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#### Abstract

The relatively new theory of peridynamics is a non-local continuum theory for the modeling of materials behaviour and is especially powerful in treating the spontaneous formation of discontinuities. This indicates that it might be useful in the dynamic modeling of dislocations, but in order to achieve this, its basic principles should be comprehended first. A literature study on the theory has been performed and a peridynamic code has been developed. Using the code in the simulation of a tensile test under quasistatic conditions has verified the linear elastic properties of the peridynamic model material and the correctness of the code. An impact test is used subsequently to explore the influence of several parameters. A dynamic fracture test has been studied next to determine the limit of the crack propagation speed, which turns out to be bounded by the Rayleigh wave speed. The insight that these results give in the properties of peridynamics opens the road to extension of the code to solve problems which have not yet been solved.


## Introduction

The peridynamic theory is a continuum theory that makes use of a nonlocal model to describe material properties. It is particularly powerful in modelling problems where spontaneous formation of discontinuities, like cracks, occurs. In most other continuum mechanics methods partial derivatives are used for the calculation of the relative displacement and force between two particles. These methods need special calculation techniques as soon as discontinuities arise in the material, because partial derivatives are undefined across the discontinuities. Moreover, the location of the discontinuity must be known in order to apply the technique correctly. By contrast, the peridynamic theory makes use of integral equations to compute the force on a particle. Therefore, spatial derivatives are not used and the equations remain valid at a discontinuity, and its location does not need to be known in advance.

The goal of this thesis is to understand the fundamentals of the peridynamic theory and to develop a computer code. In case of success, possibilities for the use of peridynamics for dislocation modelling can be considered.

This report starts with the outcome of a literature study on the peridynamic theory in Chapter 1. Here, the fundamentals of the theory are explained, as well as the terms under which it can be applied. The second chapter explains how the theory can be discretized in time and space. This leads to a numerical approach for calculations using the computer. Chapter 3 describes a tensile test to compare the results of the the newly developed peridynamic code with the linear elastic theory. Chapter 4 describes a dynamic fracture experiment carried out by a peridynamic simulation. The simulation involves a solid sphere which is pulled through a thin plate of peridynamic material (comparable to glass) and is highly fragmented afterwards. In both experiments, the influence of some particular parameters on the results is tested. In Chapter 5, a dynamic fracture test is performed. The crack propagation speed found with this experiment is compared to values found in the literature. Chapter 6 describes the problems that were encountered with both the theory and the code during the project and gives recommendations for further research on this subject. Chapter 7 summarises the results and outlines the conclusions of the project. The appendix contains the details of solving a particular integral and provides information about the input and output files of the peridynamic code.

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## Chapter 1

## Theory of peridynamics

The peridynamic model is a recently developed theory that can be described as a continuum version of molecular dynamics. A summary of its formal derivation is given in the next eight sections. The first section gives the general formulas which are the fundamentals of the theory. The next section introduces the concept of elasticity in peridynamics. By assuming certain material configurations, the number of variables is narrowed down in the third section. A linearization of the model, assuming only small deformations, is described in the fourth section. The next section investigates the conditions to assure material stability. Certain relations between the peridynamics theory and the conventional theory are described in the sixth section. In the seventh section, a prototype peridynamic brittle material is introduced by defining the necessary functions. The last section describes how boundary conditions can be applied in the peridynamic theory.

### 1.1 Peridynamic model of a continuum

In the peridynamic model, the body under investigation is divided into a continuous set of particles with a certain volume. The response of the body $\mathcal{R}$ to external forces is assumed to be dependent only on the displacement of the particles relative to the reference configuration. A particle at point $\mathbf{x}$ in the reference configuration interacts with particles $\mathbf{x}^{\prime}$ that lie within a neighbourhood $\mathcal{H}_{\mathbf{x}}$ of $\mathbf{x}$, defined with


Figure 1.1: Schematic drawing of the body, a pair of particles $\mathbf{x}, \mathbf{x}^{\prime}$ and their corresponding (displacement) vectors $\mathbf{u}(\mathbf{x})$ and $\mathbf{u}\left(\mathbf{x}^{\prime}\right)$ at a certain time $t$.
the horizon $\delta$ :

$$
\begin{equation*}
\mathcal{H}_{\mathrm{x}}=\left\{\mathrm{x} \in \mathcal{R}:\left|\mathrm{x}^{\prime}-\mathrm{x}\right|<\delta \Longrightarrow \mathrm{x}^{\prime} \in \mathcal{R}\right\} \tag{1.1}
\end{equation*}
$$

The force between two particles is denoted by the vector-valued function $\mathbf{f}$, the pairwise force function with dimensions $\left[\mathrm{N} / \mathrm{m}^{6}\right]$. This is a function of the relative position $\boldsymbol{\xi}=\mathrm{x}^{\prime}-\mathrm{x}$ and the relative displacement $\boldsymbol{\eta}=\mathbf{u}\left(\mathbf{x}^{\prime}, t\right)-\mathbf{u}(\mathbf{x}, t)$ between the particles. The physical interaction between two particles can be called a bond. The pairwise force function holds all the constitutive information of the material. Note that the relative position of the particles in the deformed configuration is $\boldsymbol{\xi}+\boldsymbol{\eta}$, as seen in Figure 1.1.

The basis of the peridynamic theory is the integral equation for $\mathbf{L}$, the force per unit reference volume of a particle $\mathbf{x}$ at time $t$ due to the interaction with all other particles:

$$
\begin{equation*}
\mathbf{L}_{\mathbf{u}}(\mathbf{x}, t)=\int_{\mathcal{R}} \mathbf{f}\left(\mathbf{u}\left(\mathbf{x}^{\prime}, t\right)-\mathbf{u}(\mathbf{x}, t), \mathbf{x}^{\prime}-\mathbf{x}\right) \mathrm{d} V_{\mathbf{x}^{\prime}} \quad \forall \mathbf{x} \in \mathcal{R}, \quad t \geq 0 \tag{1.2}
\end{equation*}
$$

or in shorthand:

$$
\begin{equation*}
\mathbf{L}_{\mathbf{u}}(\mathbf{x}, t)=\int_{\mathcal{R}} \mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) \mathrm{d} V_{\boldsymbol{\xi}} \tag{1.3}
\end{equation*}
$$

The power of the peridynamics theory lies within the fact that this function does not contain any spatial derivatives.

The acceleration of a particle $\mathbf{x}$ at any time $t$ is described by the peridynamic equation of motion:

$$
\begin{equation*}
\rho \ddot{\mathbf{u}}(\mathbf{x}, t)=\int_{\mathcal{H}_{\mathbf{x}}} \mathbf{f}\left(\mathbf{u}^{\prime}-\mathbf{u}, \mathbf{x}^{\prime}-\mathbf{x}\right) \mathrm{d} V_{\mathbf{x}^{\prime}}+\mathbf{b}(\mathbf{x}, t) \tag{1.4}
\end{equation*}
$$

Here, $\mathbf{b}(\mathbf{x}, t)$ represents the body force per unit reference volume on the particle.
The peridynamic static equilibrium equation is given by:

$$
\begin{equation*}
\mathbf{L}_{\mathbf{u}}+\mathbf{b}=0 \quad \text { on } \quad \mathcal{R}, \tag{1.5}
\end{equation*}
$$

which states that the total force on a particle is zero. If this equation is satisfied with a zero displacement and no loading force, the reference configuration will be called equilibrated. The reference configuration is called pairwise equilibrated if

$$
\begin{equation*}
\mathbf{f}(\mathbf{0}, \boldsymbol{\xi})=\mathbf{0} \quad \forall \boldsymbol{\xi} \neq \mathbf{0} \tag{1.6}
\end{equation*}
$$

A material with a pairwise force function of the form in (1.2) is called a peridynamic material without memory because it does not contain any history-dependent variables. It is also a form which is only appropriate for homogeneous bodies. The form for nonhomogeneous bodies would look like: $\mathbf{f}\left(\mathbf{u}^{\prime}-\right.$ $\left.\mathbf{u}, \mathbf{x}, \mathbf{x}^{\prime}\right)$.

The function $\mathbf{f}$ must be an even function because, owing to Newton's Third Law, the force exerted by particle 1 on particle 2 is of the same magnitude but opposite to the force exerted by particle 2 on particle 1. Moreover, the force must be in the direction of the relative position between the particles $\boldsymbol{\xi}+\boldsymbol{\eta}$. This results in the most general form of $\mathbf{f}$ :

$$
\begin{equation*}
\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi})=F(\boldsymbol{\eta}, \boldsymbol{\xi})(\boldsymbol{\xi}+\boldsymbol{\eta}) \tag{1.7}
\end{equation*}
$$

where $F$ is an even, scalar-valued function.
The form of $\mathbf{f}$ can be restricted more using definitions for certain material properties. First, a (micro-) elastic peridynamic material is defined using the concept of elasticity.

### 1.2 Elasticity

A material is defined as microelastic if the net work done, by any material particle $\mathbf{x}$ on $\mathbf{x}^{\prime}$ when $\mathbf{x}^{\prime}$ moves along a closed path, is zero. This condition can formally be written as:

$$
\begin{equation*}
\int_{\Gamma} \mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi}) \cdot \mathrm{d} \boldsymbol{\eta}=0 \quad \forall \text { closed curves } \Gamma, \quad \forall \boldsymbol{\xi} \neq \mathbf{0} . \tag{1.8}
\end{equation*}
$$

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A necessary and sufficient condition for this to hold is provided by Stokes' Theorem:

$$
\begin{equation*}
\nabla_{\boldsymbol{\eta}} \times \mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi})=0 \quad \forall \boldsymbol{\xi} \neq \mathbf{0} \tag{1.9}
\end{equation*}
$$

This statement has two consequences which are useful for the peridynamic theory. The first consequence is obtained by applying $\mathbf{f}$ from (1.7) to (1.9):

$$
\begin{equation*}
\frac{\partial F}{\partial \boldsymbol{\eta}}(\boldsymbol{\eta}, \boldsymbol{\xi}) \times(\boldsymbol{\eta}+\boldsymbol{\xi})=\mathbf{0} \quad \forall \boldsymbol{\xi} \neq \mathbf{0} \tag{1.10}
\end{equation*}
$$

This requires that the derivative of $F$ with respect to $\boldsymbol{\eta}$ must be in the direction of $\boldsymbol{\eta}+\boldsymbol{\xi}$. Integrating this derivative leads to the notion that $F$ is dependent only on the length of $\boldsymbol{\eta}+\boldsymbol{\xi}$ and of course on the choice of particles which is contained in $\boldsymbol{\xi}$. The conclusion is that the most general form of $\mathbf{f}$ for a microelastic material is given by:

$$
\begin{equation*}
\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi})=H(|\boldsymbol{\xi}+\boldsymbol{\eta}|, \boldsymbol{\xi})(\boldsymbol{\xi}+\boldsymbol{\eta}) \tag{1.11}
\end{equation*}
$$

From this result it is seen that the bonds between particles in a microelastic material can be interpreted as being a (possibly nonlinear) spring, because the force between every pair of points $\mathbf{x}$ and $\mathbf{x}^{\prime}$ is only dependent on the distance between these points in the deformed configuration $(|\boldsymbol{\xi}+\boldsymbol{\eta}|)$.

The second implication of Stokes' Theorem is that for a peridynamic microelastic material, there exists a differentiable, scalar-valued function $w$, such that

$$
\begin{equation*}
\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi})=\frac{\partial w}{\partial \boldsymbol{\eta}}(\boldsymbol{\eta}, \boldsymbol{\xi}) \tag{1.12}
\end{equation*}
$$

With the aid of this pairwise potential function $w$, the transition from microelasticity to macroelasticity can be made. Consider a particle $\mathbf{x}$ sharing a bond with a particle $\mathbf{x}^{\prime}$. The energy in this bond "belongs" for one half to particle $\mathbf{x}$ and for the other half to particle $\mathbf{x}^{\prime}$. Because of this, the macroelastic energy density $W_{\mathbf{u}}$ of any particle $\mathbf{x}$ is an integral over the energies in all the bonds that it has with other particles, divided by 2 :

$$
\begin{equation*}
W_{\mathbf{u}}(\mathbf{x})=\frac{1}{2} \int_{\mathcal{R}} w(\boldsymbol{\xi}, \boldsymbol{\eta}) \mathrm{d} V_{\boldsymbol{\xi}} \tag{1.13}
\end{equation*}
$$

This result is used in the comparison of the behaviour of elastic materials in the conventional and peridynamics theory (see section 1.6).

### 1.3 Material properties

This section introduces several forms of the pairwise force function belonging to different or combined material properties. The material properties that are considered are: isotropic, structureless and harmonic.

### 1.3.1 Isotropy

An isotropic peridynamic material is defined as a material whose response is independent of the orientation of the material or, equivalently, as a material with no special directions. In this case, $F$ in (1.7) only depends on the length of the vectors $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$ and the angle between them $\left(\cos ^{-1} \boldsymbol{\xi} \cdot \boldsymbol{\eta} /(|\boldsymbol{\xi} \| \boldsymbol{\eta}|)\right)$. A dependence on $|\boldsymbol{\eta}|$ and $|\boldsymbol{\xi}|$ can more conveniently be expressed as a dependence on $|\boldsymbol{\xi}+\boldsymbol{\eta}|$ and $|\boldsymbol{\xi}|$, who together carry the same information. Because of this, $|\boldsymbol{\xi}+\boldsymbol{\eta}|$ will be used in the remainder of this chapter. Now we can write the most general form of $\mathbf{f}$ for an isotropic material:

$$
\begin{equation*}
\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi})=I(|\boldsymbol{\xi}+\boldsymbol{\eta}|, \boldsymbol{\xi} \cdot \boldsymbol{\eta},|\boldsymbol{\xi}|)(\boldsymbol{\xi}+\boldsymbol{\eta}) \tag{1.14}
\end{equation*}
$$

### 1.3.2 Structureless materials

Another type of peridynamic materials is called structureless. For these materials, the pairwise force function $\mathbf{f}$ is only dependent on the relative position of the two particles in the deformed configuration. This means that for such a material, there is a vector-valued function $\mathbf{g}$ such that

$$
\begin{equation*}
\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi})=\mathbf{g}(\boldsymbol{\xi}+\boldsymbol{\eta}) \tag{1.15}
\end{equation*}
$$

Compressible nonviscous fluids can be seen as structureless materials. However, accurate modeling of most real fluids by peridynamics cannot be done with structureless materials, because the degrees of freedom corresponding to thermal motion of the molecules are not captured in the present theory.

### 1.3.3 Harmonic materials

If $F$ is independent of $\boldsymbol{\eta}$ for an isotropic, microelastic material, $\mathbf{f}$ can be written as:

$$
\begin{equation*}
\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi})=K(|\boldsymbol{\xi}|)(\boldsymbol{\xi}+\boldsymbol{\eta}) . \tag{1.16}
\end{equation*}
$$

When this is fed to the equilibrium equation (1.5) with $\mathbf{b} \equiv \mathbf{0}$,

$$
\begin{equation*}
\mathbf{L}_{\mathbf{u}}(\mathbf{x})=\int_{\mathcal{R}} K\left(\left|\mathbf{x}^{\prime}-\mathbf{x}\right|\right)\left(\left(\mathbf{u}^{\prime}-\mathbf{u}\right)+\left(\mathbf{x}^{\prime}-\mathbf{x}\right)\right) \mathrm{d} V^{\prime}=\mathbf{0} \tag{1.17}
\end{equation*}
$$

is obtained. Because $\mathbf{L}_{\mathbf{u}}$ is linear, the superposition principle can be used, which simplifies the equation to

$$
\begin{equation*}
\mathbf{L}_{\mathbf{u}}(\mathbf{x})=\int_{\mathcal{R}} K\left(\left|\mathbf{x}^{\prime}-\mathbf{x}\right|\right)\left(\mathbf{u}^{\prime}-\mathbf{u}\right) \mathrm{d} V^{\prime}=\mathbf{0} \tag{1.18}
\end{equation*}
$$

It can be shown that this equation holds for a displacement field that satisfies Laplace's equation $\nabla^{2} \mathbf{u}=0$. Because the displacement fields that are solutions to Laplace's equation are called harmonic functions, materials with a pairwise potential function of the form of (1.16) are called harmonic materials.

### 1.4 Linearization of the model

The peridynamic model can be linearised by holding $\boldsymbol{\xi}$ fixed and assuming that $|\boldsymbol{\eta}| \ll 1$ :

$$
\begin{equation*}
\mathbf{f}(\boldsymbol{\eta}, \boldsymbol{\xi})=\mathbf{C}(\boldsymbol{\xi}) \boldsymbol{\eta}+\mathbf{f}(\mathbf{0}, \boldsymbol{\xi}) \tag{1.19}
\end{equation*}
$$

Here, $\mathbf{C}$ denotes the second-order micromodulus tensor, given by:

$$
\begin{equation*}
\mathbf{C}(\boldsymbol{\xi})=\frac{\partial \mathbf{f}}{\partial \boldsymbol{\eta}}(\mathbf{0}, \boldsymbol{\xi}) \tag{1.20}
\end{equation*}
$$

If the condition for a microelastic material (1.9) is applied to (1.20), it turns out that $\mathbf{C}$ needs to be symmetric. If this is the case, it can be shown that there must be a scalar-valued function $\lambda$ so that $\mathbf{C}$ can be written as:

$$
\begin{equation*}
\mathbf{C}(\boldsymbol{\xi})=\lambda(\boldsymbol{\xi}) \boldsymbol{\xi} \otimes \boldsymbol{\xi}+F_{0}(\boldsymbol{\xi}) \mathbf{1} \tag{1.21}
\end{equation*}
$$

where $\lambda$ and $F_{0}$ are given by

$$
\begin{equation*}
\lambda(\boldsymbol{\xi})=\frac{1}{|\boldsymbol{\xi}|^{2}} \boldsymbol{\xi} \cdot \frac{\partial F}{\partial \boldsymbol{\eta}}(\mathbf{0}, \boldsymbol{\xi}), \quad F_{0}(\boldsymbol{\xi})=F(\mathbf{0}, \boldsymbol{\xi}) \tag{1.22}
\end{equation*}
$$

Here $F_{0}$ describes the forces present in the reference configuration and $\lambda$ can be seen as a spring constant representing the stiffness of the bonds in the microelastic material. When assuming one of the previously described material properties and/or symmetries, the equations in (1.22) will depend on fewer variables. Because $\mathbf{f}$ is an even function it follows from (1.20) that $\mathbf{C}$ is also even. Furthermore, (1.21) shows that $\lambda$ and $F_{0}$ must be even too then. If the reference configuration is pairwise equilibrated, $F_{0} \equiv 0$ and consequently, $\mathbf{f}(\mathbf{0}, \cdot) \equiv \mathbf{0}$ in (1.19).

