, for those coincident nodes on the boundary. In Figure 4.2, Equations 4.13 are utilised in the computation of shape functions for both Ω_L and Ω_s . In the case of a 2-D problem, the interface Γ takes the form of a line, whereas in 3-D a surface is shown to form a convex quadrilateral. The diagram aids the depiction of hanging nodes, for those nodes that are not coincident with Γ_L .

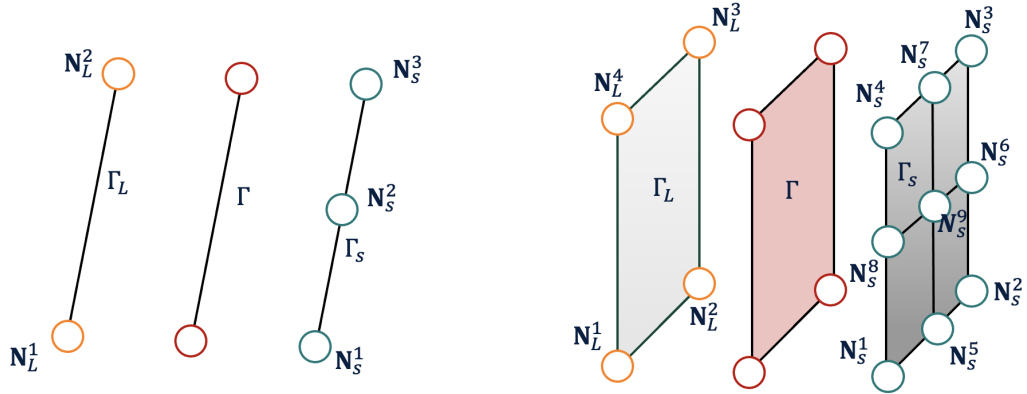


Figure 4.2: The spatial coupling algorithm requires the computation of shape functions of interface nodes that share the same geometry of Γ ; (a): 2-D problems find N_{Γ_L} and N_{Γ_s} on a line; (b): 3-D problems find N_{Γ_L} and N_{Γ_s} on a convex quadrilateral surface.

This follows the combination of LLMs with the mortar method on Ω_s , similar to González and Park [143, 144]. The interface is subsequently discretised with shape functions, $\mathbf{N}_\Gamma$, to give:

$$\dot{\mathbf{u}}_\Gamma(\mathbf{x}, t) \approx \sum_{i=1}^{\mathcal{N}_n} N_i(x_\Gamma) \dot{u}_\Gamma(t) = \mathbf{N}_\Gamma(\mathbf{x}_\Gamma) \dot{\mathbf{u}}_\Gamma(t) \quad (4.14)$$

Despite Equation 4.13 being presented for the two subdomain problem, it is noted that this formulation can be extended to a number, $\mathcal{N}_S$, of subdomains that compute

their own respective shape functions that share an external interface Γ :

$$\mathbf{N}_\Gamma(\mathbf{x}) = \delta(\mathbf{x}_\Gamma - \mathbf{x}_{\Gamma i}), \text{ for } i = 1, 2, \dots, \mathcal{N}_\mathcal{S} \quad (4.15)$$

Next, the combination of these interface shape functions with the virtual power are used to give the discretised form of the two subdomain coupling.

4.1.2 Definition of Interface Coupling Operators

As Γ_L and Γ_s do not share the same nodal positions, kinematic and kinetic continuity can no longer be enforced with the methods of Chapter 3. Subsequently, to ensure the conditions of Equations 4.11 - 4.12 are maintained, additional operations are required to compute the interface system variables. Analogous to the concepts in multigrid methods [145], as well as LLMs [94], two coupling operators are defined for each Ω_i :

$$\mathbf{N}_L \in \mathbb{R}^{\mathcal{N}_{\Gamma L} \times \mathcal{N}_\Gamma}; \quad \mathbf{N}_s \in \mathbb{R}^{\mathcal{N}_{\Gamma s} \times \mathcal{N}_\Gamma} \quad (4.16)$$

$$\mathbf{R}_L \in \mathbb{R}^{\mathcal{N}_\Gamma \times \mathcal{N}_{\Gamma L}}; \quad \mathbf{R}_s \in \mathbb{R}^{\mathcal{N}_\Gamma \times \mathcal{N}_{\Gamma s}} \quad (4.17)$$

where $\mathcal{N}_\Gamma$ is the number of nodes on the external interface Γ , $\mathcal{N}_{\Gamma L}$ and $\mathcal{N}_{\Gamma s}$ are the number of nodes of the subdomain's interface of Γ_L and Γ_s . $\mathbf{N}$ is the interpolation (or prolongation) operator that transfers acceleration onto the subdomains' interfaces, whereas $\mathbf{R}$ is the restriction of masses and forces to the discretisation of Γ . In doing so, a two way mapping is created. The virtual power δP for a two-subdomain system, in its discretised form, is written as:

$$\begin{aligned} \delta P &= \delta P_L + \delta P_s + \delta P_\Gamma \\ &= \delta \dot{\mathbf{u}}_L^T \{ \mathbf{f}_L^{\text{int}} - \mathbf{f}_L^{\text{ext}} + \mathbf{M}_L \ddot{\mathbf{u}}_L + \mathbf{N}_L^T \mathbf{f}_{\Gamma L} \} + \delta \dot{\mathbf{u}}_s^T \{ \mathbf{f}_s^{\text{int}} - \mathbf{f}_s^{\text{ext}} + \mathbf{M}_s \ddot{\mathbf{u}}_s + \mathbf{N}_s^T \mathbf{f}_{\Gamma s} \} \\ &\quad + \delta \mathbf{f}_{\Gamma L}^T \{ \mathbf{N}_L^T \dot{\mathbf{u}}_{\Gamma L} - \mathbf{L}_L^T \dot{\mathbf{u}}_\Gamma \} + \delta \mathbf{f}_{\Gamma s}^T \{ \mathbf{N}_s^T \dot{\mathbf{u}}_{\Gamma s} - \mathbf{L}_s^T \dot{\mathbf{u}}_\Gamma \} - \delta \dot{\mathbf{u}}_\Gamma^T \{ \mathbf{N}_L^T \mathbf{f}_{\Gamma L} + \mathbf{N}_s^T \mathbf{f}_{\Gamma s} \} \end{aligned} \quad (4.18)$$

where variation in $\dot{\mathbf{u}}$ and $\mathbf{f}_\Gamma$ are for velocities and coupling forces, respectively. The shape functions act on the interface defined with $\mathbf{N}^T$. By construction, an important property of the spatial coupling is given as:

$$\mathbf{N}_L^T = \mathbf{R}_L; \quad \mathbf{N}_s^T = \mathbf{R}_s \quad (4.19)$$

Algorithm 4 Coupling operator algorithm for non-matching meshes

```

1: procedure COMPUTE SHAPE FUNCTIONS FOR SUBDOMAIN INTERFACE NODES
2:   if  $t_s$  and  $t_L == 0$  then
3:     Determine the nodes on  $\Gamma_L$  and  $\Gamma_s$ 
4:     Create nodal coordinates and connectivity of  $\Gamma$ 
5:     for  $n_L \in \Gamma_L$  do
6:       Let  $\mathbf{N}_L = \mathbf{I}_{\dim((\cdot)_{\Gamma_L})}$ 
7:     for  $n_s \in \Gamma_s$  do
8:       Get global coordinates of the small node  $\mathbf{x}_s$ 
9:       for  $e \in \Gamma$  do
10:        Get interface element  $e$  local coordinates  $\xi$ 
11:        Compute the  $[N_1, N_2, \dots]$  of the small node  $n_s \in e$ 
12:        Store shape functions  $\mathbf{N}$  in the coupling operator matrix  $\mathbf{N}_s$ 

```

Consequently, once the elements of $\mathbf{N}$ are found, the restriction matrix $\mathbf{R}$ is trivial to find. Algorithm 4 summarises a method to compute this interpolation operator.

Operators $\mathbf{N}_L$, $\mathbf{N}_s$, $\mathbf{R}_L$, and $\mathbf{R}_s$ are found through establishing an independent mesh on Γ . The components of the interpolation $\mathbf{N}_L$, $\mathbf{N}_s$ matrices contain the shape functions of the nodes with respect to the externally defined mesh Γ . A linear isoparametric mapping is used, where Γ is discretised with line elements in 2-D, or quadrilateral elements in 3-D. For the case of the line element, a subdomain interface node requires computing shape functions N_1 and N_2 for the two Γ nodes that construct the line. The equations are familiar to finite element developers as:

$$N_1(\xi) = \frac{1}{2}(1 - \xi) \quad (4.20)$$

$$N_2(\xi) = \frac{1}{2}(1 + \xi) \quad (4.21)$$

for which the local coordinate is denoted ξ . Whilst this is simplistic in 2-D, the computation of shape functions on a surface for 3-D couplings is slightly more complicated due to the requirement of finding both ξ and η in the parent domain. The current algorithm in 3-D uses a bilinear mapper that analytically finds the local coordinates ξ and η [146], followed by computing traditional quadrilateral shape functions as:

$$N_1 = \frac{1}{4}(1 - \xi)(1 - \eta) \quad (4.22)$$

$$N_2 = \frac{1}{4}(1 + \xi)(1 - \eta) \quad (4.23)$$

$$N_3 = \frac{1}{4}(1 + \xi)(1 + \eta) \quad (4.24)$$

$$N_4 = \frac{1}{4}(1 - \xi)(1 + \eta) \quad (4.25)$$

It can be observed that storing each of the shape functions in $\mathbf{N}_L$ and $\mathbf{N}_s$ for all the interface nodes would require significant computational memory, especially in the case for large meshes. The following section looks to address this potential issue.

To elucidate the the operators further, the connection between two non-matching meshes is described in 2-D for the simple case in Figure 4.3.

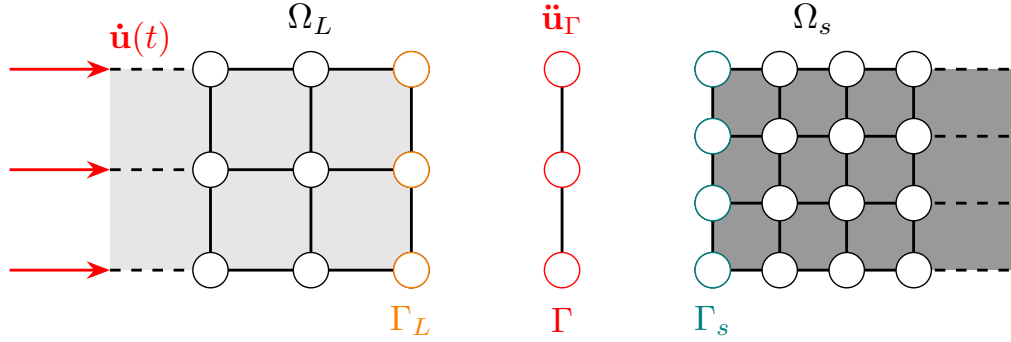


Figure 4.3: A non-matching benchmark with differently discretised domains with the Large Γ_L , small Γ_s and externally meshed interface Γ .

The number of nodes corresponding to the non-matching Γ are $\mathcal{N}_{\Gamma_L} = \mathcal{N}_{\Gamma} = 3$ and $\mathcal{N}_{\Gamma_s} = 4$, as highlighted in yellow, red and green, respectively. The interpolations matrices for this simple case allow the shape functions to be computed as:

$$\mathbf{N}_L = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}; \quad \mathbf{N}_s = \begin{bmatrix} 1 & 0 & 0 \\ 1/3 & 2/3 & 0 \\ 0 & 2/3 & 1/3 \\ 0 & 0 & 1 \end{bmatrix} \quad (4.26)$$

whereas the restriction matrices are:

$$\mathbf{R}_L = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}; \quad \mathbf{R}_s = \begin{bmatrix} 1 & 1/3 & 0 & 0 \\ 0 & 2/3 & 2/3 & 0 \\ 0 & 0 & 1/3 & 1 \end{bmatrix} \quad (4.27)$$

As a consequence of the one-to-one mapping from Γ_L to Γ , it is clear that operator $\mathbf{N}_L$ always takes the form of an identity matrix. $\mathbf{N}_s$ follows a similar trend for

coincident nodes, whereas computation of the shape functions are required for those non-matching. The restriction matrices allow for the summation of masses and forces on the interface to give:

$$\mathbf{M}_\Gamma = \mathbf{R}_L \mathbf{C}_L^T \mathbf{M}_L + \mathbf{R}_s \mathbf{C}_s^T \mathbf{M}_s = \mathbf{R}_L \mathbf{M}_{\Gamma_L} + \mathbf{R}_s \mathbf{M}_{\Gamma_s} \quad (4.28)$$

$$\mathbf{f}_\Gamma^{\text{int}} = \mathbf{R}_L \mathbf{C}_L^T \mathbf{f}_L^{\text{int}} + \mathbf{R}_s \mathbf{C}_s^T \mathbf{f}_s^{\text{int}} = \mathbf{R}_L \mathbf{f}_{\Gamma_L}^{\text{int}} + \mathbf{R}_s \mathbf{f}_{\Gamma_s}^{\text{int}} \quad (4.29)$$

$$\mathbf{f}_\Gamma^{\text{ext}} = \mathbf{R}_L \mathbf{C}_L^T \mathbf{f}_L^{\text{ext}} + \mathbf{R}_s \mathbf{C}_s^T \mathbf{f}_s^{\text{ext}} = \mathbf{R}_L \mathbf{f}_{\Gamma_L}^{\text{ext}} + \mathbf{R}_s \mathbf{f}_{\Gamma_s}^{\text{ext}} \quad (4.30)$$

Through the use of shape functions to compute the mass and forces, the partition of unity ensures that method is both mass and energy conserving. The definition of the coupling matrices, although mathematically consistent, is computationally inefficient with the storage of matrices with a high sparsity. For this reason, the procedure is optimised further for more efficient solutions.

4.1.3 Algorithmic Implementation of the Spatial Coupling

The previous definition of coupling operators are summarised in Algorithm 5. Once again, for mass-conserving problems $\mathbf{M}_\Gamma$ need only be assembled once at $t_i = 0$. In this study, the interpolation functions, $\mathbf{N}$, are computed just once at the start of the simulation. For small deformations, this is a reasonable assumption, however error could potentially accumulate for large deformations. This is due to the change in the positions of nodes $\mathbf{x}_{\Gamma_s}$ relative to $\mathbf{x}_{\Gamma_L}$. As time progresses for these scenarios, the values of the shape functions in Equation 4.13 would require re-computation. For now, the success of this algorithm is evaluated with the assumption of small deformations, as well as the nodes of Γ_s not separating from the originally defined interface Γ . The storage of $\mathbf{N}$ and $\mathbf{R}$ as sparse matrices for each subdomain results in an excessive computational expense. Algorithm 4 states the determination of those nodes on Γ_L and Γ_s . This can be implemented in several ways; the simplest being the provision of a nodal lists, prior to the solving the problem, by the user. Consequently the mass on each subdomain interface can be within vectors $\mathbf{M}_{\Gamma_L}$ and $\mathbf{M}_{\Gamma_s}$:

$$\mathbf{M}_\Gamma[i] = g(\mathbf{M}_{\Gamma_L}[i]) + \sum_{n_s=1}^4 N_i[n_s] \cdot \mathbf{M}_{\Gamma_s}[n_s] \quad (4.31)$$

Algorithm 5 Summary of Spatial Coupling for Non-Matching Meshes

```

1: procedure INTEGRATE A TWO-DOMAIN NON-MATCHING MESH PROBLEM
2:   while ( $t_s$  or  $t_L \leq t_{final}$ ) do
3:     Compute  $\ddot{\mathbf{u}}_{\Gamma_s}$  with operator  $\mathbf{N}_s$  in Eq. 3.48 on  $\Gamma_s$ ;
4:     Integrate small domain  $\Omega_s$ ;
5:     Update all elements  $\in \Omega_s$  and compute vectors  $\mathbf{f}_s^{\text{int}}, \mathbf{f}_s^{\text{ext}}$ ;
6:     Compute  $\ddot{\mathbf{u}}_{\Gamma_L}$  with operator  $\mathbf{N}_L$  in Eq. 3.48 on  $\Gamma_L$ 
7:     Integrate Large domain  $\Omega_L$ , with  $\ddot{\mathbf{u}}_{\Gamma}$  on  $\Gamma_L$ ;
8:     Update all elements  $\in \Omega_L$  and compute vectors  $\mathbf{f}_L^{\text{int}}, \mathbf{f}_L^{\text{ext}}$ ;
9:     Restrict with  $\mathbf{R}_L$  and  $\mathbf{R}_s$  to find  $\mathbf{M}_{\Gamma}, \mathbf{f}_{\Gamma}^{\text{int}}$  and  $\mathbf{f}_{\Gamma}^{\text{ext}}$  with Eqs. 4.28-4.30;

```

where mapping $g : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is a one-to-one mapping, and the summation corresponding to each Γ node i requires a maximum of four n_s nodes in 2-D, or eight in 3-D. The same can be assumed for the coupling of $\mathbf{f}^{\text{ext}}$ and $\mathbf{f}^{\text{int}}$. The coupling of kinematics is performed in similar fashion to compute $\ddot{\mathbf{u}}_{\Gamma_L}$ and summing accelerations for those n_s nodes belonging to the vector $\ddot{\mathbf{u}}_{\Gamma_s}$.

