An Atomic Interaction based Continuum Model for
Computational Multiscale Contact Mechanics

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Abstract

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A computational multiscale contact mechanics model is proposed to describe the interaction between deformable solids based on the interaction of individual atoms or molecules. The contact model, formulated in the framework of large deformation continuum mechanics, is termed the ‘Coarse-Grained Contact Model’, since it is based on the homogenizing, or coarsening of the discrete description of a large assembly of interacting atoms. The atomic interaction is distinguished into two different cases: the interaction of atoms within a small neighborhood, and the interaction of atoms over large distances. The former furnishes a constitutive relation for the continuum, like the Cauchy-Born rule, while the latter is used to model the interaction, like contact and adhesion, between distinct bodies. The proposed multiscale contact model is formulated as a variational principle and implemented within an updated Lagrangian finite element method. Three different implementations are proposed, designed to maintain computational efficiency as the length scale increases. In this respect it is shown by direct comparison, that the proposed contact model can lead to a seamless transition between nanoscale contact mechanics, as modelled by molecular dynamics, and macroscale contact mechanics, as modelled by continuum mechanics.

The Coarse-Grained Contact Model is fully normalized in order to determine its characterizing model parameters. These are used to analyze the physical and numerical behavior of the contact model. In particular the scaling of the CGC model is investigated and studied over a wide range of length scales and material properties. The consistency and accuracy of the three proposed implementations is further analyzed by a simple contact patch test. Several numerical examples are used to illustrate the applicability of the CGC model to micro/nano-scale contact/interaction problems. These results are in agreement with experimental, analytical and numerical results reported in the literature, thus validating the proposed multiscale contact model. By using a second level of homogenization, it is finally shown, that the CGC model can be applied to macroscale contact problems.
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“If in some cataclysm all scientific knowledge were to be destroyed and only one sentence passed on to the next generation of creatures, what statement would contain the most information in the fewest words? I believe it is the atomic hypothesis that all things are made of atoms - little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another. In that one sentence, you will see there is an enormous amount of information about the world, if just a little imagination is applied.”

Richard Feynman
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1 Introduction

1.1 Motivation

Much attention has been devoted to the contact description of large scale objects, either analytically [37], [49] or computationally [58], [100]. On the other hand, with the emergence of nanotechnology, the nanoscale treatment of contact and related subjects such as adhesion, indentation and tribology are becoming more prominent. In macroscopic contact modelling, the behavior of the bodies is governed by the mechanics of both continua and the unilateral constraint that the bodies may not penetrate each other. As we scale down the problem size to the nanoscale world of atoms and molecules, the physical picture changes. At this level, the particles interact with each other over relatively large distances: They repel each other if they are pushed together and attract each other as they are separated. It is this interaction of individual atoms that ultimately governs the macroscopic behavior of objects. In other words, an accurate atomic model should predict the behavior at the macroscale. However, a macroscale model, such as for contact, will in general not be appropriate to describe the nanoscale behavior.

Contact interaction at atomic or sub-atomic scales can be simulated by first-principle methods such as molecular dynamics (MD) [29], [42]. This is the predominant case in the study of interactions among flexible nanotubes [31], [43], DNA strands and proteins [82], nanoindentation [28], [80], [81], and atomic force microscopy [15], [19]. However, most of these simulations are qualitative in nature and focus on general scientific principles rather than the quantitative engineering design in nanotechnology. Even in the near future, it may not be practical to use first principle based simulations to model such systems in engineering design, due to the computational expense, complexity, and difficulty in interpreting results.

Small scale contact phenomena can be efficiently modelled by the analytical theories of Johnson, Kendall and Roberts (JKR) [48], of Derjaguin, Muller and Toporov (DMT) [25], and by the related Maugis-Dugdale model [64]. Although these models have been successfully applied to study rubber adhesion [48], MEMS stiction [108], adhesion of living cells [23], nanoindentation [28], [109], atomic force microscopy [56] and the adhesion used by the Gecko [6], they have some major limitations: They are restricted to infinitesimal deformations and contacting bodies with special, e.g. spherical, geometry. To obtain more general models, the authors of [88] and [22] have considered finite element approaches to model adhesive contact. These approaches achieve to generalize the geometry, and they have been successfully validated by the JKR and M-D models. However, in both [88] and [22] the interaction between the contacting bodies is not taken into account since one of the bodies is supposed to be rigid, thus decoupling the deformation between the two bodies in contact and simplifying the computational treatment substantially. In order to capture the interaction of largely deforming bodies during contact interaction, a more general model is called for.

In this work, we present and study a computational quasi-continuum contact mechanics model, formulated for arbitrarily shaped nanoscale solids undergoing large deformation, whose interaction is based on the interaction of individual atoms. In recent years, the atomistic potential based ‘Quasi-Continuum Model’ developed by Tadmor et al. [89], [83], [65], has been used successfully in multiscale modelling. Nevertheless, it seems to us that a systematic treatment on the contact mechanics of a quasi-continuum is still lacking. The
key to building a nanoscale contact model within a quasi-continuum framework, is the homogenization of the long range atomic interaction to obtain an effective interaction between continua. To capture this effective interaction, we propose three different computational strategies, which lead to a seamless transition from molecular dynamics to macroscale computational contact mechanics: At large scales two bodies interact via tractions acting on their contacting surfaces, whereas at very small scales the interaction expresses itself as a body force field extending over large parts of the interacting bodies. Using the proposed three methods, we have successfully formulated and implemented a quasi-continuum contact mechanics model within the framework of the finite element method [9], [14], [45], [99], [110]. The model, termed the Coarse-Grained Contact Model (CGCM), is computationally more efficient than molecular dynamics simulations, while, at the same time, is capable of predicting some of the nanoscale effects of atomic interactions.

1.2 Examples

Figure 1.1 displays several examples governed by nanoscale interactions which are suitable to be studied by the proposed model. Frame (a) shows the interaction between two crossing carbon nanotubes (CNTs) [43]. The individual atoms of the two tubes interact with each other leading to strong deformation of the tubes. At this scale, the bodies influence each other.

Figure 1.1: a. Carbon nanotube interaction; b. Nanoindentation; c. MEMS stiction; d. Atomic force microscopy; e. Gecko adhesion

other over large distances without coming into actual contact. An account of the mechanical properties of CNTs is given in [73]. Frame (b) shows a molecular dynamics simulation of the nanoindentation of an aluminum thin film [59]. The indenter itself is not shown. Within the film only dislocated atoms are displayed. These dislocations emerge to accommodate the large deformation of the crystal. A further example, shown in frame (c), is the stiction problem in micro-electromechanical systems (MEMS). During manufacturing or operation, components of the MEMS can stick together due to strong adhesive forces and render the device useless. For a review on adhesion in MEMS see [108]. Frame (d) shows an atomic force microscope [15], capable of measuring the atomic force between its tip and a surface below. It allows the examination and manipulation of the topology of the surface beneath. For example, it can be used to move and align individual carbon nanotubes, e.g. see [7], [44]. We note that macroscopically, atomic interactions are very weak and act only over tiny length scales, which are of the order of atomic distances themselves. The combined effect between billions of atoms, however, can create large forces between macroscopic bodies. An example is the adhesion employed by the gecko shown in frame (b). Its toes enable the gecko to cling to both smooth and rough surfaces, for example while rapidly climbing up walls [5], [6]. Another macroscopic examples, which is strongly influenced by nanoscale interactions is the Head-Disk instability discussed in [94].

1.3 Objectives and Scope

The first objective of this dissertation is to outline the proposed Coarse-Grained Contact Model and discuss its key ingredients. In particular we focus on the relation of the CGCM to large scale continuum mechanics and small scale molecular dynamics. This is addressed in section 2.

The second objective, following in section 3, is to formulate the governing equations of the CGC model. These can be derived both from molecular dynamics ‘below’ and from continuum mechanics ‘above’. Both approaches are taken, however the focus is placed on the latter. It is shown that the model is conservative and governed by a variational principle. In the derivation we don’t restrict ourselves to infinitesimal deformations, as is the case in many contemporary models, but account for the geometrical nonlinearity arising from large deformations. For a treatment of large deformation continuum mechanics see for example [20], [40], [63], [66]. Further, to identify the characteristic parameters of the CGC model, it is fully normalized.

The next objective, addressed in section 4, is to present a robust and efficient finite element implementation of the derived model and to compare it to existing computational contact techniques. The accuracy and consistency of the proposed contact algorithms are assessed in section 6.

In section 5 the general behavior of the CGC model is illustrated by the means of some simple analytical and numerical examples. A comparison of the proposed model with a molecular simulation is shown, which underlines the possible gains in efficiency obtained by the CGCM. The behavior of the CGC model is further studied in section 7 under the scaling of the overall geometry and the scaling of the involved energies.

The fifth objective is to demonstrate the usefulness of the proposed model by considering several realistic applications. This is addressed in section 8. In particular a comparison of the CGCM with the analytical JKR, DMT and Maugis-Dugdale theories, developed for
dry, adhesive contact, is shown.
The last objective, addressed in section 9, is the applicability of the CGC model, as the problem size is scaled up to macroscopic proportions. It is shown that under certain physical modifications, the CGC model can serve as a computational regularization technique for macroscale contact.
Finally, conclusions are drawn in section 10.
2 Modelling nanoscale Interaction

This section aims to lay the foundation of the present work and outline its key ingredients and concepts. The proposed model is introduced and a discussion on particle interaction and surface energies ensues.

2.1 The Coarse-Grained Contact Model

We proceed by presenting a conceptual overview of the proposed model. Figure 2.1 illustrates how the model fits into the approaches of classical continuum contact mechanics and molecular dynamics: At large scales the interaction between two bodies is described by a continuum approach. The bodies under study are considered to be continuous media, possibly homogeneous, whose loading-deformation relation is modelled upon some constitutive relation. In the case of hyperelasticity, the material response derives from a stored energy function $W$, which can be considered a property of the continuum. The contact of two such bodies is usually modelled as a globally constrained problem, where the constraint is the impenetrability of the two bodies. In other words the gap $g$ between the two bodies must remain positive. Analytical and numerical aspects of continuum contact mechanics can be found in [49], [100], [58] and also [57].

On the other hand, the behavior at the atomic scale is governed by interactions among individual atoms, which are modelled by interatomic potentials (see figure 2.1). Conceptually we distinguish between two such potentials: The interaction potential $\phi$, acting between atoms of two distinct bodies and therefore also termed the *intersolid* potential, and the interaction potential $\psi$, governing atoms within the solid and thus termed the *intrasolid* potential. This notation is in analogy to the behavior of carbon nanotubes, where we distinguish between the interlayer and intralayer behavior [74]. Molecular dynamics provides a powerful tool to simulate the behavior of large assemblies of atoms (or molecules), modelled...
by point masses and atomic interaction potentials. Comprehensive background information on interatomic forces is given in [46], an introduction to molecular dynamics can be found in [29], [42] and appendix A. We note, that a single cubic millimeter contains more than a billion billion \(10^{18}\) atoms and that the time scale of atomic oscillations is of the order of picoseconds \(10^{-12}\) seconds. Thus it quickly becomes impossible to solve such systems even with state-of-the-art computing technology. Furthermore, for many practical applications, the detailed knowledge of the positions and velocities of all these atoms over time, is of little interest.

An aim of multiscale modelling [71], [60], [69], [97] is to combine both the character of a continuum with the character of a discrete system. That is, one seeks to develop a model capable of seamlessly transcending from one scale to the other. The proposed quasi-continuum contact model, termed the ‘Coarse-Grained Contact Model’ (CGCM) combines features from both the continuum and the molecular approach (see figure 2.1). From the continuum model ‘above’ we take the general continuum description of the bodies under consideration. In particular we use a hyperelastic material model described by an internal potential \(W\). From the molecular approach ‘below’ we take the short range interaction potential \(\psi\), to generate the stored energy function \(W\), and use the long range interatomic potential \(\phi\), to model the interaction between the bodies. In other words \(\psi\) furnishes a constitutive relation for the solids, \(W = W(\psi)\), whereas \(\phi\) generates an external potential field, denoted by \(\Phi = \Phi(\phi)\), which envelops the solids like an ‘aura’. Physically, the intrasolid interaction can be associated with covalent, ionic, or metallic bonds, which are strong but only act over a close range. An example for the intersolid interaction is the van der Waals attraction between solids, which is relatively weak but of much longer range.

