Sahir Nawaz Butt

Computational Fracture and Fragmentation Modeling using Peridynamics: Application to Mechanized Excavation in Hard Rock

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by

M.Sc. Sahir Nawaz Butt

Dissertation

for the degree

Doctor of Engineering (Dr.-Ing.)

Department of Civil and Environmental Engineering
Ruhr University Bochum, Germany

Bochum, April 2023
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Abstract

The understanding and reliable prognosis of material failure is crucial in many engineering applications. In addition to the assessment of the ultimate load of structures and the safety margin in structural design, there are cases where material failure is the primary engineering goal, such as boring and excavation processes, where the material has to be loosened and cut from the ground as efficiently as possible. One important field of application is mechanized tunneling in hard rock environments, characterized by the continuous rock excavation by means of cutting discs mounted on the cutterhead of a tunnel boring machine. Simulating the rock excavation process is challenging, as it constitutes a highly dynamic process that involves complex fragmentation and local crushing of the rock. To address these challenges, a recently developed nonlocal continuum theory suitable for modeling complex fragmentation processes has been carefully analyzed, extended, and applied to computational simulations of ground excavation to assess the influence of ground conditions, disc spacing and other parameters on the excavation efficiency of cutting discs.

The peridynamic theory has been extensively analyzed with a focus on the peridynamic horizon, which is the length scale involved in its formulation. The in-depth analyses provided valuable insights into the role of model parameters on wave dispersion properties. In particular, it was possible for the first time to establish a physical interpretation of the peridynamic horizon, a parameter that has often been debated extensively and controversially in the scientific community. Additionally, the analyses investigating dynamic fracture revealed important insights into the impact of this length scale on the crack propagation velocity and provided computational evidence of the influence of specimen geometry and size on the dynamic fracture process. An extensive analysis of the ability of the model for simulating failure under compressive loads, as is the case for mechanized rock excavation, revealed the severe limitations of existing peridynamic models. Therefore, the model has been extended by considering pore-collapse to simulate crushing under high triaxial compressive loading in porous materials and validated using indentation tests on sandstone specimens. Furthermore, for simulating compressive failure in low-porosity heterogeneous materials such as concrete or granite, another enrichment of the model has been formulated and implemented by considering a pressure-dependent fracture energy, which performed excellently in reproducing the biaxial failure strength envelope of concrete.

Following these investigations and extensions, the peridynamic model has been applied to simulate mechanized rock excavation using cutting discs. The model performance has been validated by means of comparisons with results from the Linear cutting test and predictions from an empirical model. One of the goals of the developed peridynamic model is the prognosis of the forces acting
on the cutting discs. This information has been exploited by coupling the peridynamic model with a wear model to predict also the abrasive wear of the cutting discs. This model has been successfully verified using theoretical predictions. With the confidence in peridynamic modeling capabilities derived from all these validated extensions, the model was successfully applied to simulate a number of excavation scenarios, including mixed-ground conditions and excavation using blunted cutting discs, as well as discs with varying levels of localized damage. The analysis showed that excavation in mixed-ground conditions involved repeated impact loads on the discs, causing uneven wear. Due to cutting disc blunting, the decrease in excavated rock mass was quantified, leading to an inefficient excavation process. The developed model provides a virtual laboratory where various geological and cutterhead configurations can be investigated to characterize and optimize the excavation process.
Acknowledgments

This thesis reports the main findings of my research on modeling material failure. Working on failure for an entire dissertation was an enlightening experience. It’s not every day that one gets to focus exclusively on something that most people try to avoid. As noted by Marder and Fineberg (1996), “There is also the embarrassment of explaining to colleagues that one is working on failure”. I would like to express my sincere gratitude to the people who have helped me through this journey.

First and foremost, I would like to express my gratitude to Prof. Günther Meschke, my supervisor and principal referee, for the opportunity to work on this topic and for his invaluable support, care, and guidance throughout the process. Our discussions and “therapy sessions” have taught me a great deal about scientific research and life in general. I am also grateful to Prof. Jörg Renner, my co-supervisor. Our conversations significantly deepened my understanding of rocks, and his input in the model development presented in Chapter 5 was indispensable. My appreciation is also extended to my external supervisor, Prof. Jamal Rostami from the Colorado School of Mines, for his guidance in understanding rock excavation aspects, providing opportunities for rock cutting experiments, and his input in troubleshooting the excavation simulations presented in Chapter 6.

I would like to thank Dr. Stewart Silling and Dr. David Littlewood for their input regarding the theoretical and software implementation aspects of peridynamics. I am grateful to Dr. Pablo Seleson and Dr. Jithender Timothy for their input in wave dispersion analysis presented in Chapter 3. I also extend my gratitude to Prof. Jay Fineberg for his contribution in interpreting the simulation results presented in Chapter 4. I would also like to acknowledge my colleagues and friends who helped me revise and improve the quality of this thesis and gave me the necessary push to the finish line. In particular, I would like to thank Dr. Tagir Iskhakov, M.Sc. Vladislav Gudžulić, Dr. Abdullah Alsahly, and Dr. Ahmed Marwan.

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Bochum, April 2023

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<tbody>
<tr>
<td>TBM</td>
<td>Tunnel Boring Machine</td>
</tr>
<tr>
<td>LEFM</td>
<td>Linear Elastic Fracture Mechanics</td>
</tr>
<tr>
<td>FEM</td>
<td>Finite Element Method</td>
</tr>
<tr>
<td>XFEM</td>
<td>eXtended Finite Element Method</td>
</tr>
<tr>
<td>EFG</td>
<td>Element Free Galerkin</td>
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<tr>
<td>CZM</td>
<td>Cohesive Zone Model</td>
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<tr>
<td>SPH</td>
<td>Smoothed Particle Hydrodynamics</td>
</tr>
<tr>
<td>RK</td>
<td>Reproducing Kernel</td>
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<tr>
<td>RKPM</td>
<td>Reproducing Kernel Particle Method</td>
</tr>
<tr>
<td>LPS</td>
<td>Linear Peridynamic Solid</td>
</tr>
<tr>
<td>PMB</td>
<td>Prototype Microelastic Brittle</td>
</tr>
<tr>
<td>RMSD</td>
<td>Root Mean Square Deviation</td>
</tr>
<tr>
<td>AE</td>
<td>Acoustic Emission</td>
</tr>
<tr>
<td>BTS</td>
<td>Brazilian Tensile Strength</td>
</tr>
<tr>
<td>UTS</td>
<td>Ultimate Tensile Strength</td>
</tr>
<tr>
<td>UCS</td>
<td>Ultimate Compressive Strength</td>
</tr>
<tr>
<td>LCM</td>
<td>Linear Cutting Machine</td>
</tr>
<tr>
<td>CSM</td>
<td>Colorado School of Mines</td>
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1.1 Background and Motivation

Despite the tremendous advances in solid-state physics and mathematics in the last century, mathematical modeling of evolving fractures remains challenging. Modeling discontinuities with mathematical consistency is difficult, and considering all the understood multi-scale mechanisms makes it even harder. Comprehending the mechanisms behind material failure is crucial for a variety of material science and engineering applications. By gaining a deep understanding of the factors involved, more precise models can be developed, which enable better prediction and prevention of failures. Furthermore, this knowledge is also valuable in developing efficient techniques for the cases where material failure and removal is the primary goal, as seen in mining and tunneling applications.

1.1.1 Mechanized tunnel construction

The construction of underground infrastructure has made steady progress over recent decades. Mechanized tunnel construction using a Tunnel Boring Machine (TBM) has become one of the dominant excavation methods, it has revolutionized the construction industry by allowing for the efficient and safe excavation of tunnels on a large scale. The breakthrough in the development of today’s TBM technology occurred in the mid 1950s, with the development of first hard rock TBM equipped with cutting discs (Figure 1.1, right) by Robbins (MAIDL ET AL. 2008, ROSTAMI 2008). Since then, the mechanized excavation using TBMs has become an industry standard in modern tunneling projects, due to their high advance rates, reduced environmental impact, and improved safety.

The use of TBMs has enabled the construction of long underground structures even at shallow depths where the ground has poor load bearing capacity or under the groundwater table, without causing disruption to the existing infrastructure on the ground surface. A rotating cutterhead (Figure 1.1, left) at the front of a TBM is used to excavate the tunnel face. TBMs work by using a rotating cutterhead (Figure 1.1, left) at the front of the machine to excavate the tunnel face. The cutterhead can be equipped with a range of cutting tools, which are designed to break up and remove the rock or soil at the tunnel face. The excavated material is then transported away from the tunnel face by
a conveyor belt system or other means of transport. The TBM cutting head is mounted on a series of thrust cylinders that provide the force necessary to push the machine forward. As the machine advances, the tunnel wall is supported by a variety of means, such as steel reinforcement, shotcrete, or pre-cast concrete segments (MAIDL ET AL. 2013).

Cutting tools constitute the interface between the TBM and the ground being excavated. These tools have been developed to handle a wide range of geological conditions and ground materials ranging from soft soils to hard rock. The main types of tools mounted on a cutterhead of a TBM are cutting discs, scrapers tools, and gauge cutters (MAIDL ET AL. 2013). Scrapers and gauge cutters are used in the excavation of soft ground, while cutting discs are used for fracturing hard rock. The material removal process using cutting discs is achieved by point-load or indentation failure of the rock. Indentation induced fracture is an example of dynamic fracturing (LAWN AND WILSHAW 1975). Indentation applies a force to a rock surface, causing high stresses and resulting in the formation of a crushed zone and microcracks. As the load increases, these microcracks propagate and coalesce, leading to the fragmentation of the rock (ROSTAMI 2013, YANG ET AL. 2022). The mechanics of indentation induced fracture and fragmentation are complex and depend on various factors, including the mechanical properties of the rock, the geometry of the indenting body, and the loading conditions (JEONG ET AL. 2016). Understanding the mechanics of fragmentation by indentation is important for the development of more efficient rock-breaking tools and techniques, which can improve the performance of a TBM.

Performance of a TBM, which is crucial for tunneling projects (ROSTAMI 2008), is affected by various factors, including the geological properties of the ground, the machine design, the cutting tools used, and the environmental conditions. One of the primary performance parameters for TBM is the advance rate (JING ET AL. 2021), which is the rate at which the machine progresses through the ground. Another important performance parameter is the excavation volume, which is the amount of rock or soil excavated per unit time. Other critical performance parameters include the energy
consumption of the TBM and the wear and life of cutting tools which influences the machine’s
downtime due to maintenance or repairs.

The cutting disc’s wear and life are critical factors in the TBM performance and productivity.
The cutting discs’ life is determined by several factors, including the disc’s material and design,
the abrasive nature of the rock, the cutting speed, and the machine’s operational parameters. Proper
maintenance and replacement of cutting discs are essential to ensure the TBM’s optimal performance
and avoid costly downtime. Therefore, a strong interest exists in a reliable wear prediction for
the cutting tools working in a particular ground (Hassanpour et al. 2014, Verhoef 2017).

Performance prediction models are essential tools for optimizing the TBM’s performance and
minimizing downtime during tunneling projects. Empirical performance prediction methods (Bruland
1975) typically involve analyzing historical data from previous tunneling projects and experiments to
develop statistical models that can predict the TBM’s performance under similar conditions. These models allow engineers to optimize the TBM’s design and operation to achieve the desired excavation rate and minimize downtime. However, empirical models have their limitations in gaining a deeper understanding of complex processes, such as the cutting disc and rock interaction, which involve several factors such as the strength, hardness and abrasiveness of the rock, the cutting disc design, the cutting speed, and the machine’s operational parameters. Empirical models are limited by the available data and can have problems predicting the performance in certain situations, for example, mixed ground conditions (Zhao et al. 2007, 2019), where the ground being excavated can have two or more layers of rock or soil, having significantly different mechanical properties (Toth et al. 2013). Mechanized tunneling in such conditions results in highly variable loads on the cutting discs (Moulin and Vallon 2009). These varying loads can cause abnormal cutter wear which can lead to unexpected TBM stoppage. Computational models (Butt and Meschke 2017a, Cho et al. 2010, Choi and Lee 2015, Labra et al. 2017, Moon and Oh 2012, Xu et al. 2022) provide a powerful alternative in such cases (Butt et al. 2019, 2022, Butt and Meschke 2021a), which allows incorporating new scenarios and equips researchers with a virtual laboratory where several simulations can be performed while varying different process parameters.

Computational modeling has also proved to be a powerful tool for studying, understanding, and
predicting the mechanics of fracturing and material failure involved in mechanized tunneling (Alsahly et al. 2017, Cai et al. 2007, Hoek and Martin 2014, Jing 2003, Liu et al. 2007, Stead et al. 2006), which enables a safe and efficient excavation processes. Simulation tools can help predict the behavior of the rock mass surrounding the excavation zone, preventing disasters such as spalling, deep cracking, massive roof collapse, large deformations, and rockbursts (Feng et al. 2022). Additionally, a deeper understanding of how materials fracture helps design novel excava-
tion techniques and tools, as the efficiency of an excavation process relies on effectively breaking and chipping the rock (Innaurato et al., 2007). Rock is a complex material that is inherently discontinuous, anisotropic, inhomogeneous, and inelastic, exhibiting a wide range of mechanical behaviors, including brittle, quasibrittle, and ductile fracture, as well as crushing and pore-collapse, which can cause permanent deformations (Jing 2003). Fracturing and material failure can occur at various scales, from the microscopic level of individual rock grains to the macroscopic level of entire rock masses. The specific behavior exhibited by rock depends on factors such as its type and the loading conditions it experiences. The next subsection provides a brief introduction to the material failure and fracturing process.

1.1.2 Physics of material failure

A fracture is a discontinuity in a material that initiates from the atomic scale, interacts with the microstructure, extends to the macroscopic level, is irreversible, and can activate several other modes of energy dissipation in a material. The tip of a propagating ideal crack is an intriguing and thought-provoking location, a region with infinite stresses. Under loading this discontinuity extends by converting the available elastic energy into the fracture surface energy (Knott 1973, Thomson 1986). The dynamics of a growing crack tip are governed by several key properties, including the size of the plastic zone around the tip, strain rate, crack tip velocity, crack tip geometry, and the stress intensity factor. The size of the plastic zone around a crack tip, or more generally known as the process zone, which represents the region of the material that is deformed permanently, has divided fracture models into three main categories: brittle, quasibrittle, and ductile fracture (Bažant and Planas 1998). Brittle fracture implies a very small process zone around the crack tip, and the material fails with very little inelastic deformation. In contrast, quasibrittle fracture occurs in materials that develop a process zone in front of the propagating crack tip. In this zone, several mechanisms, such as distributed micro-cracking, can get activated, exhibiting some level of ductility. Ductile fracture occurs when a material undergoes significant plastic deformations before ultimate failure. The type of fracture occurring in a body depends on the mechanical properties of the material, as well as the loading conditions that it is subjected to. Examples of materials failing with brittle, quasibrittle, and ductile fracture are glass, concrete, and aluminium, respectively.

When a crack grows in a material under rapid loading conditions, inertial forces become significant, affecting the speed at which the crack propagates. This phenomenon is referred to as dynamic crack propagation. The crack propagation speed is an essential factor to consider, as it determines the stress state and energy release rate around the crack tip, which can, in turn, affect the surrounding material (Freund 1998). For a crack propagating under tensile load (known as a mode-I crack), according to Linear Elastic Fracture Mechanics (LEFM), there exists a theoretical speed limit known as the Rayleigh wave speed ($v_r$) (Atkinson and Eshelby 1968, Broberg 1960, Yoffe 1951), which is the speed at which waves propagate along the surface of a material. Experimental investigations of dynamic crack propagation have been conducted in materials such as glass and plexiglass (Bowden et al. 1967, Fineberg et al. 1992, Ravi-Chandar and Knauss 1984b). These investigations have shown that cracks never reach the Rayleigh wave speed ($v_r$) due to the activation of dissipation mechanisms at the crack tip (Bouchbinder et al. 2014). One such mechanism is
microbranching instability, which gets activated at a crack speed of around $0.4v_r$. It involves the formation of small, unstable branches along the propagating crack that increase the crack surface roughness, leading to additional dissipation of energy (SHARON AND FINEBERG 1996). As the crack speed increases further (around $0.6v_r$), these unstable micro-branches grow into stable macro-branches that facilitate further energy dissipation. Therefore, the crack speed $v_r$ is never realized.

These discrepancies between theoretical predictions and experimental observations are due in part to incomplete understanding of all the dissipation mechanisms involved in dynamic fracture process (SHARON AND FINEBERG 1999, SHARON ET AL. 1996).

The strength of a material, which is defined as its resistance to failure, is a complex property influenced by various factors such as atomic and molecular bonding, microstructure, temperature, loading rate, specimen size, and the presence of defects and impurities. Materials are inherently heterogeneous and contain a distribution of flaws, voids, inclusions, and other defects (ASHBY AND CEBON 1993, BAZANT 1989). Under loading, these defects serve as nucleation sites for new fractures, resulting in the propagation of multiple fractures simultaneously within the material (BRIAN 1993). The interaction between these fractures depends on the loading configuration and rate, as well as the nature of the heterogeneity. Depending on the type of heterogeneity and loading conditions, various dissipation mechanisms can be activated in addition to crack propagation (GIBSON AND ASHBY 1997, GIBSON 2000). For example, a porous material like sandstone undergoes pore-collapse under compressive loads, which contributes to the total dissipated energy and can effectively delay the onset of failure (BAUD ET AL. 2004, KLEIN ET AL. 2001). In materials such as ceramics, the generation and propagation of microcracks can contribute to the total energy dissipation. These microcracks can interact with each other and cause crack deflection or branching, which increases the energy required before failure (ASHBY AND HALLAM 1986). These materials can also exhibit frictional sliding of the existing flaws under compressive loads, leading to increased dissipation (VAN VLIET AND VAN MIER 1996). In some materials, such as concrete, the energy dissipated in failure can also be influenced by the presence of reinforcing fibers, which can undergo large deformations before failure and provide additional energy dissipation mechanisms (ROSSI ET AL. 1996, VAN MIER 2017). Therefore, when a material is loaded, it undergoes several dissipation mechanisms in addition to the growing cracks. As the loading is increased, the most critical crack grows from this ensemble of cracks and eventually leads to material failure.

### 1.1.3 Computational modeling of material failure

Building and testing physical prototypes can be both expensive and time consuming. Numerical modeling provides a cost-effective way to explore design options and evaluate the performance of a product or system before it is built. Although empirical models facilitate cost-effective product development to some extent, they are limited in their ability to consider and explain complex physical phenomena. In contrast to empirical models, simulations also help us understand properties that can not be observed or measured experimentally, such as stresses or plastic strains at arbitrary points in a material body or the interaction of elastic waves with a propagating crack. Analytical solutions are available for simple cases; however, some engineering problems involve complex geometries and physical processes that do not have a closed form solution, such as fragmentation processes.
where high-speed multiple cracks branch and coalesce. In order to consider these complexities, the use of numerical simulations becomes inevitable. Moreover, numerical simulations can be used to optimize the design of a product or system by testing different configurations and parameters to find the most efficient and effective solution. This can save both time and resources in the development process.

Over the past few decades, various sophisticated continuum models have been proposed for simulating evolving fractures. These methods solve the partial differential equations of continuum mechanics using approximation functions and their derivatives, constructed either locally using a mesh or using scattered points without mesh connectivity. The first class of methods is known as mesh-based methods, such as the Finite Element Method (FEM) (BELYTSCHKO ET AL. 2014), while the second class is known as mesh-free methods (BELYTSCHKO ET AL. 1996), such as the Diffuse Element Method (NAYROLES ET AL. 1992) or the Element Free Galerkin (EFG) method (BELYTSCHKO ET AL. 1994). Discrete as well as smeared representations of cracks as strong and weak discontinuities are employed in these models to represent the discontinuity resulting from a crack.

A strong discontinuity is modeled using Cohesive zone models (BARENBLATT 1962, CAMACHO AND ORTIZ 1996, KHSAMITOV AND MESCHKE 2018, XU AND NEEDLEMAN 1994), which equip the interfaces of standard finite elements with a traction-separation law. While these models can simulate the autonomous initiation, propagation, and branching of a crack (XU AND NEEDLEMAN 1994), the crack path is highly dependent on the specific mesh topology (FALK ET AL. 2001, MOSLER AND MESCHKE 2004, ZHOU AND MOLINARI 2004), which can introduce bias. Addressing this issue using adaptive re-meshing techniques is challenging, especially in 3D. Another option is the eXtended FEM (XFEM) (BELYTSCHKO AND BLACK 1999, MESCHKE AND DUMSTORFF 2007, MOËS ET AL. 1999), which allows the crack to propagate through finite elements by incorporating enrichments with strong displacement discontinuity kinematics, thereby removing the mesh bias and enabling crack propagation in any direction. However, these methods require additional degrees of freedom and suitable crack indicators for crack tip advancement and tracking, resulting in additional complexity (ALSAHLY ET AL. 2017, RABCZUK ET AL. 2010, ZHUANG ET AL. 2011). Mesh-free methods provide an alternative solution by modeling arbitrary discrete cracks without remeshing (BELYTSCHKO ET AL. 1996, NGUYEN ET AL. 2008, SILLING AND ASKARI 2005).

A weak discontinuity is modeled using non-local averaging approaches (BAŽANT AND JIRÁSEK 2002) which regularize the surface energy of the discrete crack over a characteristic length in order to avoid mesh dependence (MOSLER AND MESCHKE 2004). These approaches enable autonomous crack initiation, growth and branching without the need to track the crack tip. To model complex fragmentation processes, it is necessary to represent crack propagation independently from the discretization with minimal or no external intervention, such as tracking of discontinuities or decisions on the direction of crack growth. Several models in this category include the crack band model (BAŽANT AND OH 1983), non-local damage model (PIAUDIER-CABOT AND BAŽANT 1987), gradient-enhanced damage models (PEERLINGS ET AL. 1998), eigen-erosion models (PANDOLFI AND ORTIZ 2012), and phase-field models (BOURDIN ET AL. 2008). Phase-field models for fracture (BORDEN ET AL. 2012, HOFACKER AND MIEHE 2013) regularize the discontinuity over a
characteristic length, defining the width of the failure zone. However, in these models, the representation of the discontinuity is not discrete, and the mechanisms governing the change of crack dynamics with respect to this internal length scale are not yet well understood.

1.1.4 Peridynamics

Peridynamics provides an alternative to the discussed models by combining the properties of a regularized damage approach and a discrete fracture approach in one model. The models discussed earlier rely on partial differential equations to describe a continuum body containing discontinuities. This brings us to the key issue; as a discontinuity is by definition "not differentiable", some mathematical gymnastics are required to reconcile these discontinuities with existing continuum differential formulations. Peridynamics (Silling 2000, Silling et al. 2007) offers a solution to this problem by reformulating the classical theory of solid mechanics. This reformulation removes the dependence on the spatial derivatives and unifies the mathematical representation of continuous and discontinuous field variables. Instead of using spatial derivatives, peridynamics employs spatial integrals to compute strain energy at a point, introducing a length scale in its formulation and making it a nonlocal theory. This length scale is known as the radius of the peridynamic horizon. It can be viewed as a consequence of the mathematical formulation; that is, there is no clear physical argument for the need of such a parameter. However, as analyzed in this dissertation, it does affect certain aspects of the physics of the problem, particularly when inertial forces are involved, such as wave propagation and dynamic crack propagation. For fracture modeling, peridynamics regularizes the dissipated energy over the horizon, similar to classical continuum methods using non-local regularization. Unlike other non-local continuum models for fracture, however, peridynamics introduces damage at the level of connections (or bonds) between material points. This bond breakage results in the evolution of a discrete fracture surface autonomously, so multiple discrete cracks can initiate, propagate and interact with each other.

Fracture modeling using peridynamics has been of particular interest among the research community. In last few years, it has been applied to analyze crack initiation and propagation and severe fragmentation in a variety of materials, including glass (Ha and Bobaru 2010, 2011), plexiglas (Butt and Meschke 2018, 2021b, Mehrmashadi et al. 2019), fiber-reinforced composites (Hu et al. 2012, Zhou et al. 2017), laminated composites (Ma et al. 2022, Wu et al. 2020), concrete (Gerstle et al. 2007, Yang et al. 2018), additively manufactured metals (Behzadinasab 2019, Behzadinasab and Foster 2019), polycrystalline materials (De MEO et al. 2016, Gu et al. 2019), ice (Lu et al. 2020, Wang et al. 2018), and rocks (Butt and Meschke 2017a, 2021a, Ha et al. 2015, Rabczuk and Ren 2017). Fracturing initiated from various physical processes has also been analyzed, including ballistic and impact loads (Silling and Askari 2004, Xu et al. 2008), explosive loads (Diyaroglu et al. 2016, Fan et al. 2016, Wang et al. 2018, Zhu and Zhao 2021), shock waves induced fracturing (Ren et al. 2015, Silling et al. 2017), hydraulic fracturing (Nadimi et al. 2016, Ni et al. 2020), thermally induced fracture (Wang et al. 2018, Xu et al. 2018), fatigue loads (Nguyen et al. 2021, Zhang et al. 2016), and corrosion induced fracturing (Chen and Bobaru 2015, De MEO et al. 2016). For a review of the progress, current state, and validation of peridynamics models,
the interested reader is referred to Bobaru et al. (2016), Diehl et al. (2019), Javili et al. (2019), Madenci and Oterkus (2014).

1.2 Objectives and contributions

The overarching objective of this thesis was to develop a robust and accurate simulation framework to model the complex fracture and fragmentation processes involved in hard rock excavation. Peridynamic continuum theory was selected as the simulation tool for this work, which is a nonlocal continuum theory with an internal length scale, the peridynamic horizon. Understanding how this parameter influences wave and fracture propagation was crucial before applying it to specific engineering problems. With this understanding, the peridynamic model was applied to modeling of rock indentation, and fracture and fragmentation resulting from rock indentation and excavation. These simulations provide insights into the mechanisms that underlie rock failure, which is essential for designing more effective rock excavation methods.

1.2.1 Wave dispersion and propagation

While the influence of peridynamic horizon on wave propagation was qualitatively understood, a quantitative analysis, which required the derivation of the dispersion relations of ordinary state-based peridynamics was lacking. To address this, the presented work aimed to answer the following questions:

− How does the peridynamic horizon and influence function quantitatively affect wave propagation?
− Can the dispersion of elastic waves be reduced or controlled?
− Is there a physical interpretation of the peridynamic horizon in the context of wave propagation?
− Can the peridynamic horizon be calibrated to mimic the wave dispersion properties of a particular material?

To provide answers to these questions, this thesis made the following contributions:

∗ Wave dispersion relations are derived for the ordinary state-based peridynamics.
∗ A physics-based interpretation of the peridynamic horizon is provided in relation to the dispersion properties and influence functions are suggested to reduce the wave dispersion.
∗ A calibration procedure is introduced for modeling the dispersion properties of heterogeneous granular materials.

These contributions advanced the understanding of how peridynamics can be used to model wave propagation, with potential applications in a range of fields, including materials science and geophysics.

1.2.2 Tension dominated failure

Several researchers used peridynamics to model dynamic fracture, but a convergence study with respect to the peridynamic horizon is still lacking. Understanding how this parameter affects the
modelling results regarding dynamic fracture properties, such as micro- and macro-branching, crack propagation speed, and velocity toughening behavior, is important for fracture modeling. Key questions about fracture modeling with peridynamics include:

- What is the influence of the peridynamic horizon on the strength of a material and the energy consumption of a propagating crack?
- Is there a qualitative difference between peridynamic fracture modeling in 2D and 3D?
- Can peridynamics reproduce the size effect inherent in Linear Elastic Fracture Mechanics (LEFM)?
- Can peridynamics capture the loading rate-dependence of failure patterns?

This thesis contributes to the understanding of dynamic fracture modeling using peridynamics in the following ways:

* A convergence study is conducted on the peridynamic horizon in 2D and 3D, which investigated micro- and macro-branching, the evolution of elastic, kinetic, and dissipated energies, crack propagation paths, and velocity toughening relationships.
* The influence of specimen size on the velocity toughening relationship is investigated, and the LEFM size effect is reproduced.
* The transition of crack surface topology with respect to the crack speed is successfully modeled.
* The influence of loading rate on crack propagation path and branching is investigated in three benchmark problems.

These contributions shed light on the effect of the peridynamic horizon on fracture modeling and provide insight into important questions about the use of peridynamics for modeling dynamic fracture.

### 1.2.3 Compression dominated failure

Although peridynamics has been extensively used to model tensile failure in various materials, there is still a need for further investigation into modeling material failure under compression. This work applies peridynamics to model rock indentation in porous rock, such as sandstone, and biaxial failure of heterogeneous materials, such as concrete. The limitations of the standard peridynamic approach are highlighted, and the model is extended to accurately simulate these processes. Some of the key questions that need to be addressed include:

- How accurately can existing models simulate the compressive failure process?
- How can the heterogeneous nature of materials be modeled?
- How can the pore-collapse phenomenon observed in porous materials be modeled?
- Are existing models sufficient to model the biaxial failure of materials?
- How can the ratio of compressive to tensile strength be controlled?

This thesis addresses these questions and contributes to the peridynamic modeling of compressive failure in materials in the following ways:

* Existing peridynamic models are investigated, highlighting accuracy and stability issues.
* The heterogeneity of rock-like materials is modeled by considering randomly distributed strengths sampled from a distribution.
A model to consider the pore-collapse phenomenon in porous rocks is developed. The pore-collapse model is validated using the indentation experiments performed on a sandstone. A pressure-dependent failure criterion is developed to simulate the compressive failure of materials exhibiting significant differences in tensile and compressive strengths. The developed pressure-dependent failure criterion is demonstrated to model the compressive strength independently of the tensile strength and is validated using the biaxial strength of concrete.

This work addresses the limitations of standard peridynamic models in simulating compression-induced failure in heterogeneous materials. The developed models significantly advance peridynamic modeling of materials and processes where failure is triggered by compressive loads.

1.2.4 Rock excavation using cutting discs

One of the most important material parameters for rock excavation processes is the compressive strength. The model developed to simulate the compressive failure of materials is applied to simulate the rock excavation process using the cutting discs of a TBM. This application of peridynamics involves high-resolution simulations investigating parameters such as the tool penetration and spacing, excavation efficiency, and abrasive wear of the cutting discs. Some of the key research questions include:

- Can the developed model for compressive failure accurately simulate the rock excavation using cutting discs?
- How can abrasive wear on cutting discs be modeled?
- How can mixed ground conditions be modeled?
- How can the localized damage of cutting discs be identified using cutting force data?

This thesis addresses these questions by the following contributions:

- The model developed for compressive failure is applied to simulate the linear cutting test and validated based on experiments performed on granite and the Colorado School of Mines (CSM) model.
- An Archard-type wear model is incorporated into the peridynamic framework to model the abrasive wear of the cutting discs.
- Excavation in the mixed ground conditions are simulated by using a Drucker-Prager type plasticity model to model the soil domain.
- Varying geometries of the cutting discs, representing the blunting due to excavation, are used to investigate the excavation efficiency.
- Synthetic data is generated using linear cutting with locally damaged discs and is further used to rank the extent of damage to the cutting discs using vibrational analysis.

The results obtained from this research demonstrate the capabilities of peridynamics for modeling rock excavation processes, and provide several proof-of-concept models, including the wear model, the model for studying mixed ground conditions, and the model for identifying the extent of damage to cutting discs. These findings will be valuable for the future development of excavation process modeling using peridynamics.
1.3 Organization of the thesis

The dissertation comprises seven chapters:
Chapter 2 provides a review of the state of peridynamic theory, material modeling approaches, contact formulation, and discretization techniques.
Chapter 3 contains the derivation of dispersion relations for state-based peridynamics and analysis of wave dispersion and propagation for different influence functions. A calibration procedure for the peridynamic horizon is introduced and validated to model wave dispersion in granular materials. The content of this chapter has been published in BUTT ET AL. (2017) and BUTT AND MESCHKE (2017b).
Chapter 4 presents an investigation into the peridynamic simulations of tension-dominated failure. Dynamic fracture properties of peridynamics are analyzed by conducting 2D and 3D simulations of crack propagation in plexiglass plates. A convergence analysis of the peridynamic horizon is performed on the velocity toughening relationship of plexiglass and compared with experiments. Simulation results are analyzed to understand the impact of the peridynamic horizon, dimensionality, and specimen size. Additionally, the model is used to simulate loading rate-dependent fracture propagation in three benchmark experiments. Some contents of this chapter have been published in BUTT AND MESCHKE (2018, 2019, 2021b).
In Chapter 5 the limitations of the standard peridynamic approach for modeling compressive load-dominated failure are identified and the need for an extended model is highlighted. A model is developed to account for the pore-collapse phenomenon in porous rocks and validated using indentation experiments conducted on sandstone. Additionally, the standard peridynamic model is assessed for simulating the biaxial failure of concrete, revealing inadequacies that motivate the development of a pressure-dependent failure criterion to model compressive failure. The developed model is then validated using the biaxial strength envelope of concrete. Some contents of this chapter have been published in BUTT AND MESCHKE (2023).
Chapter 6 provides an investigation into the rock excavation process using the cutting discs of a TBM in both homogeneous and heterogeneous ground conditions. An abrasive wear model is incorporated into the model to simulate the wear on the cutting disc due to abrasion and the cutting efficiency of worn-out cutting discs is examined. Cutting force data for locally damaged discs is generated and analyzed to identify the level of damage to the disc. Some contents of this chapter have been published in BRACKMANN ET AL. (2023), BUTT ET AL. (2019, 2022), BUTT AND MESCHKE (2017a, 2021a), PRIEBE ET AL. (2021).
Chapter 7 concludes the dissertation with a summary of the results and offers suggestions for future work.
Chapter 2

Peridynamics: Theory and formulation

This chapter provides a background of the peridynamic theory and its evolution over past two decades. Peridynamic theory was put forward by Silling (2000) to provide a continuum model capable of incorporating spatial discontinuities in kinematic fields. Peridynamics holds some similarities to the mathematical framework of Eringen’s nonlocal elasticity theory (Eringen 2002), which introduces nonlocality in the constitutive relation by computing the stress at a material point \( x \) from the strain state not only at \( x \) but also considering a weighted average of the strains in the vicinity of \( x \). In contrast, the peridynamics model introduces nonlocality in the definition of peridynamic elastic energy density. The nonlocal weighted averaging at a point \( x \) is performed directly based on the difference of the displacements at \( x \) and all other material points within a finite distance called the horizon. Hence, it circumvents the classical definition of stresses and strains as spatial derivatives of the deformations and therefore allows one to deal also with spatially discontinuous displacement fields. This feature renders peridynamics an attractive computational method to model the physics of fractures.