In the next section, the functions for $\lambda$ and $F_{0}$ will be restricted by applying criterions for material stability in addition to a newly defined equilibrium condition.

### 1.5 Material stability

The theory derived so far is not restricted enough to be sure that it has a unique solution, or in other words: to maintain material stability. The precise range of the functions $\lambda$ and $F_{0}$, explicitly defining the force function in a linear peridynamic material, has not yet been defined. In this section, a notion of 'force per unit area' in the peridynamic theory is explained first. This is needed to define an 'unstressed' reference configuration, which is less restrictive and more realistic than (pairwise) equilibration. After that, the strongest and less strong conditions for material stability can be defined using the principle of stationary potential energy. Then the consequence of these conditions to $\lambda$ and $F_{0}$ will be given.

### 1.5.1 Force per unit area

Because pairwise equilibration has the strong restriction that the force between between any pair of particles vanishes, a so-called unstressed configuration will be defined. The concepts needed for this definition will first be explained.

When a homogeneous, microelastic body $\mathcal{R}$ is divided into two parts by a plane $\mathcal{P}$ then one of these parts, $\mathcal{R}^{+}$, exerts a force on the other part, $\mathcal{R}^{-}$. This force does not only exist between the particles on the surface of each part, but also in the bonds between particles below the surface. If the total force exerted on a part is divided by the area of the plane dividing the parts, force per unit area is left over. These parts can formally be described by:

$$
\begin{equation*}
\mathcal{R}^{+}=\left\{\mathbf{x}^{\prime} \in \mathcal{R}:\left(\mathbf{x}^{\prime}-\mathbf{x}\right) \cdot \mathbf{n} \geq 0\right\} \quad \mathcal{R}^{-}=\{\hat{\mathbf{x}} \in \mathcal{R}:(\hat{\mathbf{x}}-\mathbf{x}) \cdot \mathbf{n} \leq 0\} \tag{1.23}
\end{equation*}
$$

where $\mathbf{x}$ is a point in $\mathcal{R}$ and $\mathbf{n}$ is a unit vector normal to the dividing plane $\mathcal{P}$ (see Figure 1.2). The described force per unit area can be seen as the total force acting on an (infinitesimal) point on $\mathcal{P}$, which is called $\mathbf{x}$, in the direction of $\mathbf{n}$. The total force $\mathbf{F}$ on $\mathbf{x}$ is found by integration over both $\mathcal{R}^{+}$and $\mathcal{R}^{-}$:

$$
\begin{equation*}
\mathbf{F}(\mathbf{x}, t)=\int_{\mathcal{R}^{-}} \int_{\mathcal{R}^{+}} \mathbf{f}\left(\mathbf{u}^{\prime}-\hat{\mathbf{u}}, \mathbf{x}^{\prime}-\hat{\mathbf{x}}\right) \mathrm{d} V_{\mathbf{x}^{\prime}} \mathrm{d} V_{\hat{\mathbf{x}}} \tag{1.24}
\end{equation*}
$$



Figure 1.2: A circular body $\mathcal{R}$ divided into the parts $\mathcal{R}^{-}$and $\mathcal{R}^{+}$by a plane $\mathcal{P}$, which is defined by the point $\mathbf{x}$ and the normal $\mathbf{n}$ (parallel to $\mathbf{e}_{1}$ in this case). Also, $\mathbf{n}$ together with $s$ defines a set of colinear points $\mathcal{L}$ in $\mathcal{R}^{-}$.

The integration over $\mathcal{R}^{-}$can be split up by an integration over the area $\mathcal{P}$ and the set of colinear points $\mathcal{L}$ :

$$
\begin{equation*}
\mathbf{F}(\mathbf{x}, t)=\int_{\mathcal{P}} \int_{\mathcal{L}} \int_{\mathcal{R}^{+}} \mathbf{f}\left(\mathbf{u}^{\prime}-\hat{\mathbf{u}}, \mathbf{x}^{\prime}-\hat{\mathbf{x}}\right) \mathrm{d} V_{\mathbf{x}^{\prime}} \mathrm{d} \hat{\mathrm{l}} \mathrm{~d} A \tag{1.25}
\end{equation*}
$$

where

$$
\begin{equation*}
\mathcal{L}=\left\{\hat{\mathbf{x}} \in \mathcal{R}^{-}: \hat{\mathbf{x}}=\mathbf{x}-s \mathbf{n}, 0 \leq s<\infty\right\} \tag{1.26}
\end{equation*}
$$

Dividing the total force by the area of the plane dividing the parts, the areal force density $\boldsymbol{\tau}(\mathbf{x}, \mathbf{n})$ is found:

$$
\begin{equation*}
\boldsymbol{\tau}(\mathbf{x}, \mathbf{n})=\int_{\mathcal{L}} \int_{\mathcal{R}^{+}} \mathbf{f}\left(\mathbf{u}^{\prime}-\hat{\mathbf{u}}, \mathbf{x}^{\prime}-\hat{\mathbf{x}}\right) \mathrm{d} V_{\mathbf{x}^{\prime}} \mathrm{d} \hat{l} \tag{1.27}
\end{equation*}
$$

The areal force density in peridynamics theory is the closest one can get to the concept of traction in the conventional theory. Now, a configuration is called unstressed if

$$
\begin{equation*}
\boldsymbol{\tau}(\mathbf{x}, \mathbf{n})=\mathbf{0} \quad \forall \mathbf{x} \in \mathcal{R}, \quad \forall \mathbf{n} . \tag{1.28}
\end{equation*}
$$

Integration over the sets $\mathcal{R}^{+}$and $\mathcal{L}$ is also useful when calculating the total work done by the bonds between particles. The dividing plane $\mathcal{P}$ is arbitrary, but can be a real (existing or originating) fracture surface.

### 1.5.2 Material stability conditions

An isotropic, microelastic body $\mathcal{R}$ is considered. An orthonormal basis $\left\{\mathbf{e}_{1}, \mathbf{e}_{2}, \mathbf{e}_{3}\right\}$ is given and $\mathbf{x}$ is taken as the origin with $\mathbf{n}$ pointing in the direction of $\mathbf{e}_{1}$. Furthermore, $\boldsymbol{\xi}=\mathbf{x}^{\prime}+s \mathbf{n}$ as sketched in Figure 1.2. In an unstressed reference configuration $\boldsymbol{\eta}=\mathbf{0}$ and, using (1.28):

$$
\begin{equation*}
\boldsymbol{\tau}\left(\mathbf{0}, \mathbf{e}_{1}\right)=\int_{0}^{\infty} \int_{\mathcal{R}^{+}} \mathbf{f}\left(\mathbf{0}, \mathbf{x}^{\prime}+s \mathbf{n}\right)\left(\mathbf{x}^{\prime}+s \mathbf{n}\right) \mathrm{d} V_{\mathbf{x}^{\prime}} \mathrm{d} s=\mathbf{0} \tag{1.29}
\end{equation*}
$$

Using isotropy (1.14) combined with microelasticity (1.11), the first component of $\boldsymbol{\tau}$ is evaluated: (see Appendix A)

$$
\begin{equation*}
\tau_{1}\left(\mathbf{0}, \mathbf{e}_{1}\right)=\Psi=\frac{2 \pi}{3} \int_{0}^{\infty} F_{0}(r) r^{4} \mathrm{~d} r \tag{1.30}
\end{equation*}
$$

where $r=|\boldsymbol{\xi}|$. The answer is called $\Psi$ because it will be used again later on.
$\Psi$ needs to be zero, which is certainly the case if $F_{0}(r)$ is zero. This is equivalent to the strong restriction of pairwise equilibration (see (1.6)). One might expect however, that there are significant forces within the body, even when no loading is applied. If this is the case, the configuration should still be unstressed. This implies that $F_{0}(r)$ must be a function which is negative for some interparticle distances $(r)$, and positive for others. This is physically interpreted as particles attracting or repelling each other, depending on their separation.

Further investigation on the conditions for material stability is carried out by applying the principle of stationary potential energy to peridynamic materials. First, (1.13) is used to express the total macroelastic energy $\Phi$ as

$$
\begin{equation*}
\Phi=\int_{\mathcal{R}} W_{\mathbf{u}}(\mathbf{x}) \mathrm{d} V \tag{1.31}
\end{equation*}
$$

If for a microelastic material there is a displacement field $\mathbf{u}$ that satisfies the equilibrium equation (1.5) for some loading force $\mathbf{b}$, the potential energy can be expressed as

$$
\begin{equation*}
\Pi_{\mathbf{u}}=\Phi_{\mathbf{u}}-\int_{\mathcal{R}} \mathbf{b} \cdot \mathbf{u} \mathrm{d} V \tag{1.32}
\end{equation*}
$$

The derivative of the potential energy with respect to a change in the displacement should be zero for stationary potential energy. This derivative can be expressed if $\mathbf{u}$ is supposed to change with a scalar $\varepsilon$ times a vector-field $\mathbf{v}$ and defining

$$
\begin{equation*}
\hat{\Pi}_{\mathbf{v}}=\Pi_{\mathbf{u}+\varepsilon \mathbf{v}} \tag{1.33}
\end{equation*}
$$

Now the stationary potential condition becomes:

$$
\begin{equation*}
\frac{\mathrm{d} \hat{\Pi}_{\mathrm{v}}}{\mathrm{~d} \varepsilon}(0)=0 \tag{1.34}
\end{equation*}
$$

It can be shown that the Euler-Lagrange equation for $\Pi$, which satisfies the condition above, is the peridynamic equilibrium equation (1.5).

The goal (to have conditions for a stable material with an unstressed reference configuration) has not yet been established. So now $\Pi$ is required not only to be stationary, but also to reach a minimum at $\mathbf{u}$. If displacements are assumed to be small, linearization can be applied. Then, by differentiating $\Pi$ again with respect to $\varepsilon$,

$$
\begin{equation*}
\chi_{\mathbf{v}}(\varepsilon)=\frac{\mathrm{d}^{2} \hat{\Pi}_{\mathbf{v}}}{\mathrm{d} \varepsilon^{2}}(\varepsilon) \tag{1.35}
\end{equation*}
$$

is defined and $\chi_{\mathbf{v}}(0)$ is required to be positive definite. Now it can be shown that for all choices of $\mathbf{v}$, $\mathbf{C}(\boldsymbol{\xi})$ has to be positive definite for all $\boldsymbol{\xi}$. This condition can be written as:

$$
\begin{equation*}
\boldsymbol{\eta} \cdot \mathbf{C}(\boldsymbol{\xi}) \boldsymbol{\eta}>0 \quad \forall \boldsymbol{\xi}, \boldsymbol{\eta} \neq \mathbf{0} \tag{1.36}
\end{equation*}
$$

For an isotropic material, $\mathbf{C}(\boldsymbol{\xi})$ has the form of (1.21) with eigenvalues

$$
\begin{equation*}
\lambda(r) r^{2}+F_{0}(r) \text { and } F_{0}(r) \quad \text { where } r=|\boldsymbol{\xi}| \tag{1.37}
\end{equation*}
$$

which both need to be positive to satisfy (1.36). This is a sufficient condition for an equilibrated deformation to minimise $\Pi$. Unfortunately, this condition requires $F_{0}(r)>0$ so it does not allow for the physically expected nonzero forces in the unstressed reference configuration.

Another (less strong) condition for minimising $\Pi$ can be found by looking for a non-null field $\mathbf{v}$ for which $\chi_{\mathbf{v}}(0)$ is a minimum and still positive definite at this minimum. This leads to a new Euler-Lagrange equation:

$$
\begin{equation*}
\mathbf{L} \mathbf{v}=-\beta \mathbf{v} \quad \text { on } \mathcal{R}, \quad \beta=\frac{1}{2} \cdot \frac{d^{2} \bar{\Pi}_{\mathbf{v}}}{d \varepsilon^{2}}(0) \tag{1.38}
\end{equation*}
$$

$\bar{\Pi}$ denotes the normalised version of $\Pi$ since only the direction of $\mathbf{v}$ is important. This eigenvalueequation can be interpreted if we consider applying the energy minimising field $\mathbf{v}$ to the body and suddenly releasing it. Then, since $\mathbf{L v}$ denotes a force, the acceleration field will be

$$
\begin{equation*}
\rho \ddot{\mathbf{v}}=-\beta \mathbf{v} \quad \text { on } \mathcal{R} \tag{1.39}
\end{equation*}
$$

which describes a system of standing waves. Material stability in the sense of potential energy minimisation can now be obtained by requiring that the wave speeds are real for all waves satisfying (1.39) at any wavelength. Investigating the existence of plane waves of the form

$$
\begin{equation*}
\mathbf{u}(\mathbf{x}, t)=\mathbf{a} e^{\imath(\kappa \mathbf{N} \cdot \mathbf{x}-\omega t)} \tag{1.40}
\end{equation*}
$$

in an isotropic, linear microelastic peridynamic material leads to the following implications for $\lambda$ and $F_{0}$ :

$$
\begin{equation*}
\lambda(r) \geq 0 \quad \text { and } \quad \frac{\lambda(r) r^{2}}{5}+F_{0}(r)>0 \quad 0<r<\delta \tag{1.41}
\end{equation*}
$$

This condition tolerates negative values for $F_{0}(r)$ if $\lambda(r)$ can compensate enough for it. So repulsive forces between particles in the reference configuration can be allowed if the stiffness of the spring bonds, represented by $\lambda(r)$, compensates for it.

### 1.6 Link with conventional elasticity theory

In the case of a homogeneous deformation of a body, it can be shown that $\boldsymbol{\tau}$ depends linearly on $\mathbf{n}$, using a Cauchy tetrahedron. In that case a stress tensor $\boldsymbol{\sigma}$ can be used:

$$
\begin{equation*}
\boldsymbol{\tau}(\mathbf{x}, \mathbf{n})=\boldsymbol{\sigma} \mathbf{n} \quad \forall \mathbf{x} \in \mathcal{H}_{\mathbf{x}}, \quad \forall \mathbf{n} \tag{1.42}
\end{equation*}
$$

This is a Piola-Kirchhoff stress tensor in the sense of conventional continuum theory, because $\boldsymbol{\tau}$ represents force per unit area in the reference configuration. (A Cauchy stress tensor expresses the stress relative to the present configuration.)

Another way of arriving at this stress tensor is through the connection between the macroelastic energy density $W$ (1.13) and the strain energy density $\hat{W}$ of conventional elasticity theory. They both represent the energy that the material has stored during deformation and this energy can be recovered by a reverse deformation. Therefore, it is seen again that the conventional $\boldsymbol{\sigma} \equiv \partial \hat{W} / \partial \mathbf{C}$, with $\mathbf{C}$ the right Cauchy-Green tensor $\mathbf{C}=\mathbf{F}^{T} \mathbf{F}$, is identical to $\boldsymbol{\sigma}$ in (1.42).

When, for any peridynamic material, a proper pairwise potential function is given, the corresponding conventional material can be found. This is accomplished by expressing the displacement $\boldsymbol{\eta}$ in terms of $\mathbf{C}$ and $\boldsymbol{\xi}$ and using (1.13). Then the strain energy density can be calculated:

$$
\begin{equation*}
\left.\hat{W}(\mathbf{C})=\frac{1}{2} \int_{\mathcal{R}} w\left(\sqrt{\boldsymbol{\xi} \cdot\left(\mathbf{F}^{T} \mathbf{F}\right) \boldsymbol{\xi}}, \boldsymbol{\xi}\right) \mathrm{d} V_{\boldsymbol{\xi}}\right) . \tag{1.43}
\end{equation*}
$$

Because $\hat{W}$ is only dependent on $\mathbf{F}^{T} \mathbf{F}$, this represents a legitimate hyperelastic material. For an isotropic material, it can be shown that

$$
\begin{equation*}
\hat{W}(\mathbf{C})=\boldsymbol{\Omega}\left(\lambda_{1}, \lambda_{2}, \lambda_{3}\right) \tag{1.44}
\end{equation*}
$$

where $\lambda_{1}, \lambda_{2}$ and $\lambda_{3}$ are the principal strains derived from the eigenvalues of $\mathbf{F}^{T} \mathbf{F}$.
So using the pairwise potential function for a peridynamic material, a function $\hat{W}$ can be found that represents a conventional elastic material. The other way around is not possible in general. A reason for this is the restriction on the linear elastic moduli for peridynamic materials, which will be explained next.