4.2 Numerical Examples

To demonstrate the performance of the proposed spatial coupling, several numerical examples are presented. Dynamic problems that transmit force across subdomain interfaces are described, with elastic wave propagation in a 2-D and 3-D long bar configurations, followed by a compact-tension numerical simulation.

4.2.1 Axial Wave Propagation in Non-Matching Meshes

In the following section, the elastic wave propagation in a 2-D mesh is considered. Utilising a similar coupling to Figure 4.3, the same shape functions that are found in Equations 4.26 can be used to demonstrate the accurate transmission of a pulse from Ω_L to Ω_s . Figures 4.4 - 4.6 depict the axial velocity field near the interface between Ω_L and Ω_s at three different time steps. Through plotting each row of nodes, along the axial direction, each plot shows how the outer nodes at $x = 0$ mm and $x = 1$ mm interact on Γ , as well as those non-matching nodes for $x = 0.5$ mm on Γ_L , as well as $x = 0.333$ mm and $x = 0.667$ mm on Γ_s . Through restricting Poisson ratio $\nu = 0.0$, the propagated waves are purely axial.

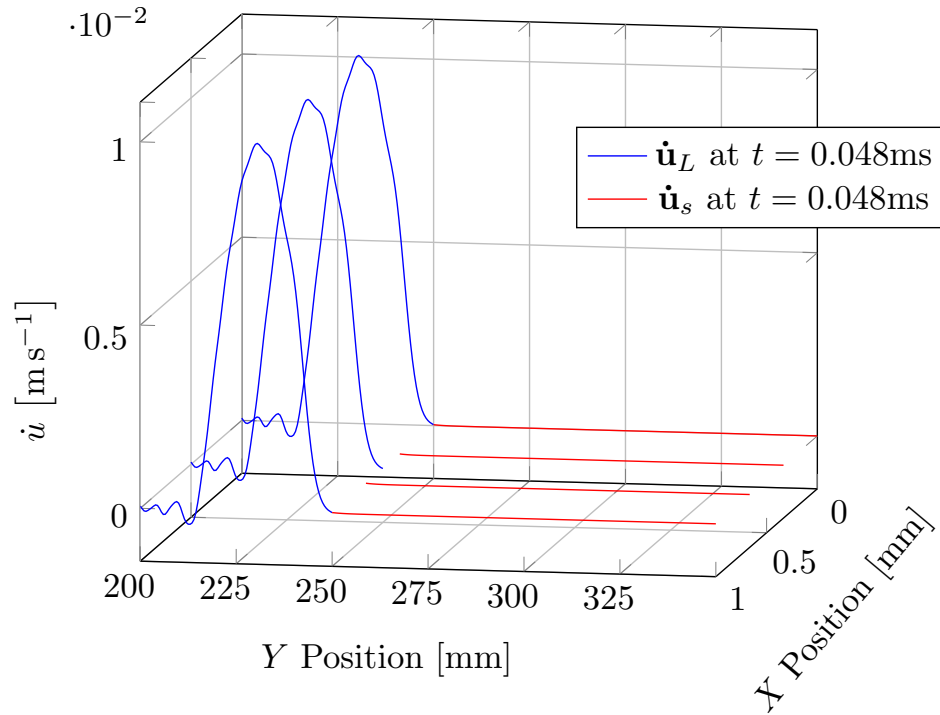


Figure 4.4: Axial wave propagation through Γ for a 2-D Non-Matching Mesh at $t = 0.048$ ms with 3 large coupling 4 small nodes.

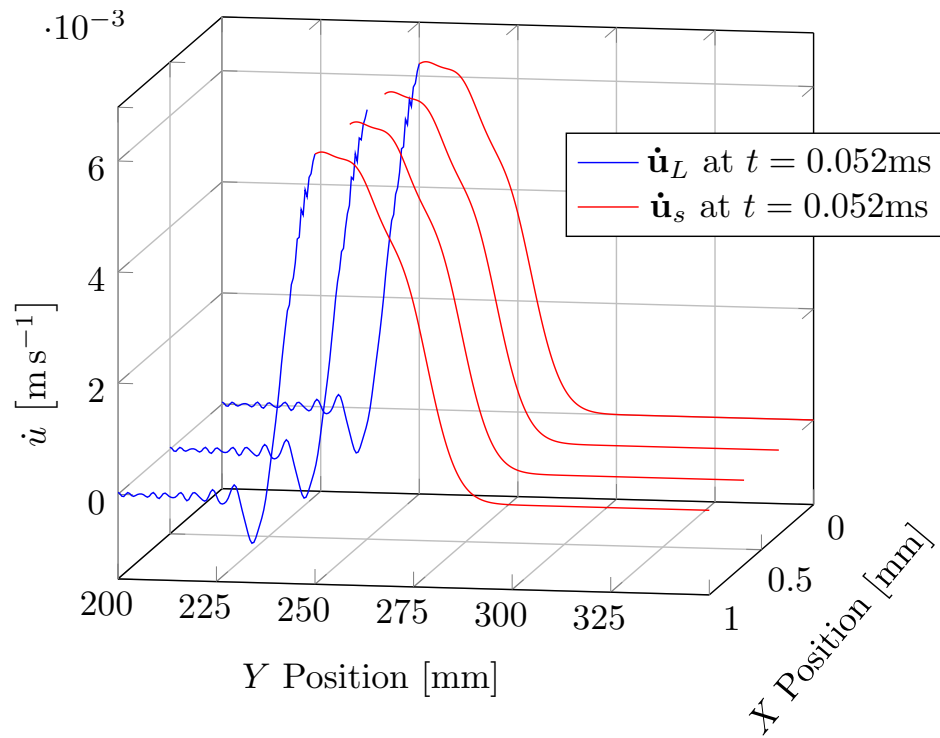


Figure 4.5: Axial wave propagation through Γ for a 2-D Non-Matching Mesh at $t = 0.052$ ms with 3 large coupling 4 small nodes.

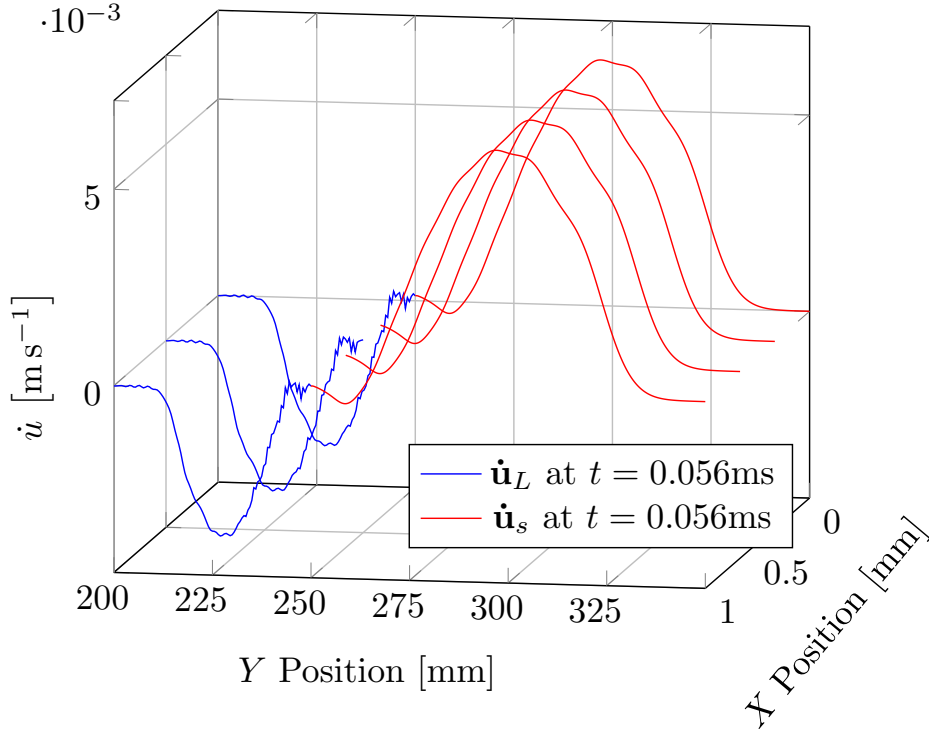


Figure 4.6: Axial wave propagation through Γ for a 2-D Non-Matching Mesh at $t = 0.056$ ms with 3 large coupling 4 small nodes.

In Figure 4.4, at $t = 0.048$ ms, the half sinusoidal boundary condition propagates and begins to interact with the non-matching interface. All three rows of nodes on Ω_L perform identically, similarly for those four rows on Ω_s . Figure 4.5 illustrates the partial transmission of the waves from Ω_L , with a dilatational wave speed of 5141.67 ms^{-1} , to Ω_s with 11301.06 ms^{-1} . This difference in impedance is evident, as the wave travels faster through Ω_s . Even as the wave interacts with non-matching Γ_L and Γ_s , each row of nodes follow the same motion on their respective subdomain. In the last of the three, Figure 4.6, shows the transmission and reflection of the waves, where the new amplitudes of the waves is determined by the ratio of the difference in impedance.

In all three simulations, numerical oscillations can be observed. These can be alleviated through refining the meshes, or through application of bulk viscosity. More importantly, the spatial coupling algorithm does not alter the spurious oscillations, maintaining identical motion on each row of nodes. Simulating monolithically throughout all plots, both subdomains are solved with the Δt_s . In the following

section, an evaluation of the kinematics on the interface, and assessment of energies is made for an axial wave propagation problem in three dimensions.

4.2.2 Mixed Element Coupling and Extension to 3-D

A key advantage of the algorithm is its independence to choice of element formulations, whilst also requiring little modification when extending from 2-D to 3-D. Following on from the previous two dimensional benchmark, a similar axial wave propagation problem can be simulated with hexahedral elements representing Ω_L and tetrahedral elements for Ω_s . The method restricts the externally assembled Γ , to the discretisation of Γ_L . So long as the compatibility condition $\Gamma = \Gamma_L \cap \Gamma_s$ is met, the algorithm is adaptable to any finite element discretisation.

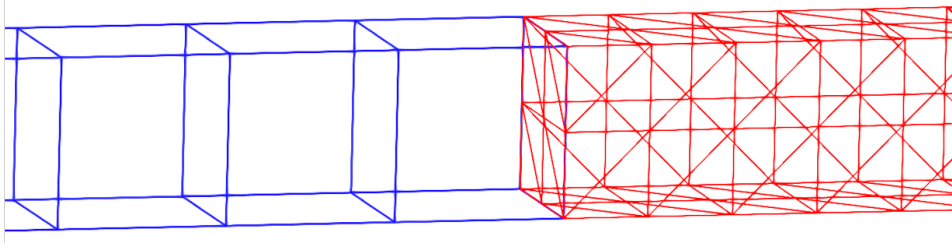


Figure 4.7: Wireframe representation of mixed element coupling mesh close to interface Γ . The interfaces Γ_L and Γ_s are represented by four nodes and nine nodes on hexahedral and tetrahedrals, respectively.

Extending to 3-D requires the definition of Γ to a convex quadrilateral surface. Whilst iterative methods by Lim et al. and Liu et al. are available to find the local coordinates (ξ, η) of the hanging node n_s [147, 148], an ongoing area of research is the use of an analytical bi-linear inverse mapper [146]. To demonstrate this capability, the material properties are now homogeneous throughout a long bar, but the element formulation Ω_L and Ω_s differ. In Figure 4.7, a diagram of the mesh close to the interface is shown. Similar boundary conditions to the previous section are maintained, where now four nodes on a linear hexahedral element are prescribed a half sine velocity boundary condition. The axial wave propagation problem is defined such that $E_L = E_s = 207$ GPa and $\rho_L = \rho_s = 7.83 \times 10^{-6}$ kgmm⁻³ in each of the subdomains. Subdomains are of consecutive lengths $L_L = 125$ mm and

$L_s = 250$ mm, with the half sine velocity boundary condition applied at $x = 0$ with a sine period $L_L/2 \cdot \sqrt{\rho/E}$. A total of 125 large hexahedral and 13717 small tetrahedral elements are used to discretise the long square cross sectioned bar. Time steps initially integrate with $\Delta t_L = 1.8317 \times 10^{-5}$ ms and $\Delta t_s = 3.1988 \times 10^{-6}$ ms with $Co = 0.1$ for both subdomains. Bulk viscosity is applied, with linear term $C_1 = 0.06$ to reduce spurious oscillations. Interfaces Γ_L and Γ_s are discretised with four and nine nodes respectively, where Γ_L takes the shape of a quadrilateral and Γ_s a set of triangular surfaces.

Figures 4.8 - 4.10 plot the time history of the three kinematic variables on Γ_L and Γ_s . The continuity of $\ddot{\mathbf{u}}_\Gamma$ is exact for coincident nodes, with very slight variation when considering the acceleration of all nine tetrahedral nodes. The acceleration $\ddot{\mathbf{u}}_\Gamma$ is held constant over six small time steps, an assumption similar to that made in the temporal work. Tetrahedral shape functions are unable to exactly capture the motion of an axial wave through a square cross section. Despite this, the results show a highly accurate transmission of the inertial force from large to small subdomain. Interface velocity $\dot{\mathbf{u}}_\Gamma$ also aligns well on both subdomains with variation in velocity $< 5 \times 10^{-6}$ ms⁻¹. $\mathbf{u}_\Gamma$ is also accurately captured, with no clear sign of the drifting phenomena amongst nodes. The addition of σ^{bv} alleviates spurious oscillation when comparing to the previous numerical example. Prescription of $\ddot{\mathbf{u}}_\Gamma$ for each Δt_s is a fair assumption for the given boundary condition, granted a smooth pulse is accurately captured for velocity and displacement.

To assess the spatial coupling, the energy throughout Ω_L and Ω_s must be computed through each subdomains' simulation. Equation 3.96 is called upon to assess the stability of the algorithm. As $\dot{\mathbf{u}}(t)$ is applied to Ω_L , a smooth increase in $W_{\text{ext},L}$ is observed, with $W_{\text{int},L}$ and $W_{\text{kin},L}$ each equating to half of the external work. A smooth transmission on Γ is observed at $t > 0.025$ ms, where the coupling of $\dot{\mathbf{u}}_\Gamma$ leads to the decrease in $W_{\text{ext},L}$ and increase in $W_{\text{ext},s}$. A similar trend for components of W_L is observed as the wave travels through Γ . Evaluating the cumulative effect of each of the components of energy gives Equation 3.96, of which Figure 4.12 shows an energy balance $\delta W_i = W_{\text{bal},i} < \times 10^{-12}$ kNmm.