2.1 Governing equations

Peridynamic theory reformulates the continuum governing equations in terms of integro-differential equations rather than partial differential equations of classical continuum mechanics (Love 1927), which suffer from singularities and discontinuities. Consider the conservation of linear momentum according to the classical theory at a material point \( x \) in the reference configuration at time \( t \):

\[
\rho \ddot{u}(x, t) = \nabla \cdot P(x, t) + b(x, t),
\]

where \( \rho \) is the density, \( u \) denotes the displacement field, \( P \) is the first Piola-Kirchhoff stress and \( b \) represents the body force density. The use of a dot on a variable refers to its time derivative. In contrast to the classical theory, peridynamic formulation of a continuum is characterized by the
direct interaction of a material point $x$ with a set of material points $x'$ in a volume defined by a cut-off radius $\delta$, known as the peridynamic horizon $\mathcal{H}_x$. This results in the following integro-differential equation for the balance of linear momentum:

$$\rho \ddot{u}(x, t) = \int_{\mathcal{H}_x} \left[ T[x, t](x' - x) - T[x', t](x - x') \right] dV_{x'} + b(x, t), \quad (2.2)$$

where $T[x, t]$ is the force state at $x$ and $T[x', t](x' - x)$ is the force, which a material point $x$ exerts on $x'$. Angular brackets are used to denote quantities that $T$ operates on.

The deformation state $Y[x, t]$ is defined as $Y[x, t](x' - x) = y' - y = (x' + u') - (x + u)$, where $y' - y$ and $u' - u$ are the deformed relative position vector and the relative displacement vector of the bond $x' - x$, respectively (Figure 2.1). Analogous to the deformation gradient of the classical continuum theory it provides information on the change of relative positions in the neighborhood of a point $x$. In the following, the relative position vector is denoted as $\xi = x' - x$ and the relative displacement vector is denoted as $\eta = u' - u$, which gives $Y[x, t](\xi) = (\xi + \eta)$.

**Figure 2.1:** Kinematics of a peridynamic body: undeformed (left) and deformed state (right).

**Balance laws**

Peridynamic equation of motion Eq. (2.2) along with the constitutive relation must satisfy the balance of linear momentum, angular momentum and energy. Here the focus is on the balance of linear and angular momentum, which requires the following conditions to hold (Silling et al. 2007):

- **Balance of linear momentum** is satisfied if the net forces on pair of particles due to each other obey Newton’s third law, i.e.,
  
  $$\left[ T[x, t](\xi) - T[x', t](-\xi) \right] = -\left[ T[x', t](\xi) - T[x, t](-\xi) \right]. \quad (2.3)$$

  It is shown in Madenci and Oterkus (2014) that for a given body, Eq. (2.3) is satisfied for arbitrary force state vectors $T[x, t](\xi)$ and $T[x', t](\xi)$.

- **Balance of angular momentum** is satisfied only if the following holds true:
  
  $$\int_{\mathcal{H}_x} Y[x, t](\xi) \times T[x, t](\xi) dV_{x'} = 0. \quad (2.4)$$

  It is evident that Eq. (2.4) is automatically satisfied if the force state vector $T[x, t](\xi)$ and the deformation state vector $Y[x, t](\xi)$ are collinear.
2.2 Constitutive modeling: Elasticity

Peridynamic material models, which govern the relationship between the deformation state $\mathbf{Y}$ and the force state $\mathbf{T}$, are divided into three main classes, namely bond-based peridynamics, ordinary state-based peridynamics and non-ordinary state-based peridynamics. This classification is based on the magnitude and direction of the force state vectors $\mathbf{T}[x, t]\langle\xi\rangle$ and $\mathbf{T}[x', t]\langle-\xi\rangle$ with respect to the deformation state vector $\mathbf{Y}[x, t]\langle\xi\rangle$. A brief introduction to these three modeling approaches is provided in the following.

![Figure 2.2: Bond-based peridynamics: Deformation of material points $x$ and $x'$ resulting in equal and opposite pair-wise force density vectors.](image)

2.2.1 Bond-based peridynamics

Bond-based peridynamics was the original version of peridynamics presented in SILLING (2000). It involves pair-wise interaction between the material points, i.e., the bond force density depends only on the deformation of the individual bond and is independent of the deformation of the neighboring points. This results in the force density vectors that are equal in magnitude as well as parallel to the deformed position vector as shown in Figure 2.2. Thus, resulting in following form of force density vectors:

$$
\mathbf{T}[x, t]\langle\xi\rangle = \frac{1}{2} f(\eta, \xi) \frac{\xi + \eta}{|\xi + \eta|}, \quad \mathbf{T}[x', t]\langle-\xi\rangle = -\frac{1}{2} f(\eta, \xi) \frac{\xi + \eta}{|\xi + \eta|},
$$

where $f(\eta, \xi)$ is a scalar force defined as, $f(\eta, \xi) = cs$. Here $c$ is a material parameter known as the micro-modulus and $s$ is the stretch which is analogous to the strain in the classical continuum, defined as:

$$
s = \frac{|\xi + \eta| - |\xi|}{|\xi|}.
$$

According to SILLING AND ASKARI (2005), $c$ can be determined by considering an infinite homogeneous body going through isotropic expansion, which leads to the following expression for three dimensional analysis:

$$
c = \frac{18}{\pi} \frac{K}{\delta^3},
$$

(2.7)
where $K$ is the bulk modulus and $\delta$ is the radius of the peridynamic horizon. It can be seen from Eq. (2.5) that the balance of angular momentum (Eq. 2.4) is automatically satisfied for this class of material models.

The resulting model is known as a Prototype Microelastic Brittle (PMB) model (Silling and Askari 2005), it has been shown to perform well for phenomena involving autonomous crack growth and branching (Ha and Bobaru 2010), however it suffers from following limitations (Silling et al. 2007):

- Particles interact only through a central potential, i.e., independent of other local conditions, which limits the material’s Poisson’s ratio to $\frac{1}{4}$ in three dimensions (and $\frac{1}{3}$ in two dimensions).
- Recasting a classical constitutive behavior (stress-strain based) in terms of peridynamic formulation can be cumbersome.
- Plastic incompressibility, which is needed in metal plasticity, cannot be achieved using bond-based peridynamics.

State-based peridynamics (Silling et al. 2007) was proposed to remedy the above shortcomings.

2.2.2 Ordinary state-based peridynamics

Ordinary state-based materials are characterized by the force density vectors which are different in magnitudes, but are parallel to the deformed position vector, as shown in Figure 2.3. Thus, these models also satisfy the balance of angular momentum (Eq. 2.4) automatically. The force state $T[x, t]$ for ordinary state-based peridynamics is characterized by a magnitude, i.e., a scalar state $t[x, t]$ and a direction, provided by the unit vector state $M[x, t]$:

$$T[x, t] \langle \xi \rangle = t[x, t] \langle \xi \rangle M[x, t] \langle \xi \rangle,$$

(2.8)
where $\mathbf{M}[\mathbf{x}, t]$ is a unit vector state, given by:

$$
\mathbf{M}[\mathbf{x}, t](\xi) = \frac{\mathbf{Y}[\mathbf{x}, t](\xi)}{|\mathbf{Y}[\mathbf{x}, t](\xi)|} = \frac{\mathbf{y}' - \mathbf{y}}{|\mathbf{y}' - \mathbf{y}|} = \frac{\mathbf{x} + \mathbf{e}}{|\mathbf{x} + \mathbf{e}|}.
$$

(2.9)

The force state $\mathcal{f}[\mathbf{x}, t]$ depends on a scalar stretch-like quantity, denoted as the extension state $\mathbf{e} [\mathbf{x}, t]$ which characterizes the kinematics of the model. Extension state $\mathbf{e}$ is defined as the difference of the length of the deformed and undeformed relative position vectors and can be further decomposed additively into an isotropic ($\mathbf{e}^i$) and a deviatoric ($\mathbf{e}^d$) extension state, it is given by:

$$
\mathbf{e}(\xi) = \mathbf{e}^i(\xi) + \mathbf{e}^d(\xi) = |\mathbf{Y}(\xi)| - |\mathbf{e}| = |\mathbf{x} + \mathbf{e}| - |\mathbf{e}|,
$$

(2.10)

where $\mathbf{x}' - \mathbf{x} = \mathbf{e}$. The isotropic extension state can be represented in terms of a scalar-valued volume dilatation $\theta(\mathbf{x}, t)$ that is defined to match the volumetric strain of a classical continuum model under isotropic loading conditions.

$$
\mathbf{e}^i(\xi) = \frac{\theta(\mathbf{x}, t) |\mathbf{e}|}{3},
$$

(2.11)

where $\theta(\mathbf{x}, t)$ is defined as:

$$
\theta(\mathbf{x}, t) = \frac{3}{m(\mathbf{x})} \int_{\mathcal{X}} \omega(\mathbf{e}|\xi|) |\mathbf{e}| \mathbf{e}(\xi) dV_{\mathbf{x}'.}
$$

(2.12)

The material parameters corresponding to $\mathbf{e}^i$ and $\mathbf{e}^d$ are determined by strain energy equivalence with the classical continuum model (Silling et al. 2007) and $\mathcal{f}[\mathbf{x}, t]$ is given by:

$$
\mathcal{f}[\mathbf{x}, t](\xi) = \frac{3K}{m(\mathbf{x})} \theta(\mathbf{x}, t) \omega(|\mathbf{e}|) |\mathbf{e}| + \frac{15\mu}{m(\mathbf{x})} \omega(|\mathbf{e}|) \mathbf{e}^d(\xi).
$$

(2.13)

Here $K$ and $\mu$ are the bulk and shear modulus, respectively. $\omega(|\mathbf{e}|)$ is the influence function, its effect is discussed in detail in Chapter 3. $m$ is the weighted volume, defined as:

$$
m(\mathbf{x}) = \int_{\mathcal{X}} \omega(|\mathbf{e}|) |\mathbf{e}|^2 dV_{\mathbf{x}'.}
$$

(2.14)

The resulting model is known as the Linear Peridynamic Solid (LPS) model.

### 2D plane-stress LPS model

For two dimensional LPS models, the formulation presented in Chapter 6 in Bobaru et al. (2016) is followed. 2D equation of motion is obtained by replacing the volume $dV_{\mathbf{x}'}$ in Eq. (2.2) by $t_{2D} dA_{\mathbf{x}'}$, where $t_{2D}$ is the plane-stress thickness and $dA_{\mathbf{x}'}$ is the area of the material point $\mathbf{x}'$. Dilatation for the plane-stress case is obtained by scaling $\theta(\mathbf{x}, t)$ from Eq. (2.12) by $\gamma$, where $\gamma = (4\mu)/(3K + 4\mu)$, and $K$ and $\mu$ are the bulk and shear modulus, respectively. The force state $\mathcal{f}_{2D}[\mathbf{x}, t]$ for two dimensional plane-stress problems is given by:

$$
\mathcal{f}_{2D}[\mathbf{x}, t](\xi) = \gamma \frac{K}{m(\mathbf{x})} \theta(\mathbf{x}, t) \omega(|\mathbf{e}|) |\mathbf{e}| + \frac{8\mu}{m(\mathbf{x})} \omega(|\mathbf{e}|) \mathbf{e}^d_{2D}(\xi),
$$

$$
\mathbf{e}^d_{2D}(\xi) = \mathbf{e}(\xi) - \gamma \frac{\theta(\mathbf{x}, t)|\mathbf{e}|}{3}.
$$

(2.15)
Linearized LPS model

Considering small displacements, the unit vector state $M(x, t)$ and the scalar extension state $e(x, t)$ can be linearized according to SII\(\text{LING}(2010)$, resulting in a linearized LPS model as:

$$M(x, t)\langle \xi \rangle = \frac{\xi}{|\xi|}, \quad e(x, t)\langle \xi \rangle = \frac{\xi \cdot (u(x + \xi) - u(x))}{|\xi|}. \quad (2.16)$$

In Eq.(2.16), the displacements are assumed to satisfy the following condition:

$$\sup_{x' \in \mathcal{H}_x} |u(x') - u(x)| << \delta. \quad (2.17)$$

This is analogous to the condition on the displacement field for allowing to adopt linearized strain measures in classical continuum, i.e., $|\nabla u| << 1$.

2.2.3 Non-ordinary state-based peridynamics

This class of peridynamic models provide the most general form of material models. Force density vectors for a pair of material points in non-ordinary state-based peridynamics can be different in magnitude as well as the direction, as shown in Figure 2.4. These models do not satisfy the balance of angular momentum by default and hence Eq. (2.4) has to be satisfied explicitly.

![Figure 2.4: Non-ordinary state-based peridynamics: Deformation of material points x and x' resulting in arbitrary force density vectors.](image)

Correspondence materials

A sub class of non-ordinary material models is the correspondence model, it was presented by SILLING ET AL. (2007) to enable the incorporation of local (classical) constitutive relations within the framework of nonlocal peridynamic theory. This is an important contribution, as the material modeling in classical continuum mechanics has much longer history and there are several well established constitutive relations which are still not available in the peridynamic theory.

A nonlocal deformation gradient was defined by SILLING ET AL. (2007) as:

$$F(x, t) = \left( \int_{\mathcal{H}_x} \omega(|\xi|) (\xi + \eta) \otimes \xi dV_{x'} \right) \cdot K^{-1}(x, t), \quad (2.18)$$
here \( K(x, t) \) is called the shape tensor. It is a second-order symmetric tensor given by:

\[
K(x, t) = \int_{\mathcal{M}_s} \omega(|\xi|) \, \xi \otimes \xi \, dV'.
\] (2.19)

Peridynamic deformation gradient (Eq. 2.18) corresponds to its local counterpart under homogeneous deformations. To approximate higher order derivatives, higher order terms from the Taylor series expansion of the deformation field can be incorporated (MADENCI ET AL. 2016). Peridynamic deformation gradient can then be used by any classical material model to compute the Piola-Kirchhoff stress \( P \) which is the work conjugate of the deformation gradient. \( P \) is further used to compute the peridynamic force state according to SILLING ET AL. (2007) as:

\[
T[x, t](\xi) = \omega(|\xi|) \, P(x, t) \, K^{-1}(x, t) \, \xi.
\] (2.20)

**Shear bond force peridynamics**

![Figure 2.5: Rigid body rotation \( \gamma \) of the total bond deformation \( \eta \) (left) and decomposition of shear and normal component of the effective bond deformation \( \eta_r \) (right).](image)

A new peridynamic formulation was introduced by REN ET AL. (2016) to incorporate shear deformations into the bond kinematics of a linear elastic solid. In order to define the shear part of the deformation, the rigid rotation \( \gamma \) must be removed from the deformation, as shown in Figure 2.5. To find the relationship between \( \xi \) and \( \xi_r \), a rotation matrix \( R \) for each particle has to be defined. As the rigid body rotation depends on the collective deformation of all particles in the neighborhood, it is necessary to compute the deformation gradient \( F \) using Eq. (2.18). Once the deformation gradient is computed, it can be decomposed using polar decomposition as follows:

\[
F(x, t) = R(x, t) \, P(x, t),
\] (2.21)

where \( R(x, t) \) is a unit rotation matrix and \( P(x, t) \) is a positive semi-definite Hermitian matrix. \( R \) and \( P \) can be computed using the singular value decomposition of \( F \) as follows:

\[
F = U \, \Sigma \, V^T, \quad P = V \, \Sigma \, V^T, \quad R = U \, V^T.
\] (2.22)

The bond \( \xi \) after rigid body rotation is given by:

\[
\xi_r = R \cdot \xi,
\] (2.23)
and the effective deformation $\eta_r$ can be computed as:

$$\eta_r = \xi + \eta - \xi_r.$$  \hspace{1cm} (2.24)

Furthermore, the deformation $\eta_r$ is additively decomposed into a normal $\eta_n$ and a shear $\eta_s$ part which are parallel and perpendicular to $\xi_r$ (Figure 2.5), respectively. Volumetric strain (dilatation) $\theta_r(x, t)$ is defined as:

$$\theta_r(x, t) = \frac{3}{m(x)} \int_{H(x)} \omega(|\xi|) \eta_r \cdot \xi_r \, dV_x,$$  \hspace{1cm} (2.25)

where $m(x)$ is the weighted volume as defined in Eq. (2.14). Isotropic and deviatoric part of the deformation can now be obtained as follows:

$$\eta^i = \frac{\theta}{3} \xi_r \quad , \quad \eta^d = \eta_r - \eta^i.$$  \hspace{1cm} (2.26)

The associated deviatoric bond strain $\varepsilon^d$ is defined as:

$$\varepsilon^d = \frac{\eta^d}{|\xi|}.$$  \hspace{1cm} (2.27)

According to REN ET AL. (2016), the force vector state can then be obtained by comparing the strain energy densities of classical continuum with the current peridynamic formulation as:

$$T[x, t](\xi) = \frac{3 \omega(|\xi|)}{m(x)} \left( K \theta_r(x, t) \xi_r + 2 \mu \eta^d \right).$$  \hspace{1cm} (2.28)

### Surface effects

Peridynamic material models are defined by strain energy equivalence with classical continuum models via the definition of a peridynamic neighborhood $H_x$. However, as material points located near a boundary do not have a complete non-local neighborhood, the effective material properties near the surface of a peridynamic model are computed to be slightly different from those in the bulk. This issue is known as surface or skin effect in peridynamics.

A number of methods have been recently proposed for correcting this peridynamic surface effect (see for e.g. MADENCI AND OTERKUS (2016), MITCHELL ET AL. (2015), TRASK ET AL. (2019)). These correction procedures specify different material properties for the affected points at the boundaries. This is usually achieved by comparing the differences in the internal force for simple loading conditions obtained from peridynamics and classical continuum. The accuracy of such techniques depends on the specific geometry and boundary conditions. Additionally, it is also unclear how these corrections influence the total energy in the system.

A consistent solution for these surface effects, i.e., independent of the problem type and geometry as well as without influencing the total energy of the system, is provided by the correspondence model (SILLING ET AL. 2007). However, correspondence formulation suffers from zero energy modes (BEHZADINASAB AND FOSTER 2020a, SILLING 2017) and stabilization techniques (WANG ET AL. 2016) again introduce some fictitious parameter which influences the total energy.
Recently, the idea of bond-associated correspondence has been put forward by Behzadinasab and Foster (2020b), Breitman and Dayal (2018), Chen and Spencer (2019). These models have enhanced stability along with the benefits of the original (nodal) correspondence model, but they do so at an extremely high computational cost.

### 2.3 Constitutive modeling: Elastoplasticity

First ordinary, state-based plasticity model for peridynamics was presented by Mitchell (2011). A non-local, $J_2$-type (pressure independent), perfect plastic yield function was proposed. The yield function depended on the yield strength of the material as well as the horizon size of the material. In this work, an elastic-plastic model will be used to model the soil material for the excavation simulations. Soil exhibits a strong dependence on the pressure, to this end, a pressure-dependent, Drucker-Prager type plasticity model, developed by Lammi and Zhou (2017), Vogler and Lammi (2014) for peridynamics, will be used.

**Figure 2.6:** Pressure-dependent peridynamic yield surface in the force state space. $F(x) = 0$ separates elastic and plastic deformations.

#### Drucker-Prager plasticity model

Pressure-dependent plastic behavior is modeled by additively decomposing both isotropic and deviatoric part of the extension state (Eq. 2.10) into an elastic and plastic part, i.e., $e^i = e^{ie} + e^{ip}$ and $e^d = e^{de} + e^{dp}$, respectively. The force state (Eq. 2.13) is then modified to consider only the elastic part of the deformation (Vogler and Lammi 2014) as:

$$F(x, t) = \kappa \omega(|\xi|) (e^i(\xi) - e^{ip}(\xi)) + \alpha \omega(|\xi|) (e^d(\xi) - e^{dp}(\xi)),$$

where, $\kappa = \frac{9K}{m(x)}$ and $\alpha = \frac{15\mu}{m(x)}$. The pressure-dependent peridynamic yield surface (Figure 2.6) at $x$ is defined as:

$$F(x) = (t_d \bullet t_d)^{1/2} - \beta p(x) - t_0(x) \leq 0.$$

Here, $t_d(\xi)$ is the deviatoric part of the force state, $\beta$ is a constant of internal friction, $p(x)$ is the peridynamic pressure and $t_0$ is a material yield strength parameter. And $t_d \bullet t_d$, according to
SILLING ET AL. (2007) is defined as:

\[
\mathbf{t}_d \cdot \mathbf{t}_d = \int_{\mathcal{H}_x} \mathbf{t}_d(\xi) \cdot \mathbf{t}_d(\xi) \, dV_x. \tag{2.31}
\]

For an associative flow rule, the plastic increment of the extension state is given by (VOGLER AND LAMMI 2014):

\[
\dot{\varepsilon}_p = \lambda \nabla F = \lambda \left( \frac{\mathbf{t}_d \cdot \mathbf{t}_d}{(\mathbf{t}_d \cdot \mathbf{t}_d)^{1/2}} + \frac{\beta |\xi|}{3} \right), \tag{2.32}
\]

where, \(\lambda\) is a scalar plastic multiplier. Furthermore, enforcing the consistency condition, i.e., \(\lambda \dot{F} = 0\), and using the identities \(\mathbf{t}_d \cdot \dot{\varepsilon}_i = 0\) and \(\mathbf{t}_i \cdot \dot{\varepsilon}_d = 0\), \(\lambda\) can be computed. According to VOGLER AND LAMMI (2014), it is given as:

\[
\lambda = \frac{\kappa \omega \nabla^i F \cdot \dot{\varepsilon}_i + \kappa \omega \nabla^d F \cdot \dot{\varepsilon}_d}{\kappa \omega \nabla^i F \cdot \nabla^i F + \kappa \omega \nabla^d F \cdot \nabla^d F}. \tag{2.33}
\]

Where, \(\nabla^i F\) and \(\nabla^d F\) are the isotropic and deviatoric part of the Fréchet derivative of the yield function, respectively.

For pressure-dependent materials, usually a non-associative plastic flow rule is utilized. A peridynamic non-associative plastic flow potential is defined as:

\[
G(x) = (\mathbf{t}_d \cdot \mathbf{t}_d)^{1/2} + \psi p(x), \tag{2.34}
\]

where \(\psi\) is a constant of dilatation. Increment of the plastic extension state is computed as:

\[
\dot{\varepsilon}_p = \lambda \left( \frac{\mathbf{t}_d \cdot \mathbf{t}_d}{(\mathbf{t}_d \cdot \mathbf{t}_d)^{1/2}} + \frac{\psi |\xi|}{3} \right), \tag{2.35}
\]

and the plastic multiplier \(\lambda\), which now depends on both yield function (Eq. 2.30) and flow rule (Eq. 2.34), is found to be:

\[
\lambda = \frac{\kappa \omega \nabla^i G \cdot \dot{\varepsilon}_i + \kappa \omega \nabla^d G \cdot \dot{\varepsilon}_d}{\kappa \omega \nabla^i G \cdot \nabla^i G + \kappa \omega \nabla^d G \cdot \nabla^d G}. \tag{2.36}
\]

The nonlocal peridynamic parameters \(t_0\), \(\beta\) and \(\psi\) are related to the classical, local Drucker-Prager parameters, according to VOGLER AND LAMMI (2014), as:

\[
t_0(x) = \tau_0 \left[ \frac{6}{m(x)} \left( \frac{\pi \delta_0^5}{3} \right)^{1/2} \right],
\]

\[
\beta(x) = \tan(\beta_{DP}) \left[ \frac{6}{m(x)} \left( \frac{\pi \delta_0^5}{3} \right)^{1/2} \right],
\]

\[
\psi(x) = \tan(\psi_{DP}) \left[ \frac{6}{m(x)} \left( \frac{\pi \delta_0^5}{3} \right)^{1/2} \right]. \tag{2.37}
\]

Here, \(\tau_0\) is the yield strength of the material, and \(\beta_{DP}\) and \(\psi_{DP}\) are the internal friction and dilatation angles, respectively, from the classical (local) Drucker-Prager model. For further details on the derivation of these parameters as well as the integration scheme, the interested reader is referred to VOGLER AND LAMMI (2014).
2.4 Constitutive modeling: Fracture

Crack initiation and propagation is modelled in peridynamics by irreversibly breaking the connections (bonds) between the material points. This results in an autonomous crack propagation at the continuum level without the explicit need of a criterion for the direction or for the length of the propagating crack.

Figure 2.7: Illustration of the fracture surface and the associated integration domain.

2.4.1 Critical-stretch failure criterion

A critical-stretch criterion was first proposed by Silling (2000) and was later on associated with a material property in Silling and Askari (2005). It is defined by considering a planer fracture surface in the interior of a large homogeneous body. In order to separate the two halves connecting the fracture surface, all the bonds connecting these two halves must be broken. For a PMB material (Silling and Askari 2005) the energy of a single bond is defined as:

\[
w(\xi) = \frac{1}{2} c s^2 |\xi|, \tag{2.38}\]

where \(s\) and \(c\) are defined in Eq. (2.6) and Eq. (2.7), respectively. When stretch \(s\) exceeds a critical value \(s_c\), known as the critical-stretch, the bond breaks irreversibly and \(w_c(\xi)\) amount of energy is released. The energy \(G_c\) required to break all the bonds per unit fracture area can then be found as:

\[
G_c = \int_0^\delta \int_0^{2\pi} \int_0^z \cos^{-1}\left(\frac{z}{\xi}\right) \left( c s^2 |\xi| / 2\right) |\xi|^2 \sin\phi \ d\phi \ d\xi \ d\theta \ dz. \tag{2.39}\]

The integration domain for the above equation is shown in Figure 2.7. After evaluating the integrals, using Eq. (2.7) and solving for \(s_c\) leads to:

\[
s_c = \sqrt{\frac{5 G_c}{9K\delta}}. \tag{2.40}\]

2.4.2 Critical-energy failure criterion

A critical-energy based bond failure criterion was developed by Foster et al. (2011) to use with the state-based peridynamics. It defines a critical threshold for the bonds to fail irreversibly. The
stored energy density of a bond $w_\xi$ is calculated by projecting the relative force vector on the relative displacement vector as:

$$w_\xi = \int_0^{\eta(t_{\text{final}})} \left( \mathbf{T}[\mathbf{x}, t]\langle \xi \rangle - \mathbf{T}[\mathbf{x}', t]\langle -\xi \rangle \right) \cdot d\eta.$$  

(2.41)

The integrand of $w_\xi$ is called the dual force density and $w_\xi$ represents the energy density of a bond due to the relative displacement of two material points $\mathbf{x}$ and $\mathbf{x}'$ from $\eta = 0$ at time $t = 0$ to $\eta(t_{\text{final}})$. For an ordinary state-based model (Section 2.2.2) using Eq. (2.8), (2.9) and (2.13), the dual force density can be computed as:

$$\mathbf{T}[\mathbf{x}, t]\langle \xi \rangle - \mathbf{T}[\mathbf{x}', t]\langle -\xi \rangle = (3K - 5\mu) \omega(|\xi|) \frac{\theta(\mathbf{x}, t)}{m(\mathbf{x})} + \frac{\theta(\mathbf{x}', t)}{m(\mathbf{x}')} \right) \right] \mathbf{M}[\mathbf{x}, t]\langle \xi \rangle.$$  

(2.42)

The energy density in a bond $w_\xi$ is assumed to be fully recoverable unless it exceeds a critical energy density level $w_c$. FOSTER ET AL. (2011) defined $w_c$ in terms of the fracture energy $G_c$, a material property that can be measured experimentally. Figure 2.7 shows a fracture plane separating the two halves of a body. The bonds between all material points A (along the dashed line $0 < z < \delta$) and all material points B in the spherical volume of radius $\delta$ are bridging a unit fracture surface. It is assumed that, when all these bonds exceed $w_c$, a fracture surface of unit area is created which results in an energy release of $G_c$:

$$G_c = \int_0^{\delta} \int_{-2\pi}^{2\pi} \int_{\sin^{-1}z/\xi}^{\cos^{-1}z/\xi} w_c |\xi|^2 \sin \phi \, d\phi \, d\xi \, dz.$$  

(2.43)

The integration domain of Eq. (2.43) is shown in Figure 2.7. For further details we refer to FOSTER ET AL. (2011), YU AND LI (2020). Solving Eq. (2.43) for $w_c$ leads to:

$$w_c = \frac{4G_c}{\pi\delta^4}.$$  

(2.44)

**2D critical-energy failure criterion**

For the two dimensional case, following DIPASQUALE ET AL. (2017), the energy required to break all the bonds per unit fracture area is given by:

$$G_c = \int_0^{\delta} \int_{-\delta}^{\delta} w_{c2D} d\phi \, d\xi \, dz,$$  

(2.45)

which leads to the critical-energy density level $w_{c2D}$ as:

$$w_{c2D} = \frac{3G_c}{2\delta^3 t_{2D}},$$  

(2.46)

where $t_{2D}$ is the thickness of the 2D body being simulated.
In Eq. (2.44) and Eq. (2.46), \( \delta \) acts as a localization limiter and guarantees a constant energy release rate independent of the discretization. Further details are provided in Dipasquale et al. (2017). In a structural simulation, once the condition \( w_\xi \geq w_c \) is satisfied for a bond, it breaks, i.e., the stiffness of the bond vanishes irreversibly and it does not contribute to the internal force any more. A damage variable \( d \) can be defined as the ratio of the number of broken bonds to the total (initial) number of bonds at a node. This damage parameter \( d \) will be used for generating contour plots along the computed crack paths in the simulations.

### 2.4.3 Deviatoric-strain failure criterion

A failure criterion for the anti-symmetric fracture surface, i.e., Mode II/III, was presented by Ren et al. (2016). This criterion is based on the maximum allowed deviatoric strain of a bond (Eq. 2.27). Assuming zero volumetric strain along an anti-symmetric crack surface, according to Ren et al. (2016) the elastic energy for a bond is given by:

\[
 w^d = \frac{9 \mu \delta}{4 \pi \delta^3} (\varepsilon^d)^2, \tag{2.47}
\]

where \( \varepsilon^d = |\varepsilon^d| \) from Eq. (2.27). The bond is damaged irreversibly when \( \varepsilon^d \) exceeds a critical deviatoric bond strain \( \varepsilon_c^d \) and \( w_c^d \) is the amount of energy released by the bond. Based on Figure 2.7, the total work \( G_c \) required to break all bonds per unit fracture area can then be computed as:

\[
 G_c = \int_0^\delta \int_0^{2\pi} \int_0^{\cos^{-1} z/\xi} w_c^d |\xi|^2 \sin \phi \, d\phi \, d\xi \, dz. \tag{2.48}
\]

Solving the integrals in Eq. (2.48), using Eq. (2.47) and solving for \( \varepsilon_c^d \) leads to the critical deviatoric bond strain as:

\[
 \varepsilon_c^d = 4 \frac{4}{3} \sqrt{\frac{G_c}{\mu \delta}}. \tag{2.49}
\]

### 2.5 Frictional contact formulation

The most common contact formulation used with the peridynamic models is the short-range force approach of Silling and Askari (2005). The normal and tangential contact forces are exerted in the deformed configuration at a node \( y \) by all nodes \( y_j \) in a close proximity satisfying \(|y_j - y| < r_c\), where \( r_c \) is a predefined contact radius. The normal contact force \( f_n(y_j - y) \), i.e., the force that \( y_j \) exerts on \( y \), is computed using:

\[
 f_n(y_j - y) = c_f \left( \frac{|y_j - y| - r_c}{\delta} \right) V_j n_n, \quad n_n = \frac{(y_j - y)}{|y_j - y|}. \tag{2.50}
\]

Where \( c_f \) is a constant representing the penalty stiffness for the repulsive forces (Littlewood 2015), \( V_j \) is the volume of the node \( y_j \) and \( n_n \) is a unit vector in the direction of normal contact. Tangential contact force \( f_t \) is then computed using the normal contact force \( f_n \) as follows:

\[
 f_t(y_j - y) = -\mu f_n(y_j - y) |n_t|, \quad n_t = \frac{v_{rel}}{|v_{rel}|}. \tag{2.51}
\]
\( \mu_f \) is the coefficient of friction and \( \mathbf{n}_t \) is a unit vector in the direction of relative tangential velocity \( \mathbf{v}_{rel} \) of the nodes \( y \) and \( y_j \). Finally, the total contact force exerted on node \( y \) is found by summing \( \mathbf{f}_n \) and \( \mathbf{f}_t \) from Eq. (2.50) and Eq. (2.51) for all \( y_j \) nodes. For further details on frictional contact modeling in peridynamics, the interested reader is referred to Kamensky et al. (2019).