If an isotropic peridynamic material undergoes a homogeneous deformation under microelastic conditions, the elastic moduli, known from conventional linear elasticity theory, can be computed. Suppose there is an orthonormal basis $\left\{\mathbf{e}_{1}, \mathbf{e}_{2}, \mathbf{e}_{3}\right\}$, then the deformation is given by $\boldsymbol{\xi}: \eta_{1}=\epsilon_{11} \xi_{1}, \eta_{2} \equiv \eta_{3} \equiv 0$, where $\epsilon_{11}$ is a constant and very small.. Now each component of the pairwise force function can be obtained, by substitution in (1.21). The first component becomes:

$$
\begin{equation*}
f_{1}=\epsilon_{11}\left[\lambda(r) \xi_{1}^{3}+F_{0}(r) \xi_{1}\right] \tag{1.45}
\end{equation*}
$$

Using this for the force, the first component of the areal force density can be computed from (1.27) in a spherical coordinate system: (see Appendix A for the change of variables and a dimension analysis)

$$
\begin{equation*}
\tau_{1}\left(\mathbf{e}_{1}\right)=\epsilon_{11} \int_{0}^{\infty} \int_{0}^{r} \int_{0}^{\cos ^{-1}(s / r)} \int_{0}^{2 \pi}\left[\lambda(r)(r \cos \theta)^{3}+F_{0}(r)(r \cos \theta)\right] r^{2} \sin \theta \mathrm{~d} \phi \mathrm{~d} \theta \mathrm{~d} s \mathrm{~d} r=(\Lambda+\Psi) \epsilon_{11} \tag{1.46}
\end{equation*}
$$

where $\Psi$ is given in (1.30) and

$$
\begin{equation*}
\Lambda=\frac{2 \pi}{5} \int_{0}^{\infty} \lambda(r) r^{6} \mathrm{~d} r \tag{1.47}
\end{equation*}
$$

Similarly, the tractions in the other directions can be calculated, which together form the stress tensor through (1.42). Assuming an unstressed reference configuration prevents the definitions of the elastic moduli from becoming ambiguous. With this assumption, the matrix form of the stress tensor becomes:

$$
[\boldsymbol{\sigma}]=\epsilon_{11}\left[\begin{array}{ccc}
\Lambda & 0 & 0  \tag{1.48}\\
0 & \Lambda / 3 & 0 \\
0 & 0 & \Lambda / 3
\end{array}\right]=\epsilon_{11}\left[\begin{array}{ccc}
l+2 \mu & 0 & 0 \\
0 & l & 0 \\
0 & 0 & l
\end{array}\right]
$$

where the latter is the stress of this deformation in the conventional theory of elasticity, with $l$ the Lamé modulus and $\mu$ the shear modulus. Using the relations between the elastic moduli from conventional theory, it is found that:

$$
\begin{equation*}
l=\mu=\frac{\Lambda}{3}, \quad E=\frac{5 \Lambda}{6}, \quad k=\frac{5 \Lambda}{9} \tag{1.49}
\end{equation*}
$$

where $\nu$ is Poisson's ratio, $E$ is Young's modulus and $k$ is the bulk modulus. This result gives, through $\Lambda$, a relation between the function $\lambda(r)$, which is not directly measurable, and measurable quantities like $E$ and $k$. This is useful when the theory is applied to real materials. For homogeneous deformation of a linear isotropic material, Poisson's ratio

$$
\begin{equation*}
\nu=\frac{1}{4} \tag{1.50}
\end{equation*}
$$

can be computed using the conversion relations between the elastic moduli of (1.49). Materials with another $\nu$ can be modeled in the peridynamic approach, but that requires fundamental changes to $\mathbf{L}_{\mathbf{u}}$. [1]

### 1.7 Modelling fracture

The peridynamic model is very powerful when discontinuities appear in the material. An example of a phenomenon which involves the spontaneous formation of discontinuities is fracture. A way of representing fracture in the peridynamic theory will now be explained.

The fact that particles on either side of a crack have no physical contact anymore means that they cannot exert a force on each other (directly). So if a peridynamic material is considered, fracture can be introduced as a vanishing pairwise force function, which can be seen as the breaking of bonds between particles.

The pairwise force function can be defined in such a way that a criterion for fracture is incorporated. This is illustrated by the force function which defines a prototype microelastic brittle (PMB) material:

$$
f(|\boldsymbol{\xi}+\boldsymbol{\eta}|, \boldsymbol{\xi})= \begin{cases}c s(t, \boldsymbol{\xi}) & s\left(t^{\prime}, \boldsymbol{\xi}\right)<s_{0} \quad 0 \leq t^{\prime} \leq t  \tag{1.51}\\ 0 & \text { otherwise }\end{cases}
$$

where $c$ is a constant and $s_{0}$ is the critical stretch for bond failure. For simplicity, the scalar force $f$ is assumed to be dependent only on the bond stretch $s$ defined as:

$$
\begin{equation*}
s(t, \boldsymbol{\xi})=\frac{|\boldsymbol{\xi}+\boldsymbol{\eta}|-|\boldsymbol{\xi}|}{|\boldsymbol{\xi}|} \tag{1.52}
\end{equation*}
$$

The pairwise force function arises from the micropotential (per unit volume squared):

$$
\begin{equation*}
w(\boldsymbol{\xi}, \boldsymbol{\eta})=\frac{1}{2} \frac{c}{|\boldsymbol{\xi}|}(|\boldsymbol{\xi}+\boldsymbol{\eta}|-|\boldsymbol{\xi}|)^{2}=\frac{1}{2} c s^{2}|\boldsymbol{\xi}|, \tag{1.53}
\end{equation*}
$$

which can be used to calculate the potential energy in a bond.
The critical bond stretch can depend on various effects that influence the fracture behaviour. For example, a time dependency of $s_{0}$ can be used to model ageing and fatigue. Environmental or manufacturing effects can be taken into account through $s_{0}$ also. However, it is held constant for now.

The parameters that characterise the PMB material are only the spring constant $c$ and the critical bond stretch $s_{0}$. To link $c$ to the measurable bulk modulus $k$, a large homogeneous body under hydrostatic extension is considered. In this case, the bond stretch $s$ is the same for every pair of points, and $\eta=s \xi$. Using (1.13) and (1.12) the macroelastic energy density can be calculated:

$$
\begin{equation*}
W=\frac{1}{2} \int_{\mathcal{H}_{\times}} w \mathrm{~d} V_{\xi}=\frac{1}{2} \int_{0}^{\delta}\left(\frac{c s^{2} \xi}{2}\right) 4 \pi \xi^{2} \mathrm{~d} \xi=\frac{\pi c s^{2} \delta^{4}}{4} \tag{1.54}
\end{equation*}
$$

As discussed in the second paragraph of Section 1.6, the macroelastic energy density is equivalent to the strain energy density $\hat{W}$ for the same material in the classical theory of elasticity:

$$
\begin{equation*}
\hat{W}=\frac{9 k s^{2}}{2} \Longrightarrow c=\frac{18 k}{\pi \delta^{4}} \tag{1.55}
\end{equation*}
$$

To relate the critical bond stretch $s_{0}$ with a measurable quantity, the work needed to break all bonds per unit fracture area is calculated. The work $w_{0}$ required to break a single bond is found by

$$
\begin{equation*}
w_{0}(\boldsymbol{\xi})=\int c s \mathrm{~d} \eta=\int_{0}^{s_{0}} c s \xi \mathrm{~d} s=\frac{c s_{0}^{2} \xi}{2}, \quad \xi=|\boldsymbol{\xi}| \tag{1.56}
\end{equation*}
$$

where $\mathrm{d} \eta=\xi \mathrm{d} s$ has been used.
The concept of a plane $\mathcal{P}$ dividing the body into two halves as explained in Section 1.5.2 is very helpful here. If the plane $\mathcal{P}$ is taken as the fracture surface, the energy per unit fracture area $G_{0}$ can be calculated in the same manner as the force per unit area:

$$
\begin{equation*}
G_{0}=\int_{0}^{\delta} \int_{z}^{\delta} \int_{0}^{\cos ^{-1}\left(\frac{s}{r}\right)} \int_{0}^{2 \pi}\left(\frac{c s_{0}^{2} \xi}{2}\right) \xi^{2} \sin \theta \mathrm{~d} \phi \mathrm{~d} \theta \mathrm{~d} \xi \mathrm{~d} s \tag{1.57}
\end{equation*}
$$

where the coordinate system described in Appendix A has been used. The range over which $\xi$ is integrated is $[0, \delta]$ because the force is assumed to exist only within the neighbourhood $\mathcal{H}_{\mathbf{x}}$ of a particle $\mathbf{x}$, which is defined by a maximum separation $\delta$ (1.1).

The energy per unit fracture area from (1.57) (or energy release rate for brittle materials) is a measurable quantity, assuming that the fracture surfaces are completely separated and that other dissipative mechanisms near the crack tip do not exist. Evaluating (1.57) and using (1.55) gives:

$$
\begin{equation*}
s_{0}=\sqrt{\frac{10 G_{0}}{\pi c \delta^{5}}}=\sqrt{\frac{5 G_{0}}{9 k \delta}} \tag{1.58}
\end{equation*}
$$

With this model, fracture can be simulated for isotropic, elastic materials. The parameters that are used are related to measurable quantities and therefore reflect the material properties of the real material. [2]

### 1.8 Boundary conditions

Boundary conditions are not inherently defined in the peridynamic theory, unlike in the conventional elastic theory, which uses differential equations. Body forces, like gravity, are brought into the model by the loading force density $\mathbf{b}$. To include a displacement loading condition, the set of boundary particles $\mathcal{R}^{*}$ in the complement of $\mathcal{R}$ is defined. Now, to account for displacement boundary conditions, (1.2) is modified to be:

$$
\begin{equation*}
\mathbf{L}_{\mathbf{u}}(\mathbf{x}, t)=\int_{\mathcal{R}} \mathbf{f}\left(\mathbf{u}^{\prime}-\mathbf{u}, \mathbf{x}^{\prime}-\mathbf{x}\right) \mathrm{d} V^{\prime}+\int_{\mathcal{R}^{*}} \mathbf{f}\left(\mathbf{u}^{*}-\mathbf{u}, \mathbf{x}^{*}-\mathbf{x}\right) \mathrm{d} V^{*} \tag{1.59}
\end{equation*}
$$

where $\mathbf{u}^{*}$ is the specified displacement field for the particles in $\mathcal{R}^{*}$.
To define a stress on the boundary, the force on the particles in $\mathcal{R}^{*}$ is set to the required value $\mathbf{f}^{*}\left(\mathbf{x}^{*}, t\right)$. This leads to a displacement field $\mathbf{u}^{*}$, which is used in (1.59) again.

## Chapter 2

## Numerical approach

To simulate the behaviour of a material with the peridynamic model, the theory described before needs to be discretized in time and space. This chapter explains this discretization and the main concepts of the algorithm.

The general idea of the algorithm is to start with defining the reference configuration. This means that a lattice has to be defined in which a body can be placed. Each lattice point $\mathbf{x}$ represents a box that can contain a volume fraction $V_{\mathbf{x}}$ of the body, ranging from an empty box where there is no material, a partly filled box at the boundary of the material to a completely filled box within the material. Once the reference configuration has been defined, there are $N$ non-empty lattice points. The next step is to compute the net force $\tilde{\mathbf{f}}$ on each particle taking into account the interaction with other particles (within the same body or in another body) as well as with body forces, like gravity. With this force, the acceleration of each particle is known and it's new velocity can be calculated. Knowing the velocity for a certain timestep, the positions of the particles can be calculated. Then the procedure is repeated using the new positions.

### 2.1 Defining the reference configuration

As pointed out above, the reference configuration is defined in terms of a cubic lattice with lattice parameter $\Delta x$. Each particle $i$ at the position $\mathbf{x}_{i}$ has a volume fraction $V_{i}$.

Because the reference configuration needs to be remembered for the calculations, the current configuration is stored as $\mathbf{y}(\mathbf{x}, t)=\mathbf{x}+\mathbf{u}(\mathbf{x}, t)$. Note that the distance between two particles $p$ and $i$ is always $\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right|=|\boldsymbol{\xi}+\boldsymbol{\eta}|$ by definition. A particle $i$ at position $\mathbf{y}$ at timestep $n$ will be denoted as $\mathbf{y}_{i}^{n}=\mathbf{x}_{i}+\mathbf{u}\left(\mathbf{x}_{i}, t_{0}+n \Delta t\right)$.

As is explained in Section 1.1, a particle only interacts with particles within its horizon $\delta$. Therefore, it is convenient to define the family of particles $p$ that share a bond with particle $i$ in the reference configuration:

$$
\begin{equation*}
\mathcal{H}_{i}=\left\{p:\left|\mathbf{x}_{p}-\mathbf{x}_{i}\right| \leq \delta\right\} . \tag{2.1}
\end{equation*}
$$

### 2.2 Spatially discretized equation of motion

Equation (1.4) can be discretized using the lattice described in the previous section, resulting in the discretized equation of motion:

$$
\begin{equation*}
\rho \ddot{\mathbf{y}}_{i}^{n}=\sum_{p \in \mathcal{H}_{i}} \mathbf{f}\left(\mathbf{u}_{p}^{n}-\mathbf{u}_{i}^{n}, \mathbf{x}_{p}-\mathbf{x}_{i}\right) V_{p}+\mathbf{b}_{i}^{n} . \tag{2.2}
\end{equation*}
$$

### 2.3 Time discretization - The Verlet scheme

Integration of the equation of motion for all particles leads to the velocities and new positions of the particles. A numerical method that is often used to do this in Molecular Dynamics was developed by the French physicist Loup Verlet in 1967. There are different forms of his algorithm, but the so-called Velocity Verlet scheme will be used. This scheme makes use of the position and velocity at the previous time step to calculate the new position. Its basic steps are :

$$
\begin{aligned}
& 1: \mathbf{y}_{i}^{n+1}=\mathbf{y}_{i}^{n}+\dot{\mathbf{y}}_{i}^{n} \Delta t+\frac{\ddot{\mathbf{y}}_{i}^{n}(\Delta t)^{2}}{2} \\
& 2: \dot{\mathbf{y}}_{i}^{n+\frac{1}{2}}=\dot{\mathbf{y}}_{i}^{n}+\frac{\ddot{\mathbf{y}}_{i}^{n} \Delta t}{2} \\
& 3: \ddot{\mathbf{y}}_{i}^{n+1}=\frac{1}{m_{i}} \tilde{\mathbf{f}}_{i}^{n+1} \\
& 4: \dot{\mathbf{y}}_{i}^{n+1}=\dot{\mathbf{y}}_{i}^{n+\frac{1}{2}}+\frac{\ddot{\mathbf{y}}_{i}^{n+1} \Delta t}{2}
\end{aligned}
$$

Where $\tilde{\mathbf{f}}$ is the total force and $m_{i}=\rho\left(\mathbf{x}_{i}\right) V_{i}$ is the mass of particle $i$. Incorporating step 3 in the other steps, rewriting and reordering leads to the scheme:

$$
\begin{aligned}
& 1: \dot{\mathbf{y}}_{i}^{n+\frac{1}{2}}=\dot{\mathbf{y}}_{i}^{n}+\frac{\Delta t}{2 m_{i}} \tilde{\mathbf{f}}_{i}^{n} \\
& 2: \mathbf{y}_{i}^{n+1}=\mathbf{y}_{i}^{n}+\Delta t \dot{\mathbf{y}}_{i}^{n+\frac{1}{2}} \\
& 3: \dot{\mathbf{y}}_{i}^{n+1}=\dot{\mathbf{y}}_{i}^{n+\frac{1}{2}}+\frac{\Delta t}{2 m_{i}} \tilde{\mathbf{f}}_{i}^{n+1}
\end{aligned}
$$

### 2.4 Modelling a PMB material

The Prototype Microelastic Brittle material, introduced in Section 1.7, is now redefined in a slightly different manner for convenient programming. The criterion for bond failure is expressed in a separate function $\mu$, so that the pairwise force function becomes:

$$
\begin{equation*}
\mathbf{f}(t, \mathbf{x}, \mathbf{y})=c s(t, \mathbf{x}, \mathbf{y}) \mu(t, \mathbf{x}, \mathbf{y}) \tag{2.3}
\end{equation*}
$$

Where $s$ expressed in $\mathbf{x}$ and $\mathbf{y}$ becomes:

$$
\begin{equation*}
s(t, \mathbf{x}, \mathbf{y})=\left(\frac{\left|\mathbf{y}^{\prime}-\mathbf{y}\right|-\left|\mathbf{x}^{\prime}-\mathbf{x}\right|}{\left|\mathbf{x}^{\prime}-\mathbf{x}\right|}\right) \tag{2.4}
\end{equation*}
$$

The history-dependent scalar boolean function $\mu$ is defined as:

$$
\mu(t, \mathbf{x}, \mathbf{y})=\left\{\begin{array}{lll}
1 & s\left(t^{\prime}, \mathbf{x}, \mathbf{y}\right)<s_{0} & 0 \leq t^{\prime} \leq t  \tag{2.5}\\
0 & & \text { otherwise }
\end{array}\right.
$$

This means that the state of the bonds (unbroken or broken) can be remembered by storing the boolean $\mu$. Note that a bond in the model cannot be repaired after it is broken. Moreover, new bonds are never created during the simulation.

At this point, everything is defined to express the complete discretized equation of motion for a PMB material:

$$
\begin{equation*}
\left(\rho\left(\mathbf{x}_{i}\right) V_{i}\right) \ddot{\mathbf{y}}_{i}^{n}=c \sum_{p \in \mathcal{H}_{i}}\left(\frac{\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right|-\left|\mathbf{x}_{p}-\mathbf{x}_{i}\right|}{\left|\mathbf{x}_{p}-\mathbf{x}_{i}\right|}\right) \mu\left(t, \mathbf{x}_{i}, \mathbf{y}_{i}\right) V_{i} V_{p} \frac{\mathbf{y}_{p}-\mathbf{y}_{i}}{\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right|}+\mathbf{b}_{i}^{n} V_{i} . \tag{2.6}
\end{equation*}
$$

The potential bond energy $W_{i}^{\text {bond }}$ in the bonds that particle $i$ shares with its neighbours is calculated using (1.53):

$$
\begin{equation*}
W_{i}^{\text {bond }}=\frac{1}{2} \sum_{p \in \mathcal{H}_{i}} c\left(\frac{\left(\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right|-\left|\mathbf{x}_{p}-\mathbf{x}_{i}\right|\right)^{2}}{\left|\mathbf{x}_{p}-\mathbf{x}_{i}\right|}\right) V_{i} V_{p} \tag{2.7}
\end{equation*}
$$

When a bond breaks, its potential bond energy at the moment of failure is added to the fracture energy $W_{\text {frac }}$.