Thus the essence of the CGCM is an atomic potential enriched hyperelastic continuum with a surrounding long range field, which governs the interaction, like adhesion and contact, among different solids. We stress that this continuum model is based on two distinct components: The generation of an internal potential \(W\) from \(\psi\), and the generation of an enveloping field \(\Phi\) based on \(\phi\). The former has been studied extensively by the original Quasi-Continuum Method [89], [65], and we will, for this reason, focus more of our attention on the latter aspect. The treatment of this second component has a long history in the calculation of continuum van der Waals forces [41], [46], [90]. However, to the best of our knowledge, the combination of both components into a single model, its formulation within the setting of large deformation continuum contact mechanics, its implementation into a suitable numerical approach, like the finite element method, and the investigation of its general behavior, have not been studied before. Thus the motivation of the proposed CGC model is to combine the governing atomistic physics of nanoscale contact with the efficiency obtained by computational continuum modelling such as the finite element method.

It is further noted, that for some applications, the internal response \(W\) can also be taken from an empirical, not atomistic, constitutive approach [66]. In this fashion it becomes apparent that the CGC model approaches the traditional continuum model for increasing scales, i.e. as the ‘aura’ \(\Phi\) vanishes to be replaced by the contact constraint. It is because of this, that the model takes two conceptual variations: the molecular motivated model, where both the internal response and the enveloping field are based on the quasi-continuum treatment of the atomic behavior, and the continuum motivated model, where both \(W\) and \(\Phi\) are motivated form the usual continuum modelling. The motivation of the proposed contact model from both these directions is discussed in this work. In the theoretical development
of section 3 we have chosen to follow the latter approach. The derivation from molecular
dynamics is discussed in appendix A. From the atomic perspective, the CGC model can
be seen as a coarsened, or smeared-out picture of the atomic world, both in terms of the
internal response, captured by $W$, and in terms of the interaction between bodies, captured
by $\Phi$, which gives the model its name.

### 2.2 Molecular Interaction Potentials

The interaction between two molecules can originate from different physical phenomena.
A comprehensive account is given by the monograph of Israelachvili [46]. Consider figure
2.2, which is an excerpt of a similar figure taken from chapter 2 of [46]. It illustrates the

![Figure 2.2: Pairwise intermolecular interaction potentials in vacuum [46]](image)

interaction energy between charged, dipolar and non-polar particles. For instance the first
case gives the interaction energy

$$\phi(r) = \frac{Q_1 Q_2}{4\pi \varepsilon_0 r}$$

between two charged particles, e.g. ions, with charges $Q_1$ and $Q_2$, separated by $r$. Here $\varepsilon_0$
is the electric permittivity in vacuum. (Further, in the figure, $u$ denotes the electric dipole
moment, $\alpha$ denotes the electric polarizability, $k$ denotes Boltzmann’s constant, $T$ denotes
absolute Temperature, $h$ denotes Planck’s constant and $\nu$ denotes the electronic absorption
frequency.) A detailed derivation of the formulas listed in figure 2.2 is given in [46]. For all
cases displayed, the force between the particles follows from the derivative of the potential
with respect to $r$. In vacuum, this force is repulsive for the Coulomb energy and attractive
for all other cases. The interaction potentials are modified when the interaction occurs
within a medium. In some instances, interactions which are attractive in one media can
become repulsive within another. An example is a drop of oil in water. Ordinarily the forces between the oil molecules are attractive and the drop does not dissolve. However, if soap is added to the water the forces within the oil become repulsive and the drop dissolves.

The van der Waals interaction is given by the sum of the Debye induction energy, the Keesom orientation energy and the London dispersion energy, all of which are attractive in vacuum and proportional to $1/r^6$. In contrast to covalent, ionic or metallic bonds, which are short range and are the predominant interaction within solids (associated with $\psi$), van der Waals interactions are long range and a suitable origin for intersolid interactions modelled by $\phi$. Due to its proportionality to $1/r^6$, van der Waals interaction is often modelled by the Lennard Jones potential

$$\phi(r) = \frac{A}{r^{12}} - \frac{B}{r^6}, \quad (2.2)$$

where the repulsive $A/r^{12}$ term is empirical and models the repulsion which occurs when atoms are in close proximity. The list in figure 2.2, which is not exhaustive, describes the interaction between molecule pairs. These form the building blocks of multi-particle potentials, which usually depend on all the mutual distances and angles, and tend to become much more complicated. An example is given by the Brenner-Tersoff potential, [93], [17], commonly used for carbon systems, like diamond or graphite.

Interaction potentials can also be used to describe interactions between macroscopic particles, e.g. to model a rigid indenter [52], to model the interaction of blood cells [61], or to study particle flows [111]. A further example are cohesive finite elements [102], [67], developed for the study of crack propagation. There an interaction potential is used to model the intrasolid bonding between finite elements.

### 2.3 Limitations of the proposed Contact Model

The CGC model is envisioned for contact/interaction problems at very small scales, i.e. of the order of micrometers and below. As is shown by the numerical examples of this work, the model is capable of describing the characteristic features of such problems, as they are observed experimentally and predicted by analytical theories like the JKR model. Like any other model, however, the CGCM has its limitations. Some of these may be removed by expanding and refining the current model.

One obvious limitation is that the model cannot track the motion of individual atoms, since their behavior is smeared out, or averaged into an effective continuum. To improve this deficiency the CGCM can be coupled with molecular dynamics, so that we attain a detailed picture where necessary and a coarse picture where possible.

Another restriction is that we only consider the deformation of the bodies’ surfaces but not their creation or consumption, such as occurs during fracturing or reversely, during sintering. Such changes in the free surface area lead to changes in the free surface energy. This energy arises from the fact that surface atoms (which are only partly surrounded by neighboring atoms), as seen in figure 2.1, have a different environment than bulk atoms (which are fully surrounded by neighbors). During fracturing, intersolid bonds (modelled by $\psi$) are broken so that former bulk atoms become surface atoms. During sintering, non-bonded surface atoms (interacting with $\phi$) bond together (so that $\phi$ turns into $\psi$) and thus former surface atoms become bulk atoms. Although presently lacking, such processes can be incorporated into the framework of the CGC model (e.g. by including the surface energy.
contribution). Another lacking consideration are chemical reactions, like oxidation, which can occur at the free surfaces. We finally note that within this work we are not considering inelastic behavior, energy dissipation and thermal effects. Such effects may also be readily included in the present formulation.
3 Theory of the Coarse-Grained Contact Model

In this section the theory of the CGC model is laid out, as governed by the principles of kinematics, equilibrium and constitution. Uniqueness and stability of the model are addressed in section 3.4 and it is further shown in section 3.5, that the general behavior of the CGC model can be characterized by two fundamental parameters.

3.1 The Weak Form

Let us now derive the weak form governing the Coarse-Grained Contact model introduced in the previous section. The derivation is based on the model problem of two interacting bodies. The extension to multibody interaction is straightforward and is discussed at the end of this section. Figure 3.1 (a) shows the kinematics of two interacting bodies in the framework of finite deformation continuum mechanics. Here, \( \Omega_{10} \) and \( \Omega_{20} \) denote the reference configurations of the two bodies. Their current, deformed configurations are denoted by \( \Omega_{1} \) and \( \Omega_{2} \). The motion mapping two generic reference points \( X_1 \in \Omega_{10} \) and \( X_2 \in \Omega_{20} \) to the current locations \( x_1 \in \Omega_{1} \) and \( x_2 \in \Omega_{2} \) is denoted by \( x_1 = \varphi_1(X_1, t) \) and \( x_2 = \varphi_2(X_2, t) \). Associated with the two motions \( \varphi_1 \) and \( \varphi_2 \) are the two deformation gradients \( F_1 = \text{Grad} \varphi_1 \) and \( F_2 = \text{Grad} \varphi_2 \), where the gradient operator \( \text{Grad}(...) \) is taken with respect to the reference configurations \( \Omega_{10} \) and \( \Omega_{20} \). The two bodies are subjected to the essential and natural boundary conditions (not shown in figure 3.1)

\[
\begin{align*}
\varphi_I &= \bar{\varphi}_I, \quad \text{on } \Gamma_{I,u} \quad \text{for } I = 1, 2, \\
\sigma_I n_I &= \bar{t}_I, \quad \text{on } \Gamma_{I,t} \quad \text{for } I = 1, 2,
\end{align*}
\]

(3.1)

where \( \bar{\varphi}_I \) and \( \bar{t}_I \) are the values of the prescribed boundary displacement and traction, \( \sigma_I \) is the Cauchy stress tensor and \( n_I \) the outward unit normal of \( \partial \Omega_I \). Further, \( \Gamma_{u,I} \) and \( \Gamma_{t,I} \) denote the displacement and traction boundaries in the current configuration which are required to satisfy \( \Gamma_{I,u} \cup \Gamma_{I,t} = \partial \Omega_I \) and \( \Gamma_{I,u} \cap \Gamma_{I,t} = \emptyset \). Moreover, we require the initial conditions

\[
\begin{align*}
\varphi_I(X_I, 0) &= \varphi_0(X_I), \quad \varphi_I(X_I, 0) = V_0(X_I), \quad \text{in } \Omega_I,
\end{align*}
\]

(3.2)
where \( \dot{\varphi}_I = \frac{\partial}{\partial t} \varphi_I(X_I, t) \) denotes the material time derivative of \( \varphi_I \) and where \( \varphi_0(X_I) \) and \( V_0(X_I) \) denote the initial configuration and velocity field of \( \Omega_I \) at \( t = 0 \). (The initial configuration of \( \Omega_I \) may or may not coincide with the reference configuration \( \Omega_{I0} \).)

As indicated in figure 3.1, the atomic (or particle) densities in the two respective configurations are denoted by \( \beta_{10} \) and \( \beta_{20} \) (in number of particles per reference volume), and \( \beta_1 \) and \( \beta_2 \) (in number of particles per current volume). The atomic density \( \beta_I \) is related to the mass density by \( \rho_I = m_I \beta_I \), where \( m_I \) is the atomic mass of body \( I = 1, 2 \). The volume differentials of the spatial configuration, \( dv_I \), and the material configuration, \( dV_I \), are related by

\[
dv_I = J_I dV_I, \quad J_I = \det F_I,
\]

where \( J_I \) is the Jacobian of the mapping \( \varphi_I \). For now, we are not considering a flux of particles from or into the bodies. It then follows that the particle and mass densities of the two configurations are in inverse relation to eq. (3.3), i.e.

\[
\beta_I = \beta_{I0}/J_I, \quad \rho_I = \rho_{I0}/J_I,
\]

and that the total number of particles (and the mass) within a given volume are conserved, i.e. we have

\[
\beta_{I0} dV_I = \beta_I dV_I = \text{const}.
\]

Within the proposed CGC model we suppose that two atoms (or molecules) located at \( x_1 \) and \( x_2 \) interact with each other via an interatomic potential \( \phi \), which depends on the current distance \( r := |x_1 - x_2| \). In general \( \phi(r) \) may be any potential suitable to describe the physical situation at hand. Several elementary interaction potentials are discussed in section 2.2. A popular candidate, which we consider in the following, is the Lennard-Jones potential

\[
\phi(r) = \epsilon \left( \frac{r_0}{r} \right)^{12} - 2 \epsilon \left( \frac{r_0}{r} \right)^6,
\]

where \( r_0 \) and \( \epsilon \) are a length and a energy scale. The force \( F(r) \) between the two atoms is then given by the gradient

\[
F(r) = -\frac{\partial \phi}{\partial r} = \frac{12 \epsilon}{r_0} \left[ \left( \frac{r_0}{r} \right)^{13} - \left( \frac{r_0}{r} \right)^7 \right].
\]