### 2.6 Spatial and temporal discretization

The widely used discrete peridynamic implementation to date is the mesh-free discretization technique presented in Silling and Askari (2005). The continuum body shown in Figure 2.1 can be represented by a finite number of nodes, where each node is associated with a cell of known volume in the reference configuration. This results in the following discrete form for Eq. (2.2):

\[
\rho \ddot{\mathbf{u}}(\mathbf{x}, t) = \sum_{i=0}^{N} \left[ T(\mathbf{x}, t)[\mathbf{x}_i] \langle \mathbf{x}_i' - \mathbf{x} \rangle - T(\mathbf{x}_i', t)[\mathbf{x} - \mathbf{x}_i'] \right] \Delta V_{x_i'} + \mathbf{b}(\mathbf{x}, t). \tag{2.52}
\]

Where \( \Delta V_{x_i'} \) is the volume of node \( x_i' \) and \( N \) is the number of nodes in the neighborhood of \( x \).

This discretization scheme results in a strong-form collocation method with a relatively low computational expense, but leads to only a first order convergence rate (Pasetto et al. 2018, Seleson and Littlewood 2016). In Tian and Du (2013), it was shown that a higher order convergence rate can be obtained using quadrature based finite difference discretizations or by employing finite element discretizations. A Reproducing Kernel (RK) enhanced approximation approach was presented in Pasetto et al. (2018) for bond-based peridynamics (Section 2.2.1) and in Hillman et al. (2020) for the peridynamic correspondence framework (Section 2.2.3). It was shown, that the introduction of RK shape functions in the solution approximation allows for arbitrary smoothness and completeness of the approximation. These higher-order techniques, however, significantly increase the implementation complexity and the computational cost.

The mesh-free discretization of the correspondence model of peridynamics (Silling et al. 2007) is well investigated for uniform grids and similarities have been drawn with Smoothed Particle Hydrodynamics (SPH) discretization (Gänzler et al. 2015) as well as with RKPM discretization with synchronized derivatives (Bessa et al. 2014, Chen et al. 2017). For the general state-based peridynamics (i.e., without using the correspondence framework) and its discretizations, especially using non-uniform grids, similar analyses do not yet seem to exist.

For direct numerical simulations, an explicit Velocity-Verlet method (Verlet 1967) for time integration is used. The approximations for the velocities and the displacements are given by:

\[
\begin{align*}
\dot{\mathbf{u}}_{n+\frac{1}{2}} &= \dot{\mathbf{u}}_n + \frac{\Delta t}{2} \ddot{\mathbf{u}}_n \\
\mathbf{u}_{n+1} &= \mathbf{u}_n + \Delta t \dot{\mathbf{u}}_{n+\frac{1}{2}} \\
\dot{\mathbf{u}}_{n+1} &= \dot{\mathbf{u}}_{n+\frac{1}{2}} + \frac{\Delta t}{2} \ddot{\mathbf{u}}_{n+1}. \tag{2.53}
\end{align*}
\]

Here, \( \Delta t \) is the critical time step computed according to the stability criterion presented in Silling and Askari (2005), and \( \mathbf{u}, \dot{\mathbf{u}} \) and \( \ddot{\mathbf{u}} \) are the displacement, velocity and acceleration vectors, respectively.
Chapter 3

Elastic wave dispersion and propagation

Wave dispersion is a phenomenon that causes different frequencies comprising a signal to propagate at different velocities within a material. This chapter focuses on the dispersion properties of a state-based Linear Peridynamic Solid (LPS) model and specifically the investigation of the role of the peridynamic horizon. The dispersion relation for one, two and three dimensional cases are derived and the effect of horizon size, mesh size (particle lattice spacing) and the influence function on the dispersion properties is investigated. It is shown how the influence function can be used to minimize wave dispersion at a fixed particle lattice spacing and it is demonstrated qualitatively by wave propagation analysis in one- and two-dimensional models of dynamic media. As a main contribution of this chapter, it is proposed to associate peridynamic non-locality expressed by the horizon with a characteristic length scale related to the material microstructure. To this end, the dispersion curves obtained from peridynamics are compared with experimental data for two kinds of sandstone.

Nonlocality in a peridynamic formulation is inevitably connected with dispersion of elastic waves in transient analyses. This topic is the subject of discussion since the first proposal of a peridynamics model for dynamic analyses (Silling 2000), in which a general dispersion relation for bond-based peridynamics has been formulated. Subsequently, numerical dispersion in bond-based peridynamic models has been addressed by Weckner and Abeyaratne (2005), who studied the effect of the long-range/nonlocal peridynamic forces on the dynamic characteristics of a one dimensional bar. Thereafter, Zimmermann (2005) compared the dispersion behavior of peridynamics with classical gradient and integral type nonlocal continua. Seleson et al. (2009) introduced a peridynamic model as an upscaling of Lennard-Jones molecular dynamics model and presented an analytical comparison of the one dimensional equations of motion as well as the dispersion relations for molecular dynamics and peridynamics. Seleson and Parks (2011) investigated wave dispersion in a generalized Prototype Micro Brittle (PMB) material model and showed, that it is a special case of state-based peridynamics. Wildman and Gazonas (2014) presented a hybrid
finite difference/peridynamics method to improve the dispersion properties of the original bond-based peridynamics model. GU ET AL. (2016) showed that numerical dispersion can be controlled by an appropriate choice of the influence function (the function giving weights to nonlocal integrals) and applied this idea to reduce dispersion in numerical analyses of wave propagation in a Split Hopkinson Pressure Bar. The dispersion characteristics of state-based correspondence models was addressed by BAŽANT ET AL. (2016), they studied state-based peridynamics along with the classical constitutive relations using the correspondence framework of peridynamics (SILLING ET AL. 2007).

The content of this chapter has been published in BUTT ET AL. (2017). The main objectives of this chapter are:

- To derive the dispersion relation for the state-based peridynamic model using the constitutive relation for a Linearized LPS.
- To investigate, how dispersion can be minimized by choosing appropriate peridynamic parameters.
- To show how the nonlocal parameters of the LPS, i.e., the radius of the horizon $\delta$ and the influence function $\omega$ can be adjusted according to desired dispersive response of the material and to provide a physics-based interpretation by relating these parameters to the microstructure of different materials.

### 3.1 Wave dispersion analysis

Peridynamics involves direct interactions of material points at a finite distance and therefore induces a non-linear wave dispersion behavior (BAŽANT ET AL. 2016, WECKNER ET AL. 2009, WECKNER AND SILLING 2011). The dispersion characteristics of the numerical scheme depends on the choice of the peridynamic parameters, i.e., the horizon, influence function and particle lattice spacing. In this section, dispersion relations are derived for one, two and three dimensional ordinary state-based peridynamic solids.

#### 3.1.1 1D dispersion relation

The linearized equation of motion at a material point $x$ in a one dimensional peridynamic bar with a unit cross-sectional area is given by:

$$
\rho(x, t) \frac{\partial^2 u(x, t)}{\partial t^2} = \int_{x-\delta}^{x+\delta} \left[ T[x, t](\xi) - T[x', t](\xi') \right] d\xi' + b(x, t),
$$

and the force state $T[x, t]$ for a one dimensional linear peridynamic solid model can be written as (SILLING 2010):

$$
T[x, t](\xi) = \frac{c_1}{m} \omega(|\xi|) \theta^{\text{lin}}(x, t) \xi + \frac{c_2}{m} \omega(|\xi|)(u(x + \xi, t) - u(x, t)),
$$

where $c_1$ and $c_2$ are the elastic peridynamic material parameters and $\omega(|\xi|)$ is the so-called influence function, that scales the nonlocal interactions within the domain of the horizon with respect to $|\xi|$. 
3.1. WAVE DISPERSION ANALYSIS

The one dimensional linearized dilatation \( \theta^{\text{lin}}(x, t) \) and the weighted volume \( m \) (Silling et al. 2007) are given by:

\[
\theta^{\text{lin}}(x, t) = \frac{1}{m} \int_{-\delta}^{\delta} \omega(|\xi|) \xi \left( u(x + \xi, t) - u(x, t) \right) d\xi ,
\]

\[
m = \int_{-\delta}^{\delta} \omega(|\xi|) \xi^2 d\xi .
\]

(3.3)

To calibrate the peridynamic material parameters \( c_1 \) and \( c_2 \), the peridynamic equation of motion is compared with the one dimensional classical wave equation:

\[
\rho(x, t) \frac{\partial^2 u(x, t)}{\partial t^2} = E \frac{\partial^2 u(x, t)}{\partial x^2} + b(x, t).
\]

(3.4)

Given a smooth displacement field, as \( \delta \to 0 \), the integral operators defining spatial interactions in Eq.(3.1) and in Eq.(3.3) converge to the classical differential operators (Emmrich et al. 2007). Thus, Eq.(3.1) gives:

\[
\rho(x, t) \frac{\partial^2 u(x, t)}{\partial t^2} = (c_1 + c_2) \frac{\partial^2 u(x, t)}{\partial x^2} + b(x, t).
\]

(3.5)

Comparing Eq.(3.4) and Eq.(3.5), it can be observed that \( c_1 + c_2 = E \) and \( c_1 = c_2 = E/2 \) is chosen. It must be noted that the manner in which \( c_1 \) and \( c_2 \) are calibrated with respect to \( E \) does not influence the qualitative behavior of wave dispersion. Finally, the force state for a one dimensional linear peridynamic solid is given by:

\[
T[x, t][\xi] = \frac{E}{2m} \omega(|\xi|) [\theta^{\text{lin}}(x, t) \xi + (u(x + \xi, t) - u(x, t))].
\]

(3.6)

To obtain the dispersion relation, a plane wave of the form \( u(x, t) = u_0 e^{i(kx - \omega t)} \) is substituted into Eq.(3.3), with \( k \) as the wave number and \( \omega \) as the angular frequency. By using the fact that odd functions integrated in a symmetric domain give zero, the following equation is obtained:

\[
\theta^{\text{lin}}(x, t) = \frac{1}{m} \int_{-\delta}^{\delta} \omega(|\xi|) \xi (e^{ik\xi} - 1) d\xi u(x, t)
\]

\[
= \frac{1}{m} \left[ \int_{-\delta}^{\delta} \omega(|\xi|) \xi \cos(k\xi) - 1 \right] d\xi + i \int_{-\delta}^{\delta} \omega(|\xi|) \xi \sin(k\xi) d\xi \right] u(x, t)
\]

\[
= \frac{2i}{m} \int_{0}^{\delta} \omega(|\xi|) \xi \sin(k\xi) d\xi u(x, t).
\]

(3.7)

In the absence of body forces, substituting Eq.(3.7) and Eq.(3.6) along with the plane wave equation
in Eq. (3.1), the one dimensional dispersion relation is obtained:

\[
\omega^2(k) = \frac{-E}{2\rho m} \left[ \int_{-\delta}^{\delta} \omega(|\xi|)(e^{ik\xi} + 1)\xi \left( \frac{2i}{m} \int_{0}^{\delta} \omega(|\xi|)\xi \sin(k\xi) \, d\xi \right) + 2 \int_{-\delta}^{\delta} \omega(|\xi|)(e^{ik\xi} - 1) \, d\xi \right] + \frac{2E}{\rho m} \left[ \frac{1}{m} \left( \int_{0}^{\delta} \omega(|\xi|)\xi \sin(k\xi) \, d\xi \right)^2 + \int_{0}^{\delta} \omega(|\xi|)(1 - \cos(k\xi)) \, d\xi \right].
\]  

(3.8)

In the next step, the horizon is discretized into \( n \) material points (lumped masses/lattice points), such that \( \delta = n\Delta x \). \( \Delta x \) is the distance between particles. The discretized form of Eq. (3.8) is then obtained by substituting the integral operator in Eq. (3.8) by a summation over the elements \( \Delta x \) as
follows:

\[
\omega^2(k) = \frac{2E}{\rho m} \left[ \frac{1}{m} \left( \sum_{j=1}^{n} \omega(j \Delta x) \sin(k j \Delta x) j \Delta x^2 \right)^2 + \sum_{j=1}^{n} \omega(j \Delta x)(1 - \cos(k j \Delta x)) \Delta x \right].
\]

(3.9)

The discretized (using finite element or finite difference methods) classical wave equation (Eq.3.4) is also dispersive because the continuous mass in the medium is lumped at the nodes that interact over finite distances. This source of dispersion is an artifact of a discretization induced non-locality in discrete systems. According to Eq.(3.9), the dispersion behavior can be influenced by the size of horizon \(\delta\), the accuracy of the spatial integration (i.e., number of material points in the horizon \(n\)) and the shape of the influence function \(\omega\).

**Analysis**

The effect of the horizon size \(\delta\) as well as the nodal density \(n\) is investigated here in the sense of the so-called \(\delta\)- and \(n\)-convergence in peridynamics analysis (H A N D B O B A R U 2010). The normalized frequency, \(\omega_n = \omega/\sqrt{E/\rho}\) according to Eq.(3.9) is plotted against the wave number \(k\) in Figure 3.1. The group velocity \(c_g\) and the phase velocity \(c_p\) can be computed by the tangent \(d\omega_n/dk\) and the secant \(\omega_n/k\) of the curves presented in Figure 3.1 respectively. For simplicity, in this convergence study, \(\omega(|\xi|) = 1\) is assumed. In case of \(\delta\)-convergence, i.e., Figure 3.1a and Figure 3.1b, the number of points in the horizon \(n\) is fixed, while decreasing systematically the horizon size. As \(\delta \to 0\), the numerical solution approaches the classical continuum mechanics solution (i.e., the local theory) plotted as a dotted straight line. On the other hand, for \(n\)-convergence, the number of points in the horizon is increased while keeping the value of \(\delta\) constant. As \(n \to \infty\), the numerical approximation approaches the analytical solution of peridynamics, which can be highly dispersive depending on the size of the horizon \(\delta\), as shown in Figure 3.1c and Figure 3.1d.

![Figure 3.2: Different choices for the influence function \(\omega(|\xi|)\): \(\omega_1\), \(\omega_2\) and \(\omega_3\) with three different values of \(p\).](image)
Besides the nodal density and the peridynamic horizon, also the choice of the influence function \( \omega(|\xi|) \) is expected to affect the dispersion characteristics. Influence functions govern the manner in which these nonlocal interactions are weighted. In order to assess the effect of the shape of the influence function \( \omega(|\xi|) \) on the dispersion curves, following functions are investigated:

\[
\begin{align*}
\omega_1(|\xi|) &= 1, \\
\omega_2(|\xi|) &= \left(\frac{|\xi|}{\delta}\right)^2, \\
\omega_3(|\xi|) &= \omega_0 \exp\left(-\frac{p^2|\xi|^2}{\delta^2}\right). \\
\end{align*}
\]

\( \omega_3 \) was originally used by Eringen (2002) as a kernel in his nonlocal elasticity theory. It is normalized by calculating \( \omega_0 \) as:

\[
\int_{\mathcal{H}_x} \omega(|\xi|) dV_\xi = 1, \quad \omega_0 = \pi^{-N/2} \left(\frac{p}{\delta}\right)^N,
\]

for \( N \) dimensions (\( N = 1, 2, 3 \)). The shape of the influence functions \( \omega_1, \omega_2 \) and \( \omega_3 \) (parametrized in terms of \( p \)) are shown in Figure 3.2. For \( \omega_3 \), one observes that, as \( p \) increases, the non-local interactions localize. \( \omega_2 \) is chosen here to investigate the case when large weights are given to the long ranging interactions in comparison to the short-range interactions.

Even for constant lattice spacing and the horizon size, considerable differences of the dispersion characteristics arise from the choice of the influence function. The effect of the chosen influence function on the dispersion relation is shown in Figure 3.3a and Figure 3.3b, the frequency \( \omega_n/(2\pi/\delta) \) from Eq.(3.9) and the phase velocity, given by the relation \( \tau_p = \omega_n/k \), are plotted as a function of number of (2\pi-periodic) wavelengths per horizon, i.e., \( k/(2\pi/\delta) \), respectively. For all cases in Figure 3.3, the particle lattice spacing and the number of points in the horizon are kept constant with \( n = 3 \) and \( \Delta x = 0.5 \times 10^{-3} \) m. In comparison to \( \omega_1 \), the dispersion curve obtained for \( \omega_2 \) is highly dispersive as long-range interactions are given more weight in comparison to short-range interactions. For the case of \( \omega_3 \), a range of dispersion curves, which strongly depend on the value of \( p \), are obtained. As \( p \to \infty \), the model is dominated by local (and nearly local) interactions.
and the resulting dispersion curve mimics the response of the classical wave equation. At a fixed value of $n$ and $\Delta x$, the phase velocity decreases at different rates for different choices of influence functions, and there are zero energy modes present. The frequency goes to zero, when the number of wavelengths per horizon are equal to an integer multiple of the number of nodes in the horizon, i.e., $\varpi_n = \tau_p = 0$ when $k/(2\pi/\delta) = i \times n$, where $i = 1, 2, 3...$ (Figure 3.5). These zero energy modes are discussed further in the next section. It must be noted that the relevant range of engineering interest in Figure 3.5 is $k/(2\pi/\delta) < 0.1$.

### 3.1.2 2D dispersion relation

The peridynamic equation of motion at a material point $x$, in a two dimensional plate with unit thickness, is given by:

$$\rho(x, t) \frac{\partial^2 u(x, t)}{\partial t^2} = \int_{\mathcal{H}} [T[x, t] \langle x - x' \rangle - T[x', t] \langle x' - x \rangle] \, dA_{x'} + b(x, t).$$  \hspace{1cm} (3.12)

The scalar force state $t$ for a two dimensional LPS is derived from considering strain energy equivalence with classical continuum for both plane stress and plane strain conditions in LE ET AL. (2014). For the plane strain case, $t$ is given by:

$$t = \frac{18K + 2\mu}{9m} \theta_{\text{lin}}(x, t) \frac{\omega(|\xi|)}{m} \cdot x + \frac{8\mu}{m} \omega(\xi) \cdot u(x + \xi, t) - u(x, t),$$  \hspace{1cm} (3.13)

where the symbol $\cdot$ denotes the dot product of two states (see Eq. 2.31) as defined in SILLING ET AL. (2007). $\omega$ and $x$ are scalar states, with $\omega(\xi) = \omega(|\xi|)$ and $x(\xi) = |\xi|$.

The linearized force state $T$ is obtained using Eq.(2.8), Eq.(2.16) and Eq.(3.13) as:

$$T[x, t][\xi] = \frac{18K - 30\mu}{9m} \theta_{\text{lin}}(x, t) \frac{\omega(|\xi|)}{m} \xi + \frac{8\mu}{m} \omega(|\xi|) \frac{\xi \otimes \xi}{|\xi|^2} \cdot (u(x + \xi, t) - u(x, t)),$$  \hspace{1cm} (3.14)

where $\theta_{\text{lin}}$ is the linearized dilatation for the two dimensional plane strain case. According to LE ET AL. (2014), it is obtained as:

$$\theta_{\text{lin}}(x, t) = \frac{2}{m} \int_{\mathcal{H}} \omega(|\xi|) \xi \cdot (u(x + \xi, t) - u(x, t)) \, dA_{\xi}.$$  \hspace{1cm} (3.15)

By inserting the plane wave equation $u(x, t) = u_0 e^{i(kn \cdot x - \omega t)}$ into Eq.(3.15), with $n$ corresponding to the unit vector in the direction of propagation, the following equation can be obtained using similar arguments as in Eq.(3.7).

$$\theta_{\text{lin}}(x, t) = \frac{2i}{m} \int_{\mathcal{H}} \omega(|\xi|) \xi \sin(kn \cdot \xi) \, dA_{\xi} \cdot u(x, t).$$  \hspace{1cm} (3.16)

Substituting the plane wave equation in Eq.(3.12) (neglecting body forces) along with Eq.(3.14) and Eq.(3.16), the following eigenvalue problem is obtained:

$$\rho \varpi^2 u(x, t) = M(k, n) \cdot u(x, t),$$  \hspace{1cm} (3.17)
with
\[
M_{ij}(k, \mathbf{n}) = \frac{2}{m} \left[ \frac{18K - 30\mu}{9m} \left( \int_{\mathcal{F}_L} \omega(|\xi|) \sin(kn_l \xi_l) \xi_l \, dA_\xi \right) \int_{\mathcal{F}_L} \omega(|\xi|) \sin(kn_l \xi_i) \xi_j \, dA_\xi \right] 
+ 8\mu \int_{\mathcal{F}_L} \omega(|\xi|) (1 - \cos(kn_l \xi_i) \xi_j \xi_l) \, dA_\xi \right].
\] (3.18)

\( M_{ij}(k, \mathbf{n}) \) is a diagonal tensor if the integration domain and the influence function are symmetric, i.e., the material is isotropic and \( M_{ij} = 0 \) when \( i \neq j \). A cartesian coordinate system is introduced in Eq.(3.18), and the waves propagating in the positive \( x \) direction, i.e., \( \mathbf{n} = [1 \ 0]^T \), are sought. The Eigenvalues of \( M \) are given by \( \lambda_{11} = \rho \bar{\omega}_p^2 \) and \( \lambda_{22} = \rho \bar{\omega}_s^2 \), where \( \bar{\omega}_p \) and \( \bar{\omega}_s \) are the frequencies of the pressure and the shear waves (in \( x \) and \( y \) directions, respectively), for this particular choice of \( \mathbf{n} \). The frequency of the pressure wave \( \bar{\omega}_p \) can be written as a function of the wave number \( k \) as:
\[
\bar{\omega}_p(k)^2 = \frac{32}{\rho m} \left[ \frac{18K - 30\mu}{9m} \left( \int_0^\delta \int_0^\delta \sqrt{\xi^2 - \xi_l^2} \omega(|\xi|) \sin(k \xi_1) \xi_1 \, d\xi_2 \, d\xi_1 \right) \right]^2 
+ 2\mu \left( \int_0^\delta \int_0^\delta \sqrt{\xi^2 - \xi_l^2} \omega(|\xi|) (1 - \cos(k \xi_1)) \frac{\xi_2^2}{|\xi|^2} \, d\xi_2 \, d\xi_1 \right).
\] (3.19)

For the analysis of numerical dispersion, a mesh-free discretization is introduced in Eq.(3.19) in analogy to Eq.(3.9). For simplicity, a cubic lattice is chosen with the same lattice spacing in \( x \) and \( y \) direction, i.e., \( \Delta x = \Delta y = d \), (in general, they do not have to be the same) and obtain \( |\xi| = \sqrt{(i \Delta x)^2 + (j \Delta y)^2} = d \sqrt{i^2 + j^2} \). The horizon is discretized as \( \delta = nd \), where \( n \) is the number of points in the horizon along \( x \) or \( y \) axes. The discrete form of Eq.(3.19), introducing the aforementioned discretization, is obtained as:
\[
\bar{\omega}_p(k)^2 = \frac{32}{\rho m} \left[ \frac{18K - 30\mu}{9m} \left( \sum_{i=1}^n \sum_{j=1}^n \sqrt{\xi^2 - \xi_l^2} \omega(d \sqrt{i^2 + j^2}) \sin(id) \, id \right) \right]^2 
+ 2\mu \sum_{i=1}^n \sum_{j=1}^n \omega(d \sqrt{i^2 + j^2}) (1 - \cos(id)) \frac{i^2}{i^2 + j^2} \, d^2.
\] (3.20)

A linear interpolation for volume correction is used for the nodes which are partially inside the peridynamic horizon, i.e., when the summation limit in Eq.(3.20), \( j = \sqrt{n^2 - i^2} \) is not an integer number.

**Analysis**

The effect of the coefficient \( p \) in the influence function \( \omega_3 \) on the dispersion characteristics of both pressure and shear waves is shown in Figure 3.4 for two different values of \( p \) (\( p = 2.5 \) and \( p = 0.5 \)). The particle lattice spacing and the number of nodes in the horizon are kept constant at a value
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Comparison of normalized frequencies of pressure and shear wave with $p = 2.5$.

Comparison of normalized frequencies of pressure and shear wave with $p = 0.5$.

Comparison of normalized phase velocities of pressure and shear wave with $p = 2.5$.

Comparison of normalized phase velocities of pressure and shear wave with $p = 0.5$.

**Figure 3.4:** Pressure and shear wave dispersion for the influence function $\omega_3$ with two different shape parameters $p = 2.5$ and $p = 0.5$ in a 2D LPS.

of $d = 0.5 \times 10^{-3} m$ and $n = 4$ respectively, and the material parameters used are $K = 160$ GPa, $\mu = 79$ GPa and $\rho = 8000$ kg/m$^3$. The dispersion curves for two different shape parameters $p = 2.5$ and $p = 0.5$ are depicted in Figure 3.4a and Figure 3.4b, respectively. The characteristics of the two dimensional results are similar to the one dimensional case presented in Figure 3.3. Zero energy modes are also observed for the two dimensional case and will be discussed later in this subsection. The phase velocities of the pressure and the shear waves, defined as $\tau_p = \omega_p(k)/k$ and $\tau_s = \omega_s(k)/k$ respectively, are normalized with respect to the velocity of the pressure wave of the classical continuum model $c_p = ((K + \frac{4}{3}\mu)/\rho)^{1/2}$ and plotted as a function of $k/(2\pi/\delta)$ in Figure 3.4c and Figure 3.4d. It can be observed, that in the limit, as $k \to 0$, the phase velocities of the peridynamic waves approach the velocities of the classical continuum waves, i.e., $\tau_p / c_p \to 1$. 


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(a) Normalized frequencies of pressure and shear waves
(b) Normalized phase velocities of pressure and shear waves

Figure 3.5: Zero-energy modes in the dispersion curves of a 2D LPS.

The phase velocity continues to decrease for both wave types in both cases with increasing wave number. After a certain value of $k/(2\pi/\delta)$ (1.5 for $p = 2.5$ and 1.0 for $p = 0.5$), the velocity of the shear wave $c_s$ becomes larger than the velocity of the pressure wave $c_p$.

Zero energy modes, as discussed in Section 3.1.1, are also observed in higher dimensions (Figure 3.5). The frequency and group velocity ($d\omega/dk$) are $2\pi n/\delta$-periodic. The phase velocity decreases with an increasing wave number, with $2\pi n/\delta$-periodic zero-energy modes in between. These zero energy modes are present because the displacements generated by a harmonic wave with wavelength $\delta/n$ are the same at all points. The vibrational mode associated with this wavelength is a uniform translation of points, which does not lead to any vibrations (JIRASEK 2004). A linear peridynamic solid acts as a filter for high frequencies (Figure 3.5b).

3.1.3 3D dispersion relation

The scalar force state $t$ for a three dimensional LPS is derived by SILLING ET AL. (2007) as:

$$
t = \frac{3K}{m} \theta_{xx} + \frac{15\mu}{m} \omega \mathbf{d}.
$$

(3.21)

The linearized force state $\mathbf{T}$ for a 3D LPS is obtained using Eq.(2.8), Eq.(2.16) and Eq.(3.21) as:

$$
\mathbf{T}[\mathbf{x}, t]\langle \xi \rangle = \frac{3K - 5\mu}{m} \omega(|\xi|) \theta_{lin}(\mathbf{x}, t) \xi + \frac{15\mu}{m} \omega(|\xi|) \frac{\xi \otimes \xi}{|\xi|^2} (\mathbf{u}(\mathbf{x} + \xi, t) - \mathbf{u}(\mathbf{x}, t)),
$$

(3.22)

where $\theta_{lin}$ is the 3D linearized dilatation obtained by linearizing Eq.(102) in SILLING ET AL. (2007):

$$
\theta_{lin}(\mathbf{x}, t) = \frac{3}{m} \int_{\mathcal{F}_x} \omega(|\xi|) \xi \cdot (\mathbf{u}(\mathbf{x} + \xi, t) - \mathbf{u}(\mathbf{x}, t)) dV\xi.
$$

(3.23)

Three dimensional dispersion relations are obtained in a similar way as for the two dimensional case. Substituting the plane wave equation along with Eq.(3.22) and Eq.(3.23) in Eq.(2.2), the tensor
\( M^{3D} \) for a three dimensional linearized LPS model is obtained as:

\[
M_{ij}^{3D}(k, n) = \frac{3}{m} \left[ \frac{3K - 5\mu}{m} \left( \int_{\mathcal{H}_x} \omega(|\xi|) \xi_i \sin(k n_l \xi_l) \, dV \right) \int_{\mathcal{H}_x} \omega(|\xi|) \xi_j \sin(k n_l \xi_l) \, dV \right] + 10\mu \int_{\mathcal{H}_x} \omega(|\xi|) (1 - \cos(k n_l \xi_l)) \frac{\xi_i \xi_j}{|\xi|^2} \, dV \right].
\]

Assuming a wave propagating with the wave vector \( n = [1 \ 0 \ 0]^T \) in a cartesian coordinate system, the eigenvalues of \( M^{3D} \) are given by \( M_{11}^{3D} = \rho \omega_p^2 \) and \( M_{22}^{3D} = M_{33}^{3D} = \rho \omega_s^2 \), which represent the dispersion relations for the pressure wave in \( x \) direction and for the shear waves in \( y \) and \( z \) directions, respectively.

### 3.2 Wave propagation analysis

For direct numerical simulation of wave propagation in one and two dimensional linearized peridynamic solids, an explicit Velocity-Verlet method (Eq. 2.53, Section 2.6) for time integration is used. The Ricker wavelet is used as the input excitation function for both one and two dimensional cases. It is expressed as:

\[
u(t) = a \left( 1 - 2\pi^2 f^2 \left( \frac{1}{f} - t \right)^2 \right) \exp \left( -\pi^2 f^2 \left( \frac{1}{f} - t \right)^2 \right) n, \tag{3.25}
\]

where \( a \) is the amplitude, \( f \) is the frequency and \( n \) is the unit vector related to the direction of propagation of the signal. A time step of \( \Delta t = 1 \times 10^{-7} \) s is used for both simulations. This time step size satisfies the stability criteria defined in Silling and Askari (2005).

#### 3.2.1 1D wave propagation

Consider a one dimensional elastic bar, with a constant cross-sectional area of 0.01 m\(^2\) and material parameters given as \( E = 210 \) GPa and \( \rho = 8000 \) kg/m\(^3\). It is excited at \( x = 0 \) by the wavelet corresponding to Eq.(3.25) from \( t = 0 \) to \( t = 0.125 \) ms with \( a = 1 \times 10^{-3} \) m and \( f = 8 \times 10^3 \) cycles/sec. The opposite end (\( x = 1 \)) is fixed. The results of the numerical simulation of the propagating wave are shown in Figure 3.6 for three time instants. \( \omega_3 \) is used as the influence function, with \( p = 2.5 \) in Figure 3.6a and \( p = 0.5 \) in Figure 3.6b, representing a mildly and strongly dispersive medium, respectively. In both cases, the particle lattice spacing and number of points in the horizon are kept constant at a value of \( \Delta x = 0.5 \times 10^{-3} \) m and \( n = 4 \), respectively. The peridynamic medium presented in Figure 3.6a is also slightly dispersive for this signal, which is concluded from the change of the shape of the signal at \( t = 1.5 \) ms. Dispersion can be further eliminated by reducing \( \delta \) or by increasing \( p \). Dispersion can be almost eliminated, if the size of the horizon is chosen to be much smaller than the smallest wavelength present in the signal.
3.2.2 2D wave propagation

For two dimensional wave propagation, consider an elastic quadratic slab with dimensions $1.5 \times 1.5 \text{ m}$ and thickness $2 \times 10^{-3} \text{ m}$. The material parameters are assumed as $K = 160 \text{ GPa}$, $\mu = 79 \text{ GPa}$ and $\rho = 8000 \text{ kg/m}^3$. The slab is discretized with a cubic lattice, with a lattice spacing of $d = 1 \times 10^{-3} \text{ m}$ and the horizon size is $\delta = 3.1 \times 10^{-3} \text{ m}$. Same excitation as used in the case of one dimensional wave propagation, is used here. It is applied in the centroid of the slab, i.e., at $x = y = 0.75 \text{ m}$ and propagating in $y$ direction, i.e., with $\mathbf{n} = [0 \ 1]^T$ in Eq.(3.25). In Figure 3.7 the $y$ component and in Figure 3.8 the $x$ component of the displacement field, representing the pressure and shear waves for this excitation, are shown. The influence function is set to $\omega_3$. Two values of $p$ are investigated: $p = 2.5$ and $p = 0.5$, representing a mildly and a strongly dispersive medium.
3.2. WAVE PROPAGATION ANALYSIS

3.2.3 Discussion

Smaller wavelengths travel slower than longer wavelengths in a peridynamic medium. This difference in the speed of propagation is governed by the dispersion relation, which depends on the particle lattice spacing and horizon and the shape of the influence function. For a given signal, as the wave propagates, these smaller wavelengths in the signal lag behind the propagating group and appear as trailing waves, as shown in Figure 3.6(b), Figure 3.7(b) and Figure 3.8(b).