### 2.5 Short-range forces

If the only forces acting on a particle are the bond forces, a particle becomes a free, non-interacting particle as soon as all the bonds with other particles are broken. This is not a good representation of reality, as particles can freely move through other particles in this situation. Therefore, short-range forces are introduced by a short-range potential:

$$
\begin{equation*}
W_{S}\left(\mathbf{y}_{p}-\mathbf{y}_{i}, \mathbf{x}_{p}-\mathbf{x}_{i}\right)=\frac{c_{S}}{2 \delta}\left(\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right|-d_{p i}\right)^{2} \text { for }\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right| \leq d_{p i} \text { and } 0 \text { otherwise. } \tag{2.8}
\end{equation*}
$$

From this potential the repulsive short-range force $\mathbf{f}_{S}$ can be derived:

$$
\begin{equation*}
\mathbf{f}_{S}\left(\mathbf{y}_{p}-\mathbf{y}_{i}, \mathbf{x}_{p}-\mathbf{x}_{i}\right)=\min \left\{0, \frac{c_{S}}{\delta}\left(\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right|-d_{p i}\right)\right\} \frac{\mathbf{y}_{p}-\mathbf{y}_{i}}{\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right|}, \tag{2.9}
\end{equation*}
$$

where $d_{p i}$ is the short-range interaction distance at which the particles $i$ and $p$ are in 'contact'. The force constant $c_{S}$ is a multiple of the spring constant $c$, taken as $c_{S}=15 c$ in practice. The short-range interaction distance is chosen as:

$$
\begin{equation*}
d_{p i}=\min \left\{d_{C}\left|\mathbf{x}_{p}-\mathbf{x}_{i}\right|, d_{F}\left(r_{p}+r_{i}\right)\right\}, \quad d_{C}=0.9 \quad \text { and } \quad d_{F}=1.35 \tag{2.10}
\end{equation*}
$$

where $r_{i}$ is the node radius of particle $i$, chosen to be half the lattice constant for a discrete lattice. For a cubic lattice, $r_{p}+r_{i}=\Delta x$ (see Figure 2.1). In this figure, the cube of 26 particles $p$ close around particle $i$ are green. These particles have $d_{p i}=0.9\left|\mathbf{x}_{p}-\mathbf{x}_{i}\right|$. All particles further away from $i$ are red and have interaction distance $d_{p i}=1.35 \Delta x$. A green particle $p$ will be repelled as soon as it gets more than ten percent closer to $i$ than in the reference configuration. This definition allows for a little bit of overlap between the blue particle and the green particles. A red particle $p$ will be repelled if $p$ and $i$ get closer than $1.35 \Delta x$ to each other. This means that the red particles will be repelled by the blue particle before they actually 'touch' each other. This approach is needed because the short-range neighbourlist will not be updated during the simulation.


Figure 2.1: Two views of the short-range neighbours of a particle $i$ (blue). The close neighbours with $d_{p i}=0.9\left|\mathbf{x}_{p}-\mathbf{x}_{i}\right|$ are coloured green and the far neighbours with $d_{p i}=1.35 \Delta x$ are coloured red.

The short-range force adds the following term to the discretized equation of motion (2.6):

$$
\begin{equation*}
\sum_{p \in \mathcal{H}_{i}^{S}} \min \left\{0, \frac{c_{S}}{\delta}\left(\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right|-d_{p i}\right)\right\} V_{i} V_{p} \frac{\mathbf{y}_{p}-\mathbf{y}_{i}}{\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right|} \tag{2.11}
\end{equation*}
$$

The potential short-range energy of particle $i$, arising from the short-range potential, is calculated by:

$$
\begin{equation*}
W_{i}^{S}=\sum_{p \in \mathcal{H}_{i}^{S}} \frac{c_{S}}{2 \delta}\left(\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right|-d_{p i}\right)^{2} V_{i} V_{p} \tag{2.12}
\end{equation*}
$$

for particle pairs under contact. Here, $\mathcal{H}_{i}^{S}$ is the family of particles $p$ that are within a short range of particle $i$ : [3]

$$
\begin{equation*}
\mathcal{H}_{i}^{S}=\left\{p:\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right| \leq d_{p i}\right\} \tag{2.13}
\end{equation*}
$$

Defining $\mathcal{H}_{i}^{S}$ this way results in a short-range family that consists of only those particles that really experience a short-range force with $i$. The disadvantage of this definition is that after (nearly) every timestep a new particle can get within short-range distance of $i$, so the family needs to be repopulated all the time. By taking a short-range horizon $\delta_{S}$, the short-range neighbourhood of $i$ can be defined as:

$$
\begin{equation*}
\mathcal{H}_{i}^{S}=\left\{p:\left|\mathbf{x}_{p}-\mathbf{x}_{i}\right| \leq \delta_{S}\right\} \tag{2.14}
\end{equation*}
$$

It is assumed here that all particles that will get within short-range distance of $i$ during the simulation are in the neighbourhood $\mathcal{H}_{i}^{S}$, defined by $\delta_{S}=2 d_{F} \Delta x$ (this gives a neighbourhood of both the red and the green particles shown in Figure 2.1b). If it turns out that this assumption is not correct then the short-range family should be repopulated at certain time intervals, but not as often as would be necessary in the case of (2.13).

### 2.6 Loading forces

External forces are brought into the model by the loading force density $\mathbf{b}$, as explained in Section 1.8. This section handles the numerical implementation of a few kinds of loading forces: an indenter or projectile, gravity and displacement loading.

### 2.6.1 An indenter or projectile with prescribed velocity

To model the impact of an indenter or projectile on the body, the following parameters are needed: the position $\left(\mathbf{y}_{\text {ind }}\right)$, velocity $\left(\dot{\mathbf{y}}_{\text {ind }}\right)$, acceleration $\left(\ddot{\mathbf{y}}_{\text {ind }}\right)$ and geometry of the indenter. If the indenter is prescribed with a certain, possibly increasing, velocity, its position can be calculated with $\mathbf{y}_{\text {ind }}(t+1)=$ $\mathbf{y}_{\text {ind }}(t)+\Delta t \dot{\mathbf{y}}_{\text {ind }}$ for every timestep. Otherwise, the forces on the indenter must be calculated every timestep and the Velocity Verlet scheme can be used. Taking a spherical indenter with radius $R_{\text {ind }}$, the repulsive force that it exerts on a particle $i$ is modeled as:

$$
\begin{equation*}
\mathbf{F}_{i}\left(\mathbf{y}_{i}, \mathbf{y}_{\text {ind }}\right)=k_{\text {ind }}\left(R_{i n d}-r\right)^{2} \frac{\mathbf{y}_{i}-\mathbf{y}_{\text {ind }}}{\left|\mathbf{y}_{i}-\mathbf{y}_{i n d}\right|} \text { for } r<R_{\text {ind }} \text { and } \mathbf{F}=\mathbf{0} \text { otherwise } \tag{2.15}
\end{equation*}
$$

where $r$ is the distance from the outside of the particle to the centre of the indenter and $k_{i n d}$ is the force constant in $\mathrm{N} / \mathrm{m}^{2}$. If the particle is approximated by a sphere, $r$ can be calculated using the nodal radius $r_{i}: r=\left|\mathbf{y}_{i}-\mathbf{y}_{i n d}\right|-r_{i}$. The potential energy $W_{i n d}^{P}$ of the indenter, due to interaction with a particle $i$, is given by:

$$
\begin{equation*}
W_{i}^{P, i n d}=\frac{k_{i n d}}{3}\left(R_{i n d}-r\right)^{3} \tag{2.16}
\end{equation*}
$$

Because the indenter is moving with a constant velocity, it is injecting energy to the system. This energy is calculated by integrating the power that the indenter delivers over time. This power is defined by:

$$
\begin{equation*}
P_{i n d}^{n}=\sum_{i} \mathbf{F}_{i}^{n} \cdot \dot{\mathbf{y}}_{i n d}^{n} \tag{2.17}
\end{equation*}
$$

so the total work done by the indenter at timestep $n$ is given by:

$$
\begin{equation*}
W_{i n d}^{n}=P_{i n d}^{n} \Delta t . \tag{2.18}
\end{equation*}
$$

To know if the indenter interacts with a particle in the body, iteration over all particles is needed for every timestep. If a set of particles $\mathcal{H}_{\text {ind }}$ is defined in such a way that it consists of as few particles as possible, but at least all the particles that will come into contact with the indenter, much calculation time can be saved.

### 2.6.2 Displacement loading

Displacement loading is analogous to the boundary conditions often used in other theories. Two kinds of displacement loading are implemented. A (changing) velocity can be prescribed to a certain set of particles, as well as a (changing) force.

The boundary condition is applied to a set of particles $\mathcal{R}^{*}$ as described in Section 1.8. In case of a prescribed velocity, $\mathbf{L}_{\mathbf{u}}(\mathbf{x}, t)$ in (1.59) is set to zero in the direction that is bounded. Then the displacements are calculated directly from their prescribed velocity. In case of a prescribed force, the second term in (1.59) is replaced by the prescribed force for each bounded particle.

When the simulation is initialised, all particle indexes to which a boundary condition applies are stored in a list, together with a reference to the boundary condition that belongs to it. Now every time the simulation comes to line 13 of Algorithm 1 (The steps of the simulation algorithm are described in the Algorithms 1 to 4), the boundary conditions are applied to the particles stored in the list.

```
Algorithm 1 Simple PMB Peridynamic model
    Generate lattice with lattice constant \(\Delta x\), define timestep \(\Delta t\), total time
    Initialise the peridynamic material - size, position (velocity), critical stretch \(s_{0}\), spring constant \(c\),
    horizon \(\delta\), density
    Initialise displacement loading \(\mathbf{f}^{*}\), body force \(\mathbf{b}\) and set \(\ddot{\mathbf{y}}=\dot{\mathbf{y}}=0\)
    Generate neighbourlists for short-range and pairwise forces
    Calculate and store initial distances \(d\) and bond states \(\mu\) between all particles
    for all timesteps \(\Delta t\) do
        for all \(N\) particles \(i\) do
            Verlet Step \(1\left(\dot{\mathbf{y}}\left(t+\frac{1}{2}\right)=\dot{\mathbf{y}}+\frac{1}{2} \Delta t \ddot{\mathbf{y}}\right)\)
            Verlet Step \(2\left(\mathbf{y}(t+1)=\mathbf{y}(t)+\Delta t \dot{\mathbf{y}}\left(t+\frac{1}{2}\right)\right)\)
            Set force \(\mathbf{f}=0\)
            \(\{\mathbf{f}+=\) Calculate pairwise force function on \(i\) (Algorithm 2) \(\}\)
            \(\{\mathbf{f}+=\) Calculate short-range forces on \(i\) (Algorithm 3) \(\}\)
            \(\{\mathbf{f}+=\) Calculate loading force on \(i\) (Algorithm 4) \(\}\)
            \(\{\mathbf{f}+=\) Calculate body force (s) on \(i\}\)
            \(\{\) Move projectile \(\} \mathbf{y}_{\text {ind }}(t+1)=\mathbf{y}_{\text {ind }}(t)+\Delta t \dot{\mathbf{y}}_{\text {ind }}\)
            \(\ddot{\mathbf{y}}=\mathbf{f} / m_{i}\)
            Verlet Step \(3\left(\dot{\mathbf{y}}(t+1)=\dot{\mathbf{y}}\left(t+\frac{1}{2}\right)+\frac{1}{2} \Delta t \ddot{\mathbf{y}}\right)\)
            \(\{\) Kinetic energy \(\} W_{\text {kin }}=\sum_{i=1}^{N} \frac{1}{2} m_{i} \dot{\mathbf{y}}_{i}(t+1)^{2}\)
        end for
    end for
```


### 2.7 Implementing neighbourlists

All the forces on a particle, described in the previous sections, are due to a family of particles in its own vicinity. When the total force on a particle is calculated, there is no need to loop over all the particles in the body, because most of them do not exert a force by definition. A lot of calculation time can be saved by keeping track of the neighbours of a particle during the simulation.

```
Algorithm 2 Pairwise long-rang forces
    \(W_{\text {bond }}=0\)
    for all particles \(p \in \mathcal{H}_{i}\) sharing a bond with \(i\) do
        if Bond between \(p\) and \(i\) is intact then
            \(d=\left|\mathbf{x}_{p}-\mathbf{x}_{i}\right|\)
            \(r=\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right|\)
            \(s=\frac{r-d}{d}\)
            \{Check if critical bond stretch between \(p\) and \(i\) is reached \}
            if Bond stretch above critical bond stretch \(\left(s>s_{0}\right)\) then
            Break bond between \(i\) and \(p\) and vice versa
            \(\{\) Fracture energy \(\} W_{\text {frac }}=W_{\text {frac }}+c V_{i} V_{p} \frac{(r-d)^{2}}{2 d}\)
            else
                    \(\mathbf{f}=\mathbf{f}+c s V_{i} V_{p} \frac{\mathbf{y}_{p}-\mathbf{y}_{i}}{r}\)
            \(\{\) Potential bond energy \(\} W_{\text {bond }}=W_{\text {bond }}+c V_{i} V_{p} \frac{(r-d)^{2}}{2 d}\)
            end if
        end if
    end for
```

```
Algorithm 3 Short-range contact forces
    \(W_{S}=0\)
    for all particles \(p \in \mathcal{H}_{i}^{S}\) do
        \(r=\left|\mathbf{y}_{p}-\mathbf{y}_{i}\right|\)
        if \(p\) within short-range interaction distance \(d_{p i}\) between \(p\) and \(i\left(r<d_{p i}\right)\) then
            \(\mathbf{f}=\mathbf{f}+\frac{c_{S}}{\delta}\left(r-d_{p i}\right) V_{i} V_{p} \frac{\mathbf{y}_{p}-\mathbf{y}_{i}}{r}\)
            \(\{\) Short-range potential energy \(\} W_{S}=W_{S}+\frac{c_{S} V_{i} V_{p}}{2 \delta}\left(r-d_{p i}\right)^{2}\)
        end if
    end for
```

```
Algorithm 4 Loading forces
    \(W_{\text {ind }}^{P}=0\)
    for all particles \(i\) do
        \{Calculate overlap of \(i\) with indenter, where \(i\) is taken as a sphere \(\}\)
        \(r_{i}=\Delta x / 2\) (Nodal radius)
        \(r=\left|\mathbf{y}_{i}-\mathbf{y}_{\text {ind }}\right|-r_{i}\)
        if \(i\) overlaps with the indenter \(\left(r_{i}<R_{i n d}\right)\) then
            \(\mathbf{f}_{\text {ind }}=\mathbf{f}_{\text {ind }}+k_{\text {ind }}\left(R_{\text {ind }}-r\right)^{2} \frac{\mathbf{y}_{i}-\mathbf{y}_{\text {ind }}}{\left|\mathbf{y}_{i}-\mathbf{y}_{\text {ind }}\right|}\)
            \(\{\) Indenter potential energy \(\} W_{i n d}^{P}=W_{\text {ind }}^{P}+\frac{k_{\text {ind }}\left(R_{\text {ind }}-r\right)^{3}}{3}\)
        end if
        \(\mathbf{f}=\mathbf{f}+\mathbf{f}_{\text {ind }}\)
        \(\{\) Indenter power \(\} P_{\text {ind }}=\mathbf{f}_{\text {ind }} \cdot \dot{\mathbf{y}}_{\text {ind }}\)
        \(\{\) Work done by indenter \(\} W_{\text {ind }}=W_{\text {ind }}+P_{\text {ind }} \Delta t\)
    end for
```

Because all pairs of particles exert the same but opposite force upon each other, a so-called 'half' neighbourlist is used, which stores each particle pair only once. The force on a particle due to a neighbouring particle can then be added to them both.

Because the pairwise (long-range) forces act in a different neighbourhood than the short-range forces, multiple neighbourlists must be stored. The long-range neighbourhood $\mathcal{H}_{i}(2.1)$ is defined by the material parameter $\delta$, the horizon of a particle. Because the initial separation between particles is needed to calculate the force between the particles later on, this separation is stored in an array parallel to the
neighbourlist.
The short-range force acts in two different ways, depending on the initial separation of the particles, as explained in Section 2.5. The distinction between them lies in the short-range interaction distance $d_{p i}$, so this distance is stored in an array parallel to the short-range neighbourlist. They are called the 'close' $\left(d_{C}\right)$ and the 'far' $\left(d_{F}\right)$ short-range interaction. The short-range neighbourhood $\mathcal{H}_{i}^{S}$ is taken as two times $d_{F}$ times the lattice constant.


| id | 1 |  |  | 2 |  |  | 3 |  |  | 4 |  |  | 5 |  | 6 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Index | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 |
| neighbour id | 2 | 3 | 4 | 3 | 4 | 5 | 4 | 5 | 6 | 5 | 6 | 7 | 6 | 7 | 7 |

Table 2.1: Table representation of the arrays that administrate a neighbourlist. In this example, the neighbourlist for the row of seven (blue-coloured) particles shown above is administrated.

The administration of the neighbourlists is shown in Table 2.1. The seven particles each have their own id, as is drawn schematically above the table. The table represents the two arrays that will be needed to store the neighbourlist. The arrays are linked through the 'Index' value. One array stores the Index for every particle id (first and second row in the table). The other stores the ids of the neighbours of that particle, starting at Index.

To find the neighbours of the particle with id 1 , one starts with the first two rows. Index indicates that the desired neighbours can be found in the second array starting at Index 1. The neighbours of particle 2 are found starting at Index 4, so the neighbours of particle 1 can be found at Index 1, 2 and 3. Indeed, the neighbours 2,3 and 4 are found at these Indexes.

As another example, the neighbours of particle 4 can be found at Index 10-12 in the second array. One finds here the particles 5,6 and 7 . Because a half neighbourlist is used, not all 6 neighbours are found in this case. The connection between particle 4 and its other neighbours (1, 2 and 3 ) is already covered by storing particle 4 as a neighbour of 1,2 and 3 (at resp. Indexes 3,5 and 8 ). The storage of a pairwise variable, like the initial separation in case of the long-range interaction, is done in an array as big as the second array, where the neighbour id at every point is replaced by the required variable.

### 2.8 Damage

In the peridynamic theory, damage is caused by the breaking of bonds. While damage and fracture are main issues in the theory, a way to quantify damage is needed. Local damage $\varphi(\mathbf{x}, t)$ at a point $\mathbf{x}$ can be defined by using the bond state stored in $\mu(t, \mathbf{x}, \mathbf{y})$ and taking the volume average, as proposed in [2]:

$$
\begin{equation*}
\varphi(\mathbf{x}, t)=1-\frac{\int_{\mathcal{H}_{i}} \mu(t, \mathbf{x}, \mathbf{y}) \mathrm{d} V_{\mathbf{y}}}{\int_{\mathcal{H}_{i}} \mathrm{~d} V_{\mathbf{y}}} \tag{2.19}
\end{equation*}
$$

Defining damage this way means that $0 \leq \varphi \leq 1$, where 0 represents a particle with completely intact bonds, and 1 represents a free particle. The damage will be visualised by colouring the particles with a blue to red scheme, where a blue particle has all bonds intact and a red one is a free particle. In Figure 2.2 a , a row of seven particles is shown, each with its bonds still intact. The horizon is $3 \Delta x$, so each particle has three neighbours on the right and on the left, or less if the particle is near the edge of the row.

The first (rightmost) particle is now moved such that all its (three) bonds are broken and the particle turns red, see Figure 2.2b. The second particle had 4 bonds initially. Now one is broken, resulting in the lightblue colouring representing a damage of $1 / 4=0.25$. The third has damage $1 /(3+2)=0.2$ and the fourth $1 /(3+3)=0.167$. Repeating this process by moving the second particle also, the damage is (from right to left): $1,1,2 / 5,2 / 6,1 / 6$ and the rest has zero damage (Figure 2.2c).