One can see that \( r = r_0 \) is the equilibrium distance between the atoms, i.e. the distance where \( F = 0 \), and that \( \epsilon \) is the energy of the well at \( r = r_0 \). The well depth \( \epsilon \) corresponds to the energy required to pull the two atoms apart from \( r = r_0 \) to \( r = \infty \). A normalized graph of \( \phi(r) \) and \( F(r) \) is shown in figure 3.1 (b). To set \( \phi \) apart from the intrasolid potential \( \psi \), let us also write \( r_\phi := r_0 \) and \( \epsilon_\phi := \epsilon \). The parameters \( r_0 \) and \( \epsilon \) are material constants that have been listed in the literature for various elements. In case the two atoms belong to two distinct materials \( a \) and \( b \) with parameters \( r_0^a, r_0^b, \epsilon_a \) and \( \epsilon_b \) the equilibrium distance and well depth of the combined system can be computed from the arithmetic and geometric mean [33]

\[
r_0^{ab} = \frac{r_0^a + r_0^b}{2}, \quad \epsilon_{ab} = \sqrt{\epsilon_a \epsilon_b}.
\]

Given \( \phi(r) \) the total interaction between bodies \( \Omega_1 \) and \( \Omega_2 \) follows from the integration over all points \( x_1 \in \Omega_1 \) and \( x_2 \in \Omega_2 \). Within the CGC model, the two-body interaction is thus
modelled by the potential

$$
\Pi_C := \int_{\Omega_1} \int_{\Omega_2} \beta_1 \beta_2 \phi(r) \ dv_2 \ dv_1 ,
$$

(3.9)

or equivalently, from eq. (3.5),

$$
\Pi_C = \int_{\Omega_{10}} \int_{\Omega_{20}} \beta_{10} \beta_{20} \phi(r) \ dV_2 \ dV_1 .
$$

(3.10)

Note that by choosing the integration domains $\Omega_1 \subseteq \Omega_1$ and $\Omega_2 \subseteq \Omega_2$, as shown in figure 3.1 (a), we are allowing for the possibility that the bodies only interact via these subsets. This is motivated by the fact that the potential $\phi$, like the Lennard-Jones potential shown in figure 3.1 (b), usually has a cutoff radius $r_c$ beyond which $\phi$ is considered negligible. The dependence of $\Pi_C$ on the deformation of the two bodies $\Omega_1$ and $\Omega_2$ leads to a strong nonlinear coupling between the bodies. We further note that even though $\phi$ may only have one absolute minimum (see figure 3.1 (b) in case of Lennard-Jones) the integration in eq. (3.9) can, depending on the shape of $\Omega_1$ and $\Omega_2$, lead to countless local minima of $\Pi_C$, as is illustrated in section 3.4. Another prominent feature of $\Pi_C$ is that it is strongly controlled by the gap between $\Omega_1$ and $\Omega_2$ since the interaction is strongest between closest points.

The study of the continuum interaction energy $\Pi_C$ has a long history. The first work dates back to the 1930s by the prominent contributions of Bradley [16] and Hamaker [41], who evaluated integral (3.9) for simple, rigid geometry such as two spherical domains $\Omega_1$ and $\Omega_2$. Recently, the interaction energy $\Pi_C$ has also been considered in the study of carbon nanotubes. Assuming rigid geometry, Girifalco [33] uses $\Pi_C$ to compute the interaction between separate nanotubes. In the computational works of Arroyo et al., [2], [3] and [4], an expression analogous to eq. (3.9) is considered to model the non-bonded atomic interaction within the nanotubes. Qian et al. [74] uses the interaction energy $\Pi_C$ to model the interlayer response of multiwalled carbon nanotubes. To the best of the author’s knowledge, a general finite deformation contact theory for small scales and its nonlinear finite element implementation for arbitrarily shaped bodies, as is studied here, has not been given before. We also believe that, especially in three dimensions, the interaction energy $\Pi_C$ has to be approximated further to increase efficiency of large scale computations. Such approximations are introduced in section 4, which discusses the FE implementation of the CGCM.

We suppose that the system shown in figure 3.1 (a) is conservative, so that there exists a total potential energy given by

$$
\Pi = \Pi_{\text{int}} + \Pi_C - \Pi_{\text{ext}} ,
$$

(3.11)

where $\Pi_{\text{int}}$ and $\Pi_{\text{ext}}$ are the internal and external energy contributions. The internal response of the two deforming bodies ($I = 1, 2$) is considered as hyperelastic, so that we have

$$
\Pi_{\text{int}} = \sum_{I=1}^{2} \Pi_{\text{int},I} , \quad \Pi_{\text{int},I} = \int_{\Omega_{I0}} W_I(F_I) \ dV_I ,
$$

(3.12)

where $W_I(F_I)$ is the stored energy function (per reference volume) of body $\Omega_I$. It follows from a chosen constitutive relation modelling the material response. Within this work we distinguish between two types of constitutive models: empirical and atomistic models.
The first class is formed by models primarily based on experimental data such as the Neo-Hookean and similar models, e.g., see [66]. The second class is formed by models based on the underlying atomic structure, which is governed by the intrasolid potential $\psi$. Constitutive models are discussed in further detail in the following section.

For a quasi-static motion the equilibrium equation of a conservative system follows from the principle of stationary potential energy, which states that at equilibrium the system has stationary potential energy for the true motion $\varphi$ among all kinematically admissible variations $\delta \varphi$. It follows that the variation of $\Pi$ satisfies

$$
\delta \Pi = \delta \Pi_{\text{int}} + \delta \Pi_C - \delta \Pi_{\text{ext}} = 0 , \quad \forall \ \delta \varphi_1, \delta \varphi_2 ,
$$

which yields the weak form of the equilibrium equation. Here, we suppose that the variation of the external energy $\Pi_{\text{ext}}$ is given by

$$
\delta \Pi_{\text{ext}} = \sum_{I=1}^{2} \delta \Pi_{\text{ext},I} , \quad \delta \Pi_{\text{ext},I} = \int_{\Omega_I} \delta \varphi_I \cdot \rho_I \dd \bar{b}_I + \int_{\Gamma_{t,I}} \delta \varphi_I \cdot \bar{t}_I \dd a_I ,
$$

where $\bar{t}_I$ is the traction field prescribed on the boundary $\Gamma_{t,I} \subset \partial \Omega_I$ of body $I = 1, 2$ and $\bar{b}_I$ is the prescribed body force field in body $I$. We consider the fields $\bar{t}_I$ and $\bar{b}_I$ in a form such that $\delta \Pi_{\text{ext}}$ is derivable from a potential $\Pi_{\text{ext}}$. The variation of the internal energy $\Pi_{\text{int},I}$ of body $I$ can be written as

$$
\delta \Pi_{\text{int},I} = \int_{\Omega_I} \text{grad}(\delta \varphi_I) : \sigma_I \dd v_I ,
$$

where $\text{grad}(\ldots)$ denotes the gradient operator with respect to the current configuration and where $\sigma_I$ is the Cauchy stress. It follows from a particular choice of $W$ as is considered in the following section. Let us now derive the variation of the interaction energy $\Pi_C$ given by (3.9) or (3.10). Using chain rule and identity (3.5) the variation of $\Pi_C$ becomes

$$
\delta \Pi_C = \int_{\Omega_1} \int_{\Omega_2} \beta_1 \beta_2 \left( \frac{\partial \phi(r)}{\partial x_1} \cdot \delta \varphi_1 + \frac{\partial \phi(r)}{\partial x_2} \cdot \delta \varphi_2 \right) \dd v_2 \dd v_1 ,
$$

which can also be written as

$$
\delta \Pi_C = - \int_{\Omega_1} \delta \varphi_1 \cdot \beta_1 b_1 \dd v_1 - \int_{\Omega_2} \delta \varphi_2 \cdot \beta_2 b_2 \dd v_2 =: \delta \Pi_{C,1} + \delta \Pi_{C,2} ,
$$

where we have defined the body forces

$$
b_1(x_1) := - \frac{\partial \Phi_2}{\partial x_1} , \quad \Phi_2 := \int_{\Omega_2} \beta_2 \phi(r) \dd v_2 ,
$$

$$
b_2(x_2) := - \frac{\partial \Phi_1}{\partial x_2} , \quad \Phi_1 := \int_{\Omega_1} \beta_1 \phi(r) \dd v_1 .
$$

Physically, eqs. (3.17) and (3.18) are interpreted in the following way: Each body $\Omega_I$ ($I = 1, 2$) is surrounded by a field $\Phi_I$, termed the ‘aura’ of body $\Omega_I$. (The aura is indicated by the dashed line in figure 2.1.) The aura of one body generates a body force within the other body. In other words the presence of body $\Omega_2$ exerts a body force field, $b_1$, on body $\Omega_1$, whereas $\Omega_1$ exerts the field $b_2$ on $\Omega_2$. We see that $\delta \Pi_C$ has the same structure as the
first part of \( \delta \Pi_{\text{ext}} \), however, we emphasize that \( \mathbf{b}_I \) and \( \mathbf{b}_I \) are conceptually different: The body force \( \mathbf{b}_I \) arises from the interaction of the two bodies within the system, whereas \( \mathbf{b}_I \) is imposed externally onto the system. An example for the latter are the body forces arising from an immersing gravity field.

To simplify expression (3.18), let us define the unit direction \( \hat{r} \) between points \( x_1 \) and \( x_2 \) as
\[
\hat{r} := \frac{r}{r}, \quad r := x_1 - x_2, \quad r := |r|,
\]
and note that
\[
\frac{\partial \phi(r)}{\partial x_1} = \frac{\partial \phi}{\partial r} \frac{\partial r}{\partial x_1} = -F(r) \hat{r}, \quad \frac{\partial \phi(r)}{\partial x_2} = \frac{\partial \phi}{\partial r} \frac{\partial r}{\partial x_2} = F(r) \hat{r},
\]
where the force function \( F(r) = -\frac{\partial \phi}{\partial r} \) of the Lennard-Jones potential is given by eq. (3.7).

Pulling the gradient into the integration, eq. (3.18) can then also be written as
\[
\mathbf{b}_1(x_1) = + \int_{\Omega_2} \beta_2 F(r) \hat{r} \, dv_2,
\]
\[
\mathbf{b}_2(x_2) = - \int_{\Omega_1} \beta_1 F(r) \hat{r} \, dv_1.
\]

We remark that the force \( F(r) \) acting at the two points \( x_1 \) and \( x_2 \) is equal in magnitude and opposite in direction. However in general, the body forces \( \mathbf{b}_1 \) and \( \mathbf{b}_2 \) acting at \( x_1 \) and \( x_2 \), are neither equal in magnitude nor act in opposing directions. The resultant force on both bodies, obtained from integrating \( \mathbf{b}_I \) over body \( \Omega_I \), are again equal in magnitude and act in opposing direction.