It is proposed that these dispersive effects can be reduced by using the radius of horizon $\delta$ and the shape parameter $p$ at a fixed lattice spacing $\Delta x$. To quantify the effects of dispersion when using different values of $\delta$ and $p$, the Root Mean Square Deviation (RMSD) is used. It is defined as:

$$\text{RMSD} = \left( \frac{1}{n} \sum_{i=1}^{n} | U_i^t - U_i^t | \right)^{\frac{1}{2}},$$  \hspace{1cm} (3.26)
where $U^t_i$ and $U^t_i$ are the displacements at node $i$ at time $t$ obtained from a classical continuum (non dispersive) analysis and from peridynamics, respectively. The temporal evolution of the RMSD for a wave propagating through a one dimensional LPS are shown in Figure 3.9 for three different choices of $\delta$ and $p$. As Figure 3.9a shows, reducing the horizon size while keeping the particle lattice spacing fixed reduces dispersion and it is also computationally cheaper. From Figure 3.9b, it is observed, that dispersion can also be reduced by increasing $p$. It is noted, that dispersion can also be reduced by refining the particle lattice spacing, while keeping a fixed number of particles in the horizon, i.e., considering the case of $\delta$-convergence (see Figure 3.1a and Figure 3.1b). However, this would increase the computational cost.
3.3 Physical interpretation of the peridynamic horizon

Elastic wave dispersion due to node-skipping interactions in a peridynamic model can be minimized with an appropriate choice of influence functions and peridynamic horizon. Motivating the idea of associating elastic wave dispersion in the LPS model with actual dispersion observed in heterogeneous materials is explored, to provide a link between actual physical properties and the peridynamic parameters.

Peridynamics is a macroscopic theory of material mechanics. The wave dispersion analysis of a linear peridynamic solid presented in the previous sections has shown, that non-local interactions of peridynamic nodes/particles lead to wave dispersion, an aspect that is also experimentally observed for real materials with heterogeneities (Gранe 1961, Winkler 1983). Even though, the inter-particle interactions in a peridynamic continuum a priori has no physical background, it can be argued that the material it represents at a macroscopic scale can be assumed to be one with a microstructure. The elastic behavior of a material with microstructure can be modeled using classical continuum mechanics assuming macroscopic homogeneity and using effective material properties (Timothy and Meschke 2016a,b). However, for strongly varying stress and strain fields with wavelengths close to the size of the heterogeneity, using effective material properties within a classical continuum theory is fundamentally wrong as it ignores the tortuous transfer of internal forces across grains resulting in strong strain gradients for an applied external loading. This disparity in up-scaling of such material behavior can be accounted for by introducing non-locality into continuum theories (Bažant 1991, Drugan and Willis 1996, Willis 1985) that are characterized by a non-linear elastic wave dispersion relations.

Thus, the intrinsic property of peridynamics to model non-linear elastic wave dispersion suggests, that by specifying appropriate values for the parameters $p$ and $\delta$, the 'peridynamic solid' should be able to mimic a heterogeneous material with respect to elastic wave dispersion. Fur-
thermore, this also allows one to provide a physical meaning to the peridynamic horizon $\delta$ and the weighting function shape parameter $p$. It must be noted that BAŽANT ET AL. (2016) suggest, that the ‘fictitious’ node-skipping interactions in peridynamics are physically unjustified except at the atomic scale. This is true, assuming that the peridynamic nodes represent particles. However, instead of considering the peridynamic nodes as particles, it is proposed to associate the length scale of the horizon with the particle size. The wave dispersion behavior of peridynamics is a feature and not a deficiency in comparison to classical continuum models. This feature of peridynamics is leveraged with respect to wave dispersion to model real heterogeneous materials.

Calibration procedure and validation

Figure 3.10: Sensitivity of the dispersion curves with respect to the horizon size, using a constant $\omega_1$ and a Gaussian $\omega_3$ influence function, and comparison with the experimental data for Massilon sandstone (WINKLER 1983).

To relate the peridynamic parameters to a physically measurable quantity, experimental dispersion relations and the elastic parameters from WINKLER (1983) and ZHANG AND BENTLEY (1999) are used, respectively, for two sandstones (Berea and Massilon sandstone) at different levels of confining pressures (10, 20 and 40 MPa). The dispersion curves for longitudinal waves obtained from using the influence function $\omega_1$ for different values of the peridynamic horizon $\delta$ are plotted in Figure 3.10a. In this figure, the experimental dispersion data measured on Massilon sandstone at a confining pressure of 20 MPa (WINKLER 1983) is also included. It is observed, that for a horizon of $\delta \approx 250 \, \mu m$, the numerical dispersion curve replicated well the dispersion data for Massilon sandstone.

Next, the influence of the shape of the influence function using $\omega_3$ according to Eq.(3.10) is investigated. Figure 3.10b shows the dispersion plots for different values of $\delta$, assuming a shape parameter $p = 1$ and includes also the dispersion data from Massilon sandstone. From this Figure, the dispersion relation obtained from $\delta \approx 270 \, \mu m$ is found to fit the experimental data. Fixing the peridynamic horizon as $\delta = 270 \, \mu m$, the optimal shape of the influence function $\omega_3$ is identified by
Figure 3.11: Sensitivity of the dispersion curves with respect to the shape parameter $p$ at a fixed horizon size $\delta = 270 \mu m$, and comparison with the experimental data for Massilon sandstone (WINKLER 1983).

In analogy to the calibration procedure for Massilon sandstone, using the influence function $\omega_3$, the value of peridynamic horizon $\delta$ and the shape parameter $p$ are calibrated for Berea sandstone, using the experimental dispersion data given in WINKLER (1983). The best fit was determined by setting the horizon $\delta = 180 \mu m$ and the shape parameter $p = 2.0$. It must be noted that the size of the peridynamic horizon determined for both materials is only slightly larger than the average grain-size of the materials. The grain size of Berea sandstone used in the experiment is $\approx 150 - 200 \mu m$ and for Massilon sandstone $\approx 200 \mu m$. This must be compared with a horizon $\delta = 180 \mu m$ calibrated...
for Berea sandstone and 270 µm for Massilon sandstone. It is concluded, that in both cases, the peridynamic horizon has the same order of magnitude as the characteristic size of the heterogeneity, i.e., the grain size.

Having calibrated the peridynamic model parameters for both Berea and Massilon sandstone for one level of confining pressure (20 MPa), Figure 3.12 compares dispersion plots (frequency vs. phase velocity of the longitudinal waves) obtained from the peridynamics model and the experimental tests for Berea (Figure 3.12a) and Massilon sandstone (Figure 3.12b), respectively, for additional levels of confining pressure which have not been included in the calibration procedure. An excellent agreement is observed in all cases.

While in the previous analysis, the particle lattice spacing was kept constant and set to one third of the horizon, now the influence of the particle lattice spacing on the dispersion plots is investigated. In Figure 3.13, the velocity is plotted as a function of the frequency for various lattice spacings, ranging from Δx = 10 µm to Δx = 75 µm. Only a small change in the dispersion curves is observed as the lattice spacing is reduced. This confirms, that the aforementioned conclusions regarding the relation of the peridynamic horizon to the microstructure holds independently of the discretization.

### 3.4 Summary

Dispersion relations for a state-based linearized LPS have been derived in this chapter. State-based peridynamics is highly dispersive due to its nonlocal characteristics and it was proposed that these nonlocal interactions can be minimized by choosing a combination of the size of the peridynamic horizon and the shape of the influence function in a way that the peridynamic solution approaches the classical continuum (non-dispersive) solution, for a given set of frequencies of excitation. The possibility of modeling these nonlocal interactions provides a way to at least approximately fit the peridynamic dispersion curve to experimental dispersion curves, unlike the classical theory which has a linear dispersion relation. The peridynamic horizon δ and the shape parameter p have been...
calibrated to two different types of sandstone, for which experimental dispersion curves are available. The model was then validated by comparing the experimental and numerical dispersion plots for different levels of confining pressures. It was observed, that in both cases, the size of the peridynamic horizon is in the range of the characteristic size of the heterogeneities, i.e., the grain size of the material. For heterogeneous materials with a granular microstructure, the proposed identification procedure enables one to provide a physical interpretation to these parameters, which have been introduced originally as purely model related parameters without any physical background.
Chapter 4

Tension dominated failure

In peridynamic models for fracture, the dissipated fracture energy is regularized over a non-local region denoted as the peridynamic horizon. This chapter investigates the influence of this parameter on the dynamic fracture process in brittle solids, using two as well as three dimensional simulations of dynamic fracture propagation in a notched plate for two loading cases. The predicted crack speed for the various scenarios of the initially stored energy, also known as the velocity toughening behavior as well as characteristics of the crack surface topology obtained in different crack propagation regimes in 3D computational simulations are compared with the experimentally observed crack velocity and fracture surfaces for Polymethyl Methacrylate (PMMA) specimens. Furthermore, the influence of the specimen size on the dynamic fracture process using two dimensional peridynamic simulations is investigated. The fracture strengths and the velocity toughening relationship obtained from different specimen sizes are compared with the Linear Elastic Fracture Mechanics (LEFM) size effect relationship and with results from experiments, respectively. In addition, the performance of the peridynamic model in simulating the influence of loading rate on three benchmark problems dominated by tensile loads is tested. Fracture patterns obtained from simulations at varying loading rates for the Kalthoff-Winkler test, L-specimen test, and CT-specimen test are compared with experimental results.

Some of the contents of this chapter have been previously published in Butt and Meschke (2021b). The chapter utilizes the ordinary state-based peridynamics model (Section 2.2.2) in conjunction with the critical-energy based criterion (Section 2.4.2) to model fracture dominated by tensile loads. The main objectives of this chapter are:

- To investigate the influence of the peridynamic horizon on the dynamic fracture process using two- and three-dimensional simulations.
- To perform a convergence study on the velocity-toughening relationship of PMMA with respect to the peridynamic horizon.
- To investigate the mechanisms involved in dynamic crack propagation, such as micro- and macro-branching.
- To examine the influence of specimen size and geometry on fracture propagation.

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• To explore the capabilities of the peridynamics model in simulating loading rate-dependent fracture propagation in three benchmark experiments.

4.1 Dynamic fracture

During dynamic crack propagation, the stress field around the crack tip, the energy absorbed in the fracture process, as well as the topology of the fracture surface changes as a function of the crack tip velocity. There are bifurcation points in the stress fields at certain levels of crack propagation velocities after which velocity toughening mechanisms, such as micro-branching get activated and cause an increased dissipation rate due to additional surface creation SHARON ET AL. (1996). This leads to contradictions between the theoretical predictions and experimental observations. In the following a brief overview of the analytical, experimental as well as computational analyses performed to characterize dynamic crack propagation is provided.

Theoretical and experimental analysis

Linear elastic Fracture mechanics (LEFM) is an established theoretical framework to characterize and predict the initiation as well as the subsequent motion (position and velocity) of a moving crack, which started with the pioneering work of Inglis INGLIS (1913) and Griffith GRIFFITH (1921). LEFM predicts that cracks can not propagate arbitrarily fast, there are speed limits that they have to obey. The investigation of the stress field around a dynamically moving brittle crack of fixed length performed YOFFE (1951) suggested an explanation for this speed limit based on the bifurcation of the dynamic stress state around the moving crack tip. She showed that, as the crack speed increases to 60% of the shear wave speed, the maximum circumferential stress shifts from 0° (i.e., the plane in front of the crack) to ±60°. However, the resulting dynamic stress intensity factor from Yoffe’s solution was independent of the crack tip velocity, which is incorrect. This was later corrected by BROBERG (1960), who considered a crack that starts propagating at constant velocity from a zero initial length. The resulting ratio of dynamic to static stress intensity factor for the same crack length from Broberg’s analysis decreases with increasing crack velocity and vanishes at the Rayleigh wave speed \( v_r \), which is the theoretical velocity limit for a mode-I crack. This result was later confirmed by ATKINSON AND ESHELBY (1968). Afterwards, FREUND (1972a,b) analyzed dynamic crack propagation with a constant as well as a non-constant velocity while considering the interactions between the stress waves and cracks. The dynamic stress intensity factor obtained by FREUND (1972a) was in agreement with BROBERG (1960) and ATKINSON AND ESHELBY (1968), i.e., the terminal velocity for a mode-I crack is \( v_r \).

One of the contradictions between the predictions of LEFM (FREUND 1972a) and the observations from experiments (BOWDEN ET AL. 1967, RAVI-CHANDAR AND KNAUSS 1984b, SHARON ET AL. 1996) is related to the terminal velocity of cracks. According to LEFM, a crack should continuously accelerate up to the Rayleigh wave speed \( v_r \). However, in experiments triggering a mode-I crack, this value is never realized. The limiting crack velocity observed in experiments for soda-lime glass is about 0.51\( v_r \) (BOWDEN ET AL. 1967), around 0.7\( v_r \) for PMMA (SHARON ET AL. 1996) and about 0.45\( v_r \) for Homalite-100 (RAVI-CHANDAR AND KNAUSS 1984b). This
discrepancy is attributed to the assumption of a single sharp crack in the theoretical analyses. In experiments, however a single sharp crack is observed only up to a certain velocity and after that, an increased roughening of the fracture surface accompanied by an increase in the dissipation rate is detected. LEFM predictions (Freund 1972a) for brittle dynamic fracture are shown to be valid, as long as the assumption of a single propagating crack is replicated in the experiments (Sharon and Fineberg 1999). From postmortem fracture surface examinations (Fineberg et al. 1992, Quinn and Quinn 2007, Ravi-Chandar and Knauss 1984a), it has been shown, that the surface roughness of a propagating crack is an increasing function of the crack tip velocity. This increasing fracture surface roughness is attributed to the different micro-structural processes occurring at the crack tip as well as in the process zone in front of it. Ravi-Chandar and Knauss (1984a) attributed this fracture surface roughness to three main sources: the material heterogeneity (voids or inclusions), the material micro-structure and the interaction of the stress waves with the propagating crack (leading to the so-called Wallner lines (Quinn and Quinn 2007)). Fineberg et al. (1991, 1992), Sharon and Fineberg (1996) reported a well defined transition in the motion of the crack tip, from a smooth propagation to an oscillatory propagation above a critical velocity. They proposed the existence of a dynamic instability (micro-branching instability) above a critical crack tip velocity, which governs the crack tip oscillations and showed that these oscillations were correlated to periodic micro-structures observed on the fracture surface.

Computational analysis

A number of different classes of continuum models have been put forward to bridge the gap between dynamic fracture experiments and computational simulations. These continuum models are mostly governed by the partial differential equations of continuum mechanics. These partial differential equations are solved using approximation functions and their derivatives, which are constructed either locally using a mesh or using scattered points without any mesh connectivity. The first class of methods is known as mesh-based methods, such as Finite Element Method (FEM), while the second is known as mesh-free methods, such as the Diffuse Element Method Nayroles et al. (1992) or the Element Free Galerkin (EFG) method Belytschko et al. (1994). For a review of mesh-free methods, the interested reader is referred to Chen et al. (2017), Li and Liu (2002). To represent the discontinuity resulting from a crack, discrete as well as smeared representations of cracks as strong and weak discontinuities are employed in these models.

Cohesive zone models (CZM) Camacho and Ortiz (1996), Xu and Needleman (1994) equip interfaces of standard finite elements with a cohesive law to model crack propagation. These models provide autonomous initiation, propagation and branching of a crack Xu and Needleman (1994), however, the crack path is highly dependent on the particular topology of the discretization Falk et al. (2001), Zhou and Molinari (2004). A framework for interface elements using a variational (phase-field like) formulation was recently presented in Khisamitov and Meschke (2018). In Xu and Needleman (1994) some features of fast crack propagation were captured, such as crack branching and the existence of limit velocity for cracks. Impact damage in brittle materials was modeled in Camacho and Ortiz (1996) using a linearly decaying cohesive relation, discussing the existence of an intrinsic time scale related to the critical crack opening displacement.
and the elastic wave velocity even when using a rate-independent cohesive relation. More recently, Zhou et al. (2005) presented a rate-dependent cohesive law and compared the crack propagation velocities with a rate-independent cohesive relation which over-estimated the crack propagation velocities. Some critical artifacts of dynamic fracture simulations using cohesive zone models are also presented in Falk et al. (2001).

FEM in conjunction with cohesive elements experiences mesh bias when representing a discrete crack (a strong discontinuity). This mesh-dependence can be addressed by using adaptive re-meshing techniques which, however, become particularly challenging in 3D. Circumventing the use of a mesh in mesh-free methods facilitates modeling arbitrary cracks without re-meshing (Belytschko et al. 1996, Nguyen et al. 2008). A second option for having a discrete representation of cracks without the need for re-meshing is accomplished by the eXtended FEM (XFEM) (Belytschko and Black 1999, Moës et al. 1999), which allows the crack to propagate through the finite elements, employing enrichments with a strong displacement discontinuity kinematics. This removes the mesh bias and allows the crack to propagate in any direction. However, it requires additional degrees of freedom and suitable crack indicators for the advancement of the crack tip as well as crack tracking which adds additional complexity (Rabczuk et al. 2010). In particular, additional criteria for crack branching, coalescence and arrest are required. A loss of hyperbolicity criterion was presented in Belytschko et al. (2003) to predict the onset of branching.

For modeling complex fragmentation processes in brittle materials it is desirable to represent crack propagation independently from the discretization with minimal or no external intervention such as tracking of discontinuities or decisions on the direction of crack growth. A number of numerical models for fracture simulations rely on non-local averaging approaches to regularize the surface energy of the discrete crack over a length in order to avoid mesh dependence. The non-local approaches generally provide an autonomous crack initiation, growth and branching and one does not need to track the crack tip. Some models in this category include the non-local damage model (Piaudier-Cabot and Bazant 1987), gradient enhanced damage models (Peerlings et al. 1998), eigen-erosion models (Pandolfi and Ortiz 2012), phase-field models (Bourdin et al. 2008) and peridynamics (Silling 2000). The similarities and differences between the gradient damage and phase-field damage models are analyzed in de Borst and Verhoosel (2016). Phase-field models for dynamic fracture (Borden et al. 2012, Hofacker and Miehe 2013) regularize the discontinuity over a characteristic length, which defines the width of the failure zone. Hence, the representation of the discontinuity is not discrete anymore. In Bleyer and Molinari (2017), micro-branching instability was modeled using a phase-field model. It was reported that the length and the frequency of the micro-branches depends on the phase-field internal length scale. Some of the features of dynamic fracture propagation, such as a limiting crack speed, toughening of the material with increasing crack speed and crack branching, were qualitatively reproduced in Bleyer et al. (2017). The effect of the internal length scale of the phase-field on the crack propagation velocity and dissipated energy is discussed in Borden et al. (2012). However, the mechanisms which govern the change of the dynamics of cracks with respect to this internal length scale still do not seem to be well understood.

Besides continuum models, atomistic simulations Abraham et al. (1997), Abraham and
4.1. DYNAMIC FRACTURE

GAO (2000) have been used to investigate dynamic fracture processes. In BUEHLER AND GAO (2006), it was argued that the large deformations at the crack-tip leads to the transition of the material around the crack tip to a hyper-elastic zone. This hyper-elastic zone sets a local value of the Rayleigh wave velocity around the crack tip which limits the crack propagation velocity.

Peridynamic analysis

A mesh-free method based on bond-based peridynamic continuum presented in SILLING AND ASKARI (2005) was able to reproduce dynamic fracture and fragmentation of brittle solids subjected to impact loads. Bond-based peridynamics utilizes central force potentials between material points to characterize the force interactions. This leads, however, to a fixed Poisson’s ratio of $1/4$ for 3D $1/3$ for 2D problems. State-based peridynamics (SILLING ET AL. 2007) does not suffer from this limitation. It can also incorporate constitutive relations from the classical continuum theory (i.e., constitutive relations involving a deformation gradient) using the correspondence framework in peridynamics (SILLING ET AL. 2007). However, the correspondence framework suffers from zero energy mode instability (BEHZADINASAB AND FOSTER 2020a, SILLING 2017), stabilization conditions and stabilizing terms to the strain energy density have been proposed as remedies in SILLING (2017), TUPEK AND RADOVITZKY (2014), WANG ET AL. (2016). Bond-based peridynamics uses a critical-stretch based criterion for bond failure (SILLING 2000). It is noted, that for state-based peridynamics, a critical-energy based failure criterion, which takes into account the total bond energy (i.e., isotropic as well as the deviatoric part of the deformation) was introduced in FOSTER ET AL. (2011). A comparison between the critical-stretch and critical-energy failure criteria is presented in DIPASQUALE ET AL. (2017), ZHANG AND QIAO (2018).

Dynamic crack propagation and branching in brittle materials, using a bond-based peridynamic model with critical-stretch failure criterion, was investigated in HA AND BOBARU (2010, 2011). Crack branching and overall fracture patterns were shown to be in qualitative agreement with the experiments. Using a convergence study with respect to the horizon size, they showed, that the crack velocity profile stays below the Rayleigh wave speed and that it converges to the maximum crack velocity observed in experiments, once the horizon reaches sub-millimeter values. A peridynamics model was also used to analyze the dynamic fracture of shale and rock material in BUTT AND MESCHKE (2021a), CHENG ET AL. (2019). In AGWAI ET AL. (2011), a comparative study between cohesive zone models, the XFEM and peridynamics was provided and the crack propagation patterns and velocities were compared. The crack velocities obtained using all three methods were overestimated compared to the experiments, but remained below the Rayleigh wave velocity. Dynamic brittle fracture and crack branching was investigated in BOBARU AND ZHANG (2015) using bond-based peridynamic simulations performed using various transient boundary conditions. A stress wave pile-up mechanism at the crack tip, which deflects the damage away from the symmetry line in front of a mode-I crack, was investigated as the possible reason for crack branching.

A simulation tool which is able to reproduce and validate the relationship between the crack velocity and the fracture energy release rate observed in brittle dynamic fracture experiments, without incorporating an a priori phenomenological crack velocity or strain rate dependency, does not ex-
ist. Such phenomenological rate-dependent criteria have been used to influence the crack velocity in conjunction with interface elements (CZM), (see, e.g. ZHOU ET AL. (2005)), non-local continuum damage models WOLFF ET AL. (2015), phase-field models DOAN ET AL. (2017) as well as peridynamics BUTT AND MESCHKE (2018). In this chapter a phenomenological rate-dependent criterion is not used; instead a simple critical-energy based damage criterion is used. Hence, the dependence of the dissipated fracture energy on the crack propagation velocity is obtained purely from the interaction of the crack tip with the simulation domain.

4.2 Simulation setup: Plate under tension

The simulations are performed on a rectangular PMMA specimen with dimensions of 32 mm in length, 16 mm in height, and 0.5 mm in thickness. The crack is supposed to initiate from an initial notch with a length of 3 mm, as shown in Figure 4.1a. The material parameters for PMMA used in all simulations are presented in Table 4.1.

![Geometry of the plate specimen, with an initial notch of 3 mm at y = 8 mm.](image)

![Y-displacement field under initial quasi-static loading.](image)

**Figure 4.1:** PMMA specimen used in the simulations: (a) Simulation setup; (b) Initial loading

<table>
<thead>
<tr>
<th>Material parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s Modulus, $E$ (Pa)</td>
<td>$3.09 \times 10^9$</td>
</tr>
<tr>
<td>Poisson’s ratio, $\nu$</td>
<td>0.35</td>
</tr>
<tr>
<td>Density, $\rho$ (kg/m$^3$)</td>
<td>1180</td>
</tr>
<tr>
<td>Fracture energy, $G_c$ (J/m$^2$)</td>
<td>300</td>
</tr>
<tr>
<td>Rayleigh wave speed, $v_r$ (m/s)</td>
<td>906</td>
</tr>
</tbody>
</table>

**Table 4.1:** Material properties used for PMMA.

In peridynamic analyses, as discussed in Chapter 3, two kinds of convergence studies can be performed. One is $\delta-$ convergence (HA AND BOBARU 2010), which is performed by keeping the nodal density $n$ (number of discrete points along the radius of the peridynamic horizon) constant, while the horizon size $\delta$ is systematically decreased, i.e., $\delta \rightarrow 0$, the solution in this case approaches the classical continuum solution (SILLING AND LEHOUCQ 2008). $\delta$ and $n$ are related to each
other by \( \delta = n \Delta x \), where \( \Delta x \) is the mesh size. The second is \( n \)-convergence (Seleson and Littlewood 2016), where the horizon \( \delta \) is kept fixed and the nodal density \( n \) is increased. As \( n \to \infty \) the solution approaches the analytical solution of peridynamics for the particular horizon size. In this work the focus is on \( \delta \)-convergence, considering four values for the peridynamic horizon (\( \delta = 280, 210, 140, \) and \( 70 \) \( \mu m \)) with an approximate mesh size \( \Delta x = 80, 60, 40, \) and \( 20 \) \( \mu m \), respectively. This results in \( n = 3.5 \) for all simulations. For \( n \) lower than 3, it has been observed, that the cracks starts following the mesh, resulting in staircase fracture patterns. As very high values of \( n \) may become computationally expensive, a feasible choice of \( n = 3.5 \) is made. This discretization leads to around \( 0.08, 0.142, 0.32 \), and 1.28 million material points in two dimensions and \( 0.48, 1.138, 4.16 \), and 32.0 million material points in three dimensions for \( \delta = 280, 210, 140, \) and \( 70 \) \( \mu m \), respectively. All simulations in this chapter are carried out using an extended version of the open-source software Peridigm (Littlewood 2015, Parks et al. 2012).

In the experiments from Fineberg et al. (1991, 1992), Sharon et al. (1996), the specimens were loaded incrementally every \( 10^{-20} \) s at very low strain rates in order to dampen the elastic waves induced by the loading. Applying such a slow loading in a full dynamic simulation would be extremely time consuming. In order to eliminate the effect of elastic waves due to transient loads, a combination of an implicit quasi-static and an explicit dynamic solver is used. In the quasi-static part of the solution, the specimen boundaries are subjected to prescribed displacements such that a desired level of elastic strain energy per unit area is stored in front of the crack tip. Subsequently, the simulation switches to an explicit dynamic solver, while keeping the displacement at the specimen boundaries fixed, and the crack is allowed to propagate. For the explicit dynamic solver, a time step of \( 1.0 \times 10^{-9} \) s is used for all simulations in order to avoid any influence of the temporal discretization. A similar combination of solvers has also been used in Bleyer et al. (2017), Butt and Meschke (2019), Zhou et al. (2005) for the same purpose.

In each simulation, a displacement \( \Delta U \) (Figure 4.1a) is applied in \( y \) direction on the top and bottom surfaces of the specimen quasi-statically (while keeping the crack stationary), i.e., ignoring the inertia effects in the simulation domain (Figure 4.1b). The specimen is unconstrained in \( x \) direction. This loading condition provides a constant value of stored elastic energy \( G \) per unit area prior to fracture in front of the initial notch:

\[
G = \frac{E(2\Delta U)^2}{2h} = \frac{2E\Delta U^2}{h}.
\]  

(4.1)

Once the crack propagates completely through the specimen, \( G \) would be approximately the total amount of energy dissipated in the fracture process. After achieving the desired value of elastic energy \( G \) by applying \( \Delta U \) according to Eq. (4.1), the analysis switches to an explicit dynamic solver without changing the boundary conditions and henceforth, the crack is allowed to propagate dynamically taking inertia effects into account.

The crack propagation speed \( v_c = \dot{a} \) is computed by tracking the crack tip every 100 solution steps, i.e., the computed crack speed is averaged over 100 time steps, where \( a(t) \) is the position of the crack tip. As simulations use a time step size of \( 1.0 \times 10^{-9} \) s, the crack velocity is computed ten times in one \( \mu s \). The crack tip is defined as the most right node in the specimen experiencing a
damage level larger than 0.4. In case of macroscopic crack branching, the faster propagating branch is tracked for determination of the crack velocity.

The rate of energy dissipated per unit crack area $\Gamma$ released during fracture propagation is computed from:

$$E_{el}(t) + E_{kin}(t) + E_{diss}(t) = C,$$

as:

$$\Gamma(t) = \frac{dE_{diss}(t)}{d\bar{a}(t)} = -\frac{dE_{el}(t)}{d\bar{a}(t)} - \frac{dE_{kin}(t)}{d\bar{a}(t)}.$$  \hspace{1cm} (4.3)

$E_{el}(t)$, $E_{kin}(t)$ and $E_{diss}(t)$ denote the total elastic, kinetic and the dissipated energy as a function of time. $C$ is the initially (quasi-statically) stored elastic strain energy and $\bar{a}(t)$ is the area created by the propagating crack as a function of time. $\bar{a}$ is computed by assuming that a single crack is propagating through the medium, i.e., without taking the additional area created by the micro-branches into account. Hence, an increase in $\Gamma$ is expected when the micro- and macro-branches start to initiate and propagate (crack roughening), see Figure 4.3.

### 4.3 2D simulations of crack propagation in PMMA

In this section, results from 2D plane-stress simulations of crack propagation in a PMMA plate are presented. Initially, monotonically increasing loads are considered to investigate the influence of the peridynamic horizon on the (quasi-static) fracture strength and the effective stiffness. In a subsequent series of simulations, a combination of an implicit quasi-static and an explicit dynamic solver will be used to load the plates to a desired level prior to fracture initiation. Comparisons between cracking patterns, crack speed, evolution of energy dissipation rate as well as the elastic and kinetic energy at different loadings, obtained for varying horizon sizes, are presented.

#### 4.3.1 Crack propagation under monotonic loading

The motivation behind these simulations is to investigate the influence of the peridynamic horizon on the fracture strength and effective stiffness. These simulations are performed at a loading rate which gives a straight propagating crack without any branches. The horizontal boundaries of the PMMA plates (Figure 4.1a) are loaded monotonically until a crack starts propagating from the initial notch. The displacement is applied at a rate of 3 mm/s.

The load-displacement relationship obtained at the top boundary (at $y = 16$ mm) is shown in Figure 4.2a. It can be seen that the effective stiffness is not sensitive with respect to the horizon size. The same holds for the fracture strength, which provides almost identical results for $\delta = 140$ and 70 $\mu$m and a marginal reduction of 4% for the largest horizon size 280 $\mu$m. The figure confirms, that by virtue of the determination of the energy density in a bond according to Eq. (2.46), the fracture energy $G_c$ is preserved independently from the horizon size. Figure 4.2b shows the temporal evolution of the crack tip position. Due to slight differences in the fracture strengths, the cracks initiated at slightly different times in the four specimens. However, the crack propagation velocity is almost same ($v_c \approx 538$ m/s) for all four sizes of the peridynamic horizons.
4.3. 2D SIMULATIONS OF CRACK PROPAGATION IN PMMA

Figure 4.2: Two dimensional crack propagation simulation with monotonically increasing displacement at boundaries: (a) force-displacement relationship at the top boundary and (b) temporal evolution of the crack tip position.

4.3.2 Crack propagation for different levels of quasi-static loadings

In these simulations, the specimens are loaded quasi-statically up to different levels while restricting the initial notch (shown in Figure 4.1a) from propagating. After reaching the desired loading value, the simulations switch from an implicit to an explicit dynamic solver and the crack is allowed to propagate. In this subsection, the influence of the peridynamic horizon is investigated on the cracking pattern, the crack tip velocity, dissipation rate, energy balance and the crack velocity toughening mechanism. This comparison is performed for four loading levels $\Delta U = 21 \mu m$, $\Delta U = 25 \mu m$, $\Delta U = 30 \mu m$, and $\Delta U = 40 \mu m$. These loading levels are related to four levels of elastic prestressing of the plate (Eq. 4.1), which lead to four different characteristics of crack propagation (smooth crack propagation, rough crack propagation, crack branching and multiple crack branching).