Figure 2.2: Damage colour scheme and the colouring of particles according to their damage.

### 2.9 Conservation of energy

In the previous sections, all the different forces acting in the system are explained. For each of these forces, the corresponding energy can be calculated. For a consistent simulation, the energy that is put into the system (by for example an indenter) should be contained in the system. In this Section, conservation of energy during the simulation will be confirmed.

The complete energy balance looks like this:

$$
\begin{equation*}
W_{i n d}=W_{i n d}^{P}+W_{k i n}+W_{b o n d}+W_{f r a c}+W_{S} \tag{2.20}
\end{equation*}
$$

where each of the terms are explained in the previous Section. To get a good understanding of the influence of each interaction on the system, a simple two dimensional case is considered. This two particle system is shown in Figure 2.3 together with the graph of the energy for a certain time range. The blue spheres are particles, the grey sphere is an indenter, moving with a constant velocity of 100 $\mathrm{m} / \mathrm{s}$ downwards. All parameters are the same as given in Section 4.1.

At $t=0$, the indenter hits the upper particle. A small peak in the indenter potential energy (purple) indicates that the indenter exerts a force on this particle. It starts to move, increasing the kinetic energy


Figure 2.3: Graph showing the terms of the energy balance of a 2 D two particle system, with $\Delta t=1.0 \times 10^{-9} \mathrm{~s}$. The state of the particles in the system at different times is shown schematically above the graph.
(green) in the system. As the upper particle moves towards the other particle, their bond is compressed. The bond interaction starts repelling both particles from each other, which can be seen in the increase of potential bond energy (blue). Because the upper particle has a large momentum, the bond force cannot immediately push the particles apart. This can be seen in the scheme above the graph, where the upper particle overlaps with the bottom one at $t=2 \times 10^{-7} \mathrm{~s}$. It even reaches the short-range interaction distance of the bottom particle, so the short-range force comes into play. This can be seen by the increase of short-range potential energy (magenta) at $t=3 \times 10^{-7}$. The kinetic energy reaches a minimum at $t=5.5 \times 10^{-7} \mathrm{~s}$. Here the bottom particle starts to accelerate, taking over the momentum from the upper particle. The bond and short-range potential energy decrease until the upper particle stands still, while the bottom particle moves away from it. Then, the indenter hits the upper particle again at about $t=1.1 \times 10^{-7} \mathrm{~s}$ after which both particles travel down with the same velocity. The described effect looks like the well-known Newton's Cradle, a pendulum which nicely demonstrates conservation of momentum and energy.

By taking a closer look at the graph at the moment the indenter hits the particle, it can be seen that the energy difference (black) does not remain zero. This means that the energy balance (2.20) is not satisfied and energy is not conserved. To figure out what is going on here, the first $1.3 \times 10^{-8}$ seconds of the energy graph are shown in Figure 2.4a. It can be seen in this graph that not all the work done by the indenter is converted to indenter potential energy or kinetic energy. Because the peridynamic theory itself does not violate the law of conservation of energy, the problem must lie in the numerical method that is used here. The calculations of kinetic energy and indenter potential energy are straightforward and do not need reconsideration. However, the calculation of the work done by the indenter may not be flawless. This calculation uses the total force that the indenter exerts on the system at the end of the timestep. Multiplying this with the velocity of the indenter gives the power delivered by the indenter. Because the indenter, and the particles it interacts with, move during the time interval, the force exerted by the indenter changes during the timestep. A better approximation of the work done by the indenter is therefore retrieved by using the average force exerted by the indenter over the time interval. This is accomplished by changing line 11 of Algorithm 4 into:

$$
\begin{equation*}
P_{i n d}=\frac{\mathbf{f}_{i n d}(t)+\mathbf{f}_{i n d}(t-\Delta t)}{2} \cdot \dot{\mathbf{y}}_{i n d} \tag{2.21}
\end{equation*}
$$

The energy graph of the same simulation but using the described averaging is shown in Figure 2.4b. Now the energy difference (nearly) stays zero as desired. A more efficient way to have a better average over the time interval is to decrease the timestep itself. Figure 2.4c shows that a decrease of the timestep by a factor of 100 makes the simulation conserving energy perfectly. It will be interesting to see at which timestep the simulation gets so bad that energy conservation becomes disastrous. Figure 2.4d, e and f show the energy graphs of simulations with timesteps of 2,3 and 4 times that of Figure 2.4a respectively. The result at $\Delta t=3 \times 10^{-9} \mathrm{~s}$ can be called acceptable, but at $\Delta t=4 \times 10^{-9} \mathrm{~s}$ (and higher) the energy difference gets out of hand. It can be concluded that for this setup, the maximum timestep is $3 \times 10^{-9}$ s.


(d) $\Delta t=2.0 \times 10^{-9} s-$ Averaging

(f) $\Delta t=4.0 \times 10^{-9} s$ - Averaging

Figure 2.4: Graphs of the energy balance of the $2 D$ two particle system for different values of $\Delta t$.

## Chapter 3

## PMB material tensile test

In this chapter, a tensile test is used to reveal the linear elastic properties of the PMB material and to measure the effect of the particle spacing and the peridynamic horizon on these properties. For movies of some of the simulations described in this chapter, please see the folder 'Movies/Tensile Test' on the PD-CD.

### 3.1 The experiment

A tensile test is performed on a rectangular bar of peridynamic material with dimensions $12 \times 12 \times 24.5$ mm . The PMB material has a density of $2200 \mathrm{~kg} / \mathrm{m}^{3}$. A cubic lattice is used with a lattice constant of $\Delta x=0.5 \mathrm{~mm}$, the horizon $\delta=1.5 \mathrm{~mm}=3 \Delta x$. The total number of particles is 30,625 . The bulk modulus $k=14.9 \mathrm{GPa}$, so $c=18 k / \pi \delta^{4}=1.6863 \times 10^{22} \mathrm{~N} / \mathrm{m}$. The simulation is carried out for a total of 40,000 timesteps of $5.0 \times 10^{-8}$ seconds.

The critical bond stretch $s_{0}$ is set to 1 to obtain a purely elastic response. The microelastic behaviour of the peridynamic material is accounted for by the long-range bond force (2.3). Short-range forces were introduced in the previous chapter for brittle materials to prevent particles from becoming free, noninteracting particles when all their bonds are broken. Because the material will act purely elastic in this simulation, short-range forces are not considered.

On the $x y$-plane on one side of the bar, a zero velocity in the $x$-direction is prescribed. On the $x y$-plane on the other side of the bar, an increasing stress is applied in the $x$-direction. To maintain quasistatic conditions, the stress follows a sigmoid function which is calculated with

$$
\begin{equation*}
F(t)=\sigma A_{0}\left\{1+\exp \left(a\left[\frac{-20}{b} t+10\right]\right)\right\}^{-1} \tag{3.1}
\end{equation*}
$$

where $A_{0}$ is the area of the plane covered by the positions of the nodes to which the boundary condition is applied. The force per particle $F$, which evidently follows the same sigmoid function as the stress, is plotted against the timestep in Figure 3.1a. It reaches its maximum value after $b$ timesteps, with $b=25,000$ timesteps in this simulation. The parameter $a$ determines the steepness of the curve and is set to 0.6.

### 3.1.1 Energy in the system

Figure 3.1 b shows the energy present in the system. The energy provided by the boundary conditions is not taken into account. As required for quasistatic conditions, the kinetic energy remains zero. All energy is stored in potential energy in the bonds. The response of the potential energy in time shows that there are small vibrations in the sample, revealing the dynamic nature of the simulation.


Figure 3.1: Graphs of (a) the stress-prescribed boundary condition against the timestep and (b) the energy in the system against the time.


Figure 3.2: Contour plots of the displacement in (a) the $x$-direction and (b) the $y$-direction at the end of the simulation.

### 3.1.2 Linear elastic behaviour

Figure 3.2a and b show contour plots of the $x$ - and $y$-displacement field of the $x y$-plane at $z=-6 \mathrm{~mm}$. The origin of the coordinate system is in the sample's top centre. Figure 3.2a depicts nicely the linear increase of displacement in the $x$-direction from the clamped side on the left to the stressed side on the right.

The contraction in the perpendicular direction is seen
clearly in Figure 3.2b. This figure also shows that the displacement in the $y$-direction does not increase linearly with $y$ everywhere. This is depicted by the dark red spots in the corners of the sample. To zoom in on this, the displacement in the $y$-direction is plotted against $y$ in Figure 3.4a, for different values of $x$ along the layer of particles with $x>0$ and $z=-6$ mm (red particles in Figure 3.3). Because of the symmetry in the problem, mirroring the graph in both the horizontal and vertical axes gives the graph for the other half of the sample. It is seen from the graph that there is nonlinear behaviour at the edges, represented by a discontinuity in all the curves at


Figure 3.3: The xy-plane of red colored particles that is used for Figure 3.4
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Figure 3.4: (a) y-displacement and (b) Poisson's ratio along the $y$-direction for different values of $x$ on the layer of particles with $x>0$ and $z=-6 \mathrm{~mm}$ (red particles in Figure 3.3).
$y=5.5 \mathrm{~mm}$. Also, the curve for the particles at the outer edge, where $x=12 \mathrm{~mm}$, has a much steeper slope than the curves for smaller values of $x$.

The nonlinear behaviour at the edges of the sample can be explained by looking at the calculation of the bond strength $c$ in Section 1.7. This parameter incorporates the elastic behaviour of the PMB material. It is coupled to the bulk modulus $k$ by taking the macroelastic energy density in case of a large homogeneous body under hydrostatic extension. This is then compared with the strain energy density in the classical theory of elasticity. The macroelastic energy density of a particle is calculated by integrating over all bonds in its neighbourhood. In the tensile test, the particles at the edges do not have the same neighbourhood size and geometry as those in the centre of the sample. This causes the nonlinear effects at the edges the sample. The effect is even stronger for particles at the corners of the sample (see the results for $x=12 \mathrm{~mm}$ ). The influence of the size and geometry of the neighbourhood will further be discussed in Section 3.2.


Figure 3.5: (a) The stress-strain curve and (b) graph of the calculated elastic modulus against the time.

For a further analysis of the simulation, the stress-strain curve is shown in Figure 3.5a. The stress is known at each timestep, because its prescribed as a boundary condition. The strain is calculated between two particles at the centres of two opposing sides, for each of the three directions. The figure shows the (almost) linear elastic behaviour of the tensile bar as it is strained until $1 \%$. With $E=\sigma / \epsilon$,
the elastic modulus $E$ can be calculated from the stress strain curve. It is plotted against the timestep in Figure 3.5b. One of the input parameters of the simulation was the bulk modulus $k$, which was taken to be 14.9 GPa. Using $E=3 k(1-2 \nu)$ and taking $\nu=1 / 4$, it can be calculated that $E$ must be 22.35 GPa in the simulation. This is confirmed by Figure 3.5b, which shows that the elastic modulus reaches a nearly constant value of 22.35 GPa after 0.75 ms . The distortion in the elastic modulus until 0.75 ms appears because the force is increasing exponentially in this time range, which causes vibrations through the material in all directions. These can also be seen in Figure 3.6a, which shows the strain against time.

Figure 3.6b depicts Poisson's ratio $\nu$ against the timestep. It is calculated by $\nu=-\epsilon_{y y} / \epsilon_{x x}$. This takes into account strains in both the $x$ - and $y$-direction, which emphasises the effect of the vibrations in the early stage of the simulation. Again, the graph settles after 0.75 ms at a nearly constant value, which is not the expected $\nu=0.25$ however. (See Section 1.6 for the reason this value is expected)

The deviation in Poisson's ratio is partly caused by the manner in which the strains are calculated. It is already shown that there is nonlinear behaviour at the edges of the sample. Because the strain is calculated from the displacement of the particles at the outside of the sample, the nonlinearity there causes an error in the calculated strain. This error appears in Poisson's ratio for the strain in both the $x$ - and $y$-direction. To get rid of these errors, the strain should be calculated from the displacement of particles some distance away from the edges. To show this, Poisson's ratio is plotted against $y$ in Figure 3.4b, for a layer in the centre of the sample (red particles in Figure 3.3) and different values of $x$. The graph shows clearly the deviation in Poisson's ratio at the edges of the sample. It can also be seen that the compression of the material is not the same for different positions along the $x$-direction. The deviation of Poisson's ratio from the expected value is in the bulk about $4-8 \%$. Although $\nu$ is nowhere exactly $1 / 4$, this value is being approached at certain places along the $x$-direction and not too close to the edge.


Figure 3.6: Graphs of (a) the strain and (b) the calculated Poisson's ratio against the time.

### 3.2 Dependence on the peridynamic horizon $\delta$

As discussed in the foregoing section, the results of the tensile test show linear behaviour, except for the nonlinear effect at the edges. This section deals with the dependence of the linearity of the tensile test on $\delta$.

The $y$-displacement along the $y$-direction of a sample with $\delta=2 \Delta x$ is shown in Figure 3.7a. It is seen that the non-linearity at the edges is much smaller than for a bigger value of $\delta$ (seen in Figure 3.4a). Although the effect is minimal, the strain in this section is calculated between particles lying 5 times the lattice parameter off the edge.


Figure 3.7: Graphs of (a) the $y$-displacement along the $y$-direction for $\delta=2 \Delta x$ as in Figure 3.4 and (b) the dependence of Poisson's ratio on the peridynamic horizon.

Figure 3.7b shows Poisson's ratio $\nu$ for different values of $\delta$. It can be seen that $\nu$ for $\delta=3 \Delta x$, calculated with the strain between particles lying inside the sample, is not very different from $\nu$ in the previous section. With the new calculation of strain, $\epsilon_{y y}$ is a bit lower, but $\epsilon_{x x}$ is lower too. All in all, it can be concluded that the effect of the non-linearity at the edges on $\nu$ turns out to be negligible. The question why $\nu$ has not the expected value of $1 / 4$ remains unanswered. The solution lies in the determinative role of the parameter $\delta$.

By changing $\delta$, the size of the neighbourhood is changed. Figure 3.8 shows one quadrant of a crosssection of the dotted particle's neighbourhood for different values of $\delta$. Note that decreasing delta means less particles in the neighbourhood but also, because of the discretized space, a change in the geometry of the neighbourhood.


Figure 3.8: Schematic representation of the particles included in the neighbourhood of the dotted particle. Each box is one particle, only one quadrant of a cross-section of the neighbourhood is drawn.

A good example of the dependency of $\nu$ on $\delta$ is that $\nu=0$ for $\delta=\Delta x$, as seen in Figure 3.7b. Figure 3.8 shows that the neighbourhood of a particle for $\delta=\Delta x$ consists of only one particle in each direction. Assume that in this figure, the horizontal axis is the $x$-direction and the vertical axis the $y$-direction. If the dotted particle is pulled to the right along the $x$-direction as in the tensile test, it will pull its left neighbour along with it. Because neighbours in the $y$-direction are pulled to the right with the same force, the relative displacement between these particles stays zero. Therefore, the particles do not interact in the $y$-direction, which means that there will be no compression occurring for this value of $\delta$. So the geometry of the neighbourhood causes $\nu$ to be zero in this case, proving the dependence of $\nu$ on $\delta$.

Another dependency of $\nu$ on $\delta$ is caused by a calculation error. Because the neighbourhood contains less particles for lower values of $\delta$, averaging over the bond energies by integration over all neighbouring particles is less accurate.

The picture gets even more complicated if one remembers that the bond strength $c$ is also dependent on $\delta\left(\delta=18 k / \pi \delta^{4}\right.$, see Section 1.7). Because all these effects are interdependent, the effect of the separate errors is difficult to show. However, the effect of the dependence of $c$ on $\delta$ can be seen from Figure 3.9. Here, the function $f(\delta)=a \delta^{-4}+b$ is plotted, representing the theoretical dependence of the elastic modulus on $\delta$. The normalisation factor $a$ is taken as $5 \times 10^{-3}$ and $b=2.235 \times 10^{10} \mathrm{GPa}$. In the same graph, the elastic modulus from the simulations is shown. It can be seen clearly that the elastic modulus follows $f(\delta)$. When comparing Figure 3.9 and 3.7 b , it is striking that at $\delta=2.5 \Delta x$, the elastic modulus differs from the theoretical value while $\nu$ is exactly the theoretical value. Moreover, it is the other way around for $\delta=1.5 \Delta x$ and $3 \Delta x$. For these values of $\delta$, the elastic modulus is equal to the theoretical value, while $\nu$ differs from the theoretical value. The cause of this phenomenon lies in the geometry of the respective neighbourhoods again. The geometry for $\delta=1.5 \Delta x$ and $3 \Delta x$ is the same. This geometry differs from the geometry for $\delta=2.5 \Delta x$. It can be concluded that the former ones represent correct linear behaviour in the direction of the stress, while the latter one represents a better behaviour in the perpendicular direction.


Figure 3.9: Graph of the elastic modulus against the peridynamic horizon, together with $f(\delta)$, the theoretical dependence of the elastic modulus on $\delta$.

### 3.3 Dependence on the lattice parameter $\Delta x$

To figure out the dependence of the lattice parameter on the linear properties of the tensile test, the test has been performed for different values of $\Delta x$. Because the sample size was kept (nearly) the same in each simulation, increasing the size of the lattice parameter yields decreasing the total number of particles.

Figure 3.10 shows that the choice of the size of the lattice parameter has a negligible effect on the results of the simulations. The values for $\nu$ stay the same for an increasing lattice parameter. Only in the regime of lattice parameters above 2.5 mm , the simulation becomes inaccurate. This is mainly caused by the bad statistics that one gets in a simulation with too few particles. In such a case, averaging over all particles does not lead to a meaningful statistical average.


Figure 3.10: Graph of Poisson's ratio against the lattice parameter, together with the theoretical value of Poisson's ratio: $\nu=0.25$.

## Chapter 4

## PMB material impact test

This chapter deals with testing the algorithm with an experiment that has been carried out before. The behaviour of a thin square plate of PMB material will be simulated when a solid sphere is pulled straight through the centre of the plate with a constant velocity. By changing the parameters and looking for extremes, the response of the simulation to certain variables will be tested. Focus will lie on the macroscopic behaviour, like the evolution of damage and fracture through the plate, as well as the shape and behaviour of the debris cloud that emerges after the impact.