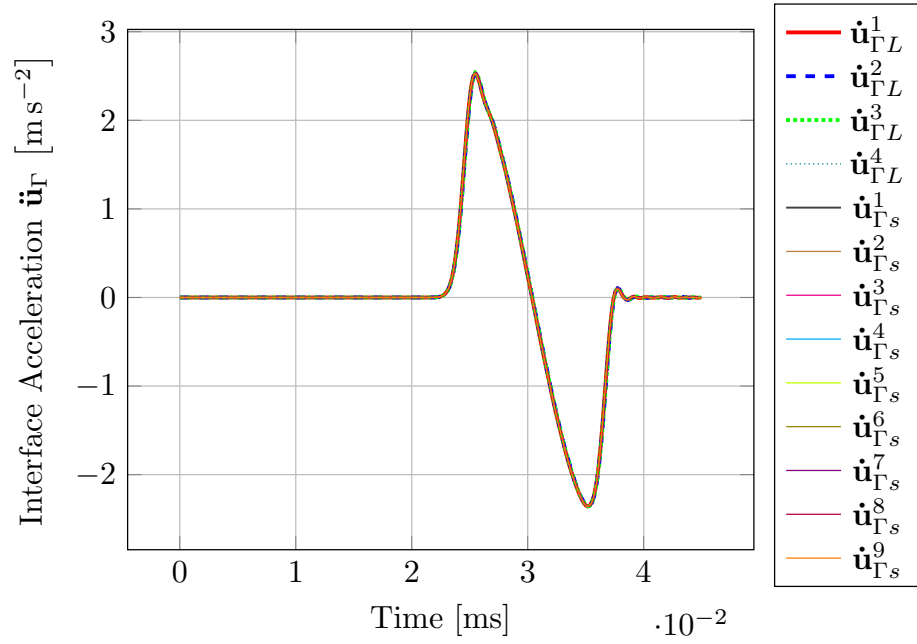


Figure 4.8: Mixed element coupling with interface acceleration $\ddot{\mathbf{u}}_{\Gamma}$ plotted through time for all nodes on Γ_L and Γ_s represented by hexahedral and tetrahedrals respectively.

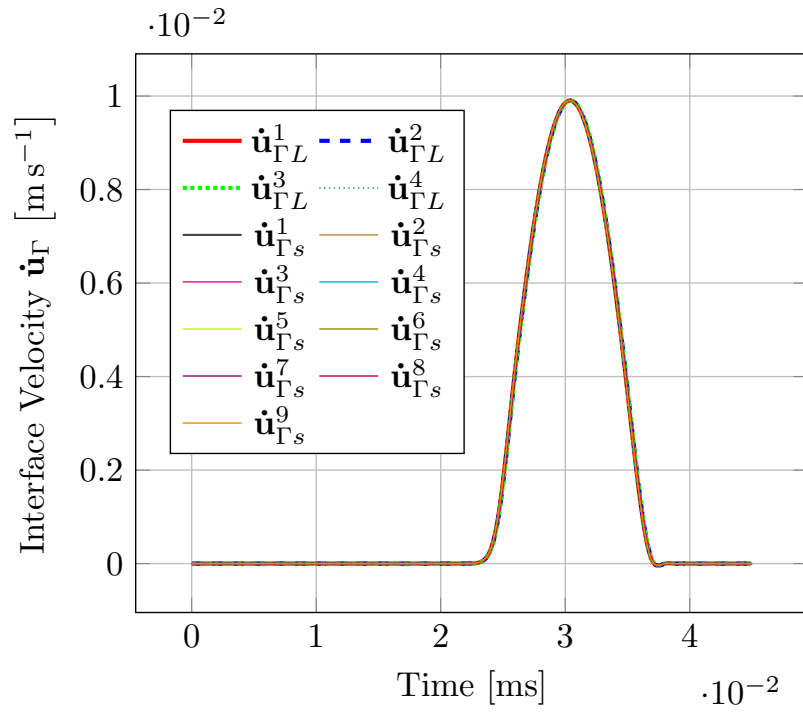


Figure 4.9: Mixed element coupling with interface velocity $\dot{\mathbf{u}}_{\Gamma}$ plotted through time for all nodes on Γ_L and Γ_s represented by hexahedral and tetrahedrals respectively.

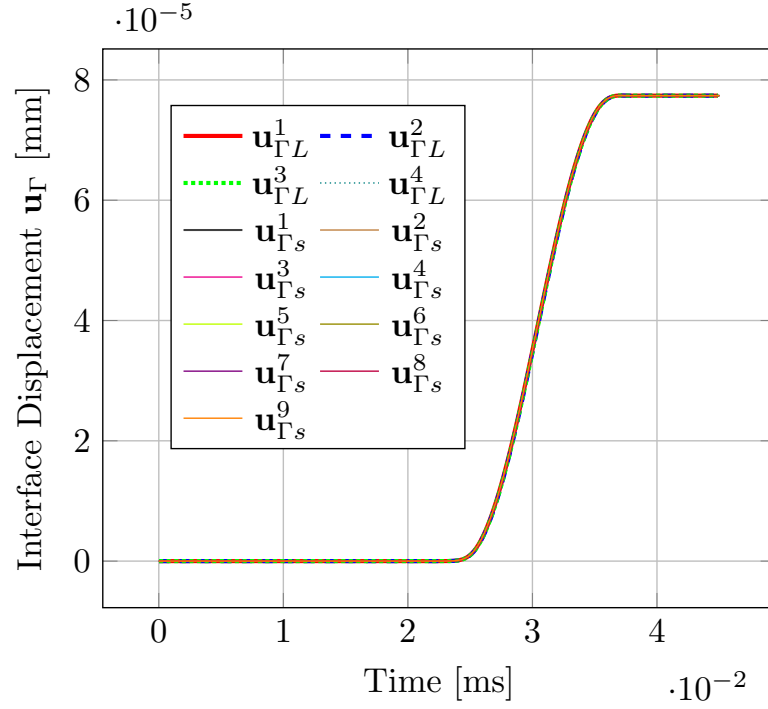


Figure 4.10: Mixed element coupling with interface displacement u_I plotted through time for all nodes on Γ_L and Γ_s represented by hexahedral and tetrahedrals respectively.

4.2.3 On Spurious Wave Reflection

As initially studied by Bažant, the use of non-uniform meshes result in the production of spurious numerical oscillations at the interface between two meshes [149]. This still proves to be a prevalent issue, and mention of its generation when spatially coupling non-matching meshes is important. Previous benchmarks depict numerical examples where the boundary condition is initially applied from Ω_L . However, in the following benchmark, a boundary condition that propagates from Ω_s is considered. The issue of spurious waves can be illustrated with a simple 1-D benchmark. The domain follows a partitioning of Ω into Ω_L and Ω_s , with homogeneous properties throughout the slender bar. Young's modulus $E = 207$ GPa and density $\rho = 7.83 \times 10^{-6}$ kgmm⁻³ is defined throughout the domains. The spatial discretisation is heterogeneous, with $L = L_L = L_s = 1.0$ mm and 125 elements used for Ω_L , whereas 500 elements for Ω_s . The corresponding mesh sizes are 0.008 mm and 0.002 mm for large and small, respectively. The boundary condition propagates from the small subdomain at

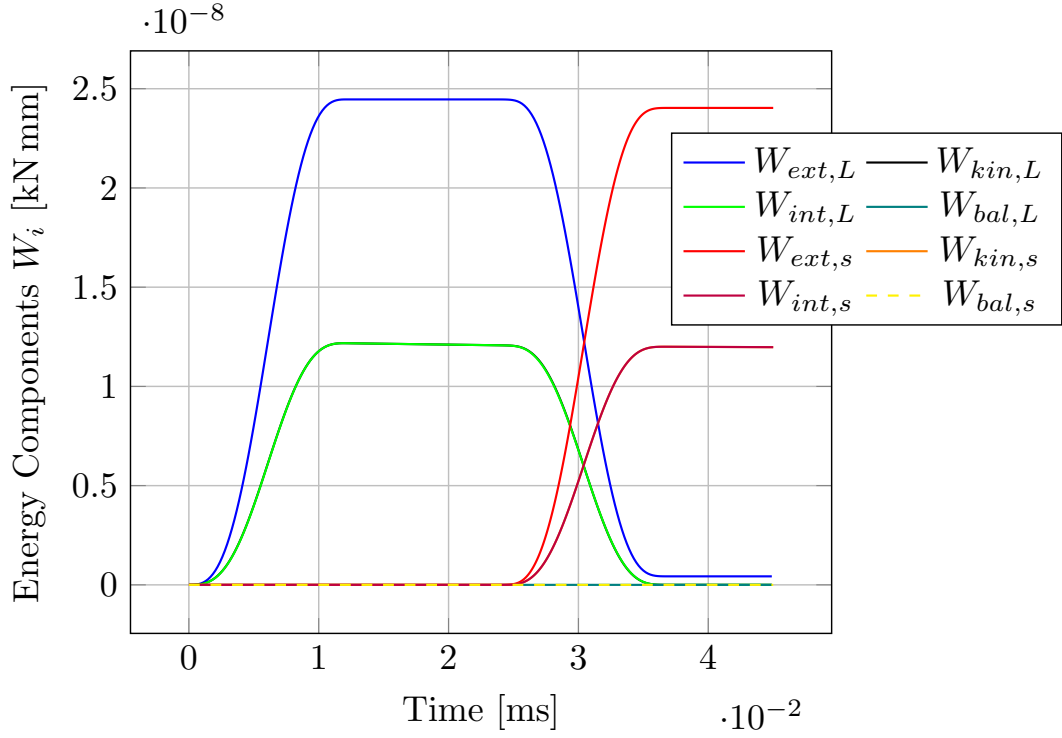


Figure 4.11: Mixed element coupling subdomain energy components for each subdomain Ω_i , where Ω_L and Ω_s are represented by hexahedral and tetrahedrals respectively.

$x = 2.0$ mm with the superposition of two sine periods. The velocity is described as:

$$\dot{u} = 0.01\sin(2\pi\omega_L t) + 0.001\sin(2\pi\omega_s t) \quad (4.32)$$

where $\omega_L = (0.5L\sqrt{\rho/E})^{-1}$ is the frequency that has been previously been shown to be captured by the large domain. The high frequency, $\omega_s = (0.01333L\sqrt{\rho/E})^{-1}$, obtaining a factor of $37.5\times$ that of ω_L . The simulation steps in time with $\Delta t_s = 1.944 \times 10^{-7}$ ms using $Co = 0.5$, and a final simulation time of 0.0003840 ms.

In Figure 4.13, two time steps are depicted; the first being $t_1 = 0.0001089$ ms, and the second $t_2 = 0.0002178$ ms. At time stamp t_1 , the propagation of the superimposed wave can be seen from Ω_s , travelling from right to left. At t_2 , the wave interacts with Γ , at $x = 1$ mm where half of the wave can be seen to propagate through to Ω_L . At this point in time, it can also be seen that Ω_L is unable to capture the higher frequency ω_s , despite ω_L propagating. The implications of this is visualised in Figure 4.14, where a spurious wave is generated and reflected back into Ω_s in the reverse direction of the initially propagating wave.

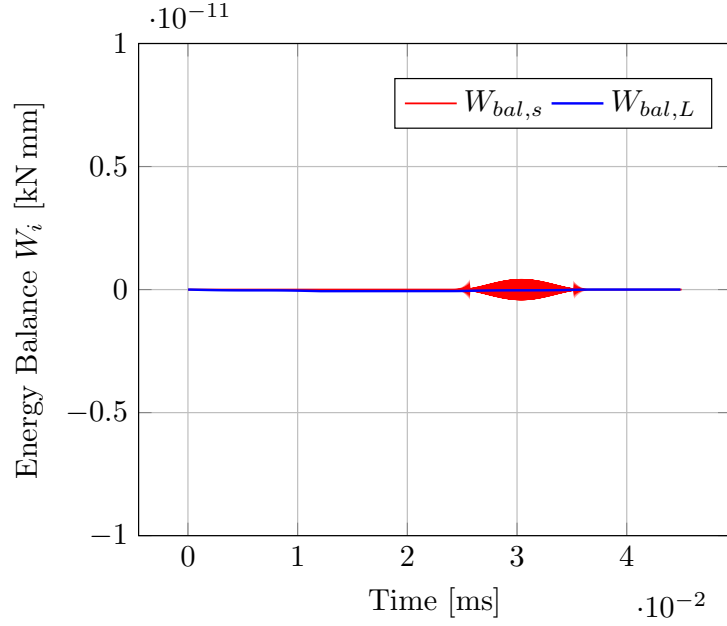


Figure 4.12: Mixed element coupling subdomain energy balance check $|W_{\text{ext},i} - W_{\text{int},i} - W_{\text{kin},i}|$ for both subdomains.

Time step $t_3 = 0.0003267$ ms also shows the propagating of the low frequency ω_L smoothly propagating through Ω_L , similarly to the previous Sections 4.2.1 - 4.2.2. However, it is this numerical artifact in Ω_s that is emphasised, with the energy subsequently trapped in this subdomain.

To mitigate this issue, a simple remedy is to refine Ω_L , where in the referenced works, a factor of < 10 was stated for which spurious oscillations were considered significant between largest element size h_e and the smallest wavelength λ . However other methods include those that apply corrective inertial terms to a coupling length in Ω_s [150]. The dissipation of this spurious energy becomes more effective as a larger coupling length is applied to the high frequencies. The application of the perfect matching layer and local absorbing boundary conditions are also noteworthy methods for tackling these issues within an elastic domain [151, 152]. In the next section, the accuracy of the spatial coupling is assessed for more elaborate meshes, whilst making efforts to ensure higher frequencies are not excited, propagating stress from the coarse mesh. Common experimental specimens are simulated, in the form of compact-tension tests.

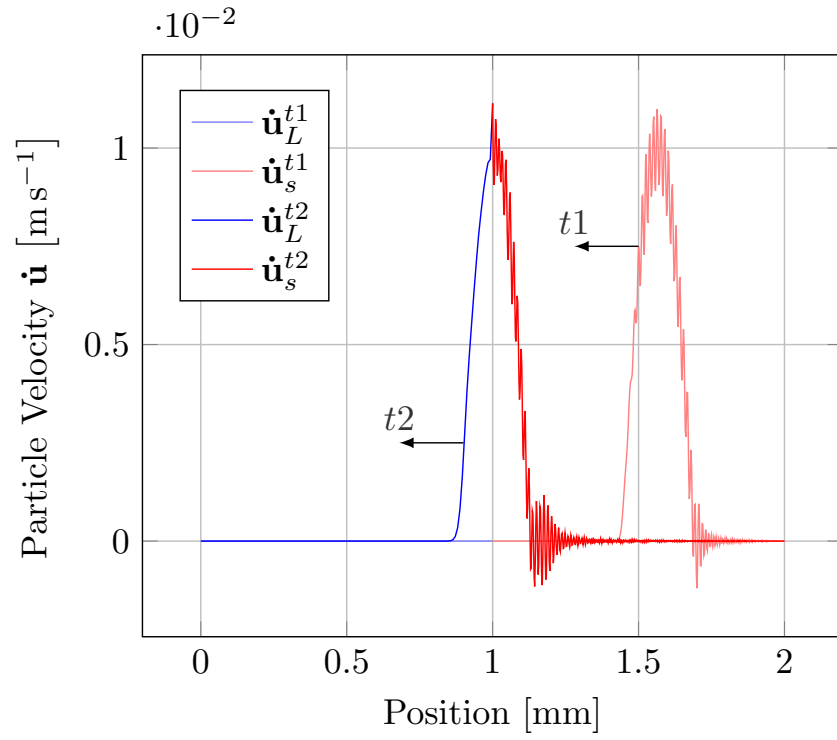


Figure 4.13: High frequency wave propagation from Ω_s to Ω_L at times $t1 = 0.0001089$ ms $t2 = 0.0002178$ ms results in spurious wave reflection.

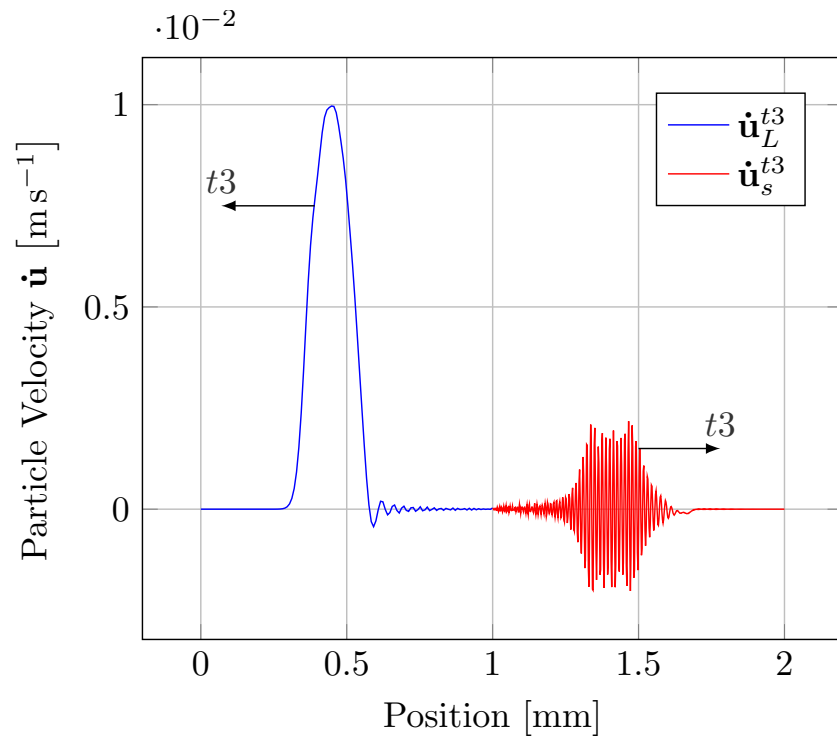


Figure 4.14: High frequency wave propagation from Ω_s to Ω_L at time $t3 = 0.0003267$ ms results in spurious wave reflection.