Fracture pattern and crack tip velocity

Figure 4.3 presents the cracking patterns obtained by simulations. It can be seen in the first row of Figure 4.3 that the crack paths obtained for the lowest loading level $\Delta U = 21 \mu m$ (which leads to the lowest crack propagation velocity) from all four horizon sizes are smooth and without any additional dissipative features. It should be noted that in the simulations $\Delta U = 21 \mu m$ is the smallest load at which cracks propagate, i.e., at $\Delta U = 20 \mu m$ cracks do not yet propagate in all specimens. With an increase in load ($\Delta U = 25 \mu m$), the crack path starts to exhibit slight roughness along the crack path (second row of Figure 4.3). At $\Delta U = 30 \mu m$ (third row of Figure 4.3), macroscopic branching attempts along the main crack can be seen. And at $\Delta U = 40 \mu m$ (fourth row of Figure 4.3), two stable daughter cracks propagate. The temporal evolution of the crack tip position and the normalized crack propagation velocity with respect to crack tip position, for all four considered loading cases in Figure 4.3, are presented in Figure 4.4. Crack propagation velocity is normalized with respect to the Rayleigh wave speed $v_r$.

For $\Delta U = 21 \mu m$, the crack tip position is almost identical for all four horizon sizes, as can be
Figure 4.3: 2D simulation of crack propagation in PMMA specimens: Final crack patterns obtained from two dimensional peridynamic simulations for four loading levels (rows) and four different horizon sizes (columns).

seen in Figure 4.4a. As the crack paths obtained for this loading value were smooth and featureless (first row of Figure 4.3), this results in smooth crack propagation velocity with a few fluctuations between 25 to 30 mm crack length, as shown in Figure 4.4b. These few fluctuations can be attributed to a slight roughness along the end of the crack path, which is hard to see for $\delta = 20, 40$ and $60 \mu m$, but is visible for $\delta = 280 \mu m$.

A rough crack path is obtained for $\Delta U = 25 \mu m$, as shown in second row of Figure 4.3. It can be observed, that the cracks start smooth and develop some roughness afterwards, connected with a slight deviation of the crack path from a straight horizontal line. This smooth crack propagation in the early stage corresponds to the smooth crack tip velocity up to 7 mm in Figure 4.4d.

For the loading level $\Delta U = 30 \mu m$, the main crack starts to develop branches along its complete path as presented in the third row of Figure 4.3. The crack velocities plotted in Figure 4.4f show high fluctuations from the beginning, which is a consequence of the non smooth crack propagation. The vertical lines in Figure 4.4f indicate crack branching events.

When the loading is increased to $\Delta U = 40 \mu m$, two stable branches develop soon after propagation starts (fourth row of Figure 4.3). Both stable branches develop further subbranches along their path. The initial branching angles for all horizon sizes are around $35^\circ$. It should be noted that, the difference between the crack propagation velocities with respect to the horizon size for straight and smooth crack propagation was negligible and this difference increased as the crack path started to roughen and branch.
4.3. 2D SIMULATIONS OF CRACK PROPAGATION IN PMMA

Dissipation rate and energy balance

The influence of the peridynamic horizon on the evolution of elastic, kinetic and dissipated energy (Eq. 4.2) as well as the instantaneous dissipation rate \( \Gamma \) (Eq. 4.3) over crack length are discussed in this section. Figure 4.5 presents the evolution of the dissipation rate \( \Gamma / G_c \) and the elastic, kinetic and dissipated energies (normalized with respect to total energy \( C \) in Eq. (4.2)) plotted over the crack tip position for the specimens shown in Figure 4.3.

By comparing Figures 4.5a, 4.5c, 4.5e, and 4.5g, it can be seen that the dissipation rate \( \Gamma \) increases with increasing \( \Delta U \). As the crack velocity increases, the normalized dissipation rate \( \Gamma / G_c \) increases from around 1.0 (Figure 4.5a) to approximately 4.0 (Figure 4.5g). This is caused by the additional surface created by crack roughening and branching at higher crack propagation velocities. The increase in dissipation with increasing crack velocity is known as crack velocity toughening, which ultimately sets the speed limit on propagating cracks.

A crack propagating smoothly should consume approximately \( G_c \) amount of energy per unit area, which is the case for the loading level \( \Delta U = 21 \mu m \) (first row of Figure 4.3). As the load level is increased to \( \Delta U = 25 \mu m \), a rough crack path is observed, however, without yet developing macroscopic branches, as presented in the second row of Figure 4.3. It can be seen that \( \Gamma / G_c \) in Figure 4.5c oscillates between 1.0 and 2.0, but never exceeds 2.0, which is the energy required to

![Graphs showing crack propagation and energy dissipation](image-url)
Figure 4.4: 2D simulation of crack propagation in PMMA specimens: Evolution of crack tip position with respect to time (left column) and normalized crack tip velocity normalized with respect to crack tip position (right column) for $\Delta U = 21\,\mu m$ in (a) and (b), $\Delta U = 25\,\mu m$ in (c) and (d), $\Delta U = 30\,\mu m$ in (e) and (f), and $\Delta U = 40\,\mu m$ in (g) and (h), respectively. Vertical lines in (f) and (h) mark the branching events. The fracture patterns obtained for these loading cases are shown in Figure 4.3.

Form two smooth fractures of unit area. $\Gamma/G_c > 2.0$ was also suggested in BLEYER ET AL. (2017), using a phase-field damage model, as an energetic criterion for macroscopic branching.

For $\delta U = 30$ and $40\,\mu m$, the crack patterns show macroscopic branches for all four horizon sizes as shown in the third and fourth row of Figure 4.3, respectively. Figure 4.5e and Figure 4.5g present the normalized dissipation rate for these two loading cases. Vertical lines in these figures correspond to the major branching events during crack propagation. In Figure 4.5e ($\Delta U = 30\,\mu m$), the dissipation rate ($\Gamma/G_c$) for all four horizon sizes is oscillating around 2.0. This is a case where one crack tip is not enough to dissipate all the energy and two equivalent macroscopic cracks (i.e., branching) would dissipate too much energy. According to Figure 4.5g, for the case $\Delta U = 40\,\mu m$, $\Gamma/G_c$ stays well above 2.0. This indicates, that two stable branches develop, which again develop their own sub branches during propagation. It is noted, that the initial crack branching occurs at almost the same position of the crack tip for all four horizon sizes.

Figure 4.5 shows, that the growth of the dissipated energy is accompanied by the growth of the
kinetic energy during the crack propagation. This is because the evolution of the kinetic energy around the tip for a straight propagating crack depends directly on the crack speed. As a mode-I crack separates the material into two pieces during dynamic fracture, the crack faces move with a certain velocity (proportional to the crack propagation velocity) perpendicular to the direction of the propagating crack, this motion contributes to the total kinetic energy of the specimen. In the context of peridynamic simulations of dynamic fracture, this will be explained for the case of a straight and smooth propagating crack, without any branches, as obtained for the loading level $\Delta U = 21 \mu m$. As the crack propagates, a damaged region is created along the crack faces. As the material is less stiff in this damaged zone as compared to the bulk material, a part of the released energy is transformed into kinetic energy in this region. This process is illustrated in Figure 4.6 at three different positions of the crack tip for different horizon sizes. Only marginal differences of the size of the concentrated kinetic energy density zone around the crack tip is observed for this loading case, which is confirmed by the small influence of $\delta$ on the evolution of the total kinetic energy in Figure 4.5b. Nonetheless, there are differences with respect to the wave dispersion properties which result in different patterns of trailing waves for each horizon size Butt et al. (2017).
Crack velocity toughening mechanism

This section focuses on the velocity toughening behavior, which governs the crack tip speed limit, and the influence of the peridynamic horizon size on it. The velocity toughening mechanism is characterized by the relationship between the energy stored prior to fracture $G$ (Eq. 4.1) and the crack propagation speed $v_c$. With increasing $G$, the crack propagation velocity increases up to an asymptotic value which sets the crack tip speed limit. Various levels of $G$ are selected from Eq. (4.1) by choosing equal intervals of $\Delta U$, for $G < 2.0 \text{ KJ/m}^2$ an interval of 5.0 $\mu$m is selected and for $G > 2.0 \text{ KJ/m}^2$ it is set to 10.0 $\mu$m.

The average crack velocities $v_c$, computed as explained in Section 4.2, and normalized with respect to $v_r$ for the selected levels of $G$ and for all considered horizon sizes, are plotted in Figure 4.7. It is noted, that at higher load levels, and for larger horizon sizes, the cracks simultaneously started propagating from initial notch as well as from the top and bottom corner of the right hand
vertical boundary (see bottom right specimen in Figure 4.15). These specimens were not considered in Figure 4.7. In addition, also experimental data from SHARON ET AL. (1996) is included in Figure 4.7 for comparison. It is noted, that results from experiments presented in the literature (e.g. FINEBERG ET AL. (1991), ZHOU ET AL. (2005)) performed on PMMA show velocity toughening characteristics in a similar range.

The fracture patterns obtained from the finest spatial resolution, i.e., for $\delta = 70 \mu m$ (in green color in Figure 4.7), for nine increasing levels of the initial stored energy $G$ are shown in Figure 4.8. A transition is observed from a single smooth propagating crack at $G = 170 J/m^2$ to a rough crack path with short lived branches along the way at $G = 348 J/m^2$ and to stable macro-branching for larger load levels from $G = 618 J/m^2$ onwards. At higher loading levels, the complexity of the fracture process increases, as the generation of daughter micro-branches evolving into new macro-branches repeats itself, eventually leading to a tree-like fracture pattern at $\delta = 100 \mu m$.

Figure 4.7 shows, that with decreasing size of the peridynamic horizon, the computed crack velocities show a converging behavior (see the results for $\delta = 70$ and $140 \mu m$). This convergence is in agreement with BOBARU AND ZHANG (2015), who also performed a $\delta$-convergence study with respect to the crack propagation speed using bond-based peridynamics with a critical stretch based fracture criterion, using a plate specimen similar to the one used in current work. They applied transient loads on the specimen boundaries and the crack faces, but without a spectrum of loading levels, which could not have been considered by using only an explicit dynamic solver. It can be observed from Figure 4.7, that the minimum crack velocity obtained for all four horizon sizes is almost identical (with differences within 1% of $v_r$). An additional observation from Figure 4.7 is, that as the energy stored per unit area $G$ increases, the difference between the average crack velocities for the smallest and the largest horizon size also increases. It is due to the difference in the spatial resolution, as the crack propagating in the finest mesh can generate a larger number of micro- and macro-branches as compared to the coarsest mesh, which is accompanied by a reduction
Figure 4.7: 2D simulation of crack propagation in PMMA specimens: Average crack velocities obtained from two dimensional simulations for four different horizon sizes $\delta$ plotted against the energy stored per unit area in front of the crack tip $G$ (Eq. 4.1) prior to fracture. The horizontal gray line marks the threshold for macroscopic branching. Experimental data from SHARON ET AL. (1996) is also added for comparison.

$\Delta U = 21 \mu m, G = 170 J/m^2$

$\Delta U = 30 \mu m, G = 348 J/m^2$

$\Delta U = 40 \mu m, G = 618 J/m^2$

$\Delta U = 50 \mu m, G = 966 J/m^2$

$\Delta U = 60 \mu m, G = 1391 J/m^2$

$\Delta U = 70 \mu m, G = 1893 J/m^2$

$\Delta U = 80 \mu m, G = 2472 J/m^2$

$\Delta U = 90 \mu m, G = 3129 J/m^2$

$\Delta U = 100 \mu m, G = 3863 J/m^2$

Figure 4.8: 2D simulation of crack propagation in PMMA specimens: Fracture patterns obtained from two dimensional simulations of crack propagation in PMMA specimens with peridynamic horizon size $\delta = 70 \mu m$. Different levels of loading ($\Delta U$) are characterized by initially stored energy ($G = 170 J/m^2 \sim G = 3863 J/m^2$).

of the average crack propagation speed. It is worth to note, that the macroscopic branches which propagate through the whole length of the specimen start around a similar level of stored energy $G = 618 J/m^2$ for all horizon sizes. This level of $G$ is marked in Figure 4.7 by a horizontal gray
4.4 3D simulations of crack propagation in PMMA

This section investigates the dynamic fracture process by performing simulations similar to Section 4.3, using, however, now a three dimensional peridynamic model of the PMMA plate shown in Figure 4.1a with a thickness of \( t = 0.5 \) mm. As discussed in Section 2.2, the LPS model suffers from surface effects, since the material points located along the boundaries have incomplete nonlocal neighborhoods. Therefore, for the three dimensional case, the parameter \( t/\delta \) becomes relevant. For the 3D simulations, it is expected, that the effective stiffness \( K_{\text{eff}} \) will depend on the peridynamic horizon because of the considerably larger number of material points along the boundary with incomplete neighborhoods as compared to the 2D case in Section 4.3.1. Hence, one goal of this section is to provide an insight on the influence of these surface effects on the fracture process.

4.4.1 Crack propagation under monotonic loading

The load-displacement relationship obtained and the temporal evolution of the crack tip position for the monotonic loading is shown in Figure 4.9. As expected, the effective stiffness (slightly) depends on the horizon size (Figure 4.9a). For the finest discretization using \( \delta = 70 \) \( \mu \)m, the effective stiffness is almost identical to the \( K_{\text{eff}} \) obtained from the two dimensional cases in Section 4.3.1. As regard to the fracture strength, slight increase with decreasing horizon size is observed. When comparing the results for the smallest horizon size, the 3D analysis (\( F_u = 127N \)) leads to a slightly smaller ultimate load as compared to the 2D case ((\( F_u = 137N \)).

Figure 4.9b shows the temporal evolution of the crack tip position. Due to the differences in the fracture strengths, the cracks start propagating at different times in the four analyses. Unlike in the 2D case presented in Section 4.3.1, the crack propagation velocities for all four peridynamic horizons also show differences in the range of 5% \( v_r \). This can be attributed to the differences in the effective elastic properties obtained for different horizon sizes. For constant density, the stiffness of a material is directly proportional to the volumetric and surface wave speed. For mode I cracks, the latter governs the maximum crack propagation velocity.
4.4.2 Crack propagation for different levels of quasi-static loadings

In analogy to Section 4.3.2, crack propagation at different levels of stored elastic energy is investigated in this section.

Figure 4.9: Three dimensional crack propagation simulation with monotonically increasing displacement at boundaries: (a) force-displacement relationship at the top boundary and (b) temporal evolution of the crack tip position.

Figure 4.10: 3D simulation of crack propagation in PMMA specimens: Crack patterns obtained from three dimensional peridynamic simulations for four loading levels (rows) and four different horizon sizes (columns).
### 4.4. 3D Simulations of Crack Propagation in PMMA

**Fracture pattern and crack tip velocity**

The cracking patterns obtained from three dimensional simulations are presented in Figure 4.10. The fracture pattern is similar to the 2D simulations. As before, a transition from smooth to a rough crack propagation is observed when increasing the load level from $\Delta U = 21 \mu m$ to $25 \mu m$. When the load level is increased to $\Delta U = 30 \mu m$, macro-branches start developing for the two large horizon sizes only, while a rough single crack with a few small micro-branches is observed for the two small horizon sizes ($\delta = 140 \mu m$ and $\delta = 70 \mu m$). For $\Delta U = 40 \mu m$, similar to the 2D simulations, macro-branching is observed for all horizon sizes.

The temporal evolution of the crack tip position and the crack propagation velocity (normalized by $v_r$) with respect to crack tip position is presented in Figure 4.11 for all four loading cases shown in Figure 4.10. For $\Delta U = 21 \mu m$, a smooth single crack with slight crack roughening when reaching the right face of the plate is realized, significant differences in the crack tip position are observed in Figure 4.11a. The maximum difference between the average crack propagation velocities obtained from the different horizon sizes is around 9% of $v_r$, while this difference was only 1% for the two dimensional case. For $\Delta U = 40 \mu m$, except for $\delta = 140 \mu m$, all analyses lead to at least two stable branches propagating through the complete length of the specimen, as shown in row 4 of Figure 4.10.
Figure 4.11: 3D simulation of crack propagation in PMMA specimens: Evolution of crack tip position with respect to time (left column) and normalized crack tip velocity normalized with respect to crack tip position (right column) for $\Delta U = 21 \mu m$ in (a) and (b), $\Delta U = 25 \mu m$ in (c) and (d), $\Delta U = 30 \mu m$ in (e) and (f), and $\Delta U = 40 \mu m$ in (g) and (h), respectively. Vertical lines in (f) and (h) mark the branching events. The fracture patterns obtained for these loading cases are shown in Figure 4.10.

In contrast to the 2D simulations, a distinct region of micro-branching is observed along the main crack (see for $\delta = 70 \mu m$ at $\Delta U = 40 \mu m$ before branching in Figure 4.10). Such micro-branches were not observed in 2D simulations, the cracks rather formed short lived macro-branches which also diverted the crack from propagating in a straight line, as can be seen in Figure 4.8. In the region of micro-branching, the crack velocity increases up to $86\%v_r$ at 8 mm crack length for $\delta = 70 \mu m$, this velocity level is shown by a horizontal dashed green line in Figure 4.11h. Around 10 mm crack length, two macro-branches start developing, this event is marked by the sudden decrease in crack velocity (around $70\%v_r$). From this observation it can be deduced, that a single crack in the micro-branching region propagates faster than compared to the individual macro-branches if it had branched.
**Dissipation rate and energy balance**

Figure 4.12 presents the evolution of the normalized dissipation rate $\Gamma / G_c$ and the normalized elastic, kinetic and dissipated energies over the crack tip position for all simulations shown in Figure 4.10. In contrast to the two dimensional case, where for smooth crack propagation $\Gamma / G_c$ was independent of $\delta$ (Figure 4.5a), the three dimensional simulations show a dependence on the peridynamic horizon (Figure 4.12a). This dependence is associated with differences in the effective stiffness and crack propagation velocities with respect to the horizon size. $\Gamma / G_c$ follows a similar trends as $K_{eff}$ (Figure 4.9a), i.e., it increases with increasing $\delta$. This also leads to a slight influence of the peridynamic horizon on the evolution of the portions of energies (Figure 4.12b).

As discussed in Section 4.3.2, the kinetic energy around a moving crack tip is directly proportional to the speed of the crack tip. And since the cracks in row 1 of Figure 4.10 ($\Delta U = 21\mu m$) propagate at different velocities (Figure 4.11a), there are differences in the kinetic energy density around the propagating crack tip with respect to $\delta$, as shown in Figure 4.13. The region of concentrated kinetic energy around the crack tip for $\delta = 70\mu m$ stays significantly smaller than the one obtained for $\delta = 280\mu m$ during the crack propagation. This leads to the differences observed in the evolution of the total kinetic energy seen in Figure 4.12b.
As discussed earlier, the dissipation rate is higher for a larger horizon, this is why macro-branching takes place in larger horizon sizes before the smaller ones in Figure 4.10. In contrast to the 2D simulations, here it can be observed that in 3D it is possible to have a single crack propagating with global $\Gamma/G_c > 2.0$, i.e., without macro-branching, as can be seen for $\delta = 70$ and 140 $\mu$m in Figure 4.12e. At $\Delta U = 40 \, \mu$m, macro-branching is observed for all four horizons (row 4 of Figure 4.10). For the 3D case a single crack can sustain significantly higher $\Gamma/G_c$, by the development of these quasi-periodic micro-branches, as compared to the two dimensional case where macro-branching occurs as soon as $\Gamma/G_c > 2.0$.

**Crack velocity toughening mechanism**

In analogy to the 2D case, the average crack velocities $v_c$ normalized with respect to $v_r$ are plotted in Figure 4.14 for different levels of $G$ stored in the specimen prior to fracture and for all considered
horizon sizes. At the load level \( \Delta U = 40 \, \mu m \) (i.e., \( G = 618 \, J/m^2 \)), initial cracks developed macroscopic branches soon after initiation, which fully propagated through the whole length of the specimen (except \( \delta = 140 \, \mu m \)). This level of \( G \) is shown in Figure 4.14 using a horizontal gray line. Compared to the 2D case, the crack speed, even for the smallest horizon size, is considerably large and almost approaches 95\% \( v_r \). As discussed in Section 4.4.2, the micro-branching mechanism observed in 3D simulations leads to a faster propagating crack tip in comparison to the speed of the individual branches if it had formed macro-branches (which is the case for the 2D simulations). A detailed discussion comparing 2D and 3D simulations is provided in Section 4.5.

The fracture patterns resulting from nine increasing levels of the initial stored energy \( G \) are presented in Figure 4.15 for the finest spatial resolution, i.e., for \( \delta = 70 \, \mu m \). The figure shows the transition from a single smooth propagating crack at \( \Delta U = 241 \, J/m^2 \), to a rough crack path at \( G = 348 \, J/m^2 \) and to the formation of micro-branches at \( G = 618 \, J/m^2 \), which finally lead to macro-branching.

**Crack surface topology: mirror-mist-hackle transition**

Figure 4.16 shows a three dimensional view of the fracture patterns obtained from six levels of \( \Delta U \), ranging from 25 to 70 \( \mu m \) after 10\( \mu s \). The transition of the surface roughness from a smooth to a rough state for the fracture obtained for \( G = 348 \, J/m^2 \) is presented in Figure 4.17. It is interesting to note, that the roughness of the simulated fracture surfaces is able to qualitatively reproduce the well-known mirror-mist-hackle transition. Fracture surfaces obtained by experiments in SHARON AND FINEBERG (1996) are also presented in the second row of Figure 4.17 for a qualitative comparison.

A surface, denoted as mirror is characterized by the propagation of a single sharp crack, creating a smooth and featureless crack surface. The misty zone is characterized by the daughter cracks which initiated (locally along the specimen thickness) but got arrested before forming a micro-
Figure 4.14: 3D simulation of crack propagation in PMMA specimens: Average crack velocities, obtained from three dimensional simulations for four different horizon sizes $\delta$ are plotted against the energy stored per unit area in front of the crack tip $G$ (Eq. 4.1) prior to fracture. The horizontal gray line marks the threshold for macroscopic branching. Experimental data from SHARON ET AL. (1996) is also added for comparison.

<table>
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<th>$\Delta U$</th>
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<tr>
<td>21 $\mu$m</td>
<td>170 J/m$^2$</td>
<td>30 $\mu$m</td>
<td>348 J/m$^2$</td>
<td>40 $\mu$m</td>
<td>618 J/m$^2$</td>
<td>50 $\mu$m</td>
<td>966 J/m$^2$</td>
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Figure 4.15: 3D simulation of crack propagation in PMMA specimens: Fracture patterns obtained for the peridynamic horizon size $\delta = 70$ $\mu$m. Different levels of loading ($\Delta U$) are characterized by initially stored energy ($G = 170$ J/m$^2 \sim G = 3863$ J/m$^2$).

branch. Finally, the hackle zone is caused by daughter cracks, which successfully form quasi-periodic micro-branches, some of which grow into macro-branches. The periodic features on the crack surface obtained in the hackle zone from the simulations are not in a quantitative agreement with the experiment, nonetheless the periodic topology is qualitatively similar.
4.4. 3D SIMULATIONS OF CRACK PROPAGATION IN PMMA

\[ \Delta U = 25 \, \mu m, \ G = 241 \ J/m^2 \]
\[ \Delta U = 30 \, \mu m, \ G = 348 \ J/m^2 \]
\[ \Delta U = 40 \, \mu m, \ G = 618 \ J/m^2 \]
\[ \Delta U = 50 \, \mu m, \ G = 966 \ J/m^2 \]
\[ \Delta U = 60 \, \mu m, \ G = 1391 \ J/m^2 \]
\[ \Delta U = 70 \, \mu m, \ G = 1893 \ J/m^2 \]

**Figure 4.16:** 3D simulation of crack propagation in PMMA specimens: Three dimensional view of the crack patterns (at \( \sim 10 \, \mu s \)) obtained from the simulation of crack propagation in a PMMA specimen with horizon size \( \delta = 70 \, \mu m \). Levels of loading are characterized by initial stored energies \( (G = 0.17 \, KJ/m^2 \sim G = 3.13 \, KJ/m^2) \).

**Figure 4.17:** 3D simulation of crack propagation in PMMA specimens: Qualitative comparison of the topology of the fracture surface obtained in PMMA from peridynamics simulations (top) and from experiment SHARON AND FINEBERG (1996) (bottom).

**Microbranching instability**

The length \( (l) \) and spacing \( (s) \) of micro-branches in peridynamic simulations are influenced by the peridynamic horizon size \( (\delta) \). Increasing \( \delta \) progressively leads to longer and farther apart micro-
branches for a fixed geometry and loading, as presented in Figure 4.18. However, the ratio between \(l\) and \(s\) remains invariant with changes in \(\delta\). The correlation between \(l\) and \(s\) for the selected horizon size is approximately 0.78, while a phase-field model by Bleyer and Molinari (2017) found it to be 0.7.

Simulations conducted on specimens with varying heights suggest that the frequency of micro-branches also depends on the rate at which elastic waves reflecting from the specimen boundaries interact with the crack tip. As the specimen height \(h\) decreases, reflected elastic waves from the specimen boundaries interact with the propagating crack tip more frequently, leading to more frequent micro-branching events, as shown in Figure 4.19. However, the correlation between \(l\) and \(s\) with changes in the specimen height remains relatively unchanged at approximately 0.72.
The findings from the peridynamic simulations indicate that the patterns of micro-branching are influenced by both the geometry of the specimen and an inherent material length scale that characterizes the dissipation mechanisms at the crack tip. In the case of peridynamics, this material length scale is the horizon size.

4.5 Interpretation of the analyses

4.5.1 Influence of the peridynamic horizon

Considering the load displacement relationship obtained from two and three dimensional crack propagation simulations of PMMA plates under monotonic loads presented in Figure 4.2a and Figure 4.9a, it is observed, that the effective stiffness almost shows no dependence on the peridynamic horizon in the 2D case, while a notable dependence is observed for the 3D case. Related to this observation, in contrast to the 2D simulations, the 3D simulations also show an influence of the peridynamic horizon on the crack propagation velocities (compare Figure 4.4 and Figure 4.11 for a loading level of $\Delta U = 21 \mu m$). This is not surprising, as the crack propagation velocity depends on the elastic wave propagation velocities, which are a function of the effective stiffness. The dependence of the effective stiffness on the horizon size for the three dimensional case is a consequence of the surface effects of peridynamic models. In the two dimensional case, the points with incomplete neighborhoods are only present at the vertical and horizontal boundaries. In the three dimensional case, in addition to the vertical and horizontal boundaries, all points along the x-y surfaces (at $z = 0$ and $z = 0.5 \text{ mm Figure 4.1a}$) also have incomplete neighborhoods.

From the relationships between $G$ and $v_c$ obtained from two and three dimensional simulations, one can observe that the difference between the crack propagation velocities with respect to $\delta$ increases with increasing $G$ (compare Figure 4.7 and Figure 4.14). As discussed earlier, the crack velocity reduces as soon as the crack branches. Crack roughening and micro-branching are also localized bifurcation attempts along the crack front which also reduce the main crack tip velocity. A crack tip propagating in a simulation domain with a very fine spatial resolution is able to form these features along the crack path more frequent as compared to a simulation with a coarse spatial resolution. Evidently, in both two and three dimensions, simulations with a high spatial resolution (e.g. $\Delta x = 20 \mu m$) is able to branch more frequent (slightly reducing crack speed at each bifurcation) as compared to simulation with a coarse discretization (e.g. $\Delta x = 80 \mu m$). Hence, as $G$ is increased, micro- and macro-branching starts, and the frequency at which the crack is able to bifurcate will depend on the spatial resolution. This leads to different crack propagation velocities observed for different peridynamic horizons at increasing loads.

4.5.2 Influence of dimensionality

As the effective stiffness for $\delta = 70 \mu m$ in 2D as well as 3D simulations is nearly identical, it can be assumed that the influence of the surface effects is not significant in this case. However, the crack propagation velocities obtained from two and three dimensional simulations for $\delta = 70 \mu m$ differ significantly, as is illustrated in Figure 4.20, in which the normalized crack propagation
Figure 4.20: Comparison of the stored energy-crack tip velocity relationship computed for 2D and 3D simulations for $\delta = 70 \mu m$. The horizontal gray line marks the threshold for macroscopic branching. Experimental data from SHARON ET AL. (1996) is also added.

Figure 4.21: Comparison of the fracture patterns obtained from 2D (left column) and 3D simulations (right column) for $\delta = 70 \mu m$.

velocities ($v_c / v_r$) obtained from 2D and 3D simulations at different levels of energy per unit area ($G$) stored in front of the initial notch are plotted. If only the effective stiffness would be governing the crack propagation velocity, one should not observe significant differences in the crack propagation velocities. Comparing again the fracture topologies for both cases, it must be concluded, that one of the major aspects that contributes to the difference of the crack propagation velocities obtained from 2D and 3D simulations is the micro-branching instability. The fracture patterns obtained from the 2D simulations presented in Figure 4.8 are qualitatively different than the ones obtained from the three dimensional simulations shown in Figure 4.15. The key qualitative differences can be best seen for $\Delta U = 30 \mu m$ and $\Delta U = 40 \mu m$ (before branching). For the ease of comparison, these two cases are presented side by side in Figure 4.21. In the 3D case the macro-crack propagates in a straight line with short lived branches on either sides, while in the 2D case a pronounced crack tip splitting is observed which results in the crack tip being diverted from propagating in a straight
4.5. INTERPRETATION OF THE ANALYSES

horizontal line.

As discussed in Section 4.4.2, macro-branching reduces the crack propagation speed of individual branches significantly as compared to a single crack propagating in the micro-branching regime. Micro-branching can be interpreted as an unsuccessful attempt by the crack tip to form a stable branch (BLEYER AND MOLINARI 2017, SHARON AND FINEBERG 1999). Bifurcation of the crack front occurs locally along the thickness of the specimen, and, given sufficient energy, this local bifurcation will expand along the thickness of the specimen to form a macro-branch. During expansion of the secondary crack along the thickness, the main crack keeps propagating. This reduces the driving force at this newly formed micro-branch and it gets arrested. When these localized bifurcations of the crack front are unable to expand through the specimen thickness, the fracture surface results in the misty zone shown in Figure 4.17. This process can happen repeatedly in a three dimensional simulation and provides a mechanism by which these simulations can even maintain $\Gamma/G_c > 2.0$ without forming stable branches (see Figure 4.12e and Figure 4.12g). In contrast, two dimensional simulations cannot provide such mechanisms for a propagating crack tip, as any bifurcation at the crack tip will lead to branching.

4.5.3 Influence of the specimen size

The differences between the crack propagation velocities obtained from the peridynamic simulations and experiments (Figure 4.20) is attributed mainly to the different sizes of the PMMA specimens used in the experiment and the simulations. In the experiments of FINEBERG ET AL. (1991), SHARON ET AL. (1996), the largest dimension of PMMA specimen used was 400 mm. In the experiment reported in ZHOU ET AL. (2005), the maximum dimension of the specimen is 320 mm. In contrast, the simulations presented here use a specimen which has the largest dimension of 32 mm.

Such large difference in the specimen size can lead to the differences observed in crack propagation velocity. The reason can be seen in the scaling for the simple case where the energy release rate $\Gamma \propto \sigma^2 l$ ($\sigma$ is the applied stress and $l$ is the instantaneous crack length). Considering two specimens where one is scaled in all dimensions (including the initial notch) to be significantly smaller than the other. A crack initiates in both specimens when $\Gamma = G_c$, i.e., when the energy release rate corresponds to the Griffith’s condition (GRIFFITH 1921). In the smaller specimen, since the initial crack length $l$ is small, the condition $\Gamma = G_c$ is realized at the cost of very high applied stresses $\sigma$. As a crack starts to propagate (assuming constant $\sigma$), the energy release rate $\Gamma$ will double when $l$ (the initial notch length) doubles, i.e., over a very short propagation distance for the small specimen and vice versa for the large specimen. In other words, the evolution of $\Gamma$ over the crack length will differ significantly for different specimen sizes (with higher $\Gamma$ for smaller specimen) and the corresponding crack tip acceleration and velocity will also differ accordingly (SHARON AND FINEBERG 1999). Additionally, depending on the size of the specimen, the elastic waves reflecting from the boundaries interact at a different frequency with the crack tip. This also influences the stress intensity at the crack tip.

The choice of specimen size used so far in this study is constrained by the computational expense. However, in order to assess the ability of the peridynamics model to correctly reproduce the fracture mechanics size effect (BAŽANT 1999) for quasi-static loading and the influence of the
specimen size on the computed toughness characteristics, a number of additional simulations were performed using additional specimen sizes. The dimensions of the PMMA specimen presented in Figure 4.1a are scaled according to a factor $\lambda$ (except the thickness, which is kept constant at 0.5 mm). Assuming $\lambda = 1.0$ for the specimen size 16 mm $\times$ 32 mm, peridynamic simulations are performed for different specimen sizes up to $\lambda = 10$ (which corresponds to the size of the specimens used in the experiments (Fineberg et al. 1991, Sharon et al. 1996, Zhou et al. 2005)). These simulations are performed using a two dimensional formulation since a 3D simulation would be computationally extremely expensive. A discretization size of $\Delta x = 40$ $\mu$m with $\delta = 140$ $\mu$m is used, which leads to 8.0 and 32.0 million material points for $\lambda = 5$ and $\lambda = 10$, respectively. A discretization size of 20 $\mu$m for $\lambda = 10.0$ would lead to 128 million material points in 2D and
3.2 billion material points for 3D analyses. Solving such a large system of equations is out of the context of this work.