For movies of some of the simulations described in this chapter, please see the folder 'Movies/Impact Test' on the PD-CD.

### 4.1 The experiment

The experiment described hereafter has been carried out in EMU and PDLAMMPS for a disc with a diameter of 74 mm and a thickness of 2.5 mm for 200,000 timesteps of $1.0 \times 10^{-9} \mathrm{~s}$. [2][3][4] This means that the forces on $\sim 100,000$ particles need to be calculated, with a neighbourlist of $5,000,000$ entries. For time saving reasons and because running the simulation on parallel processors is beyond the scope of this research, the experiment is scaled down fifty percent. Because a square plate is easier to use as a target than a disc, a square plate with a length and width of 50 mm and a thickness of 2.5 mm will be used. The dimensions of the projectile are scaled by the same amount as the target. The rest of the parameters is taken the same as in the experiments in the literature.

The material has a density of $2200 \mathrm{~kg} / \mathrm{m}^{3}$. The cubic lattice has a lattice constant of $\Delta x=0.5 \mathrm{~mm}$ and a horizon $\delta=1.5 \mathrm{~mm}=3 \Delta x$. The PMB material has parameters $k=14.9 \mathrm{GPa}, s_{0}=0.0005$ and $c=18 k / \pi \delta^{4}=1.6863 \times 10^{22} \mathrm{~N} / \mathrm{m}$. The timestep is $1.0 \times 10^{-9} \mathrm{~s}$ and taking 200,000 timesteps results in a total simulation time of $2.0 \times 10^{-4} \mathrm{~s}$. The total number of particles is 50,000 . The smaller number of particles means a loss of accuracy in the simulation which has to be kept in mind. The projectile that is used is a sphere with a radius $R_{\text {ind }}=3.38 \mathrm{~mm}$, travelling with a constant speed of $100 \mathrm{~m} / \mathrm{s}$ through the target plate's centre. The force constant $k_{i n d}$ is taken to be $1.0 \times 10^{17} \mathrm{~N} / \mathrm{m}^{2}$.

A 3D view on the results of the simulation is shown in Figure 4.1. The particles are coloured according to their damage, as described in Section 2.8. Most of the damage evolves in the first eighth of the experiment, so the figure shows only the first $2.5 \times 10^{-5} \mathrm{~s}$. After this, the area of free particles in the centre of the plate is big enough to let the projectile pass through it, so the evolution of damage at the edges of the plate is minimal.

### 4.1.1 Macroscopic behaviour

The first stages of the simulation are shown in Figure 4.1 and they show some interesting features. At the impact the target hits the centre of a square formed by four particles. The square of red particles visible in Figure 4.1 b is formed due to the evolution of damage by pushing these four particles downwards and


Figure 4.1: A view on the plate during the first $2.5 \times 10^{-5} s$ of the simulation.
sideways. There is much resistance if the particles go sideways, caused by much undamaged material, and much less if they are pushed only downwards through the thin plate. So they will 'choose' the latter option. The red square appears because the neighbours of the four particles will first be pulled down along with them, until the bonds between them are broken. The same with the next neighbours, their neighbours and so on. Around this area of free particles, a square ring of particles with less damage is visible. It is rounded at the corners because the neighbourhood of each particle is not a complete cube, but is also rounded at the corners.

Figure 4.1c shows the formation of an octagonal zone of damaged particles with a 'plus'-shaped area of red particles in the centre. This plus-shape is still a result of the point at which the projectile has hit the target combined with the particles going down which is easier than going sideways. The octagon of damaged particles is spreaded a bit in Figure 4.1d, but here it consists of only highly damaged particles. It seems that after this octagon has reached a certain size, it does not grow anymore. This size is dependent on the size of the projectile and is presumably also linked to the critical bond stretch. This will be investigated in Section 4.2. While, at this point, the projectile is not halfway the top layer of the target, it still pushes particles downwards and sideways to make a way for itself. The edges of the area of free particles are now so close to the edges of the plate that the sideways movement of the particles becomes less difficult at certain points. This results in the formation of cracks from the edges of the octagon to the edges of the plate. The Figures 4.1e and 4.1 f show that after this moment, the parts that


Figure 4.2: (a) The top monolayer and (b) side view of the target at the end of the simulation, $t=2 \times 10^{-4} s$.
are already damaged become more damaged, but new cracks do not appear.
All particles of the top monolayer (in the reference configuration) at the end of the simulation are shown in Figure 4.2a. This depicts the fracture pattern, which has a symmetry axis from the upper right corner to the bottom left corner. There also seems to be a symmetry in the opposite diagonal direction, as well as in the horizontal and vertical direction. One would expect these, based on the symmetry of the positions of the particles hit by the target. However, taking a closer look at some details, these symmetries appear not to be pure symmetries. The impurities in the symmetry can be caused by rounding errors in the calculation.

### 4.1.2 Debris cloud

The formation of the large zone of free particles causes the centre of the plate to dissolve into a cloud of particles, which is seen clearly from Figure 4.2 b . This behaviour makes sense, because once a particle is free, it will evidently move further in the direction it already went. The diamond-like shape of the cloud can be explained by looking at the cross-section of the target during the simulation.

A side view of the cross section of the target is shown in Figure 4.3. From Figure 4.3b, it can be seen that the simulation neatly handles the interaction between the projectile and the particles and between the particles themselves. The spherical projectile 'pushes out' a number of particles in a conical shape as one would expect.

This point of view also shows the quick formation of a zone of free particles in the centre and the cracks towards the edges of the plate. After this, the free particles in the centre provide a way for the projectile to travel through the plate. At first, all particles are pushed downwards, until half of the projectile has penetrated the plate. During this phase, some particles in the upper layers in the vicinity of the projectile are moving upwards. In time, this behaviour spreads along the top layer towards the edges of the red zone, resulting in the diamond-like shape of free particles seen in Figure 4.2b. This seemingly strange behaviour is investigated in Section 4.3.

(a) $t=1.0 \times 10^{-9} s$

(c) $t=2.0 \times 10^{-5} s$

(e) $t=4.0 \times 10^{-5} s$

(b) $t=1.0 \times 10^{-5} s$

(d) $t=3.0 \times 10^{-5} s$

(f) $t=5.0 \times 10^{-5} s$

Figure 4.3: Cut view of the impact during the first $5.0 \times 10^{-5}$ s of the simulation.


Figure 4.4: Top monolayer at the end of the simulation $\left(t=2.0 \times 10^{-4}\right.$ s) for different values of the critical bond stretch $s_{0}$.

### 4.2 The critical bond stretch

In this section, the influence of the critical bond stretch is investigated. This parameter defines the maximum relative separation between two bonded particles before their bond is broken. In the first simulation, described in the previous section, this bond stretch was taken to be 0.0005 . Now, additional simulations are carried out with bond stretches: $0,0.0001,0.00075,0.005,0.0015,0.0025$ and 10 . The values 0 and 10 are the extremes which should represent a plate of free particles and an indestructible plate respectively. This should be confirmed by the results in this section. The way in which both the fracture pattern and the size of the area of free particles in the centre of the plate (observed in the previous section) depend on the critical bond stretch will be investigated.


Figure 4.5: Bird's-eye view at $t=1.25 \times 10^{-4} \mathrm{~s}$ to show the increase of elastic deformation of the plate at high values of $s_{0}$.

### 4.2.1 Fracture patterns

Figure 4.4 shows the top layer of the plate at the end of the simulation $\left(t=2.0 \times 10^{-4} \mathrm{~s}\right)$. Fracture has occurred at the green particles, which are typically particles on one edge of a crack. These particles have lost half of their bonds but are still attached to a fragment with the other half.

The fracture pattern of the simulation with $s_{0}=0.0005$, already described in the previous section, can be seen in Figure 4.4 g . Comparing this with the fracture pattern of materials with a lower critical bond stretch, it is to be expected that there will be more damage at the bond level due to their weaker bonds. The results shown in Figure 4.4h and i reveal this behaviour clearly. Furthermore, all bonds should be broken at the extreme value $s_{0}=0$, because a bond cannot withstand any stretch in this situation. And indeed, Figure 4.4i shows that a plate of such a material dissolves completely into free particles.

Looking at the fracture pattern for values of the critical bond stretch higher than $s_{0}=0.0005$, it is expected that there will be less damage at the bond level. Instead of that, the projectile will press in the plate, causing it to deform elastically. This effect should be maximal for some high value of $s_{0}$ at which the plate stays completely intact.

Figure 4.4a shows the plate with the highest critical bond stretch, $s_{0}=10$. There is not a single crack in this material at the end of the simulation, as expected. Somewhere between $s_{0}=0.005$ and $s_{0}=10$, there is a value of $s_{0}$ above which the plate will stay completely intact. Which value this is will be investigated in Section 4.2.3.

Plates with $s_{0}>0.0005$ (Figures 4.4 f to a) show a decreasing number of cracks and a smaller hole in the middle for increasing critical bond stretch, which confirms that there is less damage at the bond level. The occurrence of elastic deformation is depicted in Figure 4.5. The bending can be seen clearly at the edges of the plates. Note that the particle bonds of the blue coloured areas are still intact. This will cause the plate to recover its original shape in these areas, which proofs the expected occurrence of elastic deformation.

### 4.2.2 Free particle zone

In paragraph 4.1.1, it was observed that the impact of the projectile causes the formation of a zone of free particles around the spot where the projectile hits the target. This zone gets bigger until it reaches a certain size, after which cracks form towards the edges of the plate. Because the size of the zone seems to be important in the mechanism of crack formation, this paragraph focuses on how this size, called $r_{z}$, depends on the critical bond stretch.

To measure $r_{z}$, only the top monolayer of a plate at the end of the simulation is used. By removing all particles with a damage factor above 0.9 , one ends up with only fragments of material. The size of the free particle zone is now taken to be the distance from the spot where the projectile has hit the target (the centre of the plate) to the closest edge of a fragment. The radius of the circle shown in Figure 4.6 gives $r_{z}$ by this definition.

The dependence of $r_{z}$ on $s_{0}$ is plotted in Figure 4.7. The blue line represents the maximum size of $r_{z}$, which is the distance from the centre to a corner of the plate. The red line indicates the minimum


Figure 4.6: Top monolayer of the plate with $s_{0}=0.0005$ at the end of the simulation, with all free particles omitted. The radius of the drawn circle is defined to be $r_{z}$.
size of $r_{z}$, which is the radius of the projectile. The projectile has not travelled through the plate if $r_{z}$ is smaller than this value. The value of $r_{z}$ for $s_{0}=10$ has been omitted.

The results show asymptotic behaviour at both ends of the graph. For an infinite plate with $s_{0}=0$, $r_{z}$ will also be infinite because the whole plate will consist of free particles then. In the case of a finite plate with $s_{0}=0, r_{z}$ will be the same as the 'radius' of the plate as it is in this case. For high values of $s_{0}$, the radius of the free particle zone will approach the radius of the projectile. For a certain value of $s_{0}$ higher than 0.005 , the plate will be strong enough to contain the impact of the projectile. At this value, there will be a jump in the graph of $r_{z}$, from a value around the projectile radius to zero.


Figure 4.7: Graph of $r_{z}$ against $s_{0}$ with two more lines depicting the limits of $r_{z}$.

### 4.2.3 Minimal critical bond stretch

As already mentioned in Section 4.2.1, $s_{0}$ has a minimum value for which the plate stays completely intact after the impact of the sphere. To find this minimum value, a simple estimation is used. Figure 4.8 shows a cutview of the plate just before the moment of failure. It is seen clearly that the plate is bent the most right beneath the projectile. The bottom layer of the plate at this spot endures the maximum strain, so failure will start here (see Figure 4.9). To approximate the maximum strain, it is assumed that the plate is bent completely around the projectile. A further assumption is that the length of the top layer of the plate did not change during the impact. As can be seen in the figure, the particles in this layer are bent around the indenter without much compression in the layer. Note that this behaviour is not the same as in a three-point bending test, where the top layers would be in compression and the bottom layers in tension.

Under these assumptions, the strain in the bottom layer is given by:

$$
\begin{equation*}
\epsilon=\frac{l_{i}-l_{0}}{l_{0}}=\frac{2 \pi\left(R_{\text {curv }}+d\right)-2 \pi R_{\text {curv }}}{2 \pi R_{\text {curv }}}=\frac{d}{R_{\text {curv }}} \tag{4.1}
\end{equation*}
$$

where $d$ is the thickness of the plate and $R_{\text {curv }}$ is the radius of curvature.
As shown in the figure, the radius of curvature is taken as three times the indenter radius, so $R_{\text {curv }}=$ $3 \times 3.38 \mathrm{~mm}=10.14 \mathrm{~mm}$. The thickness of the plate is not the distance between the outsides of the top and bottom particles, but the distance between the particle centres. This is because the calculation of the bond stretch in the simulation is based on the nodal positions, without taking into account the size of the node. Also, there is compression in the $z$-direction which decreases the thickness up to $80 \%$ of the original thickness. Therefore, the thickness $d$ is $80 \% \times(5-1) \times 0.5=1.6 \mathrm{~mm}$. This leads to an approximated maximum strain of 0.158 in the sample. This is the highest value that the bond stretch $s$ (2.4) reaches for this experiment using the given parameters. So for the material to withstand this strain without failure, the minimum value of the critical bond stretch $s_{0}$ needs to be 0.158 too.

A series of simulations, using different values of $s_{0}$ in the range $0.10 \leq s_{0} \leq 0.25$, has shown that the minimal critical bond stretch lies between $s_{0}=0.15$ and $s_{0}=0.16$. This outcome confirms the estimation described before.


Figure 4.8: Cutview on a part of the sample at maximum bending, depicting the bending behaviour and the radius of curvature around the centre of the sample at this moment.


Figure 4.9: Part of the cutview for $s_{0}=0.15$, showing the first three timesteps in which failure occurs.

### 4.3 Displacement field

The occurrence of upwards moving particles, as described at the end of Section 4.1.2, has raised doubts about the correctness of the simulation. To discover the cause of this phenomenon, some special cases will be tested with particular attention to the displacement field of the top layer(s).

### 4.3.1 Peridynamic microelastic material

The displacement field of a point-loaded elastic half-space is described by K.L. Johnson. For a concentrated point force $P$ acting normally to the surface at the origin, it is given by:

$$
\begin{align*}
u_{x} & =\frac{P}{4 \pi G}\left\{\frac{x z}{\rho^{3}}-(1-2 \nu) \frac{x}{\rho(\rho+z)}\right\} \\
u_{y} & =\frac{P}{4 \pi G}\left\{\frac{x z}{\rho^{3}}-(1-2 \nu) \frac{x}{\rho(\rho+z)}\right\} \\
u_{z} & =\frac{-P}{4 \pi G}\left\{\frac{z^{2}}{\rho^{3}}+\frac{2(1-\nu)}{\rho}\right\} \\
\rho & =\left(x^{2}+y^{2}+z^{2}\right)^{1 / 2} \tag{4.2}
\end{align*}
$$

where $G$ represents the tangential traction on the surface in $\mathrm{N} / \mathrm{m}^{2}$. [5] As discussed earlier: $\nu=1 / 4$.
To test if the displacement field calculated by the simulation matches with the continuum field, a block of PMB material with dimensions $24 \times 24 \times 12.5 \mathrm{~mm}$ is used (as shown in Figure 4.10). To prevent


Figure 4.10: Bird's-eye view at the simulation setup to test the displacement field of an elastic half-space. The scaling particle is coloured red and the grey spheres are the four indenters.
the sample as a whole from moving downwards along with the indenters, zero velocity in the $z$-direction is prescribed as a boundary condition on all particles in the bottom layer of the sample.

The concentrated normal force at the origin is simulated by four indenters with a radius of 2.5 mm . By taking the origin of the sample at the centre of the four indenters, the displacement field is only calculated around the origin. Therefore, the singularity of the continuum displacement field at the origin is anticipated. All other parameters are taken the same as in Section 4.1, except that the indenters are moving synchronously downwards with a prescribed velocity, which increases linearly from 0 to $10 \mathrm{~m} / \mathrm{s}$ with steps of $1.0 \times 10^{-4} \mathrm{~s}$ every timestep. This is to approach a quasistatic situation. The simulation is run for 100.000 timesteps of $1.0 \times 10^{-9} \mathrm{~s}$.

Simulations are carried out using a range of critical bond stretches: $1.0 \geq s_{0} \geq 0.0001$, to be able to compare the response of a brittle material (low critical bond stretch) with the purely elastic one ( $s_{0}>$ minimal critical bond stretch). Note that the minimal critical bond stretch is different from the value $s_{0}=0.157$ calculated in Section 4.2.3, because this experiment uses material with other dimensions and a different indenter shape and velocity.

The prefactor $P / 4 \pi G$ in (4.2) is not known explicitly for this experiment. Being a constant, it can be neglected because only the qualitative behaviour is of interest in this case. Instead, the ratio between the lengths of a displacement vector in the simulated case and the length of a displacement vector of the same scaling particle in the continuum theory is used as a prefactor to scale the continuum displacement field to the simulated one. The scaling particle (coloured red in Figure 4.10) lies at $x=3.75, y=0, z=0$ mm . It lies close enough to the indenters to distinguish small displacements but also not too close to the indenters. This is because the four indenters represent a point force which is not as concentrated as assumed in the continuum theory; a discrepancy which affects the shape of the simulated displacement field closely around the indenters.

It should be confirmed that the simulation indeed approaches quasistatic conditions. A dynamic reaction of the simulation is typified by the occurrence of elastic waves through the material. Waves with relevant proportions will show a periodicity in the kinetic energy of the system, as particles are accelerated and decelerated in a wave-like motion. In a purely static situation, the kinetic energy should remain zero. Figure 4.11 shows the energy graph of the simulation. The overview (a) shows that the energy delivered by the indenters (2.18) is transformed neatly into potential energy in the bonds (2.7) between particles. As particles are pushed closer together, a portion of this energy is stored in the shortrange potential energy (2.12). The amplitude of the kinetic energy is so small compared to the total energy in the system that the simulation can be considered (quasi)static. Zooming in at the graph (b) for low energies and considering $t \leq 9 \times 10^{-5}$ seconds, the kinetic energy shows an (irregular) wave-like shape which indicates a bit of dynamic behaviour in the simulation.


Figure 4.11: Energy graph to check the quasistatic conditions of the displacement field experiment.