4.2.4 Compact-Tension Specimen Tests with Localised Stress Gradients

In the following section, an assessment of the spatial coupling is made through dynamic modelling of the experimental compact-tension (CT) test. Typically the CT test evaluates for the failure modes and the fracture toughness of a material [153, 154]. An illustration of the geometry used in the CT test is provided in Figure 4.15. The pins (labelled with a diameter of 8 mm) of the specimen are loaded such that the stress is concentrated about the crack tip of the specimen. The proceeding study evaluates the evolution of this stress gradient, prior to any fracture, maintaining the assumption of a linear elastic material too.

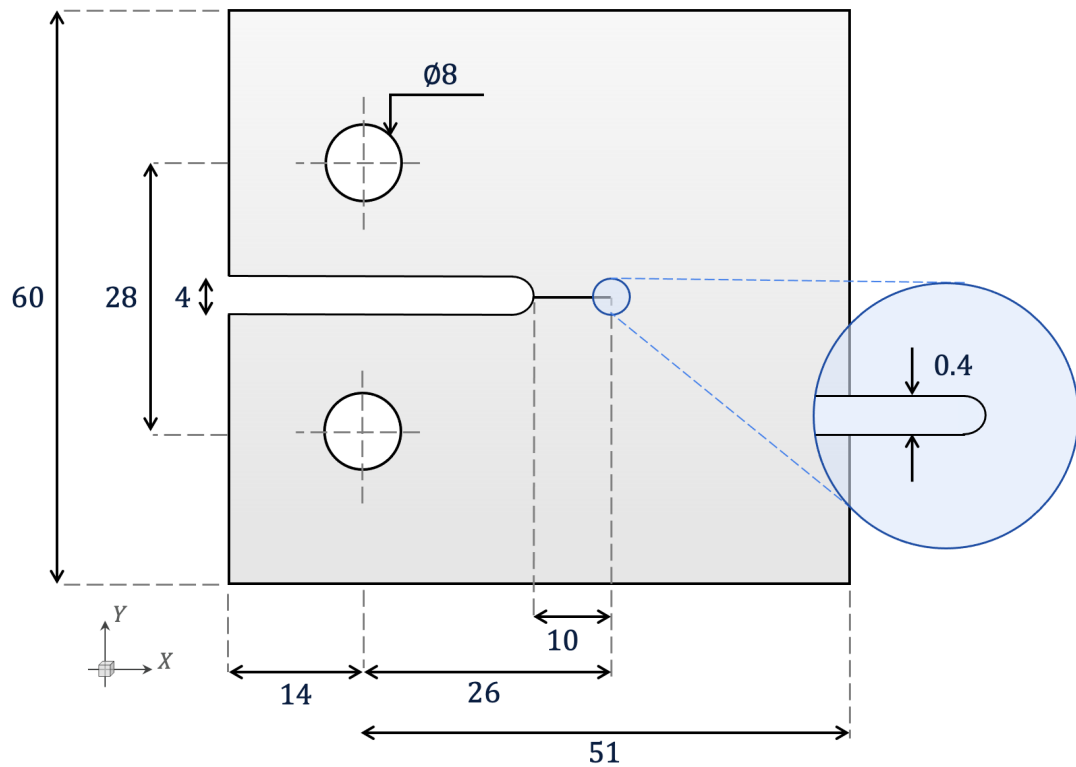


Figure 4.15: Diagram of the compact-tension geometry with dimensions given in [mm] as produced in Sommer et al. [155]

The problem is defined with a material similar to alumina with isotropic elastic properties defined with $E = 370$ GPa, $\rho = 3.9 \times 10^{-6}$ kgmm $^{-3}$ and Poisson's ratio $\nu = 0.22$. To solely evaluate the spatial coupling, the geometry is meshed with a coarse Ω_L and fine Ω_s mesh. The respective element sizes are 1 mm and 0.58 mm

for coarse and fine discretisation. First, a reference simulation is conducted with the fine discretisation utilised throughout the entire subdomain. This is compared with a second simulation; two subdomains Ω_L and Ω_s spatially coupled with a non-matching interface Γ . In both cases a velocity $\dot{\mathbf{u}}(t)$ boundary condition is applied equivalently to each of the nodes that create a semi circle on the pins. A ramp function is applied to the pins with a final magnitude of 0.2 ms^{-1} , opposing in direction for top and bottom pins. The same boundary condition is applied to both simulations, with fewer nodes prescribed in the spatially coupled case as Ω_L is discretised with larger elements. Relevant work that highlight the intricacies of boundary conditions for CT specimens, include the assessment by Triclot et al., that evaluate accurate methods in which to replicate the contact pressure on the pins [156]. For now, it is deemed appropriate to apply the same condition to all nodes on the semicircle of the pins, granted it is consistent in both reference and spatially coupled simulations. This is depicted in the meshes of Figure 4.16. The first two simulations utilise the time step derived by the fine mesh, Δt_s . A value of $Co = 0.5$ is applied to all domains, simulating until a time $t_{final} = 0.02 \text{ ms}$.

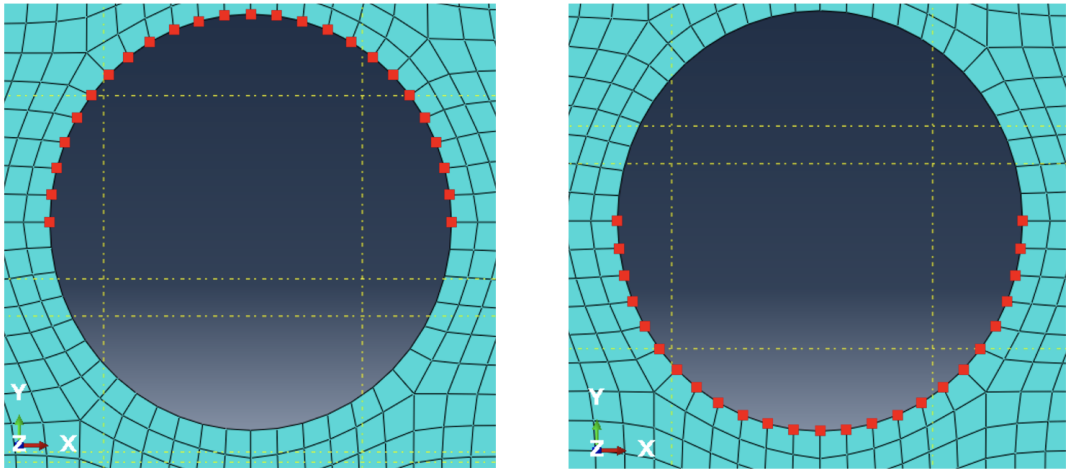


Figure 4.16: Nodal sets for prescription of velocity boundary conditions; (a): top pin nodal set applied +ve loading; (b): bottom pin applied -ve loading.

The dominant stress acts in the Y -direction, for this reason the stress distribution of σ_{yy} is plotted throughout the specimen. A comparison of stress is presented at two distinct time steps for both simulations. A clipping of the solution performed

to limit the values from -0.0005 to 0.0100 GPa, so to visualise the difference in gradients fairly. The first comparison is made at time $t = 0.01408$ ms in Figures 4.17 - 4.18, as the stress begins increasing considerably about the crack tip. The "butterfly-like" stress distribution can be seen to form at this point in the simulation. The maximum stress at $t = 0.01408$ ms for the reference simulation 0.0208 GPa, in comparison to the coupled 0.0207 GPa. A further assessment comparing the two meshes is made later.

At $t = 0.01966$ ms, Cauchy stress further increases at the crack tip, with the number of elements exceeding 0.01 GPa also increasing. Figures 4.19 - 4.20 capture this behaviour, where a very similar distribution is observed at the crack tip for the spatially coupled simulation. This shows that despite using a coarser representation Ω_L , for a significant portion of the domain, the area of interest in Ω_s can still be accurately simulated. The peak values of stress are 0.0396 GPa and 0.0410 GPa for reference and spatially coupled simulations.

Figure 4.20 emphasises a limitation in the discretisation of the domain with the coarser representation of Ω_L , a portion of Ω_L containing the chequerboard pattern, indicating potential hourglassing in Ω_L . Potential solutions to counteract the hourglassing behaviour is the application of control methods that apply artificial stiffness or viscous damping [157]. The choice to vary element formulations is also a common approach when mitigating hourglass effects. The use of higher order or fully integrated elements reduce the likelihood of hourglass modes through distributing stiffness more evenly in comparison to their linear under-integrated counterparts [12]. However, in the case of the CT specimen, both simulations do not adopt these aforementioned control methods. A more simplistic approach of mesh refinement is applied to the coarse region to minimise this artifact. Granted the accurate reproduction of the stress gradients at the crack tip, the energy associated to hourglassing can be assumed to be small. Despite this, to rigorously compare the two simulations, the error must be evaluated throughout the entire mesh.

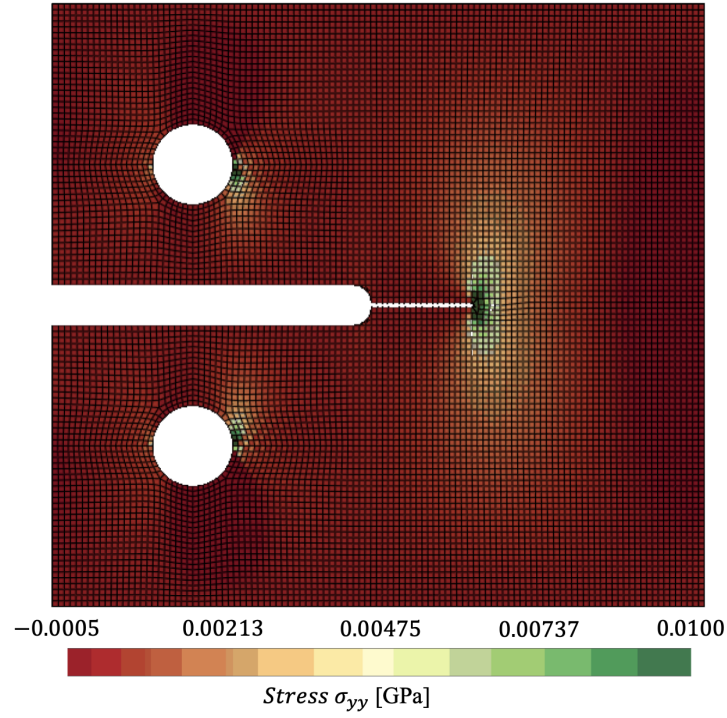


Figure 4.17: Dynamically loaded compact tension specimen σ_{yy} distribution: reference (monolithic) simulation at time $t = 0.01408$ ms.

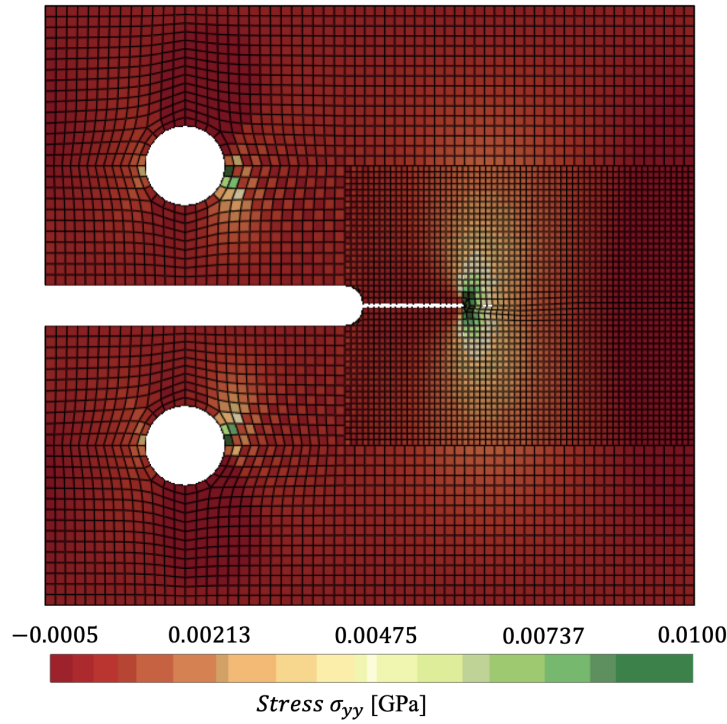


Figure 4.18: Dynamically loaded compact tension specimen σ_{yy} distribution: spatially coupled simulation with non-matching Γ at time $t = 0.01408$ ms.

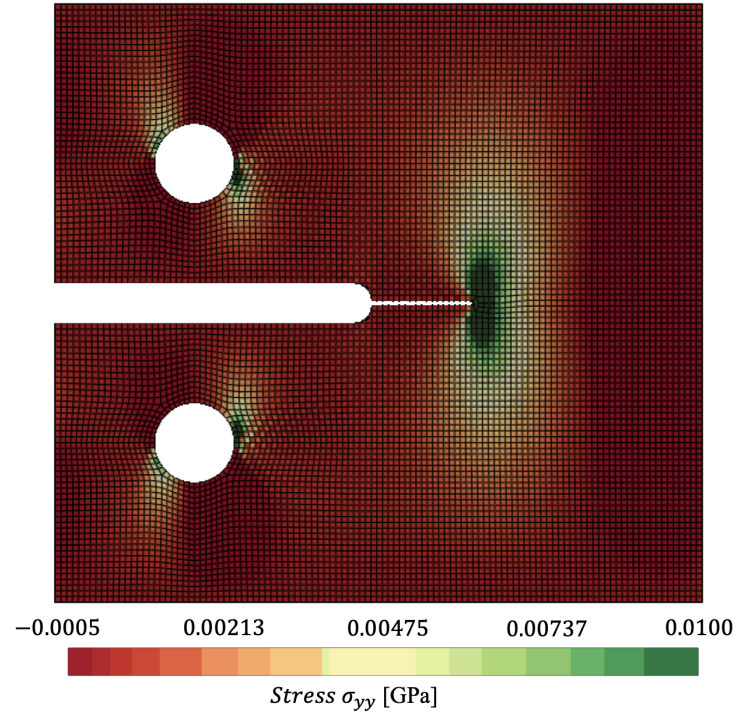


Figure 4.19: Dynamically loaded compact tension specimen σ_{yy} distribution: reference (monolithic) simulation at time $t = 0.01966$ ms.

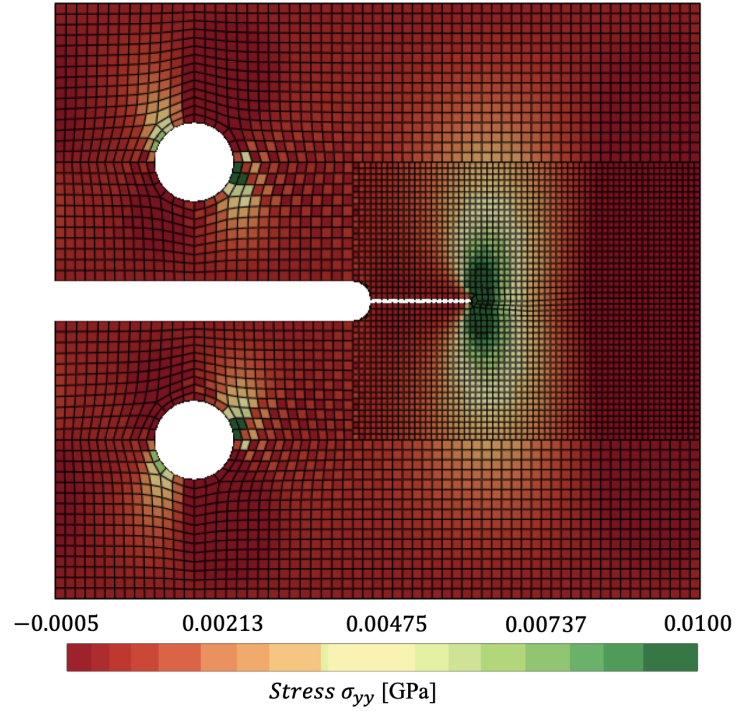


Figure 4.20: Dynamically loaded compact tension specimen σ_{yy} distribution: spatially coupled simulation with non-matching Γ at time $t = 0.01966$ ms.