Two sets of simulations are performed for various values of the size parameter $\lambda$. The first set is concerned with monotonic loading, similar to Section 4.3.1, considering $\lambda = 0.1, 1.0, 5.0,$ and $10.0$. Loading is applied at a rate of $3 \text{ mm/s}$. These simulations are performed to investigate the relationship between the failure stress $\sigma$ and the specimen size $\lambda$. According to Linear Elastic Fracture Mechanics, the fracture strength $\sigma$ for specimens of different sizes $\lambda$ should follow the scaling $\sigma = c/\sqrt{\lambda}$. On a log – log scale, this gives a straight line relationship, with a slope of $-1/2$, between $\sigma$ and $\lambda$. $c$ is the strength for $\lambda = 1.0$, obtained for $\delta = 140 \mu \text{m}$ as $c = 8.535 \text{ MPa}$ (Figure 4.2a). The expected strength scaling of the LEFM is compared with the strengths obtained from the peridynamic simulations (on a log – log scale) in Figure 4.22. This figure confirms, that the strength scaling obtained from peridynamic simulations for different $\lambda$s is able to reproduce the LEFM size effect (BAŽANT 1999).

In the second set of simulations, the velocity toughening behavior is investigated, i.e., the relationship between $G$ and $v_c$, for $\lambda = 1.0, 5.0,$ and $10.0$. Figure 4.23 compares the computational results for the different specimen sizes with the experimental data from SHARON ET AL. (1996) (in black color). It shows a reduction of the crack propagation speed with increasing $\lambda$. For $\lambda = 10.0$, which agrees with the actual size of the specimen tested in the laboratory, we can start to see an agreement between the experimental values (SHARON ET AL. 1996) and the simulations for higher levels of $G$. However, for low values of $G$, the computed crack speed is still higher than observed in the experiment. A possible cause for this deviation is the larger influence of small-scale material nonlinearities (MEHRMASHHADI ET AL. 2019) at lower values of $G$, which become insignificant compared to the total fracture induced dissipation at higher values of $G$. These analyses demonstrates the dependence of the relationship between $G$ and $v_c$ on the specimen size for a given material. This dependence on the specimen size has been discussed in DALLY ET AL. (1985), KALTHOFF (1983), KNAUSS AND RAVI-CHANDAR (1985), however further computational as well as experimental investigation into the characterization of this effect is needed.

### 4.6 Benchmarks with rate-dependent loading

In this section, the performance of the peridynamics simulation model is evaluated by simulating three well-known benchmark tests dominated by tensile loads: the Kalthoff-Winkler, L-, and CT-specimen tests. These tests are commonly used to study loading rate-dependence on crack propagation path, and the simulation results are compared with experimental findings to assess the accuracy of the peridynamics model.

#### 4.6.1 Kalthoff-Winkler test

Kalthoff-Winkler experiment (KALTHOFF AND WINKLER 1988) is performed by impacting a projectile on a maraging steel (18Ni1900) plate with two initial notches as shown in Figure 4.24. The projectile impacts the plate with an initial velocity $v$, this sends a compressive wave towards the interior of the specimen where this wave causes a mode-II loading at the notches. Depending on
the impact velocity, two failure modes are observed. At very high impact velocities, shear bands emanate from the initial notch. This case will not be considered here. While at low impact velocities ($\sim 33 \text{ m/s}$), a mode transition occurs instead, resulting in mode-I cracks starting from the notch at an angle of $\sim 68^\circ$. This benchmark has been investigated by various authors (Guo and Gao 2019, Silling 2003, Song et al. 2008) and reproducibility of this angle is an important feature for accurate modeling of dynamic brittle fracture.

![Diagram of specimen](image)

**Figure 4.24:** Geometry of the specimen for Kalthoff-Winkler test. The thickness of the plate in 9 mm.

![Simulation](image)

**Figure 4.25:** Simulation of the Kalthoff-Winkler test with an impact velocity $v$ (considering the two-fold symmetry) of 16.5 m/s. Evolution of the crack path shown from left to right.

![Final crack path](image)

**Figure 4.26:** Final crack path from simulation of Kalthoff-Winkler test for various impact velocities. Impact velocities $v$ (considering the two-fold symmetry) from left to right are; 8.25, 12.375, 20.625, and 24.75 m/s.
4.6. BENCHMARKS WITH RATE-DEPENDENT LOADING

Material properties utilized in the simulations are presented in Table 4.2. Additionally, the half-plate model is employed to take advantage of the plate’s two-fold symmetry (SONG ET AL. 2008). An initial condition of an impact velocity of 16.5 m/s is applied to the plate. The fracture patterns obtained for this case are shown in Figure 4.25. The angle of fracture ($\theta \sim 69^\circ$) is reproduced within an acceptable range by the simulations. It was observed by GUO AND GAO (2019) that with an increase in impact velocity, this angle is reduced. The simulations considering a range of impact velocities (8.25 - 24.75 m/s) are presented in Figure 4.26. The findings are in agreement with the results of GUO AND GAO (2019), i.e., a decrease in the angle of the crack path is observed. Moreover, for higher impact velocities, crack branching is observed after a certain distance of crack propagation.

### Table 4.2: Material properties used for the Kalthoff-Winkler test.

<table>
<thead>
<tr>
<th>Material parameter</th>
<th>Value</th>
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<tr>
<td>Young’s Modulus, $E$ (Pa)</td>
<td>$190 \times 10^9$</td>
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<tr>
<td>Poisson’s ratio, $\nu$</td>
<td>0.3</td>
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<tr>
<td>Density, $\rho$ (kg/m$^3$)</td>
<td>8000</td>
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<tr>
<td>Fracture energy, $G_c$ (J/m$^2$)</td>
<td>$2.213 \times 10^4$</td>
</tr>
</tbody>
</table>

The material properties utilized in the simulations are presented in Table 4.2. Additionally, the half-plate model is employed to take advantage of the plate’s two-fold symmetry (SONG ET AL. 2008). An initial condition of an impact velocity of 16.5 m/s is applied to the plate. The fracture patterns obtained for this case are shown in Figure 4.25. The angle of fracture ($\theta \sim 69^\circ$) is reproduced within an acceptable range by the simulations. It was observed by GUO AND GAO (2019) that with an increase in impact velocity, this angle is reduced. The simulations considering a range of impact velocities (8.25 - 24.75 m/s) are presented in Figure 4.26. The findings are in agreement with the results of GUO AND GAO (2019), i.e., a decrease in the angle of the crack path is observed. Moreover, for higher impact velocities, crack branching is observed after a certain distance of crack propagation.

**4.6.2 L- and CT-specimen test**

Experiments investigating the influence of loading rate on fracture behavior were performed on concrete specimens by OŽBOLT ET AL. (2013, 2016). It was reported by OŽBOLT ET AL. (2011) that there is a progressive increase in resistance as the velocity of propagating crack increases, and at higher velocities, the crack branches. Simple tests, such as L- and CT-specimen experiments, are proposed to calibrate and verify numerical models. In this subsection, the performance of the peridynamic model to reproduce the salient features observed in these tests will be investigated. The geometries of both L- and CT-specimens used in the simulations are presented in Figure 4.27.

![Figure 4.27](image-url)  
**Figure 4.27:** The geometry of the L- and CT-specimens, as well as the boundary conditions and load $F(t)$ used in the simulations. The thickness of the L-specimen is 50 mm, and for the CT-specimen, it is 25 mm.
Figure 4.28: Comparison of the fracture patterns obtained from simulations and experiments for the L-specimen with a loading rate of 740 mm/s (top row) and 1000 mm/s (bottom row).

Figure 4.29: Application of the boundary conditions on the CT-specimen (in grey) via the metal frame (in blue).

<table>
<thead>
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<td>Young’s Modulus, $E$ (Pa)</td>
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<td>Poisson’s ratio, $\nu$</td>
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<td>Density, $\rho$ (kg/m$^3$)</td>
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<td>Fracture energy, $G_c$ (J/m$^2$)</td>
<td>58.56</td>
</tr>
</tbody>
</table>

Table 4.3: Material properties of concrete used in the L-specimen test.

The material parameters used for simulating the L-specimen according to OŽBOLT ET AL. (2016) are presented in Table 4.3. For the L-specimen, the bottom part with a length of 100 mm
is fixed in a fixture, while a point load is applied at a distance of 50 mm from the left edge. Two displacement-controlled loading rates are investigated in this study: 740 mm/s and 1000 mm/s. The fracture paths obtained from the simulations for the two loading rates are shown in Figure 4.28 and compared with the experimental results. A good agreement between the fracture patterns is observed for both loading rates. The simulations show slight damage at the location where the point load is applied, which is not observed in the experiments. However, it does not significantly affect the overall fracture pattern.

<table>
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<td>Young’s Modulus, $E$ (Pa)</td>
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<td>Poisson’s ratio, $\nu$</td>
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<td>Density, $\rho$ (kg/m$^3$)</td>
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<td>Fracture energy, $G_c$ (J/m$^2$)</td>
<td>65</td>
</tr>
</tbody>
</table>

Table 4.4: Material properties of concrete used in the CT-specimen test.

For the CT-specimen, the boundary conditions are applied via a steel frame, as shown in Figure 4.29. Material parameters used for this test are slightly different from those used for the L-specimen and are presented in Table 4.4. For the dimensions and material properties of the steel frame, please refer to OŽBOLT ET AL. (2013). The fracture patterns obtained from the two loading
rates considered here (1.4 m/s and 4.3 m/s) are compared with the experiments in Figure 4.30. In the
experiments, a single crack initiates from the initial notch and propagates towards the right boundary
of the specimen at a loading rate of 1.4 m/s. At a loading rate of 4.3 m/s, the crack initiates from
the notch and branches after a certain distance. The two branches propagate towards the right and
bottom boundaries of the specimen. The simulations can capture both the single crack propagation
and the branching of the crack very well. For the loading rate of 4.3 m/s, the upper crack branch
continues propagating towards the right boundary and branches again just before reaching the edge.
Notably, the simulations can even capture this secondary branching.

4.7 Summary

The influence of the peridynamic horizon ($\delta$) on the velocity toughening relationship and the frac-
ture behavior of PMMA under a spectrum of loadings was investigated in this chapter. Two loading
scenarios were considered: i) crack propagation under monotonically increasing loads, and ii) crack
propagation in quasi-statically preloaded plates. In the 2D simulations of the monotonic loading
case, it was found that the effective stiffness, as well as the crack propagation velocity, are in-
dependent of $\delta$ and the fracture strengths converge as $\delta$ decreases. However, in contrast, the 3D
simulations show a slight dependence of the effective stiffness and crack propagation speed on $\delta$. In
the second loading case, two sources that influence the crack propagation speed with respect to the
size of the peridynamics horizon are identified. The first mechanism is the crack surface roughening
and micro-branching, which reduce the main crack propagation speed at each bifurcation attempt.
The second cause is a consequence of the nonlocal nature of the peridynamic formulation and the
influence of missing non-local neighborhoods along the surfaces.

The influence of specimen size on fracture propagation was analyzed using 2D simulations. The
peridynamics model was shown to reproduce the theoretical fracture mechanics size effect law. For
the crack velocity toughening relationship, as the specimen size in the simulations was increased to
match the size of the specimen actually used in the experiment, an agreement of the average crack
propagation velocities obtained for higher levels of the initially stored energy $G$ was observed. This
result showed that the crack velocity toughening behavior is dependent on the size of the specimen
and should not be considered as a material property, as it is usually assumed in numerical models.
Further experimental and computational studies are needed to characterize this size effect.

The simulation results obtained in this chapter demonstrate the capability of peridynamics to
accurately model the fracture process. The high-resolution 3D peridynamics simulations success-
fully reproduced the micro-branching instability and its dependence on specimen geometry, as well
as the transition of fracture surface topology, including the mirror, mist, and hackle regimes. The
performance of the peridynamic simulation model was further analyzed in this chapter for loading
rate-dependent tension-dominated fracture benchmark problems, including the Kalthoff-Winkler, L-
and CT-specimen tests. The influence of loading rate on fracture propagation was investigated, and
the simulation results were found to be in good agreement with the experiments.
Chapter 5

Compression dominated failure

Heterogeneous solids, such as rocks and concrete, contain a distribution of flaws. When subjected to tensile loads, cracks initiate from these flaws and propagate according to the Linear Elastic Fracture Mechanics (LEFM) criterion. This results in diffuse damage until one or more cracks reach a critical length, at which point the most critical crack propagates unstably, leading to failure. However, under compression, flaws in these materials undergo a complex sequence of failure processes. These include crack closure, pore-collapse, crack initiation in various modes, crack sliding, and wing crack formation (Ashby and Hallam 1986, Basu et al. 2013, Klein et al. 2001, Nemat-Nasser and Horii 1982). Due to the activation of these mechanisms, failure under compression results in diffuse damage. This means that damage is observed at various locations, unlike in tensile failure where only one crack localizes. The activation of additional mechanisms and the formation and interaction of multiple cracks under compression result in an order of magnitude higher dissipation compared to tensile failure. This leads to significant variations in tensile and compressive strengths (Lockner 1995). Hydrostatic pressure plays a crucial role in compressive failure by governing the activation of several of the aforementioned mechanisms. Therefore, it is a critical factor in the failure process.

This chapter investigates failure under compression-dominated loading conditions in heterogeneous materials using the ordinary state-based peridynamic model (Section 2.2.2) along with the standard critical-energy failure criterion, presented in Section 2.4.2. In Chapter 4, the model was thoroughly investigated for tension-dominated fracture problems, including failure strengths and crack dynamics, and it performed well for those cases. However, this chapter explores the limitations of this model for cases where the dominant loading is in compression. It will be shown that for compressive failure, where additional nonlinear dissipation phenomena, such as pore-collapse, are present, the model underpredicts the strengths. To investigate this further, the simulation model is applied to the indentation test of a porous rock. Qualitative features of indentation are analyzed through Acoustic Emission (AE) data obtained from experiments performed on Bentheim sandstone. The standard critical-energy failure criterion is shown to be incapable of capturing all processes involved in indentation. AE data guides the understanding of the limitations of the simulation model.
motivating the extension of the model for failure of porous rocks. Later on, the biaxial failure of concrete is simulated using the standard approach, and as expected, the model underpredicts the strengths in the compressive regime. These limitations motivate a further extension of the model to consider additional dissipation under compressive loads for non-porous heterogeneous materials. Some contents of this chapter have been published in Butt and Meschke (2023). The main objectives of this chapter are:

- To identify and address the limitations of the standard peridynamic model in simulating compression-dominated failure, using the rock indentation test and biaxial strength test on concrete.
- To extend the peridynamics model by incorporating pore-collapse as a dissipation mechanism, which is observed in heterogeneous porous materials such as sandstone.
- To validate the extended pore-collapse model by conducting indentation tests on Bentheim sandstone.
- To further extend the peridynamic model by incorporating pressure-dependent fracture energy, to simulate compressive failure in low-porosity heterogeneous materials such as concrete.
- To validate the extended pressure-dependent critical-energy failure criterion using the biaxial strength tests on concrete.

5.1 Consideration of material heterogeneity in peridynamic simulations

In Chapter 4, simulations on PMMA plates were conducted assuming a perfectly homogeneous simulation domain. However, rocks and concrete have inherent heterogeneity and random defects that must be accounted for in the model. To address rock heterogeneity in the simulations, strength parameters such as fracture energy are sampled from a probability distribution. Weibull’s distribution has been found to describe the distribution of micro-defects in rocks well according to the literature (Hudson and Fairhurst 1969, Liu et al. 2018). Therefore, the simulations in this chapter will consider strength parameters sampled from a Weibull distribution Weibull (1951). The probability density function for Weibull’s distribution is given by:

\[ P(\sigma) = \frac{m}{\sigma_0} \left( \frac{\sigma}{\sigma_0} \right)^{m-1} \exp \left[ -\left( \frac{\sigma}{\sigma_0} \right)^m \right], \]  

(5.1)

where, \( \sigma \) is the sampled parameter, \( \sigma_0 \) is the mean value of the parameter to be sampled and \( m \) is known as the shape parameter. The shape parameter \( m \) represents the level of homogeneity of the material Tang (1997), where larger \( m \) represents a more homogeneous material and vice versa (Figure 5.1). Simulations use a value of \( m = 3 \) for the shape parameter according to Liu et al. (2018). The open-source software Peridigm (Littlewood 2015, Parks et al. 2012) was extended to consider the distributed strengths in the simulation domain. This extended version of Peridigm is used to carry out the simulations presented in this chapter.
5.2 Rock indentation

Rock fragmentation due to indentation represents the fundamental process of mechanical rock breaking and is commonly encountered in most rock excavation processes such as mining and tunneling operations. The type of loading can vary with respect to the tool shape, loading direction, and loading rate. However, in principle, an indentation process causes subsurface fractures, which coalesce with adjacent fractures, resulting in the formation of rock fragments. As the rock surface is loaded with the indenting tool, stresses develop in the rock, which increase with the increasing load. At the tool-rock contact, the surface irregularities get deformed under the indenter, developing a crushed zone. On the rock surface, a crater is formed. As the indentation load reaches a critical value, the rock fractures, and one or more chips are formed by lateral cracks propagating to the free surface. If the tool moves along the rock surface, as with a cutting disc or a drag bit, a groove is formed, caused by similar events as for the crushed zone and crater formation in the case of indentation.

Historically, the basic indentation principle has been explored since the Stone Age. However, the mathematical ingredients required to quantitatively study the indentation process, i.e., the contact between two bodies, were developed by Hertz (1881), who analyzed the contact between two curved bodies and described the subsequent cone shaped crack that initiates at the contact region. This treatment was extended by Boussinesq (1885), who solved for the stress field in a linear elastic half space induced by a point load. Since then, indentation tests have been investigated using various shapes and sizes of the indenters on different rock types in several research works (Cook et al. 1984, Kou 1995, Lindqvist 1982, Wagner and Schümann 1971). These studies have investigated the force-penetration and pressure-penetration relationships as well as the formation of cracks. Indentation testing has also been used to measure a number of material properties, such as
hardness (Johnson 1987, Lawn and Wilshaw 1975), yield stress (Tabor 1980), and fracture toughness (Scholz et al. 2004). In addition, indentation tests have been used to assess rock drillability and cuttability (Szwedzicki 1998, Teale 1965). The maximum indentation pressure is a crucial parameter in interpretation of indentation tests; it is interpreted as the specific energy for removing a unit rock volume in cutting experiments with a Non-Truncated Tip Indenter (Teale 1965).

5.2.1 Indentation experiments

The deformation processes involved in indentation tests have been monitored experimentally using electron scanning microscopy (Lindqvist et al. 1984), digital image correlation (Zhang et al. 2012), acoustic emission (Chen and Labuz 2006, Yin et al. 2014) and infrared thermography (Liu et al. 2018). Numerical simulations, based on the discrete element method (Huang and Detournay 2013) and the finite element method (Liu et al. 2002), have also been performed. These experimental and numerical investigations have shown that the rock fragmentation due to indentation involves several progressive deformation mechanisms including elastic deformations at the initial loading stage, then volumetric compaction, plastic deformation, and finally macro fracturing. The validation of a simulation model can be derived from its ability to reproduce these significant features observed in the indentation tests.

Figure 5.2: Geometry of the indenter used in the indentation experiments (Yang et al. 2022).

The experiments considered here were carried out by Yang et al. (2022) and these results will be used to provide a further validation for the numerical model. The tests were performed on
5.2. ROCK INDENTATION

Figure 5.3: Cumulative temporal-spatial distribution of AE hypocenters (circles) at different percentages of peak force (a-d), end of test (e) and photograph after indentation test (f). The marker size indicates the relative magnitude of AE energy. Crosses indicate sensor locations. The color bar indicates time relative to the one at peak force (reproduced from YANG ET AL. (2022)).

<table>
<thead>
<tr>
<th>Material parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>Young’s Modulus, $E$ (Pa)</td>
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<td>Poisson’s ratio, $\nu$</td>
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<tr>
<td>Density, $\rho$ (kg/m$^3$)</td>
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</tr>
<tr>
<td>Fracture energy, $G_c$ (J/m$^2$)</td>
<td>10</td>
</tr>
<tr>
<td>Porosity, $\phi$ (%)</td>
<td>24</td>
</tr>
</tbody>
</table>

Table 5.1: Material properties for Bentheim sandstone.

cylindrical specimens of Bentheim Sandstone. A total of six specimen sizes were considered with diameters of 30, 50 and 84 mm and heights 50 and 100 mm, corresponding to aspect ratios ranging from 0.3 to 1.7. Bentheim sandstone is composed of approximately 95% quartz, 3% kaolinite, and 2% microcline (KLEIN ET AL. 2001). The material parameters for Bentheim sandstone are presented in Table 5.1. The truncated tip indenter used in these experiments was manufactured from hardened steel (Figure 5.2). The indentation pressure resulting from the indentation loads is calculated using:

$$p = \frac{F}{4\sqrt{2} R_{\text{ind}} d - d^2 \left( a_0 + \frac{d}{\tan \alpha} \right)}.$$  \hspace{1cm} (5.2)

Here, $F$ is the indentation load, $d$ is the indentation depth, $R_{\text{ind}}$ is the radius of the indented tip, $a_0$
denotes the half width of the indenter tip, and $\alpha$ is the angle between the indenter and the specimen surface (here $40^\circ$).

The damage in the specimen during the indentation tests was monitored using an AE system, which allows to track the sequence of the damage processes in real time. AE data is presented in Figure 5.3, which shows the progressive damage happening at various percentages of the peak load until the formation of a macro fracture. The AE data indicates the formation of a diffused damage zone at the contact initiation of the indenter-specimen interface, then growth of the diffuse damage zone from it, and finally a macro crack from the diffused damaged zone which splits the specimen in half.

5.2.2 Simulations using the standard peridynamic framework

This section provides a brief excursion into the modeling strategies used for indentation tests. The focus lies on simulations that were either unsuccessful in reproducing main features of the indentation tests or were unable to fully simulate this problem due to numerical instabilities that motivated the critical enrichments by consideration of additional physical mechanisms involved in the rock indentation process.

Simulations using the standard critical-energy failure criterion

In this section, the critical-energy damage model (Section 2.4.2) along with the ordinary state-based peridynamic material model (Section 2.2.2) is employed to simulate the indentation experiments discussed in the previous section. However, the model fails to account for the dissipation mechanisms involved in the indentation experiments leading up to the formation of the central fracture (Figure 5.3), resulting in severely underestimated failure loads as shown in Figure 5.4. In the simulations, almost no damage is observed until the peak load is achieved. In contrast, the AE data shows a lot of activity leading up to the peak load, indicating the occurrence of diffused damage under the indenter. The lack of consideration for crushing due to pore-collapse in this model causes the excess elastic energy to form several cracks initiating from the tool contact location, which ultimately leads to the formation of several small fragments.

Quantitatively, the current simulation model underestimates the peak load by around 58%. Qualitatively, the absence of pre-peak diffused damage under the indenter observed in the experiments (Figure 5.3) highlights the need to upgrade the current model. Such an upgrade should consider the various pressure-dependent mechanisms that lead to diffused damage under the indenter, ultimately leading up to the peak load where the central fracture is formed.

Simulations using the peridynamic correspondence framework

Correspondence models are the class of non-ordinary state-based peridynamic models (Section 2.2.3) which make use of the classical deformation gradient ($F$) in their material model formulations SILLING ET AL. (2007). $F$ has several advantages in material modeling, such as the additive and multiplicative splits which allow for the decomposition of various deformation modes. The decomposed deformation modes can then be used further to formulate various strength envelopes, such
as Mohr-Coulomb’s criterion, which use different mathematical relationships among these decomposed modes. For the peridynamic correspondence formulation the deformation gradient is computed using Eq. (2.18) and Eq. (2.19). Once $\mathbf{F}$ is computed, then any classical material model can be used for the evaluation of the stress state. These models work fine for the case of linear elasticity.
as well as plastic deformations, however, once the damage and fracturing is considered, the shape tensor $K$ (Eq. 2.19) can become singular due to excessive damage. And if $K$ is singular, then $F$ cannot be computed. The necessary condition for non-singular $K(x)$ is to have at least three non-coplaner points connected at $x$. It will be shown in this subsection that this condition is typically met in cases where single cracks propagate from well-defined notches. However, in the case of diffused damage and fragmentation, this condition is rarely satisfied, and $K(x)$ becomes singular, making the computation of $F$ (Eq. 2.18) unfeasible and causing the simulation to stop.

Shear bond force peridynamics REN ET AL. (2016) (Section 2.2.3) is part of the correspondence
model family, it uses the peridynamic deformation gradient to decompose the deformation at the bond level into a normal and shear component. This model is also able to distinguish between mode-I and mode-II fracture (Section 2.4.3), which is practical for modeling rocks as several classical failure criteria use such split to model pressure-dependent shearing phenomena.

The model was aimed to be verified for simple mode-I as well as mode-II fracture benchmarks with a single notch, as shown in Figure 5.6. For simplicity, both mode-I and mode-II are assumed to have the same fracture energy $G_c = 50 \text{ J/m}^2$. The load displacement relationships obtained for both cases are presented in Figure 5.7 and are compared with the LEFM solutions TADA ET AL. (1985). Qualitatively, it can be observed that the crack propagation starts in front of the initial notch and propagates towards the other end of the specimen. However, the quantitative results are overestimated by 15% for mode-I and around 22% for the case of mode-II crack propagation. One of the sources of this overestimation is the dynamic effects which are not considered in the LEFM solution. In contrast to the simulations with excessive fragmentation, these simulations finished without running into stability problems due to singular matrices.

A remedy for the singular $K$ matrix on damaged material points is to simply ignore these points from the simulation. This remedy provides satisfactory results for the case where only a few cracks are present, however this is not a stable or a robust solution. For the case of excessive fragmentation or diffused damage, this remedy does not work and simulation tends towards instabilities. Figure 5.8 shows the damaged zone obtained from the indentation test using this model up to the point where the simulation stopped due to instabilities. Almost all the material points forming the crushed zone under the indenter had to be ignored from the simulation (Figure 5.8). These material points are important for propagating the loads inside the rock specimen where the damage gets localized and a macro fracture forms. By ignoring these material points the load transfer within the rock sample is disrupted and a localized fracture is not obtained. These results render the use of
correspondence models impractical for the case of the indentation and rock excavation. Therefore, further development of the classical state-based peridynamic models is required.

5.2.3 Model extension: Pore-collapse

This section extends the ordinary state-based peridynamic model used in Section 5.2.2 to consider the pore-collapse phenomenon in Bentheim sandstone. The mechanical properties and deformation characteristics of Bentheim sandstone were studied under triaxial loads by Klein et al. (2001). It is a relatively homogeneous porous rock, these pores collapse under compressive loads and lead to stiffening of the material, this effect can be seen by comparing the volumetric strain predicted by a constant bulk modulus with the one obtained in the experiments under hydrostatic compression (Figure 5.9). This stiffening under compressive pressure due to pore-collapse contributes to a significant energy dissipation and this is a major reason why the simulation model with only mode-I fracture criterion (Section 5.2.2) underestimates the failure loads.

![Figure 5.9: Relationship between hydrostatic pressure and volumetric strain from Klein et al. (2001), and a first- and a third-order polynomial fit to the experimental data.](image)

The stiffening effect due to pore-collapse is modeled by using the experimental relationship between the hydrostatic compression and volumetric strain (Figure 5.9) instead of just using a constant Bulk modulus. According to Klein et al. (2001), this relationship has one inflection point leading up to a compressive volumetric strain of 3.0% and after that this relationship becomes linear again. So, the range of the volumetric strains from 0% to −3.0% is fitted with a third-order polynomial (Figure 5.9) and for compressive volumetric strain greater than 3.0% a linear relationship is adapted. Additionally, these volumetric deformations are assumed to be fully irreversible, as pore-collapse is an irreversible process.

For the modification of the state-based linear elastic model, presented in Section 2.2.2, an addi-
tive split is defined for the dilatation (Eq. 2.12) under compression as:

$$\theta(x, t) = \begin{cases} \theta^e(x, t) & \text{if } \theta(x, t) > 0 \\ \theta^e(x, t) + \theta^pc(x, t) & \text{if } \theta(x, t) < 0 \end{cases}$$  (5.3)

Here $\theta^e(x, t)$ is the reversible elastic part of the volumetric strain and $\theta^pc(x, t)$ is the irreversible volumetric strain representing pore-collapse under compression. The irreversible pore-collapse is assumed to get activated after $\theta^e(x, t) = -0.0025$, the volumetric strain when the hydrostatic pressure-volumetric strain relationship exhibits the first change of the slope and deviates from a linear trend (Figure 5.9). For simplicity, $\theta^e(x, t)$ is assumed to have a constant value of $-0.0025$ after the initiation of the pore-collapse.

The scalar force state $\xi(x, t)$ from Eq. (2.13) is modified to consider only the elastic part of the dilatation as:

$$\xi(x, t) = \frac{3}{m(x)} p(x, t) \omega(|\xi|) |\xi| + \frac{15\mu}{m(x)} \omega(|\xi|) \xi^d(\xi),$$  (5.4)

where $p(x, t)$ is the pressure which is computed according to:

$$p(x, t) = \begin{cases} K \theta(x, t) & \text{if } \theta(x, t) > 0 \\ K_1 + K_2 \theta(x, t) + K_3 \theta(x, t)^2 + K_4 \theta(x, t)^3 & \text{if } -0.03 < \theta(x, t) < 0 \\ K_5 + K_6 \theta(x, t) & \text{if } \theta(x, t) < -0.03 \end{cases}$$  (5.5)

Here, $K$ is the Bulk modulus, $K_1, K_2, K_3 \& K_4$ are calibrated for a third-order polynomial and $K_5 \& K_6$ are calibrated for a first-order polynomial using the experimental data from KLEIN ET AL. (2001), as shown in Figure 5.9. The applicable range of volumetric strain for the third- and first-order polynomial are shown in Eq. (5.5). The calibrated values of these parameters for Bentheim sandstone are as follows:

$$K_1 = 2.078 \times 10^6$$
$$K_2 = 6.511 \times 10^9$$
$$K_3 = -3.952 \times 10^{11}$$
$$K_4 = -6.3 \times 10^{12}$$
$$K_5 = 4.17 \times 10^7$$
$$K_6 = 13.95 \times 10^9.$$  (5.6)

Finally, the critical-energy failure criterion presented in Eq. (2.42) (Section 2.4.2) also has to be modified, according to the additive split presented in Eq. (5.3), to consider only the elastic part of the volumetric strains as follows:

$$\mathbf{T}(x, t) \xi - \mathbf{T}(x', t) (-\xi) = \left[ (3K - 5\mu) \omega(|\xi|) |\xi| \left( \frac{\theta^e(x, t)}{m(x)} + \frac{\theta^e(x', t)}{m(x')} \right) + 15\mu \omega(|\xi|) e(\xi) \left( \frac{1}{m(x)} + \frac{1}{m(x')} \right) \right] \mathbf{M}(x, t) \xi.$$  (5.7)
This model was implemented in the open-source software *Peridigm* (Littlewood 2015, Parks et al. 2012). In the next subsection, the indentation tests will be revisited, this time employing the pore-collapse model presented here.

*Figure 5.10:* Simulation of the indentation test with a specimen of 30 mm diameter and 50 mm height. The associated evolution of damaged and cracked regions are filtered out for visualization in the top row and the volumetric plastic strain, representing the collapsing pores ($\theta_{pc}$), greater than 0.1% are colored in green. The load levels a-d are marked in Figure 5.11 for comparison.

*Figure 5.11:* Indentation load-tool penetration and indentation pressure-tool penetration relationship computed from the simulation results shown in Figure 5.10.
5.2. ROCK INDENTATION

Figure 5.12: Simulation of the indentation test with a specimen of 30 mm diameter and 100 mm height. The associated damaged and cracked regions are filtered out for visualization in the top row and the volumetric plastic strain, representing the collapsing pores ($\theta^p$), greater than 0.1% are colored in green. The load levels a-f are marked in Figure 5.13 for comparison.