Figure 4.12: Graph of the displacement in the $z$-direction at $t=10 \times 10^{-5} \mathrm{~s}$ against the position on the $x$-axis of one row of particles in the upper layer of a microelastic material, for different values of the critical bond stretch.

The large fluctuations in kinetic and indenter potential energy at $t>9 \times 10^{-5}$ seconds have a different cause. Here, the particle that is pushed by the indenter has approached the particle beneath it up to the limit. This means that this particle is stuck between the potential of the indenter above it and the combination of the long-range and short-range potential of the particle beneath it. This is the recipe for an unstable situation. Ultimately, rounding errors will cause the enclosed particle to jump to the left or the right side, which is a non-unique solution. (?? An example can be seen in the movie unstable-situation.avi on the PD-CD. ??)

The displacement in the $z$-direction at $t=10 \times 10^{-5}$ seconds, for particles along the x -axis on the surface of the sample, is shown in Figure 4.12. The graph shows the displacement for different values of the critical bond stretch along with the graph of the continuum situation. The black line represents the behaviour in the continuum theory, normalised on the results for $s_{0}=1$ in the way previously described. Because four indenters were used, the displacement field from the simulations is not defined between $x=-0.25 \mathrm{~mm}$ and $x=0.25 \mathrm{~mm}$.

For highly brittle materials $\left(s_{0}<0.01\right)$ it is seen that particles have moved upwards. This is not the case for materials with $s_{0} \geq 0.01$, which however still show brittle behaviour. The big 'nod' in the curve for these materials at $x= \pm 0.75 \mathrm{~mm}$ (the particle next to the indenter) indicates that the particles underneath the indenter have lost (some of) their bonds with surrounding particles. This is confirmed by the damage value of these particles. Therefore, these materials do not respond purely elastic and the results should not be compared with the continuum theory.

Materials with $s_{0} \geq 0.5$ do not show this brittle behaviour and it is seen that for these materials, the simulated displacement behaves qualitatively the same as the continuum version. However, the indent in the continuum case is much narrower around $x=0$ than the simulated ones. This is because the four indenters used in the simulation do not apply a force as concentrated as assumed for the continuum version.

It can be concluded that the upwards movement of particles is not part of the elastic response of the peridynamic microelastic material.


Figure 4.13: Close up on the cutview of Figure 4.3f at $t=5 \times 10^{-5}$ s, which depicts the upwards displacement of the free particles in the upper layers.

### 4.3.2 Brittle material without short-range forces

In the previous section, it turned out that there is no upwards displacement in the elastic case. Figure 4.13 shows a zoom in on the cutview of Figure 4.3f. It is seen here (by their red colour) that the particles that have moved upwards are free particles, so they have no long-range interaction (2.3) anymore. This makes the short-range interaction (2.9) the main suspect for causing the upwards displacement. The effect of this short-range force will be investigated by not taking into account the short-range forces in the simulation of a PMB material. The same setup as in the previous section is used, except that the sample is made brittle again by setting $s_{0}=0.0002$.

Figure 4.14 shows a vectorplot of the displacements of a set of particles along the $x$-axis in the vicinity of the indenters at $t=6.2 \times 10^{-5} \mathrm{~s}$. All particles are coloured according to their damage and have a row number and column letter for easier reference. One immediately sees that some of the particles in row 1 have a substantial upwards displacement. This pleads the short-range force free of suspicion, because


Figure 4.14: Vector plot of the displacements of a set of particles in the vicinity of the indenters at $t=6.2 \times 10^{-5} \mathrm{~s}$. Particles are shown at their initial positions and are coloured according to their damage. The indenters are coloured grey.
this simulation only handles the long-range bond interaction.
Now the question is why it did not happen in the elastic case, where the long-range force was also present. The explanation is the brittleness of the material in this case. Looking at Figure 4.14, one can regard the displacement vectors as some sort of average of the long-range bond force, because this is the only inter-particle force causing the displacement. Then it is seen that as I1 is pushed down, J2 is pushed diagonal to the bottomright. This compresses the bond between J2 and L1, causing L1 to move up- and rightwards. In the elastic case, this movement will be held back by particles in the surrounding of L1. In this case however, the bonds will break, considering that the indenters move fast enough so the displacement of L1 will be big enough. Similar things happen between sets of particles comparable with $\{\mathrm{I} 1, \mathrm{~J} 2, \mathrm{~L} 1\}$. It can be concluded that the combination of long-range forces and brittleness of the material causes the upwards displacement of particles in the upper layers of the material.

The amount of upwards displacement in a simulation is highly dependent on the critical bond stretch. The lower $s_{0}$, the easier particles in the top layers can break their bonds and continue their way upwards. Considering that this effect is not so big in real experiments, a more realistic result will be achieved by making the critical bond stretch dependent on the maximum compression reached in a bond. If compression makes a bond stronger, particles that are pushed upwards due to compression will not break their bonds so easily. This dependency of $s_{0}$ on the relative displacement has already been used by Silling et al. [2]

One might have noticed that in Figure 4.14, the particles directly under the indenters (H1 and I1) have moved slightly towards each other. In a case with only one indenter, the particle beneath it would have moved straight down. This is not the case here because the symmetry axis lies between column H and column I. So the force acting from the right on the particles in column I is different from the force acting from the left.

## Chapter 5

## Dynamic fracture test

Now that the linear elastic properties of the peridynamic material and the correctness of the developed code have been verified in the previous chapters, some more simulations are carried out. In this chapter, a dynamic fracture experiment is described. First, a brief introduction to the subject is given. Then the setup of the experiment used is explained, including comments about introducing an initial crack in the model, reinforcing the edges of the material and analyzing crack speed. In the second section, the test is performed without an initial crack, to learn about the elastic properties of the material with the boundary conditions used. Finally, failure of the notched material is simulated and the crack speed is measured and compared with the expected value from the literature.

For movies of some of the simulations described in this chapter, please see the folder 'Movies/Crack Test' on the PD-CD.

### 5.1 How fast cracks can propagate

The established theory of dynamic fracture states that the limit speed of a straight crack in a perfect homogeneous solid under mode I tension is the Rayleigh wave speed. This is because the energy needed to break atomic bonds needs to be transferred to the crack tip. This can only go as fast as the speed of sound on the crack's surface. Recent studies of mode I and II cracks with atomistic simulations have shown that a crack tip can move faster than this theoretical barrier of the material speed of sound. This involves simulations with millions of atoms on a crack at the interface between materials with different elastic properties [6, 7].

Earlier results on both experimental and simulated mode I failure of a homogeneous solid showed a limit speed of two thirds of the Rayleigh wave speed due to zigzagging of the crack [8]. The research described in this chapter deals with a mode I crack in a Peridynamic Microelastic Brittle material. The maximum speed of the crack is expected to be two thirds of the Rayleigh wave speed.

The Rayleigh wave speed $c_{R}$ is calculated as: $c_{R}=h c_{S}$, where $c_{S}=\sqrt{\frac{E}{\rho 2(1+\nu)}}$ is the shear wave speed. The prefactor $h$ was first introduced in 1954 by Bergmann et al. [9] and modified by Pham Chi Vinh and Peter G. Malischewsky [10]:

$$
\begin{equation*}
h=\frac{0.57536+1.0097 k}{0.65858+k}, \quad \text { where } k=\frac{\nu}{1-\nu} . \tag{5.1}
\end{equation*}
$$

### 5.2 The experiment

The test is performed on a block of PMB material with dimensions $180 \times 3.5 \times 24 \mathrm{~mm}$ and a critical bond stretch $s_{0}=0.01$. The bottom plane, $z=-24 \mathrm{~mm}$, is bounded in the $z$-direction by prescribing $v_{z}=0$. Contraction in the $x$ - and $y$-direction is allowed. A velocity boundary condition is applied on
the upper plane, $z=0 \mathrm{~mm}$. To prevent this plane from breaking off due to a too large displacement in the first few timesteps, the velocity increases following a sigmoidal path (see Figure 5.1a).

The simulation runs for 25,000 timesteps with $\Delta t=2.0 \times 10^{-8}$. The sigmoidal strain rate on the boundary reaches its final value at $t=4 \times 10^{-4} \mathrm{~s}$. The rest of the parameters are the same as in the setup of the tensile test described in Section 3.1. The total number of particles is 120,960 .

The main differences of this setup with the tensile test described in Chapter 3 are the brittleness of the material, a prescribed strain rate on the boundary instead of a prescribed stress and moreover a higher strain rate (compare the Figures 5.1 b and 3.6 a - the strain in this test after 0.5 milliseconds is 5 times higher than in the tensile test). Because these differences can cause a more dynamic response than the quasistatic conditions of the tensile test, the elastic properties for this particular setup (without an initial crack) will be investigated in Section 5.3.


Figure 5.1: Graphs of (a) the prescribed velocity in the $z$-direction on the plane $z=0 \mathrm{~mm}$ and (b) the subsequent strain in the $z$-direction against the time.

### 5.2.1 Determination of crack speed

An initial crack with a length of 4 mm is introduced on the $x y$-plane $z=-12 \mathrm{~mm}$ as shown in Figure 5.2. This is done by breaking all the bonds that cross the crack plane. Because the sample is strained in the $z$-direction, the crack will propagate in the $x$-direction. The crack speed is found by selecting,


Figure 5.2: Initial crack of 4 mm at $z=-12 \mathrm{~mm}$ in a $180 \times 3.5 \times 24 \mathrm{~mm}$ sample.
for every timestep, the particle $\mathbf{x}$ that is closest to the tip of the crack. If a new particle $\mathbf{x}^{*}$ is detected closer to the crack tip in a subsequent timestep, this indicates that the crack has moved. Now the crack speed can be found by taking the distance in the crack propagation direction: $x-x^{*}$ and dividing it by the time between selecting particle $\mathbf{x}$ and particle $\mathbf{x}^{*}$. The rules which the algorithm uses to select a new particle are:

- The damage is greater than 0.3 , which indicates that the particle is on a crack edge.
- $x-x^{*} \geq 0.5 \Delta x$, where $\Delta x$ is the particle spacing. This condition is used to prevent that a particle with the same $x$ but different $y$-coordinate is selected, which would make the crack speed go to zero.
- $\frac{z}{1-\epsilon_{z}} \leq-12 \mathrm{~mm}$ (below the crack plane). This confines the selected particle to the bottom edge of the crack.

(a)

(c)

(b)

(d)

Figure 5.3: Crack propagation in a $30 \times 6 \times 12 \mathrm{~mm}$ sample with $s_{0}=1$. The red particle, indicating the crack tip position, is selected by the algorithm to determine the crack speed.

These rules lead to an accurate determination of the crack tip position (red particle) as can be seen for a small sample with a high value of $s_{0}$ shown in Figure 5.3a-d.

### 5.2.2 Determination of applied stress

The stress applied to the sample is not known directly because the boundary condition is a prescribed velocity and a calculation of stress is not (yet) implemented in the code. The traction applied at the boundary is therefore measured by the response of the material on the bounded plane. By taking the total force on the set of bounded particles, exerted by the rest of the material in the direction opposite to the applied velocity, and dividing that by the area this set of particles spans, the traction is retrieved in a direct way. This stress is used to draw the stress-strain curve and to retrieve the effective elastic modulus in the simulation with Hooke's law: $E=\sigma / \epsilon$. This elastic modulus is then used to calculate the Rayleigh wave speed of the material.

### 5.2.3 Edge reinforcement

A serie of simulations has been carried out on a sample with dimensions $90 \times 6 \times 12 \mathrm{~mm}$ to determine useable values for both the strain rate and $s_{0}$. To have a short simulation time, the strain rate should not be too low. However, if the strain rate is too high, the edges of the sample will break off before the crack has reached the end of the sample. Such a case is shown in Figure 5.4. To increase the maximum value of the strain rate, the planes to which the boundary conditions are applied are enforced. This enforcement is implemented by doubling the value of $s_{0}$ for all particle pairs for which at least one particle is in a bounded plane.

For the simulation shown in Figure 5.4, the critical bond stretch $s_{0}=1$. This means that a bond will break if it is $100 \%$ strained. The corresponding velocity boundary condition $v_{z}$ on the upper plane was $v_{z}=100 \mathrm{~m} / \mathrm{s}$. Because a more brittle sample is needed to compare the results with those of [8], $s_{0}$ is set to $0.01(1 \%$ strain $)$. Therefore, $v_{z}$ should be lowered with the same ratio to $1 \mathrm{~m} / \mathrm{s}$. Because the


Figure 5.4: Failure of a crack propagation simulation caused by edges breaking off before the crack has reached the end of the sample.
sample used for the crack propagation test is twice as long as the sample used here, $v_{z}$ is lowered further to $v_{z}=0.8 \mathrm{~m} / \mathrm{s}$. With these parameter values, the crack arrives at the end of the sample before the (enforced) bounded planes break off.

### 5.3 Elastic properties

The drastic boundary conditions, that load the sample up to the limit of breaking off the bounded planes, cause a much more dynamic response than the quasistatic conditions of the tensile test did in Chapter 3. Moreover, prescribing a velocity $v_{z}(t)$ with a sigmoidal shape (as shown in Figure 5.1) at the boundary causes the strain rate to increase until the end of the test. This is in contrast with the tensile test, where the force on the boundary was prescribed (see Figure 3.6a), which resulted in a zero strain rate at the end of the test. The implications of this difference are depicted in the Figures 5.5 a and b, showing the elastic modulus and Poisson's ratio against the time. The results are from the simulation described in the previous section, but without an initial crack. Although there is no initial crack, failure occurs after about 0.4 ms by means of bounded planes breaking off the sample. In the first 0.15 ms , the velocity boundary condition is increasing exponentially. This causes the vibrations in the sample seen in both graphs for this time span; this phenomenon was also seen in the tensile test. After this, the elastic modulus settles at a value of $2.2 \times 10^{10} \mathrm{~N} / \mathrm{m}^{2}$. This value corresponds to the value found in the tensile test, so the elastic properties of the material have not changed much despite the new boundary conditions. However, in Figure 5.5b it can be seen that $\nu$ decays from 0.33 to 0.3 after 0.15 ms . Although these values do not differ much from the value $\nu=0.28$ found in the tensile test, the time dependence shows that the material responds more dynamically in this case (as predicted).

The main goal of the simulations described in this paragraph was to see if the elastic properties have changed due to the drastic boundary conditions. The dynamic response shows that the change in the boundary conditions influences the response of the system, but the elastic moduli have changed only $1-4 \%$. Based on the results described in this paragraph, $E$ is found to be $2.2 \times 10^{10} \mathrm{~N} / \mathrm{m}^{2}$ and $\nu=0.30$. These values will be used in the calculation of the Rayleigh wave speed in the next section.


Figure 5.5: Graphs of (a) the elastic modulus and (b) Poisson's ratio against the time.

### 5.4 Crack propagation speed

This section describes the results of the dynamic fracture experiment with the setup explained in the previous section. The crack propagation through the sample is demonstrated in the Figures 5.6a,b and c. It immediately strikes that this sample is much more brittle than the samples shown in the figures


Figure 5.6: Crack propagation in a $180 \times 3.5 \times 24 \mathrm{~mm}$ sample with $s_{0}=0.01$. The particles are coloured according to their damage, as described in Section 2.8.
5.3 and 5.4. The crack propagates without a noticeable deformation of the sample. It is propagating in a straight line but also broadening in the $z$-direction along its path.

Before it has reached the end of the sample, the bounded edges do break off. The fact that the boundaries are reinforced can be seen from the figures, because the extra cracks at the top and bottom at the end of the sample appear three particles away from the outer planes; this is exactly the size of the bounded particles' neighbourhood containing the reinforced bonds.

Figure 5.7a shows the stress strain curve for this experiment. It can be seen that there is an elastic regime up to a stress of $1.1 \times 10^{8} \mathrm{~Pa}$, after which failure starts. Figure 5.7 b shows the crack speed together with the Rayleigh wave speed. The Rayleigh wave speed is calculated with the equations described in Section 5.1 and the elastic moduli determined in Section 5.3. It is seen that the crack speed exceeds the predicted value of two thirds of the Rayleigh wave speed, but it does not exceed the limit of the Rayleigh


Figure 5.7: Graphs of (a) the stress-strain curve and (b) the crack speed against the time. Graph (b) also shows the $1 / 3$, $2 / 3$ and $3 / 3$ fractions of the Rayleigh wave speed.
wave speed itself. After increasing from $t=0.32 \mathrm{~ms}$, the crack speed slowly approaches the Rayleigh wave speed after $t=0.4 \mathrm{~ms}$.

The predicted value of two thirds of the Rayleigh wave speed is not the limit for the crack speed in this simulation. However, the conditions under which Abraham found this limiting value were different [8]. His simulation was on an atomic scale and used two million atoms in a 2D configuration. This gave the crack more room in the direction perpendicular to the propagation direction. It therefore had the opportunity to move with a zigzag motion. This bounded the crack speed to two thirds of the Rayleigh wave speed. In the peridynamics simulation, 'only' 120.960 particles were used in a 3D configuration. Moreover, the scale of the peridynamics simulation is in millimeters, while the atomic scale is a factor $10^{7}$ smaller. These aspects provide a sample with a region through which the crack can propagate with a rather different length scale than the atomistic simulations used in [8]. In conclusion it can be said that, although this peridynamic simulation does not predict crack branching or crack instabilities, it still shows that the speed of a propagating crack in a solid is limited by the Rayleigh wave speed of the material.

## Chapter 6

## Problems, limitations and recommendations

This chapter summarizes several problems which have shown up during the research, and highlights the pecularities of peridynamics.

## Non-local boundary conditions

As explained in Section 1.8, boundary conditions are applied to a set of particles $\mathcal{R}^{*}$. In practice, this means that the boundary conditions are applied on particles lying in a plane defining the outside of the sample. This would be a valid method in a local theory. However, since peridynamics is a non-local theory, the boundary conditions should be applied differently. The proper way to do this is probably to apply the boundary condition to all the planes lying within a distance $\delta$ from the bounded plane.

## More realistic brittle behaviour

The impact test has shown the unrealistic behaviour of a brittle plate which dissolves into free particles travelling both along with and opposite to the direction of impact. It has been shown that this behaviour is dependent on the value of the critical bond stretch $s_{0}$. The proposition to solve this problem, due to Silling et al. [2], is to make $s_{0}$ dependent on the minimum stretch among all the other bonds of a particle.