The root mean squared error (RMSE) is computed at each of the common time steps to numerically evaluate the difference in meshes. To align with the above results, σ_{yy} is assessed at similar time steps with the following:

$$\text{RMSE} = \sqrt{\frac{1}{\mathcal{N}_e^{\text{ref}}} \sum_{e=1}^{\mathcal{N}_e^{\text{ref}}} (\sigma_{yy,e}^{\text{ref.}} - \sigma_{yy,e}^{\text{coup.}})^2} \quad (4.33)$$

where $\mathcal{N}_e^{\text{ref}}$ denotes the total number of elements in the reference simulation, averaging all elements' e contribution for reference (ref) and coupled (coup.) simulation. The coupled simulation contains fewer elements in Ω_L , when compared to the same region in the reference simulation. To still allow for comparison, the values of stress are linearly interpolated to the positions of the reference mesh. The RMSE error is plotted for $t = 0.01408$ ms in Figure 4.21, where very little difference in the two simulations can be found with the coupled simulation. More noticeable error is observed in Figure 4.22, especially in the regions of the coarse mesh around the pins and the back face at coordinates $X = 65$ mm. Despite this, nearly the entire domain captures the behaviour of the stress distribution within $< 5\%$, including the crack tip which sees < 0.002 GPa error compared to the maximum stress of 0.0410 GPa.

4.2.5 Comparison of Stress Intensity Factor

Specific to the application of the compact-tension test, another numerical evaluation can be made to assess the success of the spatial coupling method. The computation of the stress intensity factors (SIF), K , are used to characterise the stress around the crack tip. The analytical solution for in-plane, K_I , and shear, K_{II} , crack opening stress intensity factors can be found in the following works as [158] with rectangular coordinates giving:

$$\sigma_{yy} = \frac{K_I}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \left(1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right) - \frac{K_{II}}{\sqrt{2\pi r}} \sin \frac{\theta}{2} \left(2 + \cos \frac{\theta}{2} \cos \frac{3\theta}{2} \right) \quad (4.34)$$

where r represents the radial distance from the crack, and θ the angle relative to the crack plane. The second mode is found with the following:

$$\sigma_{xx} = \frac{K_I}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \left(1 + \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right) + \frac{K_{II}}{\sqrt{2\pi r}} \left(\cos \frac{\theta}{2} \sin \frac{\theta}{2} \cos \frac{3\theta}{2} \right) \quad (4.35)$$

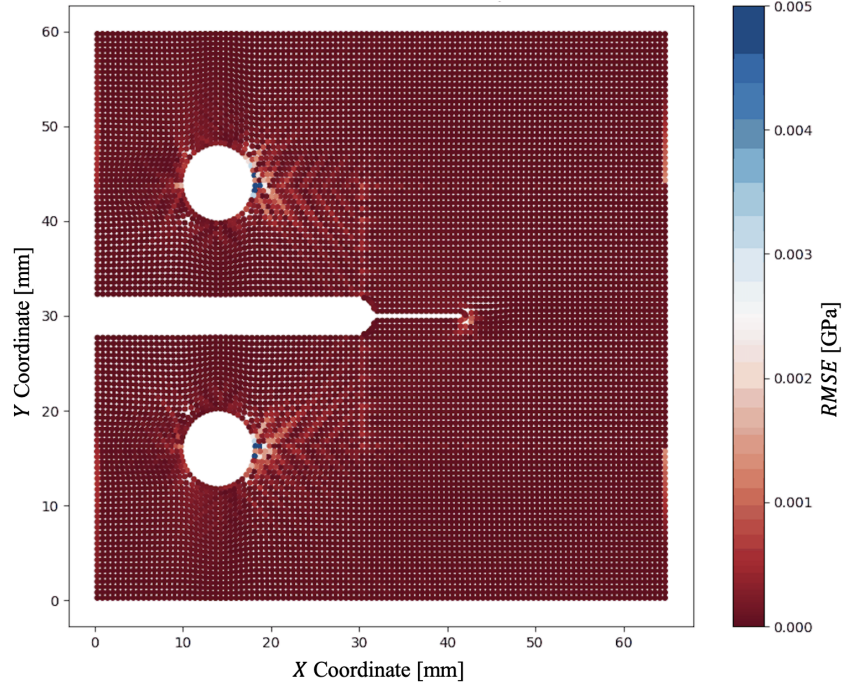


Figure 4.21: Error measure (RMSE) comparing reference and spatially coupled CT Specimen simulation at time $t = 0.01408$ ms.

The values of stress σ_{xx} and σ_{yy} are taken directly from the finite element simulation where a stress field is computed from values at each of the integration points. The stress at the crack tip is extrapolated with the value at the nearest element. This analysis uses $r^{\text{ref.}} = 0.1294$ mm, $\theta^{\text{ref.}} = 1.040^\circ$, $r^{\text{coup.}} = 0.1320$ mm and $\theta^{\text{coup.}} = 1.015^\circ$ with the slight variation in the spatial discretisation of Ω_s . Methods are plentiful in their estimation of K , a rather intuitive method is the stress extrapolation method [159, 160]. Using Equations 4.34 and 4.35, stress values in the vicinity of the crack tip can be used to simultaneously solve for K_I and K_{II} . To further explain this, assuming an evaluation at $\theta = 0$, the relationship between the SIF and stress at the crack tip in the first mode gives:

$$K_I = \lim_{r \rightarrow 0} [\sigma_{11}(r, \theta) \sqrt{2\pi r}] \quad (4.36)$$

Other methods have shown to be more accurate, with the J-integral and the virtual crack closure technique (VCCT) [161–163], accounting for multiple stress points around an integral defined surrounding the crack. Despite this, the stress extrapolation method serves as a reasonable comparison for methods, and can be

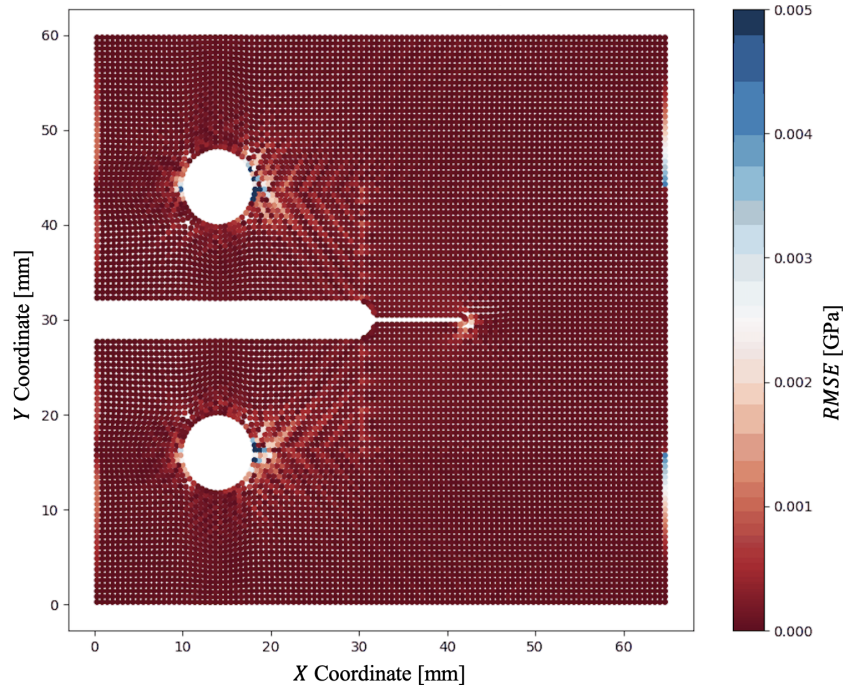


Figure 4.22: Error measure (RMSE) comparing reference and spatially coupled CT Specimen simulation at time $t = 0.01966$ ms

used as a consistent approach to evaluate monolithic and coupled solution. As Figure 4.23 illustrates, the values of stress for both the reference and coupled simulations align well. In Table 4.1, the values of SIF are compared for mode 1 and 2.

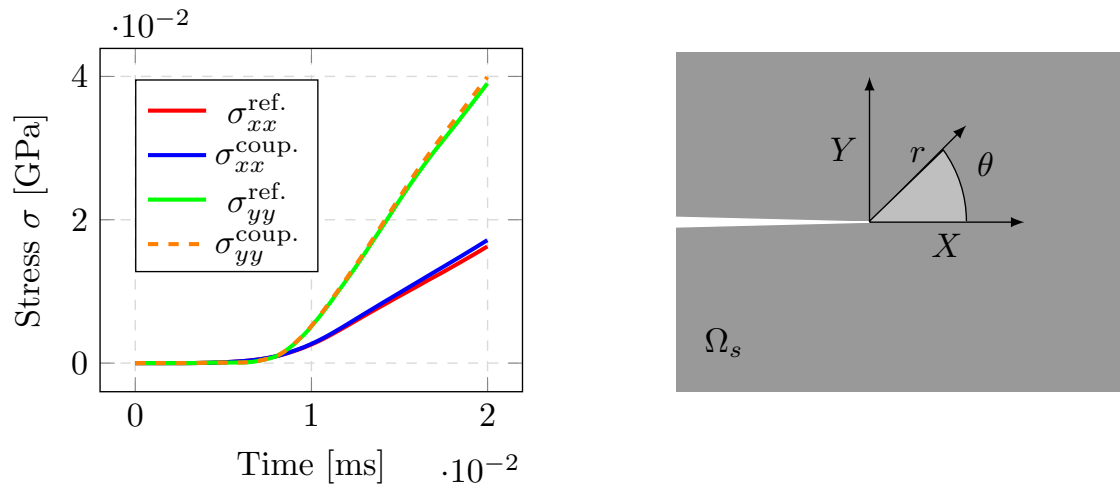


Figure 4.23: (a): Stress evolution with crack tip at coordinates (42.0, 30.0) extrapolated from nearest element comparing reference (fine mesh) and coupled (coarse and fine mesh) simulation through time. (b): The crack tip where rectangular coordinates are used in Equations 4.34 - 4.35 to estimate stress intensity factor (SIF).

Table 4.1: Comparison of stress intensity factors for the compact-tension specimen test with reference mesh and spatially coupled mesh at $t = 0.02$ ms.

Simulation	K_I [MPa·m ^{$\frac{1}{2}$}]	K_{II} [MPa·m ^{$\frac{1}{2}$}]
Reference (monolithic)	0.02714	-0.002857
Spatial coupling	0.02810	-0.003036

The results describe a slight overestimation in absolute values of K for the spatially coupled solution. This difference of 3.5% and 6.3% for K_I and K_{II} is reasonable granted the approximation of the stress extrapolation method. It should also be mentioned, accounting for the contribution of stress from multiple Gauss points would likely reduce this error, reducing the effects of the subtle difference in mesh discretisation in the two meshes. For this the aforementioned J-integral or VCCT method could be called upon in the future. Despite this, the analysis of SIF draws similar conclusions to the previous Section 4.2.4, with good alignment in stress close to the crack tip, as well as the quantitative assessment of K for both modes. Next, a combination of both spatial and temporal algorithms is made to further leverage the speedup for the couplings in the CT specimen.

4.3 Combining Spatial Coupling Algorithms with Multi-Time Stepping

The final key aspect to demonstrating the spatial coupling is the combination with multi-time step integration. Through coupling both in space and time, this section looks to illustrate a remarkable speedup in simulation time without sacrificing accuracy significantly. The culmination of aforementioned Algorithms 1 and 5, provide the building blocks for the final Algorithm 6. Notably, little adaptation is needed from both algorithms to combine the two separate methods. The salient features of time step ratios and reduction factors α_i are maintained, with the crucial difference being the addition of the interpolation $\mathbf{N}_i$ and restriction $\mathbf{R}_i$ operators.

The central theme of computational efficiency is examined utilising the previous dynamic model of the CT specimen. Advantageously, no additional pre-processing

Algorithm 6 Summary of Combined Algorithm for a Large step from N to $N + 1$

```

1: procedure A TWO-DOMAIN SPATIAL AND TEMPORAL INTEGRATION STEP
2:   while  $t_{ratio}^{n+k+1} \leq 1$  or  $(t_{ratio}^{n+k} \leq 1$  and  $t_{ratio}^{n+k+1} \leq 1 + TOL)$  do
3:     Compute  $\ddot{\mathbf{u}}_{\Gamma_s}$  with spatial operator  $\mathbf{N}_s$ 
4:     Integrate small domain  $\Omega_s$  with  $\ddot{\mathbf{u}}_{\Gamma_s}$  and compute  $\mathbf{f}_s^{\text{int}}, \mathbf{f}_s^{\text{ext}}$ 
5:     Compute trial times  $t_{T_s}^{n+k}, t_{T_L}^{N+1}$  and time step ratios  $t_{ratio}^{n+k}, t_{ratio}^{n+k+1}$ 
6:     Compute time step reduction factors  $\alpha_L, \alpha_s$ 
7:     if  $\alpha_L \geq \alpha_s$  then
8:        $\Delta t_L = \alpha_L \cdot \Delta t_L$ 
9:     else
10:       $\Delta t_s = \alpha_s \cdot \Delta t_s$ 
11:      Compute  $\ddot{\mathbf{u}}_{\Gamma_s}$  with spatial operator  $\mathbf{N}_s$ 
12:      Integrate small domain  $\Omega_s$  with  $\ddot{\mathbf{u}}_{\Gamma_s}$  and recompute  $\mathbf{f}_s^{\text{int}}, \mathbf{f}_s^{\text{ext}}$ 
13:      Recompute trial times  $t_{T_s}^{n+k}, t_{T_L}^{N+1}$  and time step ratios  $t_{ratio}^{n+k}, t_{ratio}^{n+k+1}$ 
14:      Compute  $\ddot{\mathbf{u}}_{\Gamma_L}$  with operator  $\mathbf{N}_L$ 
15:      Integrate Large domain  $\Omega_L$  with  $\ddot{\mathbf{u}}_{\Gamma_L}$  and compute  $\mathbf{f}_L^{\text{int}}, \mathbf{f}_L^{\text{ext}}$ 
16:      Summate kinetics with  $\mathbf{R}_L, \mathbf{R}_s, \mathbf{C}_L, \mathbf{C}_s$  to find  $\mathbf{M}_\Gamma, \mathbf{f}_\Gamma^{\text{int}}$  and  $\mathbf{f}_\Gamma^{\text{ext}}$ 
17:      Recompute trial times  $t_{T_s}^{n+k}, t_{T_L}^{N+1}$  and time step ratios  $t_{ratio}^{n+k}, t_{ratio}^{n+k+1}$ 

```

steps are required to enable the asynchronous integration between the coarse ($h_e = 1$ mm) and fine ($h_e = 0.58$ mm) mesh. Consequently, a third simulation is added to the comparison of the alumina CT specimen, re-purposing the mesh visualised in Figures 4.18 and 4.20. However, now Ω_L is able to integrate in time with its own respective time step. The subdomains step with $\Delta t_L = 3.082 \times 10^{-5}$ ms and $\Delta t_s = 5.315 \times 10^{-6}$ ms, resulting in a time step ratio $m = 5.80$. Simulating the same numerical experiment, but utilising Δt_L and Δt_s , produces results very similar to that of the solely spatially coupled meshes.

In Figure 4.24, the plots for $t = 0.01408$ ms and $t = 0.01966$ ms are visualised from left to right. The corresponding plots from the previous section can be seen in Figure 4.18 and 4.20. Consequently, it is a fair assumption to claim that the error achieved $< 5\%$ can also be achieved with the combined method. The spatial discretisation has a much larger effect on error than the temporal discretisation, granted the time step obeys the CFL condition.