Figure 5.13: Indentation load-tool penetration and indentation pressure-tool penetration relationship computed from the simulation results shown in Figure 5.12.
5.2.4 Simulations using the extended pore-collapse model

The pore-collapse model developed in the last subsection is now used for the indentation test on the specimen with 30 mm diameter and 50 mm height. The material properties used in these simulations are shown in Table 5.1. To consider the material’s heterogeneity, the Weibull distribution is used to randomly sample fracture energy ($G_c$), with a shape parameter of $m = 3$, as described in Section 5.1 and shown in Figure 5.1. The indenter and the rock specimen are discretized with a mesh size of 0.41 mm and 0.65 mm and a peridynamic horizon size of 0.81 mm and 4.55 mm, respectively. Temporal evolution of the fracture process during the indentation test and the final failure pattern...
Figure 5.16: Simulation of the indentation test with a specimen of 50 mm diameter and 100 mm height. The associated damaged and cracked regions are filtered out for visualization in the top row and the volumetric plastic strain, representing the collapsing pores ($\theta_{pc}$), greater than 0.1% are colored in green. The load levels a-e are marked in Figure 5.17 for comparison.

Figure 5.17: Indentation load-tool penetration and indentation pressure-tool penetration relationship computed from the simulation results shown in Figure 5.16.

is presented in Figure 5.10. The simulations capture the successive formation of a crushed zone at the tool-rock interface and the initiation of a central macroscopic tensile fracture which splits the
specimen. A qualitative agreement is observed with the acoustic emission data from the experiment (Yang et al. (2022)) shown in Figure 5.3. The quantitative validation relies on the comparison of the force-penetration as well as the indentation pressure-penetration relationship (Eq. 5.2) obtained from the experiments and the simulations. This data is presented in Figure 5.11, a good agreement between the experiments and the simulation results can be observed. These results provide a qualitative as well as a quantitative validation for the pore-collapse model presented in Section 5.2.3.

Development of a crushed zone before the peak load is observed in the simulation for a sample with 30 mm diameter and 100 mm height (a, b, and c in Figure 5.12). As the tensile stresses at the perimeter of this zone exceed a critical value, a tensile crack is formed. After a certain length of this tensile crack propagation, the crack tip bifurcation takes place and the crack branches, as shown in the last column of Figure 5.12. The loading stiffness, the peak load as well as the peak indentation pressure predicted by the simulation are in a good agreement with the experiments (Figure 5.13). By comparison of the indentation load-penetration relationship obtained for the two specimens with 30 mm diameter (Figure 5.11 and Figure 5.13), it can be concluded that the peak load does not have a strong dependency on the height of the specimen.

To investigate the influence of the specimen diameter on the peak load as well as the fracture pattern, two additional aspect ratios of the specimens are considered with a diameter of 50 mm and heights of 50 and 100 mm. It can be observed from the fracture patterns obtained for the specimens with a height of 100 mm (Figure 5.12 and Figure 5.16), that the central fracture tends to branch. This can be attributed to the fact that in a longer specimen the crack has to propagate a longer distance, and as the crack becomes longer the stress intensity increases which results in an increase of the crack propagation velocity, as the crack propagation velocity reaches some critical value the crack branching occurs (Butt and Meschke (2018, 2021b)). The indentation force- and indentation pressure-penetration relationships obtained for the two specimens with 50 mm diameter are presented in Figure 5.15 and Figure 5.17, respectively. Comparing these peak loads with the ones obtained for the specimens with 30 mm diameter, it can be observed that the failure load strongly correlates with the diameter of the specimen. Smaller the diameter of the indentation specimen, lower is the peak load and vice versa.

5.3 Uniaxial and biaxial strength of concrete

In this section, simulations of uniaxial and biaxial failure of concrete are presented. The standard critical-energy damage model (Section 2.4.2) is analyzed to reproduce the ultimate tensile and compressive strength (UTS and UCS) of concrete, with a focus on the ratio of UCS to UTS. After conducting the uniaxial tests, the model is applied to simulate the complete biaxial strength envelope for concrete (Gerstle et al. 1980, Kupfer et al. 1969). The limitations of the standard modeling strategy are highlighted by the obtained results, which motivate the need for further extensions to consider higher dissipation under compressive loads. To address this issue, a pressure-dependent fracture energy model is presented and incorporated into the peridynamic framework. The model is validated using the aforementioned tests. Concrete is chosen as the material for this study due to the availability of experimental data.
Figure 5.18: Stress-strain relationship obtained for a concrete specimen using the standard critical-energy failure criterion.

Figure 5.19: Front, side and back view of the concrete specimen failed under tensile loads.

Figure 5.20: Front, side and back view of the concrete specimen failed under compressive loads. The material points with a damage value greater than 0.95 are filtered out for visualization.

Simulation setup

A concrete specimen measuring 200 $\times$ 200 $\times$ 50 mm is chosen for the simulations, consistent with the dimensions of the specimens used in the experiments from KUPFER ET AL. (1969). The material
parameters used in the simulations, as reported by Kupfer et al. (1969), are shown in Table 5.2. To account for the heterogeneity of the material, the fracture energy \( G_c \) is randomly realized from a Weibull distribution (see Section 5.1 and Figure 5.1) using a shape parameter \( m = 3 \) (Hudson and Fairhurst 1969, Liu et al. 2018). A displacement-controlled loading is applied for all cases at a rate of 0.4 mm/s. The specimen is discretized using a mesh size of \( \Delta x = 2.5 \) mm, and a peridynamic horizon size of \( \delta = 10 \) mm is used for all cases.

<table>
<thead>
<tr>
<th>Material parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s Modulus, ( E ) (Pa)</td>
<td>( 30.9 \times 10^9 )</td>
</tr>
<tr>
<td>Poisson’s ratio, ( \nu )</td>
<td>0.2</td>
</tr>
<tr>
<td>Density, ( \rho ) (kg/m(^3))</td>
<td>2300</td>
</tr>
<tr>
<td>Fracture energy, ( G_c ) (J/m(^2))</td>
<td>10</td>
</tr>
</tbody>
</table>

**Table 5.2:** Material properties for concrete used in the uniaxial and biaxial test.

Figure 5.21: Biaxial failure envelope obtained with standard critical-energy failure criterion.
5.3.1 Simulations using the standard critical-energy failure criterion

The stress-strain relationship obtained from the simulations for UTS and UCS is presented in Figure 5.18. The UTS obtained from the simulations is approximately 2.43 MPa, which agrees well with the experimental value of 2.66 MPa (KUPFER ET AL. 1969) with an error of about 7.4%. The tensile failure pattern obtained from the simulation for this case is shown in Figure 5.19. It can be observed that cracks initiated from both sides of the specimen, coalesced after propagating a certain distance, and eventually caused failure.

The failure pattern obtained for the case of compressive failure is presented in Figure 5.20. The simulation significantly underpredicts the failure strength (Figure 5.18). The UCS obtained from the simulation is only 7.71 MPa, while the experimental value is around 30 MPa, resulting in an error of approximately 74.3%. This discrepancy arises due to the lack of the additional dissipation mechanisms discussed earlier in the simulation model. The ratio of UCS to UTS from the simulations is approximately 3.17, whereas in the experiments, it is approximately 11.28.

The simulations for biaxial failure consider varying ratios of the applied loading in the longitudinal ($\sigma_{11}$) and lateral ($\sigma_{22}$) directions. The UCS and UTS are just two points on the complete biaxial failure envelope. Several biaxial loading scenarios are now considered to obtain the complete failure envelope. The failure envelope obtained from the simulations is presented in Figure 5.21, along with the experimental data from KUPFER ET AL. (1969). A comparative research project (GERSTLE ET AL. 1980) showed that the biaxial strength envelope could vary considerably depending on the testing method, specimen size, and boundary conditions. Figure 5.21 also displays the inner and outer strength envelopes obtained from the aforementioned study. A comparison of the biaxial envelope obtained from the simulations and experiments shows satisfactory agreement in the tension-tension quadrant. However, the simulations severely underpredict the strengths in the tension-compression as well as the compression-compression quadrants. This motivates further enhancements of the current model to consider additional dissipation in the compression regime.

5.3.2 Model extension: Pressure-dependent fracture energy

Fracture energy is the energy required to create a unit fracture surface. While this is true for tensile failure, where the failure is localized to one macro fracture, under compressive loads, several additional energy dissipation mechanisms get activated, such as pore-collapse, compaction, crack sliding, crack arrest, wing cracking, and shear failures, among others (BASU ET AL. 2013, ROSSI ET AL. 1996). The activation of these failure mechanisms under compression is highly dependent on the hydrostatic pressure in the material (SAMMIS AND ASHBY 1986). Due to these additional mechanisms, the compressive strength predicted by a fracture model is underestimated, and the ratio of the UCS to UTS cannot be controlled. For the standard critical-energy failure criterion in peridynamics, the ratio of UCS to UTS is always between 3 and 4, which may vary slightly with changes in Poisson’s ratio.

To obtain a quantitative agreement with experimental predictions for compressive behavior, one could add all the micro- and meso-scale mechanisms to the simulation model. However, this approach would require either a multi-scale approach (BARTHÉLÉMY ET AL. 2003) or discrete resolu-
Figure 5.22: A schematic showing the relationship between the fracture energy ($G_c$) and pressure ($p$) for different slopes $m_b$. Compressive pressure is denoted here as negative.

Figure 5.23: Stress-strain relationship obtained for a concrete specimen using the pressure-dependent critical-energy failure criterion (Section 5.3.2) for three different values of $m_b$.

tion of the microstructure (Carlsson and Isaksson 2020, Papka and Kyriakides 1998), not to mention the lengthy simulation times required to solve such a large system. In Section 5.2.3, an approach was presented that considered one of the several dissipation mechanisms in the simulation model, pore-collapse. However, for a general material that may or may not be porous, this approach is not sufficient. Therefore, this section presents a phenomenological approach that lumps all the
5.3. UNIAXIAL AND BIAXIAL STRENGTH OF CONCRETE

Figure 5.24: Biaxial failure envelopes obtained with the pressure-dependent critical-energy failure criterion with three different values of $m_b$. The stress ratios ($\sigma_{11}/\sigma_{22}$) labeled a-k here are presented in Table 5.3.

The pressure-dependent fracture energy model considers the increase in energy required to fail a material under compressive loads. This increase in fracture energy can be explained by the aforementioned dissipation mechanisms that get activated at varying length scales depending on the material microstructure. This increase in energy to failure under compression is also reflected in the UCS to UTS ratio, which serves as a guide for calibrating the pressure dependence of the fracture energy. In this work, the relationship between compressive pressure and fracture energy is assumed to be linear, although it can be nonlinear in general. A schematic of the relationship between fracture energy...
$G_c$ and pressure ($p$) is presented in Figure 5.22 for various slopes $m_b$. The slope ($m_b$) of this linear function is calibrated using the UCS of the material under investigation. It should be noted that $G_c$ remains constant for positive (tensile) pressures, and increases according to $m_b$ only for negative (compressive) pressures. This pressure-dependence is incorporated in peridynamic formulation as:

$$G_c(x, p_{avg}) \langle \xi \rangle = \begin{cases} G_c(x) \langle \xi \rangle & \text{if } p_{avg} > 0 \\ G_c(x) \langle \xi \rangle - m_b p_{avg} & \text{if } p_{avg} < 0. \end{cases}$$ (5.8)

Where, $\xi$ is the bond between the points $x'$ and $x$, and $p_{avg}$ is the average pressure, defined as $(p(x') + p(x))/2$. Furthermore, the pressure-dependent fracture energy $G_c(x, p_{avg})$ is used to compute the critical bond dual force $w_c$ according to Eq. (2.43) and Eq. (2.44) as:

$$w_c = \frac{4G_c(x, p_{avg})}{\pi \delta^4}. \quad (5.9)$$

Dimensional analysis of Eq. (5.3.2) shows that $m_b$ has units of length. It is intriguing that $m_b$ bears similarities to the friction angle in the classical Mohr-Coulomb strength criterion. Investigating possible correlations between $m_b$ and the friction angle, or some other characteristic length scale of the material, could yield valuable insights. However, in this work, $m_b$ is considered as a phenomenological quantity that is calibrated using the compressive strength of the material, and as such, its units are ignored. The procedure for calibrating the slope $m_b$ will be presented in the next subsection.

### 5.3.3 Simulations using the pressure-dependent failure criterion

The model developed in Section 5.3.2 has been implemented in the open-source software Peridigm (LITTLEWOOD 2015, PARKS ET AL. 2012). In this subsection, the UTS and UCS tests presented in Section 5.3.1 are revisited, this time using the pressure-dependent fracture energy model. Stress-strain plots obtained using this model for various values of $m_b$ are presented in Figure 5.23. It can be observed that, as expected, the tensile strength remains unchanged (UTS = 2.43 MPa) for all $m_b$ values. However, the compressive strength shows a strong dependence on the parameter $m_b$. The UCS obtained for three different $m_b$ values presented in Figure 5.23 are 24.56, 28.27, and 31.43 MPa. A compressive strength of 31.43 MPa is obtained for $m_b = 2.33 \times 10^{-5}$, reducing the error from 74.3% for the pressure-independent case (Section 5.3.1) to only 4.7%. The UCS to UTS ratio obtained from the simulations is now around 12.9, and from the experiments, it is around 11.28. The parameter $m_b$ can be further tuned to achieve an even better agreement. However, it is assumed here that the calibrated value of $m_b = 2.33 \times 10^{-5}$ is acceptable for the concrete used in the experiments (GERSTLE ET AL. 1980, KUPFER ET AL. 1969).

<table>
<thead>
<tr>
<th>Label</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>d</th>
<th>e</th>
<th>f</th>
<th>g</th>
<th>h</th>
<th>i</th>
<th>j</th>
<th>k</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{11}/\sigma_{22}$</td>
<td>1.0</td>
<td>1.49</td>
<td>2.43/0</td>
<td>-1</td>
<td>-0.12</td>
<td>-0.067</td>
<td>-0/31.43</td>
<td>0.24</td>
<td>0.43</td>
<td>0.63</td>
<td>1.0</td>
</tr>
</tbody>
</table>

**Table 5.3:** Values of the stress ratios ($\sigma_{11}/\sigma_{22}$) labeled in Figure 5.24.
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Figure 5.25: The failure patterns obtained under biaxial loading in the tension-tension quadrant (a-c) in Figure 5.24. The stress ratios \( \sigma_{11}/\sigma_{22} \) for the labels a to c are presented in Table 5.3.

Now, we return to the simulations for the biaxial strength using the pressure-dependent critical-energy model. The biaxial failure envelopes obtained using the pressure-dependent critical-energy model for various values of \( m_b \) are compared with experimental results and the simulation results using pressure-independent model in Figure 5.24. A good agreement is obtained between the experiments and simulations for \( m_b = 2.33 \times 10^{-5} \). The fracture patterns obtained at selected locations of the biaxial strength envelope, marked with a to k in Figure 5.24, are presented in Figure 5.25 for the tension-tension quadrant (a-c), in Figure 5.26 for the tension-compression quadrant (d-g), and in Figure 5.28 for the compression-compression quadrant (h-k). The stress ratios \( \sigma_{11}/\sigma_{22} \) at these selected locations are presented in Table 5.3.

The failure patterns obtained under biaxial tension loading (Figure 5.25) show that a diagonal fracture is formed for the stress ratio (a), where equal tensile loads are applied from both sides. This fracture rotates perpendicular to the maximum tensile load direction as the tensile load is reduced on one side (stress ratio b), and the fracture finally becomes vertical for stress ratio (c), which represents the uniaxial tension test. For the tension-compression regime (Figure 5.26), the failure patterns are initially tension-dominated (d and e). However, as the compressive load is increased (f and g), the specimens exhibit significant diffuse damage, resulting in a combination of shear band formation and axial splitting. Such axial splitting is observed in the experiments for compressive strength, but it was not observed in simulations using the pressure-independent failure criterion (see Figure 5.27).
**Figure 5.26:** The failure patterns obtained under biaxial loading in the tension-compression quadrant (d-g) in Figure 5.24. The stress ratios ($\sigma_{11}/\sigma_{22}$) for the labels d to g are presented in Table 5.3.

**Figure 5.27:** Comparison of the failure patterns obtained under uniaxial compression in the experiment (middle) and in the simulations using pressure-independent (left) and pressure-dependent (right) failure criterion.
Figure 5.28: The failure patterns obtained under biaxial loading in the compression-compression quadrant (h-k) in Figure 5.24. The stress ratios ($\sigma_{11}/\sigma_{22}$) for the labels h to k are presented in Table 5.3.

Under biaxial compression loading (Figure 5.28), all specimens show significant diffuse damage, and the final failure is due to shearing failure along the thickness of the specimens. These tests show both qualitative and quantitative agreement with the experiments, providing validation for the current modeling strategy.

5.4 Summary

The limitations of the standard peridynamic modeling approach in accurately simulating compression-dominated failure were investigated in this chapter. Specifically, it was shown that the indentation process in porous rock was not accurately modeled. To overcome this limitation, the standard constitutive framework was extended to include the pore-collapse phenomenon, which was modeled as
permanent deformations. The extended model was validated through qualitative comparisons with acoustic emission data and quantitative comparisons with force-penetration and pressure-penetration data from indentation experiments performed on Bentheim sandstone samples of various sizes. These results suggest that the extended simulation model has promising potential for modeling the indentation process in porous rocks. Furthermore, the standard peridynamic simulation approach was applied to model uniaxial and biaxial failure of concrete, but it significantly underpredicted the UCS and the compression-dominated region of the biaxial strength envelope of concrete. To improve the model, a pressure-dependent fracture energy model was developed and incorporated into peridynamic formulation. The resulting model was validated through simulations of UTS, UCS, and the biaxial strength of concrete, which showed good qualitative and quantitative agreement with experimental data. The developed pressure-dependent critical-energy failure criterion will be used in the next chapter to analyze excavation processes in hard rocks.
Excavation processes involving a Tunnel Boring Machine (TBM) use cutting discs (Figure 6.1, left) to fracture and excavate rock. These cutting discs are mounted on a rotating cutterhead (Figure 6.1, right) of the TBM, which is pressed against the tunnel face. As the cutting disc penetrates the rock, the pressure in the contact area between the disc and the rock surface increases and a crushed zone develops (ROSTAMI 2013). The stresses in this zone continue to increase, leading to the initiation of radial cracks (Figure 6.2, left). These cracks grow and coalesce with adjacent cracks until the rock mass is disintegrated (CHO ET AL. 2010). The interaction between the rock and a cutting disc can be characterized by three-dimensional reaction forces at the disc (Figure 6.2, right). To accurately predict the performance of a TBM, including global thrust and torque requirements, and to design new cutter heads for specific ground geology, it is necessary to estimate the cutting forces for a single disc cutter. In addition, the loads on the disc cutters cause severe wear and damage to the tools. To plan maintenance stops and avoid unexpected TBM stoppages, it is necessary to estimate the working life of cutting tools in a given geology.

This chapter applies the pressure-dependent critical-energy failure criterion developed in Section 5.3.2 to analyze hard rock excavation using cutting discs of a Tunnel Boring Machine (TBM). The chapter introduces theoretical and computational performance prediction models, including a discussion of the Colorado School of Mines (CSM) model for predicting cutting force. The experimental setup of the Linear Cutting Machine (LCM) test, which serves as the benchmark for the simulations, is explained. Simulations are performed for rock excavation in both relieved and unrelied rock cutting scenarios. Some contents of this chapter have been published in BRACKMANN ET AL. (2023), BUTT ET AL. (2019, 2022), BUTT AND MESCHKE (2017a, 2021a), PRIEBE ET AL. (2021). The main objectives of this chapter are:

- To further validate the extended peridynamic simulation model (Section 5.3.2) using the LCM experiments and the CSM model.
- To incorporate and verify an Archard-type wear model in peridynamic framework to simulate the abrasive wear of cutting discs.
- To utilize a Drucker-Prager type soil plasticity model along with the developed abrasive wear
model to simulate excavation in mixed-ground conditions.
- To investigate the influence of cutting disc blunting on excavation efficiency.
- To generate and analyze cutting force data produced using damaged cutting discs and predict
  the level of damage using a vibration-based feature extraction algorithm.

Figure 6.1: TBM disc cutters (LABRA ET AL. 2017, left) and a hard rock TBM cutter head man-
ufactured by Terratec (right).

Figure 6.2: Rock failure mechanism during excavation with a disc cutter (CHO ET AL. 2010, left)
and three dimensional cutting forces acting on a cutting disc (LABRA ET AL. 2017, right).

6.1 TBM performance in hard rock

Predicting the cutting forces of a TBM is crucial for analyzing its performance, and is influenced by
factors such as cutting disc geometry, disc spacing, rock material properties, and process parameters
like penetration rate and cutting speed. These cutting forces can be decomposed into normal, rolling,
6.1. TBM PERFORMANCE IN HARD ROCK

and side forces (Figure 6.2, right). The forces increase as the tool spacing increases, but only up to the point where the cut spacing exceeds the area of interaction between the cracks created by adjacent cuts (Villeneuve 2017). Similarly, an increase in the penetration rate results in higher cutting forces, but the rolling forces increase at a higher rate than the normal forces (Rostami 2008).

The cutting forces estimation on a single disc cutter can be achieved using full-scale rock cutting tests (Gertsch et al. 2007, Pan et al. 2019, Rostami and Ozdemir 1993), theoretical and empirical models (Bruland et al. 1995, Nelson et al. 1985, Ozdemir 1977, Rostami et al. 1996, Roxborough and Phillips 1975), or numerical simulations of the rock cutting process (Butt et al. 2019, Butt and Meschke 2017a, 2021a, Cho et al. 2013, 2010, Labra et al. 2017). Recently, there have also been advances in utilizing Artificial Intelligence to predict TBM performance (Salimi et al. 2016, Shao et al. 2013). This section provides a brief overview of the experimental setup of the LCM test, the CSM model used for cutting force prediction, and some of the simulation models used for rock excavation.

6.1.1 Linear Cutting Machine (LCM) experiment

LCM test (Rostami 1997, Rostami and Ozdemir 1993) was developed at the Colorado School of Mines (CSM) to predict the performance of a single cutting tool. In the LCM experiment (Figure 6.3), a cutting disc moves along a rock specimen at a known penetration level and tool spacing, and tool-rock interaction is characterized by the reaction forces on the cutting disc. Several cutting lines at a fixed spacing can be performed, which comprise a cutting pass (Figure 6.4), the cutting forces can then be averaged over these cutting lines. These forces are decomposed into normal, rolling, and side forces (Figure 6.2, right). These forces have a significant influence on the excavation process, as they are used to predict the global thrust and torque requirements for a TBM.

![Figure 6.3: Schematic of the Linear Cutting Machine (left) and a close up view of a cutting disc during a cutting line in the LCM test where the formation of rock chips can be observed (right).]
6.1.2 Theoretical performance prediction

Several empirical and semi-empirical models have been proposed for the estimation of the cutting forces depending on various operational parameters. Early prediction models for V-shaped cutting discs were proposed by Roxborough and Phillips (1975) and Sanio (1985). Other methods include the Norwegian method (NTNU) (Bruland 1998, Bruland et al. 1995), Nelson’s method (Nelson et al. 1985) and the CSM model (Rostami 1997, Rostami and Ozdemir 1993).

Early version of CSM model was developed by Ozdemir (1977) and was updated based on a large database of full-scale LCM tests (Rostami 1997, Rostami and Ozdemir 1993). Since its development, the CSM model has been extensively used in practice (Exadaktylos et al. 2008). It considers the rock material properties, the geometry of the cutting disc and the operational conditions to predict the cutting forces for a given tool penetration and spacing. This model, however, does not take into account the rock mass conditions such as fractures and joints. Following provides a brief overview of the CSM model.
6.1. TBM PERFORMANCE IN HARD ROCK

Cutting forces

To predict the cutting forces on a disc cutter, the CSM model proposes the following distribution of pressure as a function of contact angle ($\theta$) in the crushed zone:

$$P(\theta) = P_o \left( \frac{\theta}{\phi} \right) \psi.$$  \hspace{1cm} (6.1)

Here, $\psi$ is a constant for the pressure distribution function. Depending on $\psi$ different pressure distributions under the cutting disc can be achieved. It varies between 0.2 for V-shaped and sharp cutters and $-0.2$ for wider tip cutters. $P_o$ is the base pressure in the crushed zone which is derived from regression analysis of several LCM tests and it is found to be a function of the cutting disc spacing ($s$), penetration ($p$), radius and tip width of the cutting disc ($R$ and $T$) and the ultimate tensile and compressive strength of the rock ($\sigma_t$ and $\sigma_c$). It is defined as:

$$P_o = C \sqrt[3]{\frac{\sigma_t^2 \sigma_c s}{\phi \sqrt{RT}}},$$  \hspace{1cm} (6.2)

where $C$ is a dimensionless constant, which for a general case is defined as $C = 2.12$ (Rostami 1997). $\phi$ is the angle of contact between the rock and the cutting disc (Figure 6.5), it is defined as:

$$\phi = \cos^{-1} \left( \frac{R - p}{R} \right).$$  \hspace{1cm} (6.3)

Now, the total resulting force on the cutting disc ($F_T$) can be computed by integrating the pressure (Eq. 6.1) over the contact area as:

$$F_T = \int_0^\phi TRP(\theta) \ d\theta = \frac{TRP_0 \phi}{1 + \psi}.$$  \hspace{1cm} (6.4)
The rolling and normal forces \((F_r\) and \(F_n\)) are decomposed from the total force using the cutting coefficient \((CC)\). It is the ratio of the rolling to normal cutting force and is defined using the angle \(\beta\) as:

\[
CC = \frac{F_r}{F_n} = \tan(\beta).
\] (6.5)

A uniform distribution of pressure is assumed at the contact area, which defines \(\beta\) as the middle point of the contact area (Figure 6.5) as:

\[
\beta = \frac{\phi}{2}.
\] (6.6)

Finally, the rolling and the normal forces are obtained by projecting the total force \(F_T\) on the two directions as:

\[
F_r = F_T \cos(\beta) = \frac{TRP_o \phi}{1 + \psi} \cos \left( \frac{\phi}{2} \right),
\]

\[
F_n = F_T \sin(\beta) = \frac{TRP_o \phi}{1 + \psi} \sin \left( \frac{\phi}{2} \right).
\] (6.7)

These forces can then be used in conjunction with the design parameters of the cutterhead (number of tools and their locations) to predict the global torque and thrust requirements of a TBM. This model has been successfully applied to predict the performance of a TBM in several tunneling projects (EXADAKTYLOS ET AL. 2008, ROSTAMI 2008).

**Specific energy**

The efficiency of an excavation process is estimated in terms of the specific energy \((SE)\), which is defined as the energy required to excavate a unit volume of rock mass. For a single disc cutter, it is calculated as:

\[
SE = \frac{F_r L}{V},
\] (6.8)

where \(F_r\) is the rolling force, \(L\) is the length of the cutting distance, and \(V\) is the excavated rock volume. The cutting volume \(V\) can be expressed in terms of the tool penetration \(p\), disc spacing \(s\), and the length of the cut \(L\). This results in the following form of Eq. (6.8):

\[
SE = \frac{F_r L}{psL} = \frac{F_r}{ps}.
\] (6.9)

**Cutterhead and machine parameters**

Cutterhead design includes the selection of the head geometry, the arrangement of the cutting discs, and the optimal disc spacing. Optimum disc spacing is selected based on the maximum anticipated penetration for a given cutting disc’s load capacity. Cutting disc spacing also considers the hardest formation to be excavated to ensure that the machine can cut through at a reasonable penetration rate.
After selecting the optimal tool spacing, the number of disc cutters on the cutterhead is estimated according to Rostami (2008) as:

\[
N = \frac{D_{TBM}^2}{2s} K, \quad (6.10)
\]

where, \( N \) is the total number of disc cutters, \( D_{TBM} \) is the diameter of the TBM, and \( K \) is a factor ranging from 1.15 for large to 1.3 for smaller diameter TBMs.

Cutterhead rotational speed (RPM) is calculated using the linear velocity limit of the selected disc cutter. The typical velocity limit \( V_{\text{limit}} \) for 430 and 480 mm cutting discs are 175 and 200 m/min, respectively (Rostami 2008). Using \( V_{\text{limit}} \) and \( D_{TBM} \), the rotational speed of the cutterhead can be computed as:

\[
RPM = \frac{V_{\text{limit}}}{\pi D_{TBM}}. \quad (6.11)
\]

Using this information, it is possible to estimate the cutterhead thrust \( (TH) \), torque \( (TQ) \) and machine power \( (P) \) requirement (Pan et al. 2019) as follows:

\[
TH = N F_n,
\]
\[
TQ = 0.3 N F_r D_{TBM},
\]
\[
P = \frac{2\pi}{60} TQ RPM. \quad (6.12)
\]

By estimating the specific energy and cutterhead design parameters, it is possible to predict the thrust, torque, and power requirements for a TBM, which is crucial for ensuring efficient and effective tunnel excavation.

### 6.1.3 Computational models

Performing numerical simulations of the rock cutting process using disc cutters is challenging, as it involves modeling the severely discontinuous process of rock fragmentation. Numerical methods are prone to stability and convergence issues when a large number of discontinuities are present in the simulation domain. Additionally, the size of the rock specimens involved in these processes presents a challenge, as the simulation domain must be discretized finely enough to resolve the fragmentation and chipping process, leading to an extremely large system of equations that requires significant computational power. Nonetheless, several simulation methods have been used to simulate the rock cutting process.

Simulations of rock cutting using the Finite Element Method (FEM) have been performed by various researchers (Geng et al. 2017, Huang et al. 2016, Menezes et al. 2014). While FEM has been applied to evaluate the optimum tool spacing (Cho et al. 2010, Xu et al. 2022), cutting efficiency (Cho et al. 2013), and case-specific rock cutting scenarios (Xia et al. 2017), the large deformations involved in the excavation processes can significantly distort the mesh, leading to instabilities in the simulation. To overcome this issue, several simulation models utilize the Discrete Element Method (DEM) to simulate the rock cutting process (Choi and Lee 2015, Huang et al. 2013, Moon and Oh 2012, Rojek et al. 2011). A combination of DEM-FEM...
simulation technique for rock excavation was developed by Labra et al. (2017). DEM assumes that a continuum body can be represented by an assembly of discrete particles interacting among themselves, facilitating the modeling of discontinuities involved in the rock excavation process. However, DEM is not a continuum method, and simulation-specific calibration of parameters is required to reproduce experimentally observed material properties, which limits its applicability to general cases. Other simulation methods used to simulate the rock excavation process include General Particle Dynamics (Zhai et al. 2016), the Bonded Particle Model (Zhang et al. 2018), and Smoothed Particle Hydrodynamics (Jeong et al. 2013, Xiao et al. 2017).

A peridynamic simulation model for rock excavation has been developed during the current work (Butt et al. 2019, Butt and Meschke 2017a, 2021a). In addition to its natural ability to model fracture and fragmentation processes, the peridynamic model is a continuum model. Unlike DEM, it can directly utilize experimentally measured elastic parameters, and a calibration procedure is not required. Moreover, because peridynamics is a continuum model, it can be demonstrated that as the mesh is refined sufficiently, the solution converges. Such concepts are not well defined in DEM simulations. This makes peridynamics a powerful tool for understanding the complex fracture and fragmentation processes involved in rock cutting. The results obtained using the peridynamics approach are presented in the next section.

6.2 Peridynamic simulations of the LCM test

This section presents peridynamic simulations of the LCM test carried out on Colorado red granite using an extended version of the open-source software Peridigm (Littlewood 2015, Parks et al. 2012). The simulations consider both relieved and unrelieved rock cutting cases. Relieved and unrelieved rock cutting modes refer to the stress state present in the rock during the excavation process. In relieved cutting mode, the fractures initiated from the adjacent cutting tools interact with each other and relieve the stress state in the rock, resulting in lower levels of cutting forces. In contrast, in unrelieved cutting mode, the surrounding rock mass is intact and stresses are not relieved, leading to higher forces on the excavation tools.

The simulation model requires the initial calibration of the fracture energy \( G_c \) and the model parameter \( m_b \) according to the pressure-dependent critical-energy model (Section 5.3.2), in order to reproduce uniaxial tensile and compressive strengths (UTS and UCS), respectively. It should be noted that Brazilian tensile strength (BTS), commonly used in rock mechanics, can also be used to calibrate \( G_c \), instead of the UTS used here. After calibrating UTS and UCS, simulations of the LCM test for both relieved and unrelieved cases are performed. The material parameters used for Colorado red granite, as reported in Gertsch et al. (2007), are presented in Table 6.1. The heterogeneous nature of the rock is considered using randomly distributed strength parameters, as explained in Section 5.1.

Calibration for the compressive strength

The calibration procedure for the pressure-dependent fracture energy is adapted from Section 5.3.3. For the granite used in the simulations, a fracture energy \( G_c \) of 100 J/m\(^2\) is assumed. The specimen
6.2. PERIDYNAMIC SIMULATIONS OF THE LCM TEST

<table>
<thead>
<tr>
<th>Material parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus, $E$ (Pa)</td>
<td>$41 \times 10^9$</td>
</tr>
<tr>
<td>Poisson’s ratio, $\nu$</td>
<td>0.234</td>
</tr>
<tr>
<td>Density, $\rho$ (kg/m$^3$)</td>
<td>2650</td>
</tr>
<tr>
<td>Tensile strength, $\sigma_t$ (Pa)</td>
<td>$6.78 \times 10^6$</td>
</tr>
<tr>
<td>Compressive strength, $\sigma_c$ (Pa)</td>
<td>$158 \times 10^6$</td>
</tr>
</tbody>
</table>

Table 6.1: Material properties for Colorado red Granite (GERTSCH ET AL. 2007).