In general the motion is time dependent and we must include the kinetic energy of the system,
\[
K = \sum_{I=1}^{2} K_I, \quad K_I = \frac{1}{2} \int_{\Omega_I} \rho_I \mathbf{v}_I \cdot \mathbf{v}_I \, dv_I,
\]
where \( \mathbf{v}_I = \dot{x}_I \) is the velocity field of body \( \Omega_I \). The Lagrangian of the system is then given by
\[
L = K - \Pi.
\]

The weak form now follows from Hamilton’s variational principle, which states that the action
\[
A = \int_{t_1}^{t_2} L \, dt,
\]
attains its stationary value for the true motion among all kinematically admissible variations within the time interval \( T = \{t_1, t_2\} \) [55]. The variation of the action \( \delta A \) of each body \( \Omega_I \) is obtained as
\[
\delta A_I = \int_T \int_{\Omega_I} \rho_I \mathbf{v}_I \cdot \delta \mathbf{\dot{v}}_I \, dv_I \, dt - \int_T \delta \Pi_I,
\]
where \( \delta \Pi_I = \delta \Pi_{\text{int},I} + \delta \Pi_{\text{C},I} - \delta \Pi_{\text{ext},I} \) according to eqs. (3.13), (3.14), (3.15) and (3.17). By switching the order of integration and by using integration of parts the first contributions is written as
\[
\int_{\Omega_I} \int_T \rho_I \mathbf{v}_I \cdot \delta \mathbf{\dot{v}}_I \, dt \, dv_I = - \int_{\Omega_I} \int_T \rho_I \mathbf{\dot{v}}_I \cdot \delta \mathbf{v}_I \, dt \, dv_I,
\]
where the variation of the motion $\delta \varphi_I$ is chosen such that it vanishes at $t = t_1$ and $t = t_2$. According to Hamilton’s Principle we set $\delta A = 0$, which now yields

$$
\delta A = - \int_T \left[ \sum_{I=1}^2 \int_{\Omega_I} \rho_I \dot{v}_I \cdot \delta \varphi_I \, dv_I + \delta \Pi_I \right] dt = 0, \quad \forall \delta \varphi_I. \tag{3.27}
$$

Since this statement is true for all spatial and temporal variations $\delta \varphi_I$, the expression in parenthesis must vanish. Expanding $\delta \Pi_I$ by using eqs. (3.13), (3.15) and (3.17) we thus find the expression

$$
\sum_{I=1}^2 \left[ \int_{\Omega_I} \delta \varphi_I \cdot \rho_I \dot{v}_I \, dv_I + \int_{\Omega_I} \text{grad}(\delta \varphi_I) : \sigma_I \, dv_I - \int_{\Omega_I} \delta \varphi_I \cdot \beta_I b_I \, dv_I - \delta \Pi_{\text{ext},I} \right] = 0,
\quad \forall \delta \varphi_I, \tag{3.28}
$$

which is the governing weak form equilibrium equation of the interacting two-body system displayed in figure 3.1. We remark that we will not devote as much attention to the external virtual work contribution $\delta \Pi_{\text{ext}}$ as we will devote to the other terms. For the examples considered later we set both $b_I$ and $t_I$ to zero throughout their respective domains $\Omega_I$ and $\Gamma_{t,I}$.

We note that, in the derivation presented so far, we have taken the continuum approach, in which the Lagrangian $L$ is derived by starting from the continuum description. In view of figure 2.1 the system has thus been derived from ‘above’. Alternatively, the same set of governing equations can be derived from ‘below’, i.e. from the underlying molecular system. This derivation is included in Appendix A. A continuum which is founded on the underlying molecular system is also termed a quasi-continuum.

Before moving ahead let us consider two simple extensions to the theory presented above. First, we may consider the interaction potential to be given by

$$
\Pi_C = \int_{\partial \Omega_1} \int_{\partial \Omega_2} \tilde{\beta}_1 \tilde{\beta}_2 \phi(r) \, da_2 \, da_1, \tag{3.29}
$$

that is we consider the two body interaction to be restricted to the surface subsets $\partial \Omega_I \subseteq \partial \Omega_1$. A situation which arises for example from the interaction of two bodies with charged surfaces. In this formulation, $\tilde{\beta}_I$ denotes the atomic surface density in number of atoms per surface area. Starting from eq. (3.29), the derivation of the weak form follows the same steps as above replacing $\Omega_I$ by $\partial \Omega_I$ and $\beta_I$ by $\tilde{\beta}_I$. We thus obtain an analogous weak form statement as given in eq. (3.28), where $b_I$ is now a surface traction acting on $\partial \Omega_I$ and which is invoked by the surface of the neighboring body.

A second extension is to study the interaction between $N$ bodies. If we consider any two of the $N$ bodies to be interacting the same way as discussed above, the total multibody interaction potential will be

$$
\Pi_C = \int_{\Omega_1} \int_{\Omega_2} \beta_1 \beta_2 \phi \, dv_2 \, dv_1 + \int_{\Omega_1} \int_{\Omega_3} \beta_1 \beta_3 \phi \, dv_3 \, dv_1 + \int_{\Omega_2} \int_{\Omega_3} \beta_2 \beta_3 \phi \, dv_3 \, dv_2 - \ldots, \tag{3.30}
$$

which can also be written as

$$
\Pi_C = \frac{1}{2} \sum_{I}^N \sum_{J \neq I}^N \Pi_{C,IJ}, \quad \Pi_{C,IJ} = \int_{\Omega_I} \int_{\Omega_J} \beta_I \beta_J \phi(r) \, dv_J \, dv_I. \tag{3.31}
$$
3.2 Constitutive Models

The formulation of the CGC model is only complete if a constitutive model, governing the internal response (3.12), is specified. As mentioned earlier we will consider two classes of constitutive models: empirical models based on experimental observations, often at macroscopic scales, and atomistic models motivated by atomic interactions. For this we define the two kinematical quantities

\[ B = FF^T, \quad C = F^T F, \]

(3.32)
termed the left and right Cauchy-Green tensors. (For simplicity we have dropped the subscript \( I = 1, 2 \), used for the two bodies \( \Omega_1 \) and \( \Omega_2 \).) Within this work the following two hyperelastic models are used:

3.2.1 Empirical Models: The Neo-Hookean Model

The Neo-Hookean model is given by the stored energy function

\[ W = U(J) + \frac{\mu}{2}(I_1 - 3) - \mu \ln J, \quad U(J) = \frac{\Lambda}{2}(\ln J)^2, \]

(3.33)
where \( J = \det F \) and \( I_1 = \text{tr} B = \text{tr} C \) characterize the deformation. It is noted that there are some variants of this models which consider different volumetric response functions \( U(J) \). The parameters \( \Lambda \) and \( \mu \) are material constants, which can be written as

\[ \mu = \frac{E_Y}{2(1 + \nu)}, \quad \Lambda = \frac{2\mu\nu}{1 - 2\nu}, \]

(3.34)
where \( E_Y \) and \( \nu \) correspond to Young’s modulus and Poisson’s ratio. Given \( W \) we can introduce the following stress measures and associated tangents. The second Piola-Kirchhoff stress is given as the derivative of \( W \) with respect to the right Cauchy-Green tensor, i.e

\[ S = 2\frac{\partial W}{\partial C} = JU' C^{-1} + \mu(I - C^{-1}), \]

(3.35)
where \( I \) is the second order identity tensor. The Cauchy stress, on the other hand, follows as the derivative of \( W \) with respect to \( B \), that is

\[ \sigma = 2\frac{\partial W}{\partial B} B = U'I + \frac{\mu}{J}(B - I). \]

(3.36)
The tangent associated with \( S \) is obtained by further differentiation as

\[ C = 4\frac{\partial^2 W}{\partial C^2} = J(JU')' C^{-1} \otimes C^{-1} + 2(\mu - JU') I_C^{-1}, \]

(3.37)
and similarly, the tangent related to \( \sigma \) is found as

\[ \tau = 4\frac{\partial^2 W}{\partial B^2} B = (JU')' I \otimes I + 2(\mu - U') I. \]

(3.38)
In the last two equations we have introduced the fourth order tensors

\[
\mathbb{I}_{ijk\ell} = \frac{1}{2}(\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk}) , \\
(\mathbb{I}^{-1})_{ijk\ell} = \frac{1}{2}((C^{-1})_{ik}(C^{-1})_{j\ell} + (C^{-1})_{i\ell}(C^{-1})_{jk}) .
\]

We note that the tensors \( C, S \) and \( \mathbb{C} \) are material quantities as they refer to the material, or reference configuration \( \Omega_0 \). On the other hand, \( B, \sigma \) and \( \epsilon \) are spatial quantities applying to the spatial configuration \( \Omega \). It is seen that \( \epsilon \) is a fourth order isotropic tensor. The selection of the Neo-Hookean model is motivated by its simplicity in implementation. Regarding the atomic physics at very small scales, this model may not give a realistic picture. This motivates the following model.

### 3.2.2 Atomistic Models: The Cauchy-Born Rule

The Cauchy-Born rule, see [27], [89], [103] and references therein, is suitable to describe crystal elasticity. It assumes that the deformation is locally homogeneous, meaning that the deformation is homogeneous across a certain range of a crystal lattice and is determined by the local deformation gradient \( F \). Under this assumption the deformation of a crystal lattice behaves as shown in figure 3.2 (a). The vector \( R \) between two undeformed atomic sites is then mapped onto the vector \( r = FR \) between two atoms in the deformed configuration. With this underlying assumption we can construct a simple constitutive relation which satisfies the locality of the stress field. We therefore consider the interaction between the atoms of the solid to be governed by the potential \( \psi \), which, in general, is a function of all the atomic sites. In the following let us restrict our discussion to the two-point interaction between atom pairs. For instance \( \psi \) may be given by the Lennard-Jones potential

\[
\psi(r) = \epsilon_\psi \left( \frac{r_\psi}{r} \right)^{12} - 2\epsilon_\psi \left( \frac{r_\psi}{r} \right)^6 ,
\]

where \( r = |r| \) is the current distance between two atoms. Further \( r_\psi \) and \( \epsilon_\psi \) are the equilibrium distance and well depth of \( \psi \). Once more we emphasize the conceptual difference between the atomic potentials \( \psi \) and \( \phi \), as illustrated in figure 2.1.

Considering a given undeformed unit cell \( S_c \) with atomic density \( \beta_0 \), we can construct the energy density

\[
W(F) = \frac{\beta_0}{2} \sum_{k \in S_c} \psi(r_k) , \quad r_k = |r_k| , \quad r_k = FR_k ,
\]

Figure 3.2: a. Cauchy-Born rule; b. Fcc nearest neighbor unit cell
which is a summation over all atom pairs $k$ within $S_c$. We note that the unit cell has to be sufficiently large to include the range of possible interactions. The simplest case is to consider interaction between nearest neighbors only. For a face centered cubic (fcc) crystal the smallest possible unit cell is displayed in figure 3.2 (b). The cell contains $k = 6$ atomic bonds (shown in gray). The fcc crystal extends in space by reflection of this unit cell across its faces. In the undeformed configuration the atoms are spaced by the equilibrium distance $r_{\psi}$. Since the cell contains $4 \times \frac{1}{8}$ atoms, the atomic density for the considered cell is given by 

$$\beta_0 = \frac{\sqrt{2}}{r_{\psi}^3}. \quad (3.42)$$

Given the stored energy function $W(F)$, the second Piola-Kirchhoff Stress now follows as 

$$S = 2 \frac{\partial W}{\partial C} = \frac{\beta_0}{2} \sum_{k \in S_c} \frac{\partial \psi}{\partial r_k} \frac{R_k \otimes R_k}{r_k^2}, \quad (3.43)$$

while the Cauchy Stress follows as 

$$\sigma = 2 \frac{\partial W}{J \partial B} B = \frac{\beta}{2} \sum_{k \in S_c} \frac{\partial \psi}{\partial r_k} \frac{r_k \otimes r_k}{r_k^2}, \quad (3.44)$$

where $\beta = \beta_0/J$ is the current atomic density of cell $S_c$. Further, the material and spatial tangent are obtained as 

$$C = 4 \frac{\partial^2 W}{\partial C^2} = \frac{\beta_0}{2} \sum_{k \in S_c} \left( \frac{\partial^2 \psi}{\partial r_k^2} - \frac{1}{r_k} \frac{\partial \psi}{\partial r_k} \right) \frac{R_k \otimes R_k \otimes R_k \otimes R_k}{r_k^2}, \quad (3.45)$$

and 

$$\varepsilon = 4 \frac{\partial^2 W}{J \partial B^2} B = \frac{\beta}{2} \sum_{k \in S_c} \left( \frac{\partial^2 \psi}{\partial r_k^2} - \frac{1}{r_k} \frac{\partial \psi}{\partial r_k} \right) \frac{r_k \otimes r_k \otimes r_k \otimes r_k}{r_k^2}. \quad (3.46)$$

We note that for a cubic crystal, as is shown in figure 3.2 (b), the Cauchy-Born rule leads to a finite anisotropic cubic material law. Again, we emphasize that this constitutive model only applies as long as the deformation is homogeneous within the considered unit cell. Highly inhomogeneous deformation, e.g. in the presence of dislocations, cannot be treated by the Cauchy-Born rule and we must then adopt a nonlocal formulation accounting for the varying deformation gradient $F$ at the individual atomic sites. In general we note that, due to the summation in eq. (3.41), the stored energy $W(F)$, and thus $\Pi_{\text{int}}$, can be highly non-convex functions with many local minima, as is shown in section 3.4.