A substantial increase in computational efficiency is achieved with the combined methods of spatial and temporal coupling. In Table 4.2 each of the runtimes are summarised for the three simulations of the CT specimen. A reasonable speedup of

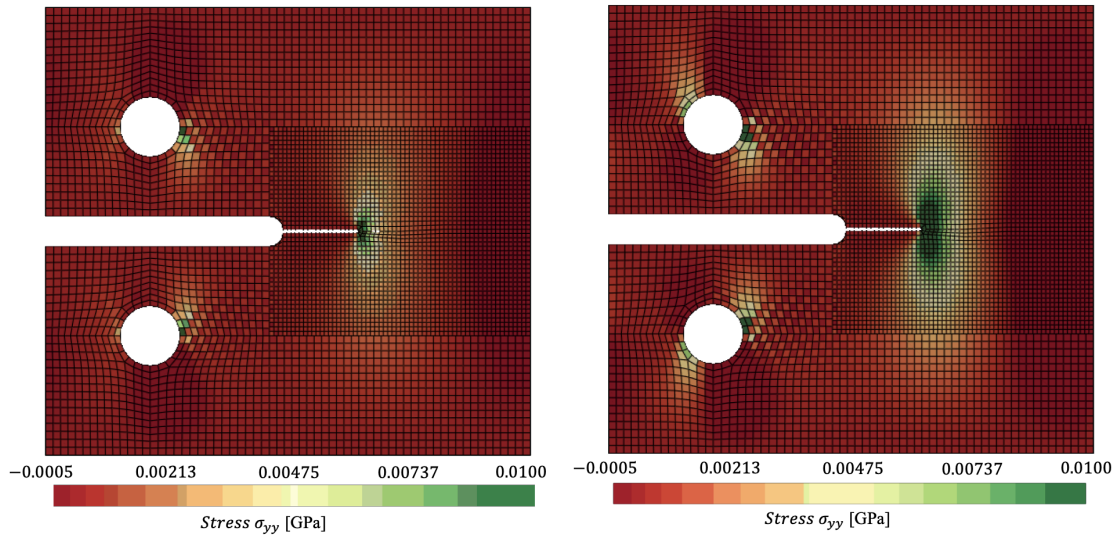


Figure 4.24: Dynamically loaded compact tension specimen σ_{yy} distribution for the spatial coupling with multi-time stepping integration - (a): at time $t = 0.01408$ ms; (b): at time $t = 0.01966$ ms.

Table 4.2: Monolithic and Multi-Time Step runtimes and speedup with spatial coupling of the compact-tension specimen test.

Simulation	Runtime [s]	Speedup
Reference (monolithic)	7,428	-
Spatial coupling	2,267	3.27×
Spatial coupling w/ MTS	572.3	12.98×

3.27× can be observed when utilising larger elements away from regions of interest; the crack tip in the case of a CT specimen. However, quite exceptionally a speedup of 12.98× is accomplished with the combined method.

Considering the similar results achieved in this section to the exclusively spatially coupled simulation, the addition of multi-time stepping to non-matching meshes seems an obvious choice. With the advancement of numerical techniques from temporal to spatial coupling, only minimal modifications are needed to adapt the original algorithms presented in Chapter 3. Following thorough evaluation of the spatial coupling and the combination of the multi-time stepping integration method, a clear demonstration in greater computational efficiency, with little difference in accuracy, is presented in this section.

5

Conclusion and Future Research

Contents

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This final chapter compiles the list of coupling algorithms presented throughout the thesis, as well as the mathematical techniques required to enable them. Numerical methods approximate the physical systems they look to describe. Consequently, assumptions are made. The implications of such assumptions specific to the couplings are described in the limitations of the work. Suggestions for work that look to address some of these, as well as algorithms that show potential in dynamically simulating heterogeneous solids are also described.

5.1 Summary of Methods

The overarching aim of the thesis is the acceleration of numerical simulations that model the dynamic loading of heterogeneous solid bodies. In Section 2.1.2, an extensive literature review revealed the robustness of explicit finite elements for capturing this short-term phenomena in solids. Their application is vast,

spanning multiple length scales. Consequently, a framework has been created around this numerical method. To facilitate the acceleration of explicit FEM, one approach is the development of coupling algorithms, both temporally and spatially. Labelled multi-time stepping, or subcycling, the majority of asynchronous methods in Section 2.2 do not enable the use of non-constant and non-integer time step ratios between subdomains. Heterogeneous systems require this ability to integrate when partitioning real world structures. Reducing the integration steps, whilst maintaining stability and continuity of the interface of subdomains have been identified as re-occurring goals for these couplings. Consequently, steps to further both of these goals are taken. The review of couplings in space that address the problem of non-matching meshes feature in Section 2.3. An apparent need for algorithms that couple subdomains without parameter sensitivity was identified. Pertinent themes in literature include the need for solving dense matrices or additional degrees of freedom. Cognisant of scalability, these methods are severely limited in solving the behaviour of large dynamical structures. A dominant concept that unifies both coupling in space and time is the practicality of implementing such algorithms. This thesis promotes the development of methods that are accurate, computationally efficient, and straightforward in their implementation.

Numerical methods that enable multi-time step integration are described in Chapter 3. The variational formulation for a partitioning into two subdomains with their own respective time step is presented. The method is described in a concise manner, in Section 3.2, ensuring the continuity of kinematics and kinetics on the interface between subdomains. Parallel formulations to Lagrange multiplier methods are made, to allow for the analysis of stability in Section 3.3. Following the study of the two-subdomain algorithm, the method is extended for multiple subdomains in Section 3.4 to enable the practical use of multi-time stepping. The increase in computational efficiency is presented with the dynamic simulation of a metamaterial, in both elastic and elasto-plastic settings.

The spatial coupling is described in Chapter 4, solving the problem of non-matching interfaces. Coupling operators that utilise the same foundation of

Lagrangian shape functions are derived in Section 4.1. Enforcing the continuity of acceleration and tractions is maintained in the spatial coupling. The interpolation and restriction operators are exemplified with a simple 2-D non-matching mesh, outlining each of the matrices that are required on the respective subdomains. However, as Section 4.1.3 illuminates, the storage of these large sparse matrices is not necessary, and methods are presented to avoid this. Without increasing the degrees of freedom of the problem, Section 4.2 presents how stress wave propagation can still be accurately captured in a heterogeneous bar and compact-tension specimen test. Assessment of energy conservation and the error between monolithic and spatially coupled simulations are provided throughout the examples. The open source implementation, used for this section is outlined in Appendix Section B. The final method amalgamates the aforementioned algorithms to develop a non-matching mesh algorithm, that also permits multi-time stepping, in Section 4.3. This combination results in a drastic reduction in computational cost, when compared to monolithic simulations.

5.2 Key Contributions

The following section summarises the main contributions of this thesis, highlighting each of the advancements in the respective types of coupling.

5.2.1 Coupling in Time

Multi-time step integration has enabled the development of the following:

- The concurrent coupling of subdomains with minimum communication between subdomains, allowing for the explicit computation of interface kinematics through evaluating acceleration $\ddot{\mathbf{u}}_I$ in Equation 3.42, and prescribing to both subdomain interfaces.
- An algorithm that circumvents the assumptions of constant and/or integer time step ratios between subdomains, therefore allowing the algorithm to be utilised in highly dynamic settings where time steps may drastically decrease.

- A comprehensive evaluation of stability with computation of the energy associated to the coupling of subdomains, and the increment in energy on the interface Γ , accounting for variation over Δt_L and Δt_s . Comparisons to Lagrange multipliers enable the quantification of these coupling forces and the acceleration in Section 3.3.1.
- A method that performs less element integration steps, when compared to the state-of-the-art [56, 57], by stepping closer to the CFL condition. The novel development of time step ratios and time step reduction factors α from Equations 3.46 to 3.51.
- An asynchronous integration method that extends to multiple subdomains, allowing for sets of finite elements with similar time steps to integrate together, regardless of their spatial adjacency. The summation of forces and mass remain unchanged conceptually as defined in Equations 3.91 and 3.92.
- A speedup of $3.25\times$ is achieved simulating the stress wave propagation of a metamaterial, namely metaconcrete, modelling both elastically and elastoplastically. The heterogeneity of the material is illustrated in Section 3.5, allowing for the dissimilar material constituents to each integrate with their own time steps.

5.2.2 Coupling in Space

Non-matching mesh algorithms have enabled the following research advances:

- Definition of coupling operators $\mathbf{N}$ and $\mathbf{R}$ for the interpolation of $\ddot{\mathbf{u}}_\Gamma$ and restriction for the computation of interface mass and forces in Equation 4.28 - 4.30. The operators do not increase the degrees of freedom of the interface or require the solution to a system of equations.
- The method is implemented in an efficient manner utilising an algorithm that does not require the storage of very large sparse matrices. As Section 4.1.3

sets out, the system variables take the form of vectors, where the mapping of indexes allow for the correct transfer in data to and from Γ .

- A method that extends from 2-D to 3-D subdomains, and permitting mixed element formulations can be found in Section 4.2.2. Spatial coupling between hexahedral and tetrahedral Lagrangian elements are simulated to accurately capture the propagation of stress waves through a slender bar.
- The combination of methods to give Algorithm 6, where very little adaptation in both temporal and spatial coupling algorithms is required. Ease of implementation is a key advantage of the method, with operations defined clearly for insertion into conventional finite element solvers.
- The computational efficiency simulating the evolution of stress gradients in a compact-tension specimen test can be increased by $12.98\times$ through implementing non-matching meshes with multi-time stepping, when compared to a monolithic simulation of fine discretisation throughout the domain.

5.3 Limitations of Work

Despite showing that the main aims and objectives of the thesis have been fulfilled, some assumptions have been made. These are reiterated below. To maximise computational efficiency when multi-time stepping, the solution at the interface between two subdomains is only computed at each large time step Δt_L . Consequently, with $\ddot{\mathbf{u}}_\Gamma^N$ maintained over N to $N + 1$, the temporal coupling is unable to capture any variation in motion on the interface for small time steps between Δt_L . This has not proven to be an issue so far with the evaluation of the force associated to this assumption shown in Section 3.3.4. On the other hand, benchmarks that excite very high frequencies with boundary conditions travelling from Ω_s to Ω_L have not been successfully captured. Variations in motion below the time step of elements on the interface result in spurious oscillations being generated. Consequently, in these scenarios the time step must be reduced. Shifting the temporal interface

to allow time steps on Ω_s to compute motion has been proposed as an initial recommendation, assuming Δt_s is sufficiently low enough to capture such behaviour. Highly heterogeneous configurations are connected to this, as described in Appendix A.2, where the constant acceleration assumption leads to an unstable simulation without the application of additional numerical strategies. Algorithm 2 presents the re-sorting of subdomains with respect to their Δt , but the subdomains themselves are determined a priori to the running of the simulation. The partitioning of a domain is obvious when modelling heterogeneous structures with large disparity in material properties, and therefore time step. This generalisation cannot be applied to all structures, especially when modelling multi-component structures that may have similar dilatational wave speeds and element sizes.

Limitations concerning the spatial coupling include the computation of the interpolation $\mathbf{N}$ and restriction $\mathbf{R}$ matrices at only $t = 0$ for computational efficiency. This assumption will not suffice when modelling large deformation or problems when the relative motion between subdomains increases to higher magnitudes. The non-matching meshes are currently assumed to be non-intersecting and planar. Therefore, the geometric representation of Γ cannot be assumed to consist of nodes that create a curved line (in 2-D) or surface (in 3-D). Should this not be obeyed, separation between subdomain interfaces can be expected with no mitigation from the existing coupling method. In both numerical examples, the brittle nature of the materials have not been captured. A linear elastic constitutive model is a fair assumption for the rates of deformation simulated. However, for more severe loading, failure and fracture models would need to be implemented.

5.4 Recommendations for Future Work

The previously mentioned limitations provide motivation to better coupling methods in both space and time. To improve the stability of the multi-time stepping algorithm for highly heterogeneous cases, adaptive methods that resolve the interface between large time steps could be implemented. In Figure 5.1, the current solution is depicted at Δt_L , whereas future work in Figure 5.2 shows how Γ_L should not necessarily

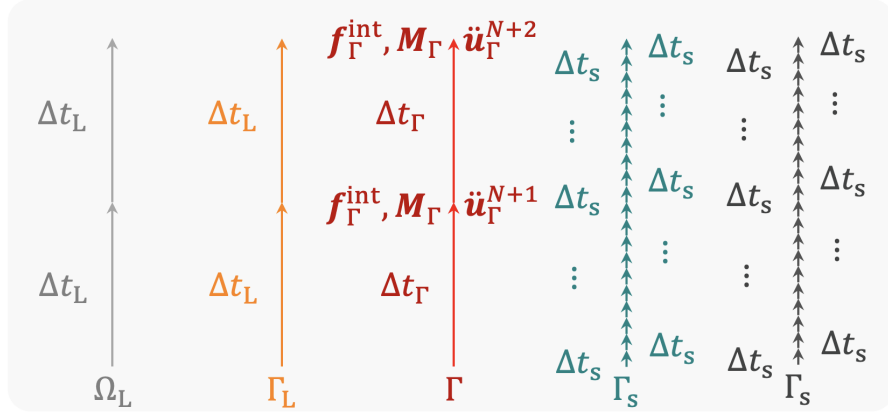


Figure 5.1: Adaptive solution of the interface for highly heterogeneous problems; current solution of the interface at large time steps Δt_L where arrows represent magnitude of time step integrated with.

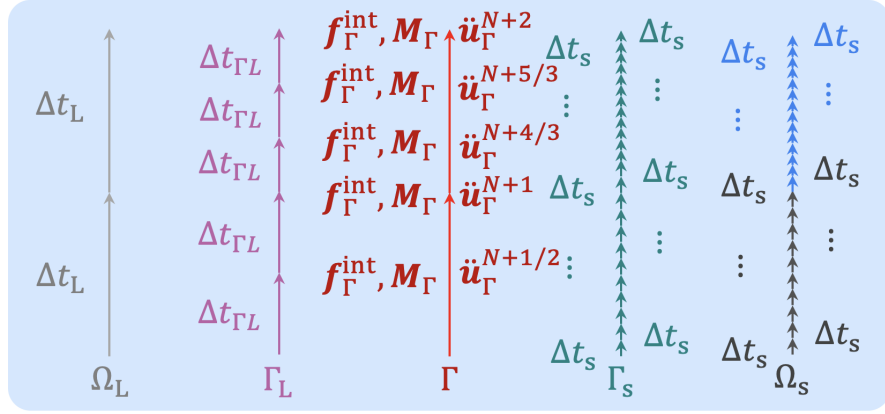


Figure 5.2: Adaptive solution of the interface for highly heterogeneous problems; future work looks to solve the interface at intermediate steps dependent on stability conditions on the interface Γ . The small interface Γ_s and subdomain Ω_s time steps could step independently of one another.

step as per the rest of Ω_L . Rather, an adaptive solution with Equations 3.43 - 3.42 could be used to maintain stability of Γ . Likewise, higher frequencies could be effectively modelled through implementing a filter on the fine scale that enforces a constant stress condition, varying in strength as distance increases from the interface. Automatic partitioning of a domain would be of great value, especially methods that group elements with similar time steps on-the-fly. By evaluating trial times t_{Ti} throughout the simulation, adaptive partitioning is a potential progression for subcycling methods. Computational mechanics cases for utilising multi-time stepping are plentiful across multiple scales, including but not limited to contact,

plasticity, fracture or impact [164–166]. In particular, for the latter, an interesting extension could be the use of multiple time steps for subdomains solved with more than one numerical method, such as coupling FEM-DEM [167] or FEM-SPH [168]. Beyond continuum-continuum coupling, asynchronous integration of multi-scale models such as those that couple on the atomistic scale could prove beneficial. As computing approaches the Exascale, work not too far afield could look to solve individual elements or degrees of freedom with on their own thread, integrating with their own respective time step.