![Tensile Strength](image1)

**Figure 6.6:** Ultimate tensile strength ($\sigma_t$) test for granite: stress-strain relationship and the obtained fracture pattern.

![Compressive Strength](image2)

**Figure 6.7:** Ultimate compressive strength ($\sigma_c$) test for granite: stress-strain relationship and the obtained fracture pattern.

is discretized with a mesh size of 5 mm and a horizon size of 15.1 mm. To account for the heterogeneous strength of the rock material, the fracture energy ($G_c$) is randomly realized from a Weibull distribution (see Section 5.1 and Figure 5.1) using a shape parameter $m = 3$ following (HUDSON...
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AND FAIRHURST 1969, LIU ET AL. 2018). This gives a UTS of $6.8 \times 10^6$ Pa, as shown in Figure 6.6.

Next, the fracture energy is fixed, and the parameter $m_b$ of the pressure-dependent fracture energy is calibrated to reproduce the compressive strength of granite. A value of $m_b = 124.5 \times 10^{-6}$ is found to reproduce a UCS of $154.5 \times 10^6$ Pa, as shown in Figure 6.7. These values for tensile and compressive strength are consistent with the material parameters presented in Table 6.1. For a discussion on the physical interpretation of $m_b$, the interested reader is referred to Section 5.3.2. This concludes the calibration procedure for the model parameters $G_c$ and $m_b$. These parameters will now be used in the next subsections for the simulations of the LCM test.

Simulation setup for the LCM test

For the simulation of the LCM test (GERTSCH ET AL. 2007), a cutting disc with a diameter of 432 mm and a tip width of 13 mm is used. The boundary conditions and dimensions of the rock specimen used in the simulations are presented in Figure 6.8. The linear cutting velocity of the disc is 1.5 m/s for all cases. The rock specimen used in the full-scale LCM experiments is $1.0 \times 0.7 \times 0.5$ m. However, simulating such a large specimen would require a significant amount of computational power. To reduce the computational effort, a smaller specimen size of $0.3 \times 0.4 \times 0.15$ m is considered. Numerical tests have shown that the selected specimen size is sufficiently large to avoid the influence of the boundaries of the specimen. This scaled-down specimen size has also been used in other numerical studies (CHO ET AL. 2010, LABRA ET AL. 2017).

The cutting disc is modeled as a rigid body and discretized using an average mesh size of 1.6 mm and a peridynamic horizon size of 5 mm. The rock specimen is discretized and the fracture energy ($G_c$) is sampled using the same parameters as used in the case of UCS calibration in the previous subsection. This discretization results in a total of $1.4 \times 10^6$ material points for the entire model. A stable time step of $1.5 \times 10^{-7}$ s is used for all simulations. Each simulation is solved using 160 parallel processes with a run time of around 15 days.

6.2.1 Unrelieved rock cutting

Unrelieved rock cutting here refers to the cutting mode in which fractures initiated from adjacent tools do not interact with the current cutting path, i.e., it represents an isolated cutting line. For the simulation of unrelieved rock cutting, the process parameters, i.e., cutting velocity and penetration rate, are taken from a real TBM drive (LABRA ET AL. 2017, 2008). According to LABRA ET AL. (2017), the TBM advance rate per rotation is considered as the penetration rate, which is 3.9 mm/rev. This penetration per revolution is taken as the penetration depth for the LCM test and is kept constant for the prescribed tool path. The LCM test also considers the spacing between disc cutters, which will be taken into account for the simulation of relieved rock cutting in the next section.

Three-dimensional cutting forces over the cutting distance and their averages obtained for this case are presented in Figure 6.9. The forces have been considered in the cutting distance range of 0.07 m to 0.23 m, discarding the results influenced by the boundaries of the specimen. The average cutting forces obtained from the simulation (Table 6.2) are consistent with the field data (LABRA ET AL. 2008) and the DEM simulation results from LABRA ET AL. (2017). The experimental value
Figure 6.8: Dimensions of the rock specimen and cutting disc as well as the boundary conditions used in the simulation of the LCM test.

Figure 6.9: Simulation result for unrelieved rock cutting and the associated cutting forces.
Table 6.2: Comparison of the average cutting forces obtained from the peridynamic simulation with the DEM simulation (LABRA ET AL. 2017) and the field data (LABRA ET AL. 2008).

<table>
<thead>
<tr>
<th>Cutting force</th>
<th>Peridynamic simulation</th>
<th>DEM simulation</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal force, $F_n$ (KN)</td>
<td>197</td>
<td>191</td>
<td>232</td>
</tr>
<tr>
<td>Rolling force, $F_r$ (KN)</td>
<td>35</td>
<td>20</td>
<td>–</td>
</tr>
<tr>
<td>Side force, $F_s$ (KN)</td>
<td>2</td>
<td>0.9</td>
<td>–</td>
</tr>
</tbody>
</table>

of normal force for a single cutting disc was obtained by dividing the total thrust of the TBM by the number of disc cutters. This represents a relieved rock cutting mode in principle. However, according to LABRA ET AL. (2017), the cutter spacing was large enough to ignore the interaction between cutting discs, and the cutting conditions were close to unrelieved rock cutting mode.

### 6.2.2 Relieved rock cutting

Relieved rock cutting takes into account the spacing between cutting discs, as the interaction of adjacent cutting paths influences the rock chipping process. Hard rock excavation with TBMs typically occurs in relieved cutting conditions, where previous adjacent cutting paths affect the excavation process. The formation of rock chips, which strongly depends on the tool spacing, ensures efficient cutting performance. Therefore, the optimum spacing between cutting discs is one of the most critical factors in the design of a hard rock TBM cutterhead.

The simulation setup used for relieved rock cutting is similar to the one presented in Section 6.2.1. These simulations consider three tool spacings, i.e., 76, 51, and 25 mm, and various tool penetration depths. The selection of these specific tool spacings is based on the availability of experimental data (GERTSCH ET AL. 2007). Simulations are conducted with three cutting disc passes at a fixed penetration and spacing, as shown in Figure 6.10. The first cutting line is used for rock conditioning to damage the rock and mimic the previous tool pass, as in the LCM test and rock cutting with a hard rock TBM cutterhead. Some simulations, especially with higher penetration depths, became unstable during the third cutting pass. To maintain objectivity, the third cutting pass is not considered in the results, and the average cutting forces presented in this section are only averaged over the second tool pass.

Simulation results show that the peridynamic approach can capture the chipping process and cutting forces in rock cutting simulations. For a tool penetration of 6 mm and spacing 76 mm, Figure 6.10 illustrates that the simulations captured the formation of rock chips between the tool passes. The average normal and rolling forces obtained for a tool spacing of 76 mm at various penetration levels are compared with the CSM model (ROSTAMI 1997, ROSTAMI AND OZDEMIR 1993) and experimental data (GERTSCH ET AL. 2007) in Figure 6.11. The normal cutting forces are in good agreement with the experiment, while the rolling forces are slightly overestimated. When the tool spacing is reduced to 51 mm, Figure 6.12 reveals that the chipping process became inefficient, even for a penetration of 5 mm. Although the normal forces for this case show a slightly different trend, they are still within an acceptable range of the experiment, and the rolling forces are slightly overestimated for higher penetration levels (Figure 6.13).
6.2. PERIDYNAMIC SIMULATIONS OF THE LCM TEST

Figure 6.10: Simulation of the LCM test for a tool penetration and spacing of 6 mm and 76 mm, respectively. Material points with a damage value greater than 0.95 are filtered out for the visualisation of the chip formation (right).

Figure 6.11: Average normal and rolling forces obtained from peridynamic simulations are compared with the CSM model and experimental data for various tool penetration levels and a tool spacing of 76 mm.

As the spacing is further reduced to 25 mm, chipping is completely suppressed (Figure 6.14). The average normal force obtained from the simulations has a very low value for some penetration
Figure 6.12: Simulation of the LCM test for a tool penetration and spacing of 5 mm and 51 mm, respectively. Material points with a damage value greater than 0.95 are filtered out for the visualisation of the excavated zone (right).

Figure 6.13: Average normal and rolling forces obtained from peridynamic simulations are compared with the CSM model and experimental data for various tool penetration levels and a tool spacing of 51 mm.

levels for this case (Figure 6.15), mainly due to the small tool spacing. The peridynamic horizon size governs the size of the damage zone around a fracture and is comparable to the tool spacing for
6.2. PERIDYNAMIC SIMULATIONS OF THE LCM TEST

Figure 6.14: Simulation of the LCM test for a tool penetration and spacing of 4 mm and 25 mm, respectively. Material points with a damage value greater than 0.95 are filtered out for the visualisation of the excavated zone (right).

Figure 6.15: Average normal and rolling forces obtained from peridynamic simulations are compared with the CSM model and experimental data for various tool penetration levels and a tool spacing of 25 mm.

In this case, which means that the cutting disc passes through this damaged zone after the first pass and experiences a weaker material. This can lead to the observed low normal forces. Nevertheless, the
overall trend of the average normal and rolling force obtained from the simulations is in agreement with the experimental data and the CSM model (Figure 6.15).

The average cutting forces obtained from the simulations in this section exhibit significant scatter due to the probabilistic nature of these simulations. As the strength parameters used to model the heterogeneous nature of the rock are randomly sampled from a Weibull distribution (Section 5.1), each simulation has a slightly different spatial distribution of material strength. These differences can result in the observed scatter. Ideally, a multi-simulation approach should be adapted for these cases to find an average solution. However, performing a large number of simulations with such high resolution would require a considerable computational effort and is outside the scope of the current work.
6.3 Wear of cutting tools

Wear is the material removal from solid surfaces that results from mechanical loads causing sliding contact. Writing with a pencil is a common example of wear in everyday life. The sketch obtained on a piece of paper is the result of the wearing process happening at the tip of the pencil. The type of material removal depends on various factors, and in general, wear mechanisms can be divided into four main classes:

**Abrasive wear** occurs when a hard, rough surface slides over a softer surface. The nature of material removal can be described by several mechanisms, including plowing, cutting, and fragmentation. Plowing occurs when hard particles displace the material laterally, resulting in grooves. Chipping is another mechanism where material is removed from the surface in the form of chips, with little or no material displaced to the sides of the grooves. Fragmentation occurs when material is separated from a surface by the penetrating hard particles causing localized fractures.

**Adhesive wear** occurs when two surfaces slide over or are pressed into each other, causing fragments to detach from one surface and adhere to the other. Adhesive wear leads to an increase in roughness due to the creation of lumps above the original surface.

**Surface fatigue wear** is a process in which the surface of a material is weakened by cyclic loading. This is due to the formation of microcracks, which can be either surface cracks or sub-surface cracks. Fatigue wear occurs when the cyclic growth of these microcracks causes material to be removed from the surface.

**Corrosive wear** occurs when the sliding of two surfaces takes place in a corrosive environment. The fundamental cause of this wear is the chemical reaction that takes place between corrosive medium and the worn surface.

Other less common types of wear include impact wear, cavitation wear, fretting wear, and erosive wear. A detailed description of wear mechanisms can be found in RABINOWICZ (1995). Wear can involve different mechanisms at various stages of the process and depend on properties of the surfaces, environmental conditions, and kinematics, such as surface roughness, temperature, sliding distance, and velocity. Reducing wear is important for excavation processes as it causes premature tool failure. Abrasive wear is selected here as the most relevant type of wear for the analysis.
Abrasive wear model

Abrasive wear is related to sliding contact and it occurs when a surface containing hard particles slides on a softer surface. The sliding causes the hard particles to dig into the softer surface and as the sliding motion continues, grooves are formed on the soft surface from where the material is removed. To estimate the wear rate, a simple model is considered in which all asperities of the hard surface are cone-shaped. Firstly, a single cone-shaped particle is considered which penetrates the surface with a normal force $\Delta F_N$ (Figure 6.18). The cone will penetrate the surface according to the hardness $H$ of the material being abraded, given as:

$$\Delta F_N = H \cdot \pi r^2. \quad (6.13)$$

The vertical projected area of this cone is $rh$. As the cone displaces a distance of $dx$, a volume $dV$ is cut out from the softer material. It is given by:

$$dV = rh \cdot dx = r^2 \tan(\theta) \cdot dx = \frac{\Delta F_N \tan(\theta) \cdot dx}{\pi H}. \quad (6.14)$$

The wear rate is defined as:

$$\frac{dV}{dx} = \frac{\Delta F_N \tan(\theta)}{\pi H}. \quad (6.15)$$

Summation of the influence of all asperities results in total worn volume as:

$$V = \frac{F_N \tan(\theta)}{\pi H} \cdot x, \quad (6.16)$$

where $\tan(\theta)$ is the weighted average of $\tan(\theta)$ values of all the individual cones, and $x$ is the total sliding distance. Equation 6.16 gives an expression that was proposed for adhesive wear by ARCHARD (1953) and later applied to abrasive wear (POPOV 2010, RABINOWICZ 1995). This is known as the Archard wear law:

$$V = k_{abr} \frac{F_N}{H} \cdot x, \quad (6.17)$$

where $k_{abr}$ is the abrasive wear coefficient, defined as the average tangent of the roughness angle divided by $\pi$. It represents the specific geometry of the abrasive surface, accounting for the angle and shape of the individual asperities. Typical values of $k_{abr}$ range from $10^{-2}$ to $10^{-5}$. Wear between a soft material and an abrasive surface, in which hard particles get embedded in the soft body, is
called *two-body wear*. Another case of abrasive wear is the wear of two bodies between which hard abrasive particles are added, known as *three-body wear*. The magnitude of $k_{abr}$ is an order of magnitude lower for the case of three-body wear. This is because the abrasive grains for the three-body case spent most of the time rolling instead of sliding which abrades the surface.

**Verification**

The abrasive wear model (Section 6.3) has been implemented in the open-source software *Peridigm* (LITTLEWOOD 2015, PARKS ET AL. 2012). The simulation model is verified based on a simple sliding test for the abrasive wear. A steel block is resting under its body weight on a rock surface, it then slides on the rock specimen for a known distance of 6.4 cm (CARBONELL 2009), as shown in Figure 6.19. The test is performed for three types of rock bases with different hardness values: Sherwood sandstone, Fell sandstone and Dealbeattie granite. The material properties used for the steel and the rocks are presented in Table 6.3. Accumulated volume loss due to abrasive wear computed using the peridynamic simulation model, is shown in Figure 6.19. Volume loss due to abrasive wear computed from the simulations is compared with the theoretical values obtained by Eq. (6.17) in Figure 6.20.

![Figure 6.19: Simulation setup and geometry of the steel and rock specimen for the wear test (left). Accumulated wear after a sliding distance of 6.4 cm on Fell sandstone (right).](image)

<table>
<thead>
<tr>
<th>Materials</th>
<th>Steel</th>
<th>Sherwood sandstone</th>
<th>Fell sandstone</th>
<th>Dealbeattie granite</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (Pa)</td>
<td>$2.0 \times 10^{11}$</td>
<td>$6.4 \times 10^{9}$</td>
<td>$3.27 \times 10^{10}$</td>
<td>$4.11 \times 10^{10}$</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.2</td>
<td>0.3</td>
<td>0.3</td>
<td>0.3</td>
</tr>
<tr>
<td>$\rho$ (kg/m$^3$)</td>
<td>7850</td>
<td>2680</td>
<td>2690</td>
<td>2670</td>
</tr>
<tr>
<td>$H$ (Pa)</td>
<td>$9.0 \times 10^{9}$</td>
<td>$4.8 \times 10^{6}$</td>
<td>$5.28 \times 10^{7}$</td>
<td>$1.48 \times 10^{8}$</td>
</tr>
<tr>
<td>$k_{abr}$</td>
<td>0.06</td>
<td>0.06</td>
<td>0.06</td>
<td>0.06</td>
</tr>
</tbody>
</table>

*Table 6.3: Material properties used for the wear model verification.*
6.4 LCM test in mixed ground conditions

Mixed or heterogeneous ground conditions occur when a tunnel face has two or more layers of rock or soil with significantly different mechanical properties. Mechanized tunneling in such conditions results in highly variable loads on the cutting discs. As the cutting disc moves from soft to hard ground, an excessive load is exerted on the cutting disc at the point of contact with the hard ground layer, as shown in Figure 6.21. This excessive load contributes to the global torque fluctuation of the TBM and may substantially increase wear rates and cause localized damage to the cutting disc and bearings, leading to unexpected TBM stoppages and delays in the project timeline.

This section focuses on the excavation process using a cutting disc in mixed ground conditions. To simulate this process, LCM tests were conducted, in which a cutting disc moves from soft soil into a hard rock domain. The simulations used a scaled cutting disc of 56 mm diameter and a rock specimen of $0.2 \times 0.15 \times 0.075$ m, as experimentalists have used such scaled cutting tests to facilitate the experimental setup and the availability of the apparatus in the laboratory (ENTACHER ET AL. 2014). Scaled tests were used due to the large computational expense associated with a full-scale test.

The soil material is modeled using an elastic-plastic Drucker-Prager type plasticity model (as discussed in Section 2.3), and the rock material is modeled using an elastic-brittle constitutive relation. The bulk and shear modulus for soil and rock material are assumed to be $K = 35.83$ GPa and $G = 16.54$ GPa, respectively. The yield strength of the soil is 100 KPa, friction angle is 30°, and the fracture energy of the rock material is $G_c = 23.7$ J/m². The objective of these analyses is to characterize the impulse load and resulting wear on the cutting disc as it moves through the interface between two materials with significantly different mechanical properties. Such repeated impulse loads can cause excess vibration in the cutterhead and increased fluctuations in torque and thrust of the TBM, which may ultimately result in premature damage to the cutting disc.

Figure 6.20: Volume loss due to abrasive wear with varying hardness of the surface under analysis.

![Volume loss due to abrasive wear with varying hardness of the surface under analysis.](image)
6.4. LCM TEST IN MIXED GROUND CONDITIONS

Figure 6.21: Schematic illustration of a mixed face tunnel and the forces acting on a cutting disc.

Figure 6.22: Peridynamic simulation of a cutting disc working in mixed ground conditions (soft soil to hard rock domain) with a penetration of $p = 2$ mm (top) and $p = 3$ mm (bottom). Plastic deformations and damage in hard rock as well as the associated cutting forces acting on the disc are presented. The vertical grey line represents the soil-rock interface.
Figure 6.23: Comparison of the abrasive wear on the cutting disc working in mixed ground conditions (Figure 6.22) at two different penetration levels (left). Total volume lost on cutting disc due to abrasive wear over the cutting length (right).

The results obtained from the simulations of the cutting disc moving from soil to rock domain are presented in Figure 6.22. Plastic deformations in the soil and the damage level in the rock, for two different penetration levels ($p = 2\ mm$ and $p = 3\ mm$), are presented in the first column of Figure 6.22. The second column shows the reaction forces at the cutting disc for the two cases. These diagrams show that the normal cutting forces are negligible when the disc cutter is in the soil domain. However, as it reaches the soil-rock interface (cutting length = 0.05 m) and continues to move into the rock domain, the cutting forces show a peak of relatively high cutting forces. As anticipated, the comparison of cutting forces at the two penetration levels in this study shows that the peak cutting force increases proportionally with the tool penetration.

The verified model for abrasive wear (Section 6.3) was utilized in conjunction with the simulations for mixed ground conditions to estimate the abraded volume on the cutting discs and localized wear occurring at the soil-rock interface. Figure 6.23 (left) displays the accumulated wear on the cutting disc, for a $180^\circ$ rotation, for two penetration levels at three different stages: in the soil domain (left column), at the soil-rock interface (middle column), and in the rock domain (right column). The figure reveals a significant increase in accumulated wear on the cutting disc as it progresses into the rock domain. Figure 6.23 (right) presents the total volume loss due to abrasive wear on the cutting disc over the cutting length for both penetration levels. A notable change in wear rate is evident as the cutting disc moves from the soil to the rock domain.

6.5 Influence of cutting disc blunting on the excavation efficiency

TBM performance prediction models (MACIAS 2016, ROSTAMI 1997) have been developed to predict the penetration rate for hard rock excavation. However, these models consider a constant geo-
metry of the disc cutter until replacement, thus disregarding the influence of the change of cutting edge geometry due to excavation loads. A well-known wear phenomenon that influences the tool geometry is the plastic deformation which blunts the cutting edge, known as mushrooming (Figure 6.24). Experiments (Brackmann et al. 2022) have shown that blunting of the cutting edge causes a reduction of the excavated rock mass.

![Figure 6.24: Cutting disc blunting after excavation (left), a 3D scan of the blunted cutting disc (middle) and the averaged cross-section of the 3D scan (right).](image)

The peridynamics model is further used to investigate the influence of cutting disc blunting on excavation efficiency. For this study, two cross-sections of cutting discs are selected; one has a flat edge with a tip width of 3.0 mm representing a pristine cutting disc, and the other has a blunted edge with a radius of 2.1 mm representing a worn-out cutting disc (Figure 6.25, left). These simulations are performed using a cutting disc with a diameter of 120 mm, as used in the experiments by Brackmann et al. (2022), and an Anröchter sandstone specimen of 0.19 × 0.07 × 0.04 m.
The bulk and shear modulus for Anröchter sandstone used in the simulations are $K = 13.81$ GPa and $G = 12.6$ GPa, respectively. The fracture energy used for the sandstone is $G_c = 57$ J/m$^2$.

Figure 6.26 shows a comparison between the excavation efficiency of both cutting discs. The cutting disc with a flat edge consistently excavates more mass compared to the blunt edge cutting disc for various penetration levels. This difference can be attributed to the lower contact stresses at the tool-rock interface in case of a blunt edge cutting disc (RAD 1975). Additionally, the accumulated wear predicted by the simulation model for the flat-edge cutting disc (Figure 6.25, right) is also in qualitative agreement with the experiment (Figure 6.24).

6.6 Identification of localized damage to cutting discs

This section presents rock cutting simulations using cutting discs with varying degrees of localized damage. Such damage to the discs can occur due to impact loads when TBMs operate in mixed ground conditions. Early identification of these damages is essential for planning maintenance downtime, a significant factor in the overall project timeline. Neglecting to address damaged cutting discs can lead to severe bearing failures and damage to the cutter head. The localized damage to the cutting disc results in periodic changes in cutting forces. A vibration-based feature extraction algorithm is presented to identify these periodic changes in the cutting forces which correlate with the extent of damage to the cutting disc.

To analyze the cutting forces and extract damage-sensitive features, four cutting discs with a diameter of 120 mm are modeled with three increasing levels of localized damages (Figure 6.27). The rock material parameters used, including bulk modulus, shear modulus, and fracture energy, were $K = 35.83$ GPa, $G = 16.54$ GPa, and $G_c = 23.7$ J/m$^2$, respectively, are based on the experiment performed by PRIEBE ET AL. (2022). Cutting force data is generated in the simulations using a fixed penetration depth of 2 mm. The normal cutting forces obtained from the simulations

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**Figure 6.26:** Comparison of rock excavation efficiency with a flat and a blunt edge cutting disc. Excavated rock mass over the rotation of the cutting disc (left) and Excavated rock mass per rotation (right) for various penetration levels.
are then used for vibration-based feature extraction to identify the extent of damage to the cutting disc. Frequency domain analysis of the cutting forces enables the extraction of damage-sensitive features (Butt et al. 2019, Prieb et al. 2021, 2022).

**Figure 6.27:** Cutting disc rings with increasing level of localized damage. Left to right: intact disc, cutting disc with 1, 2 and 3 mm localized damage.

**Figure 6.28:** Normal force obtained over three rotations of the cutting disc with a damage size of 3 mm and the moving average removed from it (left). Envelope of the data obtained via the Hilbert transform (right).

Simulations were performed with a cutting disc rotational speed of 0.377 seconds per revolution. In order to match the rotational speed of the experiment by Prieb et al. (2022), this signal was stretched by a factor of 5.305 to provide a rotational speed of 2.0 sec/rev, resulting in a cutting disc damage interaction frequency of 0.5 Hz. The simulation signal was stretched instead of performing...
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simulations with a low rotational speed because simulating with such a low rotational velocity would be computationally expensive over a long period of time. After this step, the moving average $x_{MA}$ was subtracted from the original signal $x$ using the following equation:

$$x_{MAi} = \frac{1}{2n + 1} \sum_{k=i-n}^{i+n} x_k,$$

$$x_i = x_i - x_{MAi}.$$  \hspace{1cm} (6.18)

Here, the sampling frequency of the simulation data is around 10,000 samples per second, and a window size of $2n + 1 = 1200$ was chosen based on the assumption that the interaction between the disc damage and the rock takes around 0.1 to 0.15 s. This step removes the low-frequency component of the signal and leaves behind the high-frequency component, including the damage interaction (Figure 6.28, left). Furthermore, the envelope of this data is computed using a Hilbert transform (Figure 6.28, right) with the following equation:

$$x_H = F^{-1}(F(\overline{x}) 2U) = \overline{x} + iH(\overline{x}),$$  \hspace{1cm} (6.19)

where $F$ is the discrete Fourier transform, $U$ is a Heaviside step function, and $H$ is the Hilbert transform (Cizek 1970). The generated envelope signal is then transformed into the frequency domain (Figure 6.29, left), where the maximum value in the frequency band of 0.45 to 0.55 Hz (disc revolution frequency) is taken as the damage indicator (Figure 6.29, right). The damage indicator increases with the level of localized damage to the cutting disc, demonstrating the effectiveness of the presented method in identifying the extent of damage.
6.7 Summary

The rock excavation process my means of cutting discs of a TBM using an extended peridynamic simulation model was investigated in this chapter. The simulation technique was validated by simulating relieved and unrelieved LCM tests on granite samples while considering the rock material heterogeneity through random sampling of strength parameters from a Weibull distribution. The cutting forces were found to be in good agreement with the experimental data and the CSM model predictions. In addition, the simulation model was used to perform LCM tests for mixed ground conditions where the cutting disc moves from a soil medium, modeled using a Drucker-Prager type plasticity model, to a hard rock medium. An Archard-type wear law was incorporated in the simulation model to simulate abrasive wear of the cutting discs. The mixed ground simulations revealed an abrupt increase in the cutting forces as the disc moves from soil to rock medium, resulting in uneven wear of the cutting disc. The effectiveness of the simulation model was further evaluated by investigating the excavation efficiency of cutting discs with blunted cutting edges resulting from excessive plastic deformations. The simulations revealed a decrease in excavated mass, indicating an inefficient excavation process. These findings qualitatively agree with the experimental results. Finally, the simulation model was utilized to generate synthetic cutting force data using cutting discs with varying levels of localized damage. This data was then fed to a vibration-based feature extraction algorithm to determine the extent of damage to the cutting discs. The results demonstrated the effectiveness of the proposed method in accurately identifying the damage level of the cutting discs.
Chapter 7

Conclusion and outlook

7.1 Concluding remarks

This thesis initially presented an investigation into the influence of the length scale of peridynamics on wave propagation and dynamic fracture propagation. Furthermore, the model was extended to simulate the indentation of porous rocks. Improvements were made to the model to simulate the compressive failure of concrete and rock. The enhanced model was then applied to model mechanized excavation in hard rock and mixed ground conditions using cutting discs of a TBM, while considering abrasive wear of the tools. Most of the results presented in this thesis have been published in peer-reviewed articles and conference proceedings. The list of publications can be found in the author’s CV at the end of the thesis. In the following, the most important results of the individual chapters of this thesis are summarized and an outlook on potential future work is provided.

Wave dispersion and propagation

Peridynamics is a nonlocal continuum formulation that includes a nonlocal length scale that influences wave propagation and an influence function that controls the strength of the nonlocality. Dispersion relations for ordinary state-based peridynamics were derived, and discretized dispersion relations were analyzed with respect to various influence functions. Influence functions were proposed to minimize wave dispersion in cases where it should be avoided, and root mean square deviation was used as a metric to quantify the dispersion of elastic waves. Finally, a procedure was proposed to calibrate the peridynamic horizon size to model wave dispersion in granular materials. The horizon size was found to be in the range of the material’s grain size, providing a physical interpretation of the peridynamic horizon size in the context of wave propagation.
Tension-dominated failure

To analyze the influence of the peridynamic horizon on fracture modeling properties, dynamic fracture in plexiglass plates was simulated, and elastic, kinetic, and dissipated energy were monitored under two types of loading conditions. Monotonically increasing loads were used to understand the influence of the horizon size on strength. Different levels of pre-stored elastic energy in front of the crack tip was used to understand the influence of the horizon on crack velocity toughening behavior. The analyses revealed that failure strength was independent of the horizon size, but the velocity-toughening relationship started to show dependence on the horizon size as micro- and macro-branching occurred at increasing loads. Different size specimens were analyzed for the aforementioned loading conditions to verify that peridynamics reproduces the LEFM size effect and to demonstrate that the velocity toughening relationship converges to experimental values as the specimen size increases to the range of the experiments.

The model was also applied to simulate fracture in some benchmark problems at various loading rates, including Kalthoff-Winkler’s test, L-specimen, and CT-specimen. These tests exhibit different fracturing patterns with respect to the loading rate. The simulation model predicted the fracture patterns for these benchmarks, at varying loading rates, which were in an excellent agreement with the experiments.

Compression-dominated failure

To model compressive failure in rock-like materials, the material heterogeneity was considered in these simulations using randomly distributed strengths sampled from a Weibull’s distribution. The critical-energy failure criterion used to simulate dynamic fracture in plexiglass was shown to underestimate the failure load encountered in the rock indentation process. To improve the simulation, peridynamic correspondence models were used in an attempt to incorporate classical constitutive relations to model porous materials. However, these simulations were also unsuccessful due to the instabilities that arise in the correspondence models once the fractures start to initiate. This led to the extension of the standard peridynamic constitutive formulation to consider the pore-collapse phenomenon as inelastic deformation. The extended model was able to simulate the formation of a crushed zone up to the peak load, from where a fracture initiated. This result was in qualitative and quantitative agreement with the experiments.

Furthermore, the standard peridynamic formulation was analyzed to model compressive failure in concrete. However, it was found that the compressive strength of concrete was underestimated by a factor of four and could not be modeled independently of the tensile strength using this approach. Therefore, the model was further extended to consider pressure-dependence in fracture energy dissipation, which enabled independent reproduction of the compressive strength. The extended model was used to simulate the entire biaxial strength envelope for concrete, and an agreement was obtained with the experiments in terms of failure loads and fracture patterns.
7.2. FUTURE PERSPECTIVES

Rock excavation using cutting discs

As the model was shown to be able to reproduce the compressive strength of a material, one of the most critical mechanical property with respect to rock excavation, it was subsequently applied to investigate the mechanized rock excavation process using cutting discs of a TBM. The Linear Cutting Machine (LCM) test was used as the benchmark problem to simulate the excavation process for various tool spacing and penetration levels. The resulting cutting forces were in agreement with experimental data obtained from granite samples. The model was further developed to consider abrasive wear on the cutting discs, and was utilized to simulate an LCM test under mixed-ground conditions to predict wear resulting from changes in the strength of the material being excavated. Additionally, the model was employed to analyze the excavation efficiency of cutting discs that were blunted due to significant plastic deformation. The model was also used to generate synthetic cutting force data by simulating excavation using discs with varying levels of localized damage. Subsequently, a vibration-based feature extraction algorithm used this data to identify the extent of damage to the cutting discs. The feature extraction algorithm effectively predicted the level of damage to the cutting discs.

7.2 Future perspectives

There are still many unanswered questions and unexplored directions in the field of material modeling and mechanized excavation modeling using peridynamics. While the models developed in this work provide a promising foundation, further testing is necessary to ensure their rigor in terms of accuracy, stability, and sensitivity to various parameters. Future research areas can include:

- Incorporating existing stress-based classical material models, such as the micro-plane model, directly into the ordinary state-based peridynamic framework.
- Correlating the length scale \( m_b \) of the pressure-dependent fracture energy model developed in Section 5.3.2 with a characteristic material length or with an experimentally measurable quantity, such as the angle of internal friction.
- Performing multiple simulations with different realizations of rock heterogeneity (Section 5.1) and investigate the influence of the correlation length of the random field.
- Performing simulations of the LCM test in Section 6.2 for various rock types, cutting disc geometries, and cutterhead configurations.
- Extending the wear model for cutting tools presented in Section 6.3 with additional wear modes, such as impact and fatigue wear.
- Validating the simulations for mixed ground conditions presented in Section 6.4 with a full-scale LCM experiment.

Overall, these future research directions aim to address gaps in the current state of the field and expand on the insights gained from this thesis. By further exploring these topics, the understanding of material modeling in peridynamics and its potential applications in the field of mechanized rock excavation can be advanced.


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