The Cauchy-Born rule can be easily incorporated into the framework of the finite element method. An approach combining the local and nonlocal formulations is the ‘Quasi-Continuum Method’ developed by Tadmor et al. [89], see also [54],[65] for an analysis and recent review. Another example is the ‘Interatomic Potential Finite Element Model’ (IPFEM) described in [96]. A mathematical study of the Cauchy-Born rule can be found in [30].

It is noted that the distance $r_{\psi}$ can be eliminated from the model (see appendix B) and so the Cauchy-Born rule only depends on one material constant, $\epsilon_{\psi}$, whereas a general cubic material law relies on three independent constants.
3.3 Analytical Integration

In some cases the body force \( \mathbf{b}_1 \), given by eq. (3.18), can be obtained by analytical integration. For instance let us consider the case where one body, say \( \Omega_2 \), is rigid and of simple geometry. According to eq. (3.18) the body force in body \( \Omega_1 \) is written as

\[
\mathbf{b}_1(x_1) = -\frac{\partial \Phi_2}{\partial x_1}, \quad \Phi_2 := \int_{\Omega_2} \beta_2 \phi(r) \, dv.
\]  

(3.47)

As an example let us consider the case where \( \Omega_2 = \Omega_2 \) is given by the three dimensional half-space displayed in figure 3.3 (a). Considering constant density \( \bar{\rho}_2 \) and the potential \( \bar{\phi}(r) \) to be given by eq. (3.6), the integration in \( \Phi_2 \) can be carried out analytically to find

\[
\Phi_2 = \pi \beta_2 \bar{\rho}_0 \left[ \frac{1}{45} \left( \frac{r_0}{y} \right)^9 - \frac{1}{3} \left( \frac{r_0}{y} \right)^3 \right],
\]  

(3.48)

where \( y \) is the distance away from the surface of the half-space. Equation (3.48) describes the interaction energy between the half-space and a point \( x_1 \) at distance \( y \). The vertical force acting at \( x_1 \) follows as

\[
F_{\Phi_2} = -\frac{\partial \Phi_2}{\partial y} = \pi \beta_2 \bar{\rho}_0 \left[ \frac{1}{5} \left( \frac{r_0}{y} \right)^{10} - \left( \frac{r_0}{y} \right)^4 \right].
\]  

(3.49)

We remark that, depending on the function \( \phi(r) \), other simple shapes, like for example a rigid cylinder or sphere can also be integrated analytically.

A further important case is the case of plane strain, since it requires the use of analytical integration of \( \phi(r) \). Figure 3.3 (b) shows a three dimensional body \( \Omega_2 \), with cross section \( S_2 \) which we consider to be in the state of plane strain. The body force at \( x_1 \in \Omega_1 \) can then be written as

\[
\mathbf{b}_1(x_1) = -\frac{\partial}{\partial x_1} \int_{S_2} \beta_2 \hat{\phi}(r) \, da, \quad \hat{\phi}(r) := \int_{-\infty}^{\infty} \phi(r) \, dz,
\]  

(3.50)

where \( \hat{\phi}(r) \) is the potential we obtain from integration along \( z \), the direction perpendicular to \( S_2 \). An analogous expression follows for \( \mathbf{b}_2 \), the body force in body \( \Omega_2 \). For the potential
\( \phi(r) \) given by eq. (3.6) we find

\[
\hat{\phi}(r) = \pi \epsilon r_0 \left[ \frac{63}{256} \left( \frac{r_0}{r} \right)^{11} - \frac{3}{4} \left( \frac{r_0}{r} \right)^5 \right],
\]

(3.51)

and the corresponding force becomes

\[
\hat{F}(r) = -\frac{\partial \hat{\phi}}{\partial r} = \pi \epsilon \left[ \frac{693}{256} \left( \frac{r_0}{r} \right)^{12} - \frac{15}{4} \left( \frac{r_0}{r} \right)^6 \right].
\]

(3.52)

We note that eqs. (3.51) and (3.52) above give the potential and force between a point and an infinitely long line. The distance \( r = |x_1 - x_2| \) now refers to the closest distance between the point \( x_1 \) and the line through \( x_2 \). A similar analytical integration can be carried out for axi-symmetric problems.

Furthermore if both bodies are considered rigid, with constant density and simple geometry, the interaction potential \( \Pi_C \) can be fully integrated analytically. Examples are given in [16], [41], [46] and [90]. In some cases the integration of \( \Pi_C \) can also be simplified if infinitesimal deformations are assumed. A recent example is given in [101].

The discussion of the following sections applies to both the two-point potential \( \phi \), given by eq. (3.6) and the plane strain potential \( \hat{\phi} \), given by eq. (3.51). Therefore, unless otherwise indicated, whenever we use \( \phi \) we mean both \( \phi \) and \( \hat{\phi} \).

### 3.4 Uniqueness and Stability Considerations

In this section we point out, that the conservative system shown in figure 3.1 and characterized by the potential \( \Pi \), can easily lead to non-uniqueness and instability and that these are inherent physical features of the model. Such behavior can be either caused by \( \Pi_{\text{int}} \), \( \Pi_C \) or their combination \( \Pi \).

An example of the first case, displayed in figure 3.4, is the periodic behavior exhibited by the stored energy function \( W \) of the Cauchy-Born rule (3.41) under the shown shear deformation. This periodicity follows from the fact that the environment of the central atom (shown in black) of the two crystal configurations \( P_a \) and \( P_b \) is identical. Therefore, for such a \( W \), many possible equilibrium configurations are possible. Further, the transition between such states is an unstable process, due to the non-convexity of the energy density \( W \). On the other hand if we only consider a range of deformations where \( W \) is locally convex, unique and stable solutions can be found.

To illustrate the second case, let us examine the ‘aura’ \( \Phi_\ell \) surrounding a rectangular domain \( \Omega_\ell \), as is shown in figure 3.5. The field \( \Phi_\ell \) has four local minima aligned with the sides of the rectangle. If a small, rigid particle is being attracted towards \( \Omega_\ell \) then it may come to rest in any of the four equilibrium positions given by the minima of \( \Phi_\ell \). Within a small neighborhood, these locations are stable since \( \Phi_\ell \) is convex there. On the other hand the field \( \Phi_\ell \) also has four saddle points, which are aligned with the four corners of the rectangle. These are unstable equilibrium positions for the small particle of our thought experiment. In general such minima and saddle points can be associated with asperities on the surface of \( \Omega_\ell \). (The rectangle can be though of a smooth elliptical domain with four pronounced asperities.)
locally convex

Figure 3.4: Periodicity of $W(F)$ arising from the Cauchy-Born rule

![Figure 3.5: ‘Aura’ $\Phi_l$ around a rectangular domain $\Omega_l$: a. 3D view; b. Contour plot](image)

In summary it is seen that both the internal energy $\Pi_{\text{int}}$ and the interaction energy $\Pi_C$ are possible sources of non-uniqueness and instability. When $\Pi_{\text{int}}$ and $\Pi_C$ are combined, the resulting system can be stable or unstable depending on the properties of the system. An example exhibiting unstable behavior is shown in section 5.2.

### 3.5 Normalization of the CGCM

The objective of this section is to derive a normalization scheme of the CGC model and hence identify the characterizing parameters of the model. The formulation of the CGC model can be fully normalized by selecting a reference length $R_0$, a reference energy $E_0$ and a reference mass $M_0$. In the following we examine the normalization of the quasi-static mechanical BVP, where inertia is disregarded, the initial configuration $\varphi_0$ is considered to be in static equilibrium and the initial velocity is considered zero, $V_0 = \mathbf{0}$. To normalize the model we then only need to specify the two reference quantities $R_0$ and $E_0$. The length $R_0$ is chosen from the geometry of a particular problem under investigation, while the energy
$E_0$ is chosen according to the considered constitutive model. $R_0$ is an overall, macroscopic length scale. On the other hand, the interatomic equilibrium spacing $r_0$ of potential $\phi$ (3.6) represents an intrinsic, microscopic length scale. The ratio between these two length scales is defined by

$$\gamma_L := \frac{R_0}{r_0}. \quad (3.53)$$

It is a non-dimensional parameter describing the size of the considered problem. If $\gamma_L = \mathcal{O}(1)$ the geometry is of nanoscale proportions ($\sim 10^{-9}$m and below) and contains only few interacting atoms; as $\gamma_L$ increases the geometry becomes larger and larger, containing more and more atoms. (Values for $\gamma_L < \mathcal{O}(1)$ are not considered here, as the continuum modelling breaks down at some point [62].) We note that in definition (3.53) the equilibrium distance $r_0$ of the intrasolid potential $\phi$ is chosen, since the equilibrium distance $r_\psi$ of the intrasolid potential $\psi$ can be eliminated from the CGC model, as is shown in appendix B. We define the ratio between the two distances as $\gamma_r = r_0/r_\psi$.

The reference energy $E_0$ is chosen based on the internal energy $\Pi_{\text{int}}$ (3.12). If the Neo-Hookean constitutive model (3.33) is used, the stored energy $W$ is proportional to Young’s modulus $E_Y$, which has units of energy density. In view of this proportionality we define

$$W_{\text{int},0} := E_Y, \quad (3.54)$$

as a reference quantity of the internal energy density $W$, and further, in view of integral (3.12) we define a reference quantity of the internal energy $\Pi_{\text{int}}$ as

$$\Pi_{\text{int},0} := W_{\text{int},0}R_0^3. \quad (3.55)$$

For a given deformation, i.e. known $W$, the internal energy $\Pi_{\text{int}}$ scales with the volume. This is reflected by $\Pi_{\text{int},0}$, but which is, contrary to $\Pi_{\text{int}}$, independent of the deformation. We choose $E_0 = \Pi_{\text{int},0} = E_Y R_0^3$ as the normalization parameter of the CGC model. Definitions (3.54) and (3.55) can be adapted to the Cauchy-Born rule by writing $E_Y$, which is now unspecified, as $E_Y := \beta_0 \epsilon_\psi$.

Similar to the internal energy density $W$, discussed above, we define the ‘interaction energy density’

$$W_C := c_0 \beta_0 \phi, \quad (3.56)$$

which is based on the interatomic interaction potential $\phi$ and the atomic reference density $\beta_0$. Here $c_0$ is an arbitrary constant factor, which is introduced to adjust the formulation. In order to normalize the finite element nodal force vector $f_C$, introduced in the next section, the choice $c_0 = \beta_0 r_0^3/\gamma_r$, which is a material constant, is particularly convenient. As an example, for the fcc crystal shown in figure 3.2 (b) we have $c_0 = \sqrt{2} \gamma_r^3$ according to eq. (3.42). The equilibrium energy of the potential $\phi$ is characterized by the material constant $\epsilon_\phi$. With this in mind we further define the reference quantity of $W_C$ as

$$W_{C,0} := c_0 \beta_0 \epsilon_\phi, \quad (3.57)$$

which is a material constant like $W_{\text{int},0}$. Associated with the density $W_C$, is the interaction energy $\Pi_C$ of the two solids $\Omega_1$ and $\Omega_2$ given by eq. (3.9). Due to the rapid decay of $\phi$, the energy $\Pi_C$ only penetrates a distance proportional to $r_0$ into the solids and it therefore scales by $R_0^2 r_0$, i.e. from the macroscopic point of view (for large $\gamma_L$) it scales with the
surface area $R_0^2$ of the bodies, whereas from the microscopic point of view ($\gamma_L = \mathcal{O}(1)$) it scales with the volume $r_0^3$. Depending on the scale, $\Pi_C$ is thus perceived as a surface energy or a bulk energy. In view of this scaling we define the reference value of the interaction energy $\Pi_C$ as

$$\Pi_{C,0} := W_{C,0}R_0^2r_0 = \beta_0^2\epsilon_\phi R_0^2r_0^4 .$$  \hfill (3.58)

Having defined the reference measures $W_{\text{int},0}$ and $W_{C,0}$, we introduce their ratio

$$\gamma_W := \frac{W_{\text{int},0}}{W_{C,0}} = \frac{E_Y}{c_0\beta_0\epsilon_\phi} ,$$  \hfill (3.59)

which is a problem-specific constant since $E_Y$, $\beta_0$ and $\epsilon_\phi$ are material constants. If the Cauchy-Born rule is used we further have $\gamma_W = \epsilon_\psi/(c_0\epsilon_\phi)$, which is proportional to the ratio $\gamma_\epsilon = \epsilon_\psi/\epsilon_\phi$. With $\gamma_L$ (3.53) and $\gamma_W$ (3.59) we have defined two parameters which control the behavior of the CGC model. The scaling of the model, with respect to $\gamma_L$ and $\gamma_W$ is discussed later in section 7.