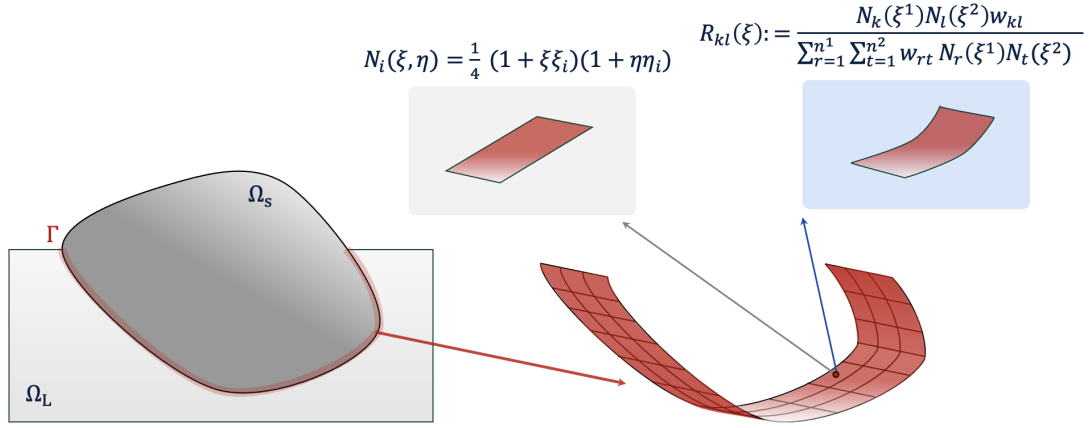


Figure 5.3: Representation of spatially coupled Γ with traditional Lagrangian shape functions could be replaced by NURBS basis functions for exact representation of the interface with NEFEM [169].

Potentially, a low hanging fruit for the spatial coupling is the evaluation of interface kinematic and kinetics with a direct mapping of Γ_s to Γ . It is postulated by increasing the degrees of freedom, the motion at the interface can be better captured. Recent works have shown that the coupling operators can be further optimised by minimising the error of the tractions [94]. Similar methods that look to optimise $\mathbf{N}$ and $\mathbf{R}$ could prove beneficial for the advancement of these types of couplings. Appropriate treatment of separable domains with physical gaps could also be treated with couplings that employ the mean-value method [93, 94]. This would increase the accuracy of such methods that externally resolve kinematics on Γ . The work presented requires planar and the same geometrical interface to be shared by interfaces, but should methods such as NURBS-enhanced finite

elements (NEFEM) or isogeometric analysis (IGA) be invoked, curved interfaces could be resolved exactly [17, 170]. This improvement is visualised in Figure 5.3, where Γ could be represented with the define knot vectors ξ and control point weights w . Replacing the traditional shape functions utilised in this thesis, recent works have identified NURBS basis functions' ability to represent the geometry of curved surfaces exactly [169, 171]. Applications for spatial algorithms are vast, in particular for heterogeneous media, where the presence of inclusions or defects could be modelled with non-matching discretisations [172]. As depicted in Figure 5.4, coupling between macro and meso-scale meshes prove an interesting topic. The raster approach of these meshes allow for a viable application of the spatial coupling described [173]. However, special attention at the interface is required to ensure that spurious reflections do not conceal the solution of stress waves propagating.

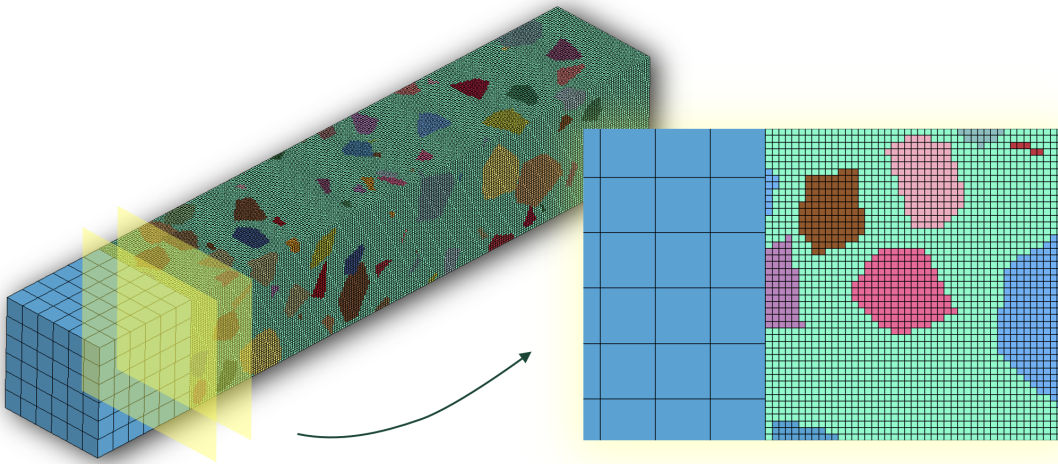


Figure 5.4: Coupling of a continuum mesh with a raster discretisation of arbitrarily packed particles as generated by Falco et al. [174]

The evolving technology of machine learning is showing potential in speeding up the solution of dynamical problems [175]. In addition, the combination of ML with traditional numerical methods could alleviate some of the artifacts produced by FEM, as a means to accurately model heterogeneous dynamic systems. Still very much a nascent topic of research, couplings with ML could be a promising solution for the seamless integration of data from both experiments and computation [176, 177].

Appendices



Further Benchmarking with Multi-Time Stepping

Contents

A.1	Convergence Plots for the Square Wave Propagation Problem	123
A.2	A Highly Heterogeneous Benchmark	125

Further details regarding the testing of the $m = \pi$ benchmark is given, with a conventional convergence plot varying both temporal and spatial parameters. An additional square wave propagation benchmark for a highly heterogeneous domain is simulated to test very high time step ratios. In such scenarios, a simple remedy is provided below to alleviate any concerns of instability on the interface of two subdomains.

A.1 Convergence Plots for the Square Wave Propagation Problem

Corresponding to Section 3.3.2, the selection of mesh discretisation and time steps are justified in the following convergence study. Running a total of 20 simulations for the $m = \pi$ benchmark, the Courant number is varied from 0.1 to 0.9, and total

number of elements varied from 120 to 1800. In Figure A.1 the mean absolute error $|\bar{\varepsilon}|$ is plotted against the total number of elements for varying values of Co . The simulation corresponds to the proposed multi-time stepping method, with bulk viscosity employed to smoothen out the solution. The error measure is estimated with the following:

$$|\bar{\varepsilon}| = \frac{1}{n} \sum_{i=1}^n |\dot{\mathbf{u}}_i - \hat{\mathbf{u}}_i| \quad (\text{A.1})$$

given the analytical solution $\hat{\mathbf{u}}_i$ for a square wave on the interface, for each time step i for the number of total time steps n , is given by:

$$\hat{\mathbf{u}}(t) = A (H(t - t_\Gamma) - H(t - (t_\Gamma + \Delta t))) \quad (\text{A.2})$$

where A is the amplitude of the wave, H is the Heaviside function, and t_Γ is the start time when the pulse first reaches the interface Γ of the two subdomains. Figure A.1 depicts the error varying both temporal and spatial quantities. Granted

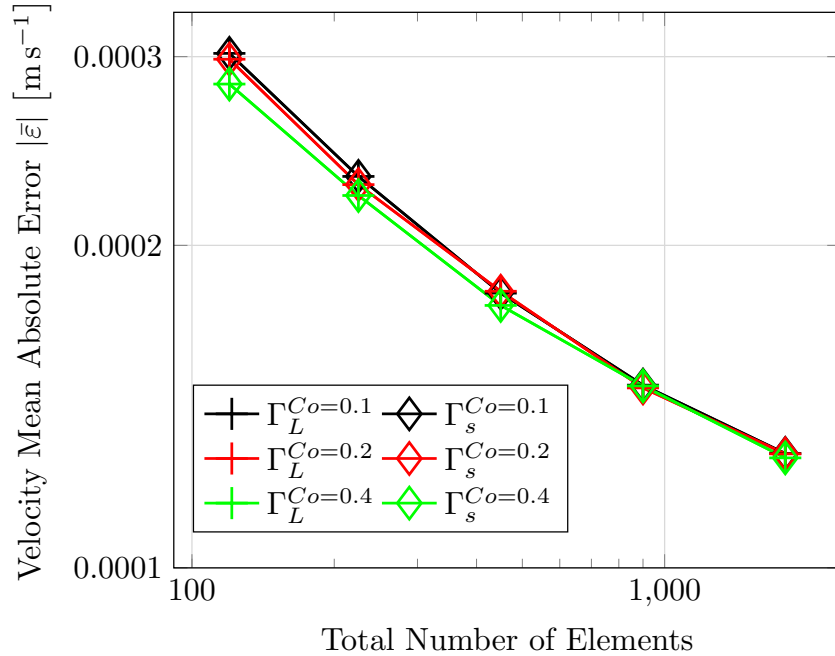


Figure A.1: Mean Absolute Error for the Square Wave Benchmark for $m = \pi$.

a simulation is stable, the log-log plot shows that error varies considerably with the mesh discretisation, but comparatively little with different values of Co . In

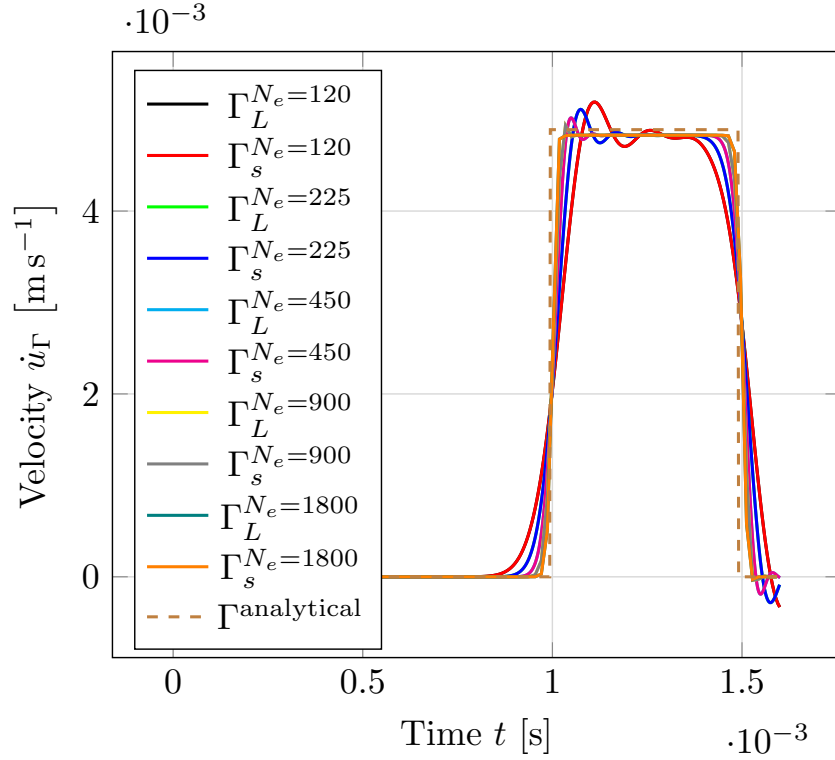


Figure A.2: Interface velocity $\dot{\mathbf{u}}_i$ values for all simulations, where $Co = 0.1$ varying Element count.

Figure A.2 analytical solution $\hat{\mathbf{u}}(t)$ is plotted with the interface velocities of the $Co = 0.1$ simulations, varying just the spatial discretisation. Due to the continuity of all three kinematic variables, difference in error on Γ_L and Γ_s is observed $< \times 10^{-12}$, for the same total number of elements. As expected, the solution improves with an increasing number of elements to represent the bar. The corresponding error $|\bar{\varepsilon}|$ decreases from 2.713×10^{-4} for 120 elements to 8.645×10^{-5} for 1800 total elements. With bulk viscosity, it can be observed that the analytical solution is accurately approximated. Granted this acceptable tolerance of error, and similar problems defined in literature [57], the problem definition is deemed convergent and appropriate for analysis of multi-time stepping methods.

A.2 A Highly Heterogeneous Benchmark

A benchmark that pushes a very high time step ratio $m = 100$ is demonstrated through varying material properties within the 1D bar in Section 3.3.2. The

two subdomains Ω_L and Ω_s are partitioned such that the elastic properties give $E_L = E_s = 0.02$ GPa and two densities $\rho_L = 8000 \text{ kgm}^{-3}$, $\rho_s = 0.8 \text{ kgm}^{-3}$. The spatial discretisation remains the same throughout the domain, where lengths $L_L = 50$ mm and $L_s = 100$ mm. Integrating with $Co_L = Co_s = 0.5$ results in time steps $\Delta t_L = 1.667 \times 10^{-6}$ s and $\Delta t_s = 1.667 \times 10^{-8}$ s. The ratio gives an $m = 100$. As stated throughout in Chapter 3, a potential limitation for the algorithm is its ability to solve severely heterogeneous domains, where instability may arise. For this, a depiction of one of the solutions is given through redefining the problem from Figure A.3 to Figure A.4. The temporal interface Γ is moved one element away from material interface, solving an extra element from Ω_L , with Δt_s . The same square wave function is applied as the $m = \pi$ benchmark with a velocity boundary condition from Ω_L . Through shifting Γ from the material interface, instability is

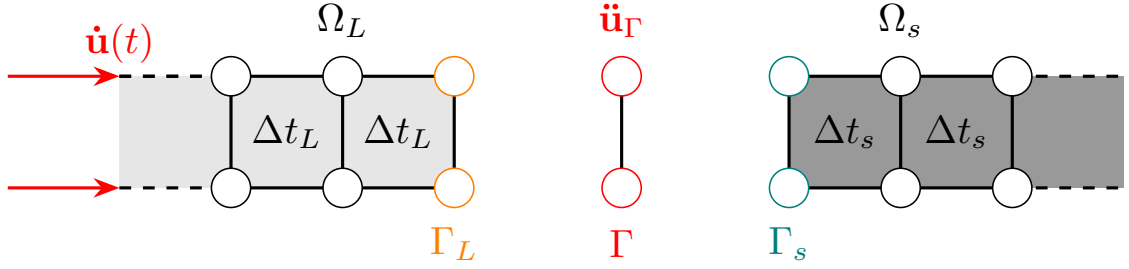


Figure A.3: Conventional definition of Γ as seen in $m = \pi$ benchmark.

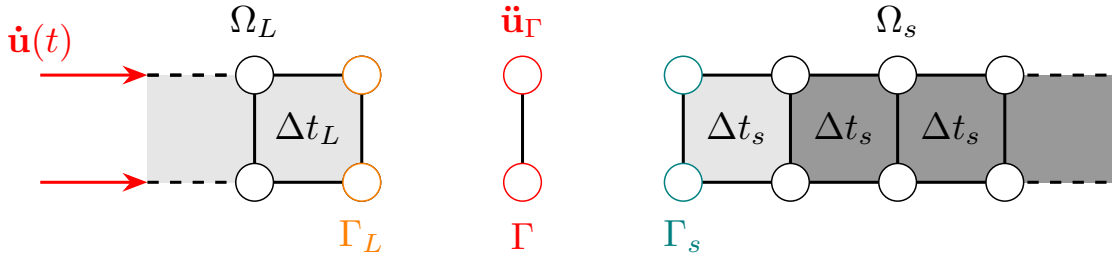


Figure A.4: Shifting Γ for Highly heterogeneous material interfaces allowing for high frequency behaviour to be resolved by Δt_s .

avoided and the square wave propagates smoothly through Ω_L . In Figure A.5 the square wave travels in the direction of the interface, with similar conclusions made at this time stamp to the original $m = \pi$ benchmark. In Figure A.6, a doubling in the transmitted wave is observed in Ω_s . Aligning with the analytical solution,

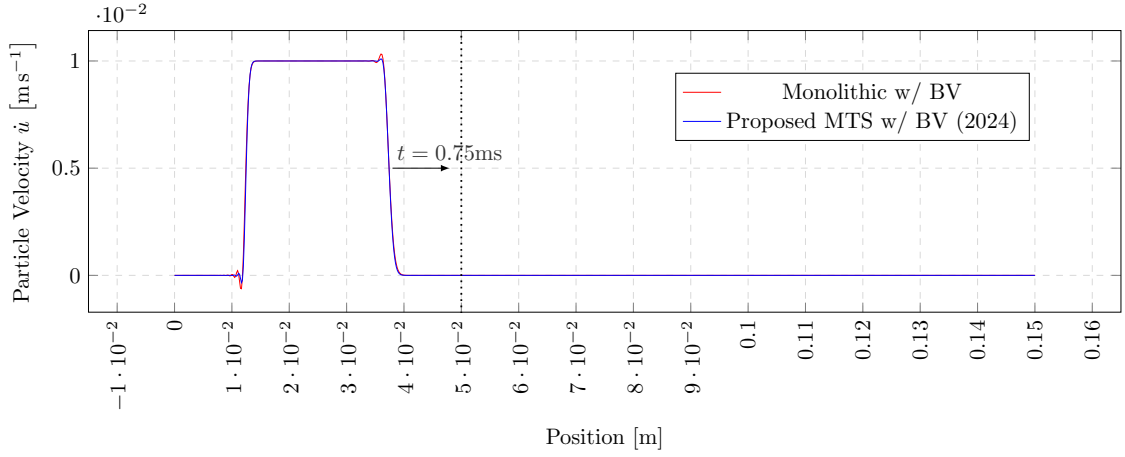


Figure A.5: Square wave propagation through a 1-D heterogeneous bar at $t = 0.75\text{ms}$ with Monolithic and the proposed method with bulk viscosity.