## Correction for surface effects

It has been seen in Section 3.1.2 that the non-linearities at the edges of the sample are caused by surface effects. The neighbourhood of particles at the edges contains less particles than those in the bulk of the sample. This makes the material less stiff at the edges. To resolve this, the particles at the edges can be given another stiffness which makes up for the part of the neighbourhood that is missing here.

## Material models

The only model that can be treated with the current version of the code is the (simple) Peridynamic Microelastic Brittle material. This has been helpful to verify the correctness of the code, but it does not account for plastic deformation, or effects like hardening and ageing. These phenomena will each need another material model represented by a new pairwise force function to be implemented in the code.

## Sample shape and material properties

Until now, the code is able to build a sample with a beam shape only. For certain experiments, it would be helpful to have the functionality to make cylinders, spheres or even irregularly shaped bodies. Additionally, multiple bodies with different material properties or even different material models can be attached to each other with certain prescribed interactions on their boundary. This would allow for simulation of multibody systems.

## Chapter 7

## Summary and conclusions

The peridynamic theory is a description of a powerful nonlocal model, specialised in the treatment of spontaneous formation of discontinuities. It treats the body under consideration as a continuous set of particles. An integral equation based on the pairwise force function $\mathbf{f}$ representing the long-range bond between particles is used to compute the relative displacements and forces between particles. The form of $\mathbf{f}$ depends on the properties of the material. Other forces, like tractions on the boundary or body forces, are introduced through a loading force density term.

Linearization of the model for small deformations leads to the definition of the so-called micromodulus tensor C. The principle of minimum potential energy is used to find conditions on $\mathbf{C}$ required to ensure material stability. Application and elaboration of the theory for homogeneous deformation of a peridynamic material provides a link between the peridynamic theory and elastic moduli for conventional continuum theory. In particular, it is found that $\nu=1 / 4$ in peridynamic theory.

A pairwise force function based on the stretch and possible failure of a bond between two particles defines the Peridynamic Microelastic Brittle (PMB) material. Fracture is incorporated by breaking the bond between two particles if the maximum critical bond stretch $s_{0}$ between the particles is exceeded.

A newly developed code treats the behaviour of a peridynamic material numerically. It makes use of a discretized version of the equation of motion in time (using a timestep $\Delta t$ ) and space (lattice parameter $\Delta x$ ), including long-range, short-range and loading forces. The long-range force only exists between particles that lie within a distance $\delta$ from each other, $\delta$ being the so-called peridynamic neighbourhood. The short-range force is introduced to prevent a particle from becoming a non-interacting particle if all its long-range bonds are broken. The loading force can consist of an indenter or of an elapsing force prescribed on a set of particles. Prescribing a displacement is also possible. The algorithm calculates the energy contribution involved in each force term. Neighbourlists keep track of particle pairs, in order to decrease calculation time. The results are visualised by representing particles as spheres which are coloured to the amount of damage, displacement or other variables of a particle.

A tensile test under quasistatic conditions reveals the linear elastic properties of a sample of PMB material. There are three length scales important for the outcome of the simulation. Free surface effects at the edges of the sample are the cause of a dependency on sample size, as the influence of these effects increases with smaller sample sizes. Because the response of the material is dependent on the size and geometry of the neighbourhood, $\delta$ is another important length scale. The third is the lattice parameter $\Delta x$. Increasing $\Delta x$ means lowering the total number of particles. This leads, for relatively large $\Delta x$ compared to the sample dimensions, to a less meaningful statistical average.

The capabilities of the theory in case of failure of the material are illustrated by means of an impact test in which a plate of PMB material is hit by a solid spherical indenter. The response of the material after the impace shows two stages. In the first stage, a zone of free particles is formed around the spot of impact and grows towards the edges. The final size of this zone is dependent on the maximum critical
bond stretch $s_{0}$, a parameter that determines the brittleness of the material. In the second stage the indenter can travel through the free particle zone, while cracks form from the edge of the free particle zone towards the edges of the sample. Compared to results of the same experiment executed by Silling et al. [2], a relatively large amount of free particles travels in the direction opposite to indentation. This phenomenon is inherent to the model used for the brittle material and is highly dependent on the maximum critical bond stretch $s_{0}$.

At and above a certain value of $s_{0}$, the plate is capable of containing the impact of the sphere without failure. A simple model is proposed to accurately predict the minimum value needed for this to happen.

Dynamic fracture behaviour is simulated with a setup using a relatively low number of particles and kinematic boundary conditions. The elastic moduli show an error of $1-4 \%$ caused by the dynamics in the system due to these boundary conditions. An algorithm is developed to measure the crack speed during the simulation. This crack speed turns out to be bounded by the Rayleigh wave speed, in accordance with the established dynamic fracture theory. The dimension of the experiment in terms of particle numbers is too low to see crack meandering, which would lower the crack speed limit.

The peridynamic theory has proven to be a powerful tool for the modeling of materials involving discontinuities. The developed code is flexible and can be configured for several kinds of experiments. Its accuracy has been tested extensively in this research, which has shown that it gives the right results for some established problems. Visualising the output delivers spectacular images and movies of material behaviour. The road is open to extend this code with more options and new peridynamic material models, so that it can be used to solve problems which have not yet been solved.

## Appendix A

## Integral evaluation

This appendix explains the integration over the spherical coordinate system that is often used in Chapter 1 of this report. Using this coordinate system, evaluation of the integral in (1.29) is worked out.
The concerned integral is

$$
\begin{equation*}
\int_{\mathcal{L}} \int_{\mathcal{R}^{+}} \mathbf{f}\left(\mathbf{u}^{\prime}-\hat{\mathbf{u}}, \mathbf{x}^{\prime}-\hat{\mathbf{x}}\right) \mathrm{d} V_{\mathbf{x}^{\prime}} \mathrm{d} \hat{l} \tag{A.1}
\end{equation*}
$$

where $\mathcal{R}^{+}$and $\mathcal{L}$ are defined in Section 1.1. For the reference configuration of an isotropic microelastic material, this integral becomes:

$$
\begin{equation*}
\int_{0}^{\infty} \int_{\mathcal{R}^{+}} F\left(\mathbf{0},\left|\mathbf{x}^{\prime}+s \mathbf{n}\right|\right)\left(\mathbf{x}^{\prime}+s \mathbf{n}\right) \mathrm{d} V_{\mathbf{x}^{\prime}} \mathrm{d} s \tag{A.2}
\end{equation*}
$$

where $\mathbf{x}^{\prime}-\hat{\mathbf{x}}=\mathbf{x}^{\prime}+s \mathbf{n}$ and $\mathrm{d} \hat{\mathbf{l}}=\mathrm{ds}$ have been used for the integral over $\mathcal{L}$. This has already been explained in Section 1.5.2 and is shown again in Figure A.1a. The spherical coordinate system which


Figure A.1: 2D schematic drawing
can be used to evaluate the integral over $\mathcal{R}^{+}$is indicated in Figure A.1b and can be described as:

$$
\begin{equation*}
\xi_{1}=r \cos \theta, \quad \xi_{2}=r \sin \theta \cos \phi, \quad \xi_{3}=r \sin \theta \sin \phi, \quad r=|\boldsymbol{\xi}| \tag{A.3}
\end{equation*}
$$

and

$$
\begin{equation*}
\mathrm{d} V_{\boldsymbol{\xi}}=r^{2} \sin \theta \mathrm{~d} \phi \mathrm{~d} \theta \mathrm{~d} r \tag{A.4}
\end{equation*}
$$

An example of the computation of an integral, using the described change of variables, is shown now for the first component of $\boldsymbol{\tau}$ in (1.29):

$$
\begin{align*}
\tau_{1}\left(\mathbf{0}, \mathbf{e}_{1}\right) & =\int_{0}^{\infty} \int_{\mathcal{R}^{+}} F_{0}(r)\left(\xi_{1}\right) \mathrm{d} V_{\boldsymbol{\xi}} \mathrm{d} s \\
& \Longrightarrow \int_{0}^{\infty} \int_{0}^{r} \int_{0}^{\cos ^{-1}\left(\frac{s}{r}\right)} \int_{0}^{2 \pi} F_{0}(r)(r \cos \theta) r^{2} \sin \theta \mathrm{~d} \phi \mathrm{~d} \theta \mathrm{~d} s \mathrm{~d} r \\
& =\int_{0}^{\infty} \int_{0}^{r} \int_{0}^{\cos ^{-1}\left(\frac{s}{r}\right)} 2 \pi F_{0}(r) r^{3} \cos \theta \sin \theta \mathrm{~d} \theta \mathrm{~d} s \mathrm{~d} r \tag{A.5}
\end{align*}
$$

Using $\cos \theta \sin \theta=\frac{1}{2} \sin (2 \theta)$ :

$$
\begin{aligned}
\int_{0}^{\cos ^{-1}\left(\frac{s}{r}\right)} \cos \theta \sin \theta \mathrm{d} \theta & =\frac{1}{2} \int_{0}^{\cos ^{-1}\left(\frac{s}{r}\right)} \sin (2 \theta) \mathrm{d} \theta \\
& =\frac{1}{2}\left[-\frac{1}{2} \cos (2 \theta)\right]_{0}^{\cos ^{-1}\left(\frac{s}{r}\right)} \\
& \left.=\frac{1}{4}\left[1-2 \cos ^{2} \theta\right)\right]_{0}^{\cos ^{-1}\left(\frac{s}{r}\right)} \\
& =\frac{1}{4}\left[2-2(s / r)^{2}\right]
\end{aligned}
$$

where $\cos (2 \theta)=2 \cos ^{2} \theta-1$ has been used. Substituting this into (A.5) gives:

$$
\begin{aligned}
\tau_{1}\left(\mathbf{0}, \mathbf{e}_{1}\right) & =\int_{0}^{\infty} \int_{0}^{r} \pi F_{0}(r) r^{3}\left[1-(s / r)^{2}\right] \mathrm{d} s \mathrm{~d} r \\
& =\int_{0}^{\infty} \int_{0}^{r} \pi F_{0}(r)\left[r^{3}-s^{2} r\right] \mathrm{d} s \mathrm{~d} r \\
& =\int_{0}^{\infty} \pi F_{0}(r)\left[s r^{3}-\frac{1}{3} s^{3} r\right]_{0}^{r} \mathrm{~d} r \\
& =\int_{0}^{\infty} \pi F_{0}(r)\left[r^{4}-\frac{1}{3} r^{4}\right] \mathrm{d} r \\
& =\frac{2 \pi}{3} \int_{0}^{\infty} F_{0}(r) r^{4} \mathrm{~d} r
\end{aligned}
$$

The validity of this answer can be made plausible by a dimension analysis. Because $\boldsymbol{\tau}$ is defined as the areal force density, it obviously has dimension $\left[\mathrm{N} / \mathrm{m}^{2}\right]$. To show that $\tau_{1}$ has the same dimension, remember that the pairwise force function has dimension $\left[\mathrm{N} / \mathrm{m}^{6}\right]$. From (1.7) it is seen that $F_{0}$ is in $\left[\mathrm{N} / \mathrm{m}^{7}\right]$. The integral for $\tau_{1}$ means $F_{0} * r^{5}$ which gives the expected dimension of force per unit area.

The dimension of $\Lambda$ in (1.47) also needs to be $\left[\mathrm{N} / \mathrm{m}^{2}\right]$. This integral means $\lambda * r^{7}$, so does $\lambda$ have dimension $\left[\mathrm{N} / \mathrm{m}^{9}\right]$ ? Looking at (1.21), $\mathbf{C}(\boldsymbol{\xi})$ has the same dimension as $F_{0}$, namely $\left[\mathrm{N} / \mathrm{m}^{7}\right]$. The same equation shows that $\lambda *\left[m^{2}\right]=\left[\mathrm{N} / \mathrm{m}^{7}\right]$, which confirms that $\lambda$ has dimension $\left[\mathrm{N} / \mathrm{m}^{9}\right]$.

## Appendix B

## Data I/O and TecPlot Tips-and-Tricks

The peridynamics code is able to calculate and output different data files. Which quantities must be calculated and printed by the program is defined in the configuration file. The main output is a TecPlot binary data file which outputs at least the position and size of all particles at defined time intervals. The looks of this file will be discussed in this Appendix, as well as the details of the other (optional) output data files. Throughout this chapter TecPlot Tips and Tricks are given to help visualise the results.

## B. 1 Basic Output file

The peridynamic code uses a fortran library (libtecio.a) which comes with TecPlot 360. This library contains functions which make it easy to output a decent binary datafile that TecPlot understands. This datafile contains the radius and $x$-, $y$ - and $z$-positions of all particles by default. Each layer of the sample (so each set of particles with the same value for $z$ ) is put in a different zone. This makes it easy to give each layer it's own colour in TecPlot.

At certain time intervals (which can be defined in the configuration file), the particle data of all layers are written to the datafile. TecPlot can distinguish between one time interval and another by giving corresponding layers the same StrandID. For a five layer thick sample, the first layer will be Zone 1, StrandID 1 and the second layer Zone 2, StrandID 2. In the second time interval, the first layer will be Zone 6 but with StrandID 1 again.

The datafile can be loaded in TecPlot choosing 'File' $\rightarrow$ 'Load Data File(s)' $\rightarrow$ 'TecPlot Data Loader'. After choosing a '.plt' or '.dat' file, TecPlot will ask which kind of graph it must draw. By choosing '3D Cartesian' one can easily make a nice 3D picture of the peridynamic sample. To do this, turn of the layers 'Mesh' and 'Edge' and activate 'Scatter'. Then push the 'Zone Style' button and select the 'Scatter' tab. Choosing a circular symbol shape is convenient because it doesn't take TecPlot a long time to draw these. Colours and other appearance values can be set here too. The size of the symbols is set by selecting layers and choosing 'Scat Size' $\rightarrow$ 'Size by Variable'. Then select the radius variable ('R') and set 'Grid Units/Magnitude' to 1 . If a square symbol is used, set it to 1.41 (Half the diagonal of a unit square: $\sqrt{2}$ ). Using spheres and lighting effects gives nice pictures for use in reports and presentations. An animation can be made by choosing 'Animate' $\rightarrow$ 'Time'.

Because StrandID's are used, TecPlot has trouble with loading a new datafile while keeping all zone styles the same. Therefore it is not possible to save a TecPlot Layout file and use it as a template for later simulations. However, the layout for one frame can be saved and reloaded. If a new datafile is loaded, one can choose 'Frame' $\rightarrow$ 'Paste Frame Style from File' to apply the stored appearance settings immediately. For some specific output options (which will be explained below), TecPlot Frame Styles are made ready (?? in the directory Development/TecplotLayout ??).

## B. 2 Main output file options

On the third line of the configuration file, a set of keywords can be given. These keywords tell the peridynamics code which quantities it has to calculate and output. Most calculations require extra simulation time, so it is recommended to ask only for necessary output.

## Damage

Putting the keyword 'damage' in the configuration file will tell the simulation to calculate the damage, which is defined in Section 2.8. The damage is printed as an extra variable in the TecPlot output file. To visualise the damage, select 'Fill Color' $\rightarrow$ 'Multi 1' in the Zone Style window. Then go to 'Plot' $\rightarrow$ 'Contour/Multicoloring' and select the damage variable. TecPlot will generate a colour scale based on the damage and will colour particles according to this scale. Some frame styles using damage are stored in the directory TecplotLayout/Reporting. Some styles (stored in the directory /before_v01i) are only suitable for datafiles generated with peridynamic code versions before V01i. In that version, the origin of the coordinate system was moved from the corner to the centre of the sample, making these frame styles useless.

## Displacement vectors

Putting the keyword 'displ_vectors' in the configuration file will tell the simulation to output displacement vectors. These will appear in the TecPlot data file under $U, V$ and $W$ representing the displacement in the $x$-, $y$ - and $z$-direction respectively. The datafile now contains the reference positions together with their displacements in time. To get the actual positions, three extra variables $x^{\prime}, y^{\prime}$ and $z^{\prime}$ can be calculated with $x^{\prime}=x+U, y^{\prime}=y+V$ and $z^{\prime}=z+W$. A nice contour plot can be obtained by using square scatter symbols and colouring them (fully) with a Multicolor, then choosing the colour scale based on a certain displacement variable. Contour plot frame styles for 3D and 2D tensile tests are stored in the directory TecplotLayout/BCs (for Boundary Conditions).

## Theoretical displacement

In Section 4.3, the displacement field in some simulations is compared with a theoretical displacement field. Both fields will be calculated and printed if the keyword 'theor_displ' is added to the configuration file. The output file will contain layers of particles and their displacement calculated by the simulation as explained in the previous paragraph. The theoretical displacement field is stored in an additional layer for each original layer, doubling the number of layers stored at each timestep. To draw a vectorplot, one activates the 'Vector' layer. TecPlot will ask which variables define the vector: $U, V$ and $W$ in this case. Vector styles can be modified in the Zone Style window. The frame styles used for the test with four indenters are stored in the directory TecplotLayout/BCs.

## Force distributions

The keyword 'forces' in the configuration file will output 6 more variables in the TecPlot file. The first three are the forces in the $x, y$ and $z$-direction for each particle. The last three represent the total force on each particle, with the sign of the force in the $x, y$ and $z$-direction respectively. This output option is used in an attempt to visualise the waves that go through the sample during the dynamic fracture test. The disappointing results can be seen in some movies in the folder 'Movies/Crack Test' on the PD-CD. They have '_Fz_', '.F-z_' etc. in the filename.

## B. 3 Other output options

Along with the variables that can be added to the TecPlot output file, there are some options which output variables in a separate file.

## Exaggerated displacement

If the keyword 'ex_displacement' is given, the peridynamic code will output an additional TecPlot file with the string '_disp' appended to the filename. This file contains the coordinates of all particles at the end of the simulation, but with all displacements exaggerated by a factor 5 . This gives a nice picture of the different fragments in the case of a fractured sample.

## Energy

The values of all the different energy terms at every timestep are printed to a separate (ASCII) datafile to which name '_energy' is appended. A GNUPlot template file that gives the same energy graphs as in Section 2.9 is stored as 'energy.gp'.

## Stress-strain curve

Giving the keyword 'stress_strain' in the configuration file will let the program output an ASCII datafile with the 'timestep', 'solution time', 'stress(x y z)' and 'strain (x y z)'. The calculations of stress and strain are discussed in Section 3.1.2.

## Crack speed

Outputting crack speed is initiated by putting the keyword 'crack_speed' in the configuration file. This will let the program initialise a particle to track the crack tip's position.

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