Before proceeding, let us comment on some consequences of the definitions above. First, let us define the continuum energy ratio

$$\gamma_{\Pi} := \frac{\Pi_{\text{int},0}}{\Pi_{C,0}} = \gamma_L\gamma_W ,$$  \hfill (3.60)

which increases linearly with the length scale $\gamma_L$, due to the fact that, from the macroscopic viewpoint, $\Pi_{\text{int}}$ increases by the volume whereas $\Pi_C$ increases with the surface area. Secondly, to assess stability one has to look at the stiffness. The deformation of the solids is of the order of $R_0$, whereas the size of the gap changes by the order of $r_0$. It thus follows that the stiffness associated with $\Pi_{\text{int}}$ is characterized by the reference quantity

$$K_{\text{int},0} := \frac{\Pi_{\text{int},0}}{R_0^2} = E_YR_0 ,$$  \hfill (3.61)

which is proportional to the derivative $\frac{\partial^2\Pi_{\text{int},0}}{\partial R_0^2}$, while the stiffness associated with $\Pi_C$ is characterized by the reference quantity

$$K_{C,0} := \frac{\Pi_{C,0}}{r_0^2} = W_{C,0}R_0^2/r_0 ,$$  \hfill (3.62)

which is proportional to the derivative $\frac{\partial^2\Pi_{C,0}}{\partial r_0^2}$. The stiffness ratio between $K_{\text{int},0}$ and $K_{C,0}$ follows as

$$\gamma_K := \frac{K_{\text{int},0}}{K_{C,0}} = \frac{\gamma_W}{\gamma_L} ,$$  \hfill (3.63)

which decreases for increasing length scales $\gamma_L$, due to the fact that, as $\gamma_L$ increases, the intersolid, contact stiffness $K_{C,0}$ increases with respect to the internal, bulk stiffness $K_{\text{int},0}$.

Several aspects of the behavior of the interacting two-body system can be explained by looking at either $K_{\text{int},0}$, $K_{C,0}$ or $\gamma_K$, as is discussed in later sections.

We summarize that we have defined two reference parameters, $R_0$ and $E_0$, to normalize the CGC model, and two scaling parameters, $\gamma_L$ and $\gamma_W$ to investigate the scaling of the model. In the following section the finite element equations are derived and they are normalized as discussed above. In section 7 we study the scaling by means of a simple model problem. We note that a given problem is characterized by relative changes in $\gamma_L$ and $\gamma_W$, their magnitudes, on the other hand, are arbitrary quantities.
4 Finite Element Discretization

This section discusses the implementation of the weak form (3.28) of the Coarse-Grained Contact Model into the finite element method. The emphasis is placed on the treatment of the interaction energy $\Pi_C$, which is the keystone of the proposed contact model. In the discretization and implementation of $\Pi_C$, we have developed three methods which are characterized by an increase in efficiency. For the treatment of the internal, external and inertial contributions to eq. (3.28) we refer to the nonlinear finite element literature, e.g. see [9], [14], [99] and [110].

To discretize the weak form (3.28) the displacement $\mathbf{u} = \mathbf{x} - \mathbf{X}$ and its variation $\delta \varphi$ are approximated by the interpolations

$$\mathbf{u}(x) \approx \sum_{A=1}^{n_{no}} N_A(x) \mathbf{u}_A, \quad \delta \varphi(x) \approx \sum_{A=1}^{n_{no}} N_A(x) \mathbf{v}_A. \quad (4.1)$$

Here $n_{no}$ denotes the total number of interpolation points, also called the finite element nodes, of the two-body system. Further $\mathbf{u}_A$ and $\mathbf{v}_A$ denote the nodal values of fields $\mathbf{u}$ and $\delta \varphi$, and $N_A(x)$ denotes the finite element shape function associated with node $A$. Eq. (4.1) can also be expressed as

$$\mathbf{u}(x) \approx \mathbf{N}(x) \mathbf{u}, \quad \delta \varphi(x) \approx \mathbf{N}(x) \mathbf{v}, \quad (4.2)$$

where $\mathbf{u}$ and $\mathbf{v}$ are global arrays containing all nodal vectors $\mathbf{u}_A$ and $\mathbf{v}_A$, and where $\mathbf{N}$ is a global matrix containing all shape functions $N_A$. In its discretized form, eq. (3.28) can then be written as

$$\mathbf{v}^T [\mathbf{M} \ddot{\mathbf{u}} + \mathbf{f}_{\text{int}} + \mathbf{f}_C - \mathbf{f}_{\text{ext}}] = 0, \quad \forall \mathbf{v}, \quad (4.3)$$

where $\mathbf{M}$ is the mass matrix of the discretized system and $\mathbf{f}_{\text{int}}$, $\mathbf{f}_C$, $\mathbf{f}_{\text{ext}}$ are the nodal force vectors associated with energies $\Pi_{\text{int}}$, $\Pi_C$, $\Pi_{\text{ext}}$. Since the equation above holds for all nodal variations $\mathbf{v}_A$ we obtain the discretized equations of motion

$$\mathbf{M} \ddot{\mathbf{u}} + \mathbf{f}(\mathbf{u}) = 0, \quad \mathbf{f}(\mathbf{u}) = \mathbf{f}_{\text{int}}(\mathbf{u}) + \mathbf{f}_C(\mathbf{u}) - \mathbf{f}_{\text{ext}}. \quad (4.4)$$

For a quasi-static problem we have $\ddot{\mathbf{u}} = 0$ and hence equilibrium is given by the nonlinear equation $\mathbf{f}(\mathbf{u}) = 0$. As such it can only be solved approximately and we shall therefore also denote the nodal force vector $\mathbf{f}$ as the residual. Further, in the absence of external loading, as is considered in the later examples, we have $\mathbf{f}_{\text{int}} + \mathbf{f}_C = 0$, so that the problem becomes a balancing between internal and interaction forces (represented by the potentials $\psi$ and $\phi$). Let us now focus on the computation of the interaction force vector $\mathbf{f}_C$; for a treatment of $\mathbf{f}_{\text{int}}$ and $\mathbf{f}_{\text{ext}}$ see appendix B. To compute $\mathbf{f}_C$, three implementation methods are proposed which are shown in a conceptual overview in figure 4.1. Consider the force $\mathbf{b}_k$ acting at point $\mathbf{x}_k$ and invoked by the presence of neighboring body $\Omega_\ell$. (In the case of two interacting bodies we either have $k = 1$, $\ell = 2$ or $k = 2$, $\ell = 1$.) Due to the cutoff range of the interaction potential $\phi$, the influence at $\mathbf{x}_k$ is restricted to the subdomain $\Omega_\ell(\mathbf{x}_k) \subset \Omega_\ell$, as is shown in figure 4.1 (1). The superposition of these subdomains for all points $\mathbf{x}_k$ yields the region $\Omega_\ell \subset \Omega_\ell$. It follows that we have the ordering $\Omega_\ell(\mathbf{x}_k) \subset \Omega_\ell \subset \Omega_\ell$ and $\partial\Omega_\ell(\mathbf{x}_k) \subset \partial\Omega_\ell \subset \partial\Omega_\ell$. The first implementation which comes to mind is the computation of $\mathbf{b}_k$ by the numerical integration over the volume $\Omega_\ell(\mathbf{x}_k)$ (see frame (1)). We term this approach as 'Method 1'
Figure 4.1: Types of interaction: 1. Volume interaction; 2. Surface interaction; 3. Point interaction

and note that it involves no approximation in the computation of $b_k$ other than the standard finite element interpolation introduced by eq. (4.1). The volume integration of Method 1 can become very costly, which motivates the following two efficient approximations, denoted as ‘Method 2’ and ‘Method 3’, and which are shown in frames (2) and (3). The idea of Method 2 is to map the region $\Omega_k(x_k)$ onto its outer boundary $\partial\Omega_k(x_k)$ and thus reduce the volume interaction to a surface interaction. Method 3 further concentrates the region $\Omega_k(x_k)$ into a single point, the closest projection point $x_P^k$. Depending on the problem, the reduction of the interaction region $\Omega_k(x_k)$ to a surface, or even a point, can lead to a huge gain in efficiency without losing much accuracy, as is demonstrated in the numerical examples of section 5.

Figure 4.1 shows one level of approximation, namely the reduction of the influencing region $\Omega_k$. A second level of approximation is the reduction of domain $\Omega_k$, the region where body forces $b_k$ are invoked. This second level, which is used in both the implementation of Method 2 and 3, is to project all the body forces $b_k$ invoked in the region $\Omega_k$ onto the outer surface $\partial\Omega_k$. This achieves a further increase in efficiency as the volume integration over $\Omega_k$ is reduced to a surface integration over $\partial\Omega_k$. We note that Method 2 and 3 are constructed such that they apply to arbitrarily shaped bodies $\Omega_k$ and $\Omega_{\ell}$. Let us now derive the three methods in detail.

### 4.1 Volume Interaction: Method 1

Let us first discuss the straightforward implementation according to the volume interaction method. Consider the interaction potential $\Pi_C$ and its variation given in eqs. (3.9) and (3.16). Applying approximation (4.2)$_2$ to eq. (3.16) we obtain

$$\delta\Pi_C \approx v^T f_C = v_1^T f_{C,1} + v_2^T f_{C,2}$$

$$= v_1^T \int_{\Omega_1} \int_{\Omega_2} N_1^T \beta_1 \beta_2 \frac{\partial \phi}{\partial x_1} \, dv_2 \, dv_1 + v_2^T \int_{\Omega_1} \int_{\Omega_2} N_2^T \beta_1 \beta_2 \frac{\partial \phi}{\partial x_2} \, dv_2 \, dv_1 ,$$

where $v_1$, $v_2$ and $N_1$, $N_2$ are the variations and shape functions associated with bodies $\Omega_1$ and $\Omega_2$. The arrays $f_{C,1}$ and $f_{C,2}$ are the global force vectors acting on the two bodies.
As is characteristic of the finite element method, the integration of eq. (4.5) is broken into small subdomains or elements. To compute (4.5) on the elemental level consider an element \( \Omega_i^e \) interacting with an element \( \Omega_j^e \) as displayed in figure 4.2 (a). According to expression (4.5), the interaction between the two elements \( \Omega_i^e \) and \( \Omega_j^e \) yields the elemental force vectors
\[
f_{C,i} = \int_{\Omega_i^e} \int_{\Omega_j^e} \mathbf{N}_i^T \beta_i \beta_j \frac{\partial \phi}{\partial \mathbf{x}_i} \, dv_j \, dv_i , \quad f_{C,j} = \int_{\Omega_i^e} \int_{\Omega_j^e} \mathbf{N}_j^T \beta_i \beta_j \frac{\partial \phi}{\partial \mathbf{x}_j} \, dv_j \, dv_i . \tag{4.6}
\]