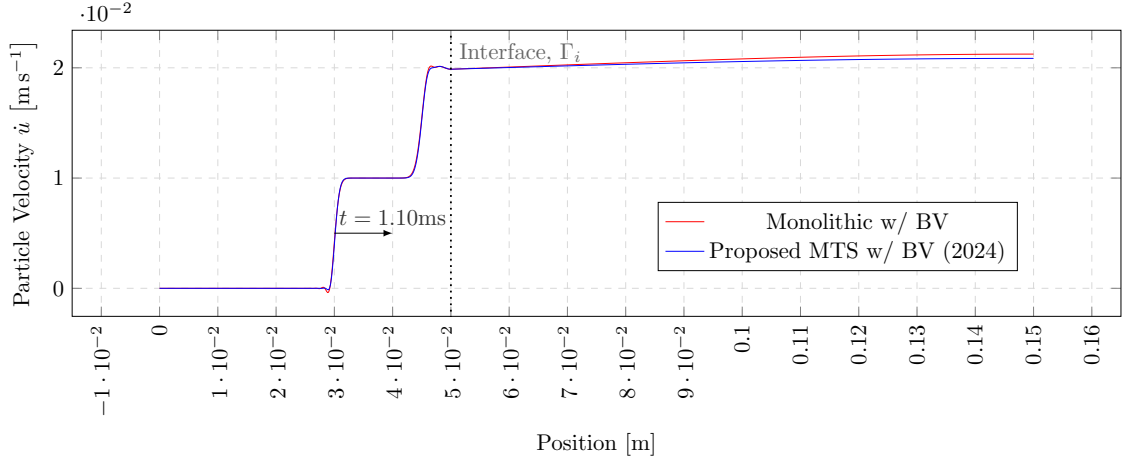


Figure A.6: Square wave propagation through a 1-D heterogeneous bar at $t = 1.10\text{ms}$ with Monolithic and the proposed method with bulk viscosity.

the multi-time stepping solution also matches the near 100% reflection of the wave back into Ω_L . This is evident in Figure A.7, where the reflected wave is of a very similar amplitude to the boundary condition that was initially applied. The highly heterogeneous configuration provides the explanation for this interaction at the interface, where the large difference in ρ_L and ρ_s gives the large impedance mismatch.

The two aforementioned remedies for solving severely high heterogeneous problems do increase the computational effort required to simulate. However it should be noted, that both still allow for less integration steps than use of a single time step, and fundamentally the proposed multi-time stepping algorithm does not require adaptation for such problems. Through adopting one of these methods, numerically

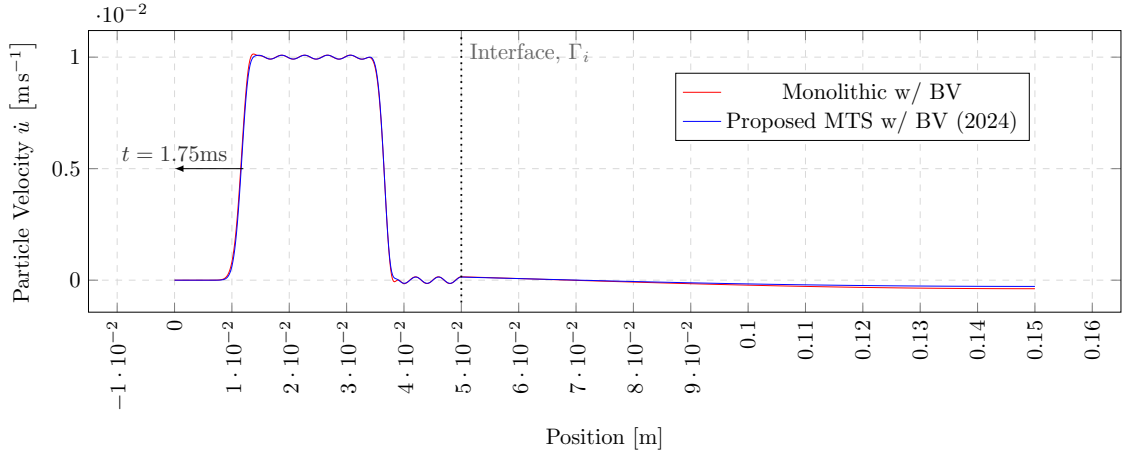


Figure A.7: Square wave propagation through a 1-D heterogeneous bar at $t = 1.77\text{ms}$ with Monolithic and the proposed method with bulk viscosity.

there is not a clear reason why time step ratios $m > 100$ could even be simulated with multi-time stepping. The benchmark can be tested from an open-source repository <https://github.com/kinfungchan/multi-time-step-integration>, containing the proposed method, as well as methods from literature [56, 57, 126].

B

Open Source FEM Framework

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Details of the framework that enabled the development of novel coupling methods are described. Clarity is provided, linking the equations required to solve a single subdomain with finite elements.

B.1 ex-fem: an open source Explicit FEM Code

In this section, a brief description of an explicit FEM (coined *ex-fem*) framework is provided. The code is written in python, following a similar modular structure to the in-house code DEST [178]. The aim of the code is to demonstrate the simplicity of coupling monolithic algorithms in an efficient, but user-friendly manner. A summary of the mathematical equations that correspond to each function is presented. Description of the coupling algorithms have preceded this appendix, hence the aim of this section is to illustrate the common operations in each subdomain. Figure B.1 depicts the tree representation of the modularity of ex-fem.

At the present time of writing, the open-source code is available with corresponding functions in 2-D, however 3-D implementations have been demonstrated

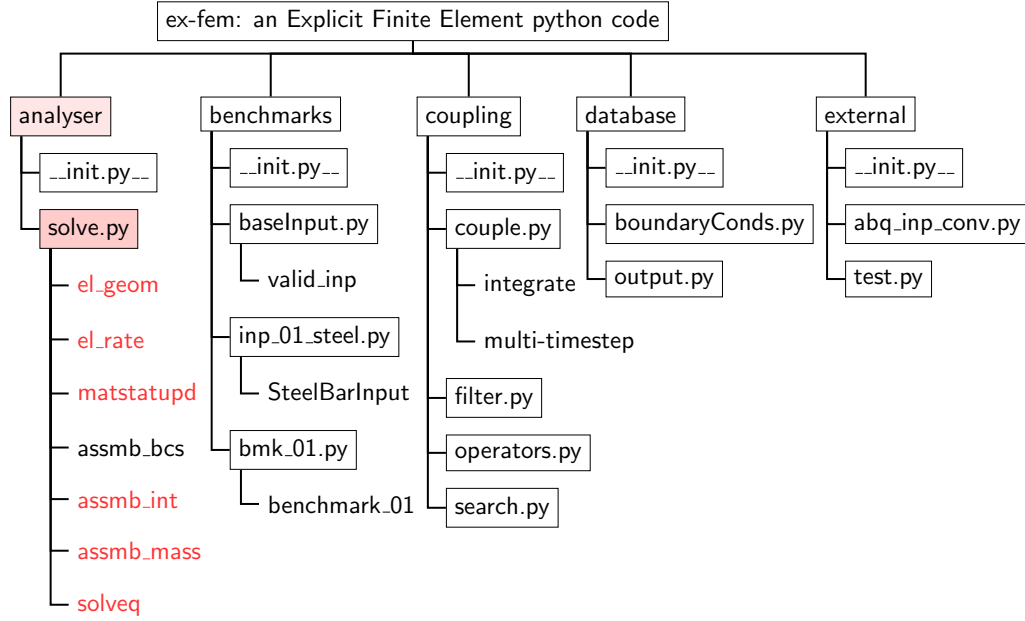


Figure B.1: Codebase structure for ex-fem, where each Ω_i calls upon its own respective analyser module for an updated Lagrangian formulation.

throughout in the aforementioned DEST. The python code is available in the following repository <https://github.com/kinfungchan/ex-fem-user> containing key ingredients for the explicit solver. For now, the prior is described for each element. The following description focuses on the `solve.py` file, containing the functionality for approximating kinetic and kinematic quantities with FEM. Each of the methods coloured red are explained in the following. It is the foundation for each Ω_i , irrespective of coupling method. The shape functions $\mathbf{N}$ are stored for each Gauss point at local coordinates (ξ, η) :

$$N_1(\xi, \eta) = \frac{1}{4}(1 - \xi)(1 - \eta) \quad (\text{B.1})$$

$$N_2(\xi, \eta) = \frac{1}{4}(1 + \xi)(1 - \eta) \quad (\text{B.2})$$

$$N_3(\xi, \eta) = \frac{1}{4}(1 + \xi)(1 + \eta) \quad (\text{B.3})$$

$$N_4(\xi, \eta) = \frac{1}{4}(1 - \xi)(1 + \eta) \quad (\text{B.4})$$

where derivative with respect to these local coordinates:

$$\frac{\partial N_1}{\partial \xi} = -\frac{1}{4}(1 - \eta); \quad \frac{\partial N_1}{\partial \eta} = -\frac{1}{4}(1 - \xi) \quad (\text{B.5})$$

$$\frac{\partial N_2}{\partial \xi} = \frac{1}{4}(1 - \eta); \quad \frac{\partial N_2}{\partial \eta} = -\frac{1}{4}(1 + \xi) \quad (\text{B.6})$$

$$\frac{\partial N_3}{\partial \xi} = \frac{1}{4}(1 + \eta); \quad \frac{\partial N_3}{\partial \eta} = \frac{1}{4}(1 + \xi) \quad (\text{B.7})$$

$$\frac{\partial N_4}{\partial \xi} = -\frac{1}{4}(1 + \eta); \quad \frac{\partial N_4}{\partial \eta} = \frac{1}{4}(1 - \xi) \quad (\text{B.8})$$

The `el_geom` method utilises Equations B.5 - B.1 to compute the Jacobian $\mathbf{J}$ for the transformation of the finite elements to global coordinates (x, y) :

$$\mathbf{J} = \begin{bmatrix} \frac{\partial N_1}{\partial \xi} & \frac{\partial N_2}{\partial \xi} & \dots & \frac{\partial N_4}{\partial \xi} \\ \frac{\partial N_1}{\partial \eta} & \frac{\partial N_2}{\partial \eta} & \dots & \frac{\partial N_4}{\partial \eta} \end{bmatrix} \begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ \vdots & \vdots \\ x_4 & y_4 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^4 \frac{\partial N_i}{\partial \xi} x_i & \sum_{i=1}^4 \frac{\partial N_i}{\partial \xi} y_i \\ \sum_{i=1}^4 \frac{\partial N_i}{\partial \eta} x_i & \sum_{i=1}^4 \frac{\partial N_i}{\partial \eta} y_i \end{bmatrix} \quad (\text{B.9})$$

with its determinant:

$$\det \mathbf{J} = |\mathbf{J}| = \frac{\partial x}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{\partial y}{\partial \xi} \frac{\partial x}{\partial \eta} \quad (\text{B.10})$$

Subsequently, $|\mathbf{J}|$ allows for the transformation of integrals over the element, to give the shape function derivatives with respect to global coordinates:

$$\begin{bmatrix} \frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial x} & \frac{\partial N_3}{\partial x} & \frac{\partial N_4}{\partial x} \\ \frac{\partial N_1}{\partial y} & \frac{\partial N_2}{\partial y} & \frac{\partial N_3}{\partial y} & \frac{\partial N_4}{\partial y} \end{bmatrix} = \mathbf{J}^{-1} \begin{bmatrix} \frac{\partial N_1}{\partial \xi} & \frac{\partial N_2}{\partial \xi} & \frac{\partial N_3}{\partial \xi} & \frac{\partial N_4}{\partial \xi} \\ \frac{\partial N_1}{\partial \eta} & \frac{\partial N_2}{\partial \eta} & \frac{\partial N_3}{\partial \eta} & \frac{\partial N_4}{\partial \eta} \end{bmatrix} \quad (\text{B.11})$$

Computations of Equations B.9 - B.11 are key in assessing the validity of elements, to ensure the avoidance of inverted or collapsed elements. The `el_rate` proceeds with computations associated to the motion and deformation of the material, in which the velocity gradient tensor $\nabla \mathbf{v}$ field is defined as:

$$\nabla \mathbf{v} = \frac{\partial \mathbf{v}}{\partial \mathbf{x}} \quad (\text{B.12})$$

followed by the rate of deformation $\mathbf{D}$ (or strain rate):

$$\mathbf{D} = \frac{1}{2} (\nabla \mathbf{v} + \nabla \mathbf{v}^T) \quad (\text{B.13})$$

and the antisymmetric part of the velocity gradient tensor, referred to as the spin $\mathbf{W}$ tensor:

$$\mathbf{W} = \frac{1}{2} (\nabla \mathbf{v} - \nabla \mathbf{v}^T) \quad (\text{B.14})$$

The rate terms are utilised in `matstatupd`, containing the constitutive model relating strain and stress. The simplest model of isotropic elasticity is implemented, where stress rate $\dot{\boldsymbol{\sigma}}$ is computed with:

$$\dot{\boldsymbol{\sigma}} = \mathbf{W}\boldsymbol{\sigma} - \boldsymbol{\sigma}\mathbf{W} + 2GD + \lambda\text{Tr}(\mathbf{D})\mathbf{I} \quad (\text{B.15})$$

with $\boldsymbol{\sigma}$ representing Cauchy stress, $G = \frac{E}{2(1+\nu)}$ as the shear modulus, $\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}$ as the first Lamé parameter and $\mathbf{I}$ an identity tensor. Following the computation of stresses, the assembly of the internal forces can be computed in `assmb_int` with:

$$\mathbf{f}_i^{\text{int}} = \begin{bmatrix} f_{xi}^{\text{int}} \\ f_{yi}^{\text{int}} \end{bmatrix} = \int_{\Omega_e} \mathbf{B}^T \boldsymbol{\sigma} dA = \int_{-1}^1 \int_{-1}^1 \mathbf{B}^T \{\boldsymbol{\sigma}\} |\mathbf{J}| d\xi d\eta \quad (\text{B.16})$$

where the strain-displacement matrix $\mathbf{B}$ contains the previously computed shape function derivatives, and dA for the difference in area. Gaussian quadrature then allows for the integral to be approximated by:

$$\mathbf{f}_i^{\text{int}} = \sum_{Q_1=1}^{\mathcal{N}_{Q_1}} \sum_{Q_2=1}^{\mathcal{N}_{Q_2}} w_{Q_1} w_{Q_2} \mathbf{B}^T(\xi_{Q_1}, \eta_{Q_2}) \{\boldsymbol{\sigma}(\xi_{Q_1}, \eta_{Q_2})\} J_\xi(\xi_{Q_1}, \eta_{Q_2}) \quad (\text{B.17})$$

where $\mathcal{N}_{Q_i}$ denotes the number of quadrature points, w_{Q_i} the weights, with corresponding coordinates ξ_{Q_i} . The mass can be computed with use of $\mathbf{N}$ in similar fashion, however for the implementation in `assmb_mass`, an efficient approach is simply the equal dissemination to each of the four nodes:

$$\mathbf{M}_i = \frac{1}{4} \rho z_0 A_0 \quad (\text{B.18})$$

where for each node, an approximation with the initial thickness as z_0 and A_0 at $t = 0$ is made. For the sake of completion, the solution of the equation of motion is reiterated, with integration in leapfrog fashion given by the following:

$$\ddot{\mathbf{u}}_i^n = \frac{(\mathbf{f}_i^{\text{ext}} - \mathbf{f}_i^{\text{int}})}{\mathbf{M}_i} \quad (\text{B.19})$$

where the velocity at $n + 1/2$ is computed as:

$$\dot{\mathbf{u}}_i^{n+1/2} = \dot{\mathbf{u}}_i^{n-1/2} + \ddot{\mathbf{u}}_i^n \cdot \Delta t^n \quad (\text{B.20})$$

and the displacement at $n + 1$ as:

$$\mathbf{u}_i^{n+1} = \mathbf{u}_i^n + \dot{\mathbf{u}}_i^{n+1/2} \cdot \Delta t^{n+1/2} \quad (\text{B.21})$$

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