Here \( f_{C,i} \) corresponds to the nodal forces acting on element \( \Omega_i^e \) due to the influence of element \( \Omega_j^e \), whereas \( f_{C,j} \) is the nodal force vector acting on \( \Omega_j^e \) due to the presence of element \( \Omega_i^e \). It is noted that here and subsequently indices \( i \) and \( j \) correspond to the two elements \( \Omega_i^e \) and \( \Omega_j^e \), and are not summed upon. In eq. (4.6) \( \beta_i \) and \( \beta_j \) correspond to the current densities at \( \mathbf{x}_i \) and \( \mathbf{x}_j \), while \( \mathbf{N}_i \) and \( \mathbf{N}_j \) are arrays containing the shape functions of element \( \Omega_i^e \) and \( \Omega_j^e \). Both \( \mathbf{N}_i \) and \( \mathbf{N}_j \) have the form
\[
\mathbf{N} = [ \begin{bmatrix} N_1 \mathbf{I} & N_2 \mathbf{I} & \ldots & N_n \mathbf{I} \end{bmatrix} ] , \tag{4.7}
\]
where \( n \) is the number of nodes per element and where \( \mathbf{I} \) is identity tensor in \( \mathbb{R}^3 \). Further, as has been noted in eq. (3.20), we have
\[
\frac{\partial \phi}{\partial \mathbf{x}_i} = -F(r) \, \bar{r} , \quad \frac{\partial \phi}{\partial \mathbf{x}_j} = F(r) \, \bar{r} , \tag{4.8}
\]
for
\[
\bar{r} = \frac{r}{r} , \quad r = \mathbf{x}_i - \mathbf{x}_j , \quad r = |r| . \tag{4.9}
\]
The total force, denoted as \( \mathbf{f}_{C,i}^e \), acting on element \( \Omega_i^e \) \( \in \Omega_2 \) due to the entire neighboring body \( \Omega_2 \) is given by the sum of the contribution \( \mathbf{f}_{C,i} \) over all elements \( \Omega_j^e \) which influence \( \Omega_i^e \), i.e. elements \( \Omega_j^e \) which lie within the influencing region \( \Omega_2(\Omega_i^e) \). Likewise to obtain \( \mathbf{f}_{C,j}^e \), the total force acting on element \( \Omega_j^e \) due to the presence of body \( \Omega_1 \), we sum over all elements \( \Omega_i^e \) \( \in \Omega_1(\Omega_j^e) \). That is, we have
\[
\mathbf{f}_{C,i}^e = \sum_{\Omega_j^e \in \Omega_2(\Omega_i^e)} \mathbf{f}_{C,i} , \quad \mathbf{f}_{C,j}^e = \sum_{\Omega_i^e \in \Omega_1(\Omega_j^e)} \mathbf{f}_{C,j} . \tag{4.10}
\]
To employ Newton’s method to solve the resulting nonlinear equation associated with eq. (4.4) we require the tangent or stiffness matrix corresponding to \( \Pi_C \). Linearizing \( f_{C,i} \) with respect to the degrees of freedom (dofs) of element \( \Omega_i^e \) and \( \Omega_j^e \) gives the two contributions

\[
k_{C,ii} = \int_{\Omega_i^e} \int_{\Omega_i^e} N_i^T \beta_i \beta_j \frac{\partial^2 \phi}{\partial x_i \partial x_j} N_j \, dv_j \, dv_i ,
\]

\[
k_{C,ij} = \int_{\Omega_i^e} \int_{\Omega_j^e} N_i^T \beta_i \beta_j \frac{\partial^2 \phi}{\partial x_i \partial x_j} N_j \, dv_j \, dv_i ,
\]

(4.11)

while the linearization of \( f_{C,j} \) with respect to the dofs of element \( \Omega_i^e \) and \( \Omega_j^e \) yields

\[
k_{C,ji} = k_{C,ij}^T ,
\]

\[
k_{C,jj} = \int_{\Omega_i^e} \int_{\Omega_j^e} N_i^T \beta_i \beta_j \frac{\partial^2 \phi}{\partial x_i \partial x_j} N_j \, dv_j \, dv_i .
\]

(4.12)

Here, the mixed derivatives can be found as

\[
\frac{\partial^2 \phi(r)}{\partial x_i \partial x_j} = \frac{F(r)}{r} I + \left[ F'(r) - \frac{F(r)}{r} \right] \bar{r} \otimes \bar{r} ,
\]

\[
\frac{\partial^2 \phi(r)}{\partial x_i \partial x_i} = - \frac{\partial^2 \phi(r)}{\partial x_i \partial x_j} = \frac{\partial^2 \phi(r)}{\partial x_j \partial x_i} .
\]

(4.13)

It is noted that in the linearization as well as in the implementation, expressions (4.6), (4.11) and (4.12) can be easily rewritten as integrals over the reference configuration of elements \( \Omega_i^e \) and \( \Omega_j^e \) by using identity (3.5). Further, the total stiffness matrices \( k_{C,ii}^e \) and \( k_{C,jj}^e \), arising from the interaction between element \( \Omega_i^e \) and body \( \Omega_2 \), and between element \( \Omega_j^e \) and body \( \Omega_1 \), are obtained by the summation

\[
k_{C,ii}^e = \sum_{\Omega_i^e \in \Omega_2} k_{C,ii} , \quad k_{C,jj}^e = \sum_{\Omega_j^e \in \Omega_1} k_{C,jj} ,
\]

(4.14)

just as seen in eq. (4.10). No summation occurs for the off-diagonal contribution \( k_{C,ij} \), and we can write \( k_{C,ij}^e = k_{C,ij} \). The global force vector \( f_C \) and associated global stiffness matrix \( K_C \) is obtained from the assembly of all contributions \( f_{C,i}^e, f_{C,j}^e, k_{C,ii}^e, k_{C,ij}^e, k_{C,ji}^e, k_{C,jj}^e \) of all elements \( \Omega_i^e \in \Omega_1 \) and \( \Omega_j^e \in \Omega_2 \). Due to the property \( k_{C,ji} = k_{C,ij}^T \), the global stiffness matrix is symmetric, as it should be, since we are considering a conservative system. The elemental assembly is discussed in appendix B.

We note that, if for both bodies \( \Omega_k(x_k) = \Omega_k, \forall x_k \in \Omega_k \), i.e., if every point in one body is influenced by every point within the other body, the resulting global stiffness matrix will be completely dense and the solution procedure will be very costly. However, for the applications envisioned here, \( \Omega_1(x_2) \) and \( \Omega_2(x_1) \) are substantially smaller than the entire domains \( \Omega_1 \) and \( \Omega_2 \), and so the global stiffness matrix retains its sparsity. Nevertheless the double volume integration of Method 1 can cause substantial computational cost, as is illustrated by the examples in section 5.4.
Symmetry Considerations

Let us briefly look at the case when the problem under consideration is symmetric and we wish to exploit this symmetry by modelling only half of the system. The case is illustrated in figure 4.2 (b). Even when modelling only half of the system we must still account for the fact that the interaction reaches across the plane of symmetry. In other words the generic points $x_i$ and $x_j$ not only interact with each other, but also interact with the mirror images $x_{j'}$ and $x_{j'}$. The plane upon which the system can be reflected is defined by the vectors $c$ and $n_r$. The reflection $x_{k'}$ of any point $x_k$ ($k = i, j$) can then be written as

$$x_{k'} = Q x_k + c,$$

with the reflection $Q$ and the constant $c$ given by

$$Q = I - 2 n_r \otimes n_r, \quad c = c_0 n_r.$$

Now, an element $\Omega_i^e$ of $\Omega_1$ (where $\Omega_1$ is half of body 1 as shown in figure 4.2 (b)) is influenced by both element $\Omega_j^e$ (of $\Omega_2$) and its reflection $\Omega_{j'}^e$. Likewise $\Omega_j^e$ is influence both by $\Omega_i^e$ and its reflection $\Omega_{i'}^e$. As an example the interaction force contribution of element $\Omega_i^e$ due to the presence of $\Omega_j^e$ can be written, similarly to eq. (4.6), as

$$f_{C,i'} = \int_{\Omega_i^e} \int_{\Omega_j^e} N_i^T \beta_i \beta_j \frac{\partial \phi(r_{j'})}{\partial x_i} \, dv \, dv, \quad \text{with} \quad \frac{\partial \phi(r_{j'})}{\partial x_i} = -F(r_{j'}) \, \tilde{r}_{j'}',$$

and where we have defined

$$r_{j'} = x_i - x_{j'}, \quad r_{j'} = |r_{j'}|, \quad \tilde{r}_{j'} = \frac{r_{j'}}{r_{j'}},$$

analogously to eq. (4.9). We note that the integration domain $\Omega_j^e$ can be mapped onto $\Omega_j^e$ using eq. (4.15). The stiffness matrix contributions associated with $f_{C,i'}$ are

$$k_{C,i'} = \int_{\Omega_i^e} \int_{\Omega_j^e} N_i^T \beta_i \beta_j \frac{\partial^2 \phi(r_{j'})}{\partial x_i \partial x_i} N_j^T \, dv \, dv,$$

$$k_{C,i'} = \int_{\Omega_i^e} \int_{\Omega_j^e} N_i^T \beta_i \beta_j \frac{\partial^2 \phi(r_{j'})}{\partial x_i \partial x_j} N_j^T \, dv \, dv.$$

with

$$\frac{\partial^2 \phi(r_{j'})}{\partial x_i \partial x_i} = -F(r_{j'}) I - \left[ F'(r_{j'}) - \frac{F(r_{j'})}{r_{j'}} \right] \tilde{r}_{j'} \otimes \tilde{r}_{j'},$$

$$\frac{\partial^2 \phi(r_{j'})}{\partial x_i \partial x_j} = \frac{\partial^2 \phi(r_{j'})}{\partial x_i \partial x_j} \frac{\partial x_{j'}}{\partial x_i} \frac{\partial x_{j'}}{\partial x_j} = -\frac{\partial^2 \phi(r_{j'})}{\partial x_i \partial x_i} Q.$$

It can be shown that the global stiffness matrix $K_C$ is still symmetric.

### 4.2 Surface Interaction: Method 2

Let us now discuss the the surface interaction method. Method 2 is motivated as an efficient approximation to Method 1 discussed in the previous section. To derive the method let us
first consider the case of plane strain, and let $\Omega_I \in \mathbb{R}^2$, for $I = 1, 2$, now refer to the plane strain cross section of the two bodies. According to figure 4.3 the volume elements of the two bodies can be expressed as

$$dv_1 = \frac{r}{r_s} dr \cos \alpha_1 da_1, \quad dv_2 = \frac{\tilde{r}}{r_s} d\tilde{r} \cos \alpha_2 da_2,$$

(4.21)

with $\cos \alpha_1 = -\hat{r} \cdot \vec{n}_1$ and $\cos \alpha_2 = \hat{r} \cdot \vec{n}_2$. Keeping $x_2$ fixed, the integration over $\Omega_1$ can then be written as

$$\int_{\Omega_1} ... dv_1 = \int_{\partial \Omega_1} \frac{1}{r_s} \int_{r_s}^{r_c} r ... dr \cos \alpha_1 da_1,$$

(4.22)

where $r_c$ is the cutoff radius associated with $\phi(r)$. The integration scheme is valid for arbitrary $r_c$ and we can set $r_c \to \infty$ for convenience. Integrating (4.22) over $\Omega_2$ we further obtain

$$\int_{\Omega_2} \int_{\Omega_1} ... dv_1 dv_2 = \int_{\partial \Omega_2} \int_{\partial \Omega_1} \frac{1}{r_s} \int_{r_s}^{r_c} r ... dr d\tilde{r} \cos \alpha_1 da_1 \cos \alpha_2 da_2.$$

(4.23)

Here it is noted that on the right hand side, the order of the surface integration can be switched, just as the volume integration on the left hand side is exchangeable. In the expressions above, $r_s$ is the distance between the two surface points $x_{s1}$ and $x_{s2}$, and we can thus define the unit direction $\tilde{r}_s$ as

$$\tilde{r}_s = \frac{r_s}{r_s} , \quad r_s = x_{s1} - x_{s2} , \quad r_s = |r_s|.$$

(4.24)

similar to definition (4.9). It is noted that $\tilde{r}_s = \hat{r}$. Let us now apply the integration rule (4.23) to the variation of $\Pi_C$ (3.16) to obtain

$$\delta \Pi_C = \int_{\partial \Omega_1} \int_{\partial \Omega_2} \frac{1}{r_s} \int_{r_s}^{r_c} \int_{r_s}^{r_c} \beta_1 \beta_2 \hat{r} \cdot \delta \varphi_1 \cdot \frac{\partial \phi(\hat{r})}{\partial x_1} dr d\tilde{r} \cos \alpha_1 \cos \alpha_2 da_1 da_2$$

$$+ \int_{\partial \Omega_1} \int_{\partial \Omega_2} \frac{1}{r_s} \int_{r_s}^{r_c} \int_{r_s}^{r_c} \beta_1 \beta_2 \hat{r} \cdot \delta \varphi_2 \cdot \frac{\partial \phi(\hat{r})}{\partial x_2} dr d\tilde{r} \cos \alpha_1 \cos \alpha_2 da_1 da_2.$$

(4.25)

Method 2 aims to simplify this expression by solving the inner two integrals (over $r$ and $\tilde{r}_s$) approximately. We therefore assume the densities $\beta_1$ and $\beta_2$, and chose the variations
\( \delta \varphi_1 \) and \( \delta \varphi_2 \), as constant along direction \( r \), so that they can all be pulled out of the inner integrals. With the help of eqs. (3.20) and (4.2) we thus obtain

\[
\delta \Pi_c \approx v^T_1 f_{c,1} + v^T_2 f_{c,2} = -v^T_1 \int_{\partial \Omega_1} \int_{\partial \Omega_2} N^T_1 \beta \beta_2 F_s(r_s) \tilde{r}_s \cos \alpha_1 \cos \alpha_2 \, da_1 \, da_2
\]

\[
+ v^T_2 \int_{\partial \Omega_1} \int_{\partial \Omega_2} N^T_2 \beta \beta_2 F_s(r_s) \tilde{r}_s \cos \alpha_1 \cos \alpha_2 \, da_1 \, da_2,
\]

(4.26)

where we have defined the force

\[
F_s(r_s) := \lim_{r_c \to \infty} \frac{1}{r_s} \int_{r_s}^{r_c} \int_{\tilde{r}_s}^{r} r \, F(r) \, dr \, d\tilde{r}_s,
\]

(4.27)

which governs the interaction between the two surface points \( x_{s1} \) and \( x_{s2} \). There are good reasons for the approximation introduced above: If the deformation within the bodies is homogeneous, it can be characterized by the surface quantities alone, so that approximation (4.26) becomes exact. Even when the deformation is strongly varying, the approximation can still be very good, namely when it is nearly homogenous within the effective cutoff range \( r_c \). The accuracy of this approximation therefore hinges on the rapid decay of \( F(r) \) and it is the combination of this decay with the variation of the deformation which determines the validity of the approximation. Its accuracy can be assessed by comparing Method 2 with Method 1, as is done in section 5, or by an analytical comparison, which is considered in section 6. The accuracy is expected to yield good results in the following two cases: during long range attraction, when the deformation is usually very small, and during short range repulsion of large scale bodies, where \( r_c \) is very small compared to the problem size.

In expression (4.26), \( f_{c,1} \) and \( f_{c,2} \) are the global force vectors acting on the surface of the two bodies. On the elemental level, the interaction occurs between the finite elements discretizing surfaces \( \partial \Omega_1 \) and \( \partial \Omega_2 \). Corresponding to eq. (4.26) we thus have the force vectors

\[
f_{c,i} = -\int_{\Gamma_i} \int_{\Gamma_j} N^T_i \beta \beta_j F_s(r_s) \tilde{r}_s \cos \alpha_1 \cos \alpha_j \, da_j \, da_i,
\]

\[
f_{c,j} = +\int_{\Gamma_i} \int_{\Gamma_j} N^T_j \beta \beta_i F_s(r_s) \tilde{r}_s \cos \alpha_1 \cos \alpha_j \, da_j \, da_i,
\]

(4.28)

acting on the two surface elements \( \Gamma_i \in \partial \Omega_1 \) and \( \Gamma_j \in \partial \Omega_2 \). Here, \( N_i \) (and likewise \( N_j \)) is the matrix containing the shape functions of element \( \Gamma_i \) (or \( \Gamma_j \)) written in the form (4.7).

The merit of Method 2 is to integrate \( F_s(r_s) \) (4.27) analytically. Since we are considering the case of plane strain here, the force function \( F \) is given by \( F(r) \) (3.52) and we thus have

\[
F_s(r_s) = \pi \varepsilon r_0^2 \left[ \frac{77}{2560} \left( \frac{r_0}{r_s} \right)^{10} - \frac{5}{16} \left( \frac{r_0}{r_s} \right)^4 \right].
\]

(4.29)

From the numerical viewpoint we have thus reduced the volume integration of eq. (4.6) to the surface integration of eq. (4.28), which can yield a huge gain in efficiency as is shown in the numerical examples of section 5. We remark that in eq. (4.28) we can replace the cosine terms by \( \cos \alpha_i = -\tilde{r}_s \cdot n_i \) and \( \cos \alpha_j = \tilde{r}_s \cdot n_j \), where \( n_i \) and \( n_j \) are the outward normals of the current surface elements \( \Gamma_i \) and \( \Gamma_j \).

To implement and linearize integrals (4.28), it is convenient to pull them back to the undeformed, reference configurations \( \Omega_{10} \) and \( \Omega_{20} \). This is achieved by using Nanson's formula

\[
n \, da = JF^{-T} N \, dA,
\]

(4.30)
where $\mathbf{N} \, dA$ is the oriented surface element in the reference configuration. (The surface normal $\mathbf{N}$ should not be confused with the shape function array $\mathbf{N}$.) The spatial integrals (4.28) can then be expressed as the material integrals

$$
\mathbf{f}_{C,i} = - \int_{\Gamma^e_{i0}} \int_{\Gamma^e_{j0}} \mathbf{N}_i^T \beta_{i0} \beta_{j0} \mathbf{F}_s(r_s) \mathbf{r}_s \, dA_j \, dA_i ,
$$

$$
\mathbf{f}_{C,j} = + \int_{\Gamma^e_{i0}} \int_{\Gamma^e_{j0}} \mathbf{N}_j^T \beta_{i0} \beta_{j0} \mathbf{F}_s(r_s) \mathbf{r}_s \, dA_i \, dA_j ,
$$

(4.31)

where $\Gamma^e_{i0}, \Gamma^e_{j0}$ and $\beta_{i0}, \beta_{j0}$ are referential quantities corresponding to the spatial counterparts $\Gamma^e_i, \Gamma^e_j$ and $\beta_i, \beta_j$. To simplify the notation we have introduced the two scalars

$$
\theta_i := \mathbf{r}_s \cdot \mathbf{F}_i^{-T} \mathbf{N}_i , \quad \theta_j := \mathbf{r}_s \cdot \mathbf{F}_j^{-T} \mathbf{N}_j ,
$$

(4.32)

where $\mathbf{F}_i, \mathbf{F}_j$ and $\mathbf{N}_i, \mathbf{N}_j$ are the deformation gradients and outward normals of elements $\Gamma^e_i$ and $\Gamma^e_j$. It is noted that the linearization of eq. (4.31) is considerably complicated by the factors $\theta_i$ and $\theta_j$. To simplify the linearization one may ignore the contribution arising from $\theta_i \theta_j$, and thus obtain an approximate tangent. Such an approximation is believed to be very good, since the main variation of eq. (4.31) is caused by $\mathbf{F}_s(r_s)$ rather than $\theta_i \theta_j$.

Let us now consider the linearization of the forces $\mathbf{f}_{C,i}$ and $\mathbf{f}_{C,j}$ (4.31) with respect to the degrees of freedom of the two elements $\Gamma^e_i$ and $\Gamma^e_j$ for fixed $\theta_i \theta_j$. This yields the four stiffness contributions (expressed as integrals over the current configuration)

$$
k_{C,ii} = - \int_{\Gamma^e_i} \int_{\Gamma^e_j} \mathbf{N}_i^T \beta_i \beta_i \frac{\partial (\mathbf{F}_s \mathbf{r}_s)}{\partial \mathbf{x}_i} \mathbf{N}_i \cos \alpha_i \cos \alpha_j \, dA_j \, dA_i ,
$$

$$
k_{C,ij} = - \int_{\Gamma^e_i} \int_{\Gamma^e_j} \mathbf{N}_i^T \beta_i \beta_j \frac{\partial (\mathbf{F}_s \mathbf{r}_s)}{\partial \mathbf{x}_j} \mathbf{N}_j \cos \alpha_i \cos \alpha_j \, dA_j \, dA_i ,
$$

$$
k_{C,ji} = \int_{\Gamma^e_i} \int_{\Gamma^e_j} \mathbf{N}_j^T \beta_i \beta_j \frac{\partial (\mathbf{F}_s \mathbf{r}_s)}{\partial \mathbf{x}_i} \mathbf{N}_j \cos \alpha_i \cos \alpha_j \, dA_j \, dA_i ,
$$

$$
k_{C,jj} = + \int_{\Gamma^e_i} \int_{\Gamma^e_j} \mathbf{N}_j^T \beta_j \beta_j \frac{\partial (\mathbf{F}_s \mathbf{r}_s)}{\partial \mathbf{x}_j} \mathbf{N}_j \cos \alpha_i \cos \alpha_j \, dA_j \, dA_i ,
$$

(4.33)

with the derivatives

$$
\frac{\partial (\mathbf{F}_s \mathbf{r}_s)}{\partial \mathbf{x}_i} = \frac{\mathbf{F}_s(r_s)}{r_s} \mathbf{I} + \left[ \frac{\mathbf{F}_s'(r_s)}{r_s} - \frac{\mathbf{F}_s(r_s)}{r_s} \right] \mathbf{r}_s \otimes \mathbf{r}_s ,
$$

$$
\frac{\partial (\mathbf{F}_s \mathbf{r}_s)}{\partial \mathbf{x}_j} = - \frac{\partial (\mathbf{F}_s \mathbf{r}_s)}{\partial \mathbf{x}_i} .
$$

(4.34)

It is noted that the arrays listed in (4.28) and (4.33) characterize the interaction between single surface elements. To obtain the interaction due to the entire surfaces, an analogous summation scheme as given in eqs. (4.10) and (4.14) is required.

We remind that Method 2 is only accurate if the deformation of the interaction zones $\bar{\Omega}_1(\mathbf{x}_2)$ and $\bar{\Omega}_2(\mathbf{x}_1)$, and thus the densities $\beta_1$ and $\beta_2$, are approximately constant along $r$. This is appropriate when the cutoff radius of $F(r)$ is very short compared to the distance over which the deformation of the body varies. Numerically, Method 2 thus reduces the volume integration to a surface integration. We can say that the interaction of the two bodies is mapped onto their surfaces. In the context of infinitesimal deformations, a similar procedure has been derived in [1] and [47].
Moreover, Method 2 can also be seen as an independent physical method to discretize eq. (3.29), i.e. the case for which the interactions are physically restricted to the surfaces. If the cosine terms are dropped and \( \bar{\beta}_i \bar{\beta}_j F_{ij} \) is replaced by \( \bar{\beta}_i \bar{\beta}_j \tilde{F} \), then eqs. (4.28) and (4.33) correspond to the discretization of the surface interaction formulation given by eq. (3.29). As a concluding remark we note that for cases other than plane strain, equations (4.28), (4.31) and (4.33) are still valid. The force function \( F_s \) (4.29), and its definition (4.27), however, will change.

### 4.3 Point Interaction: Method 3

Method 3 takes the analytical integration another step further. Consider the body force formulation of eq. (3.18). Let us rewrite this as

\[
\mathbf{b}_k(x_k) = -\frac{\partial \Phi_\ell}{\partial x_k}, \quad \Phi_\ell = \int_{\Omega_\ell} \beta_\ell \phi(r) \, dv ,
\]

for a point \( x_k \in \Omega_k \) influenced by the body \( \Omega_\ell \), as is illustrated in figure 4.4 (a). Here we have either \( \Omega_k = \Omega_1, \Omega_\ell = \Omega_2 \) or \( \Omega_k = \Omega_2, \Omega_\ell = \Omega_1 \). Let us now suppose that the curvature of surface \( \partial \Omega_\ell \) is much smaller than the curvature of the cutoff radius \( r_c \). We can then argue

Figure 4.4: Method 3: a. Approximating \( \Omega_\ell \) by a flat half-space; b. Closest point projection

that, from the point of view of \( x_k \), the body \( \Omega_\ell \) can be approximated by a flat half-space (shown hatched in frame (a)) located at the closest point projection, \( x_k^P \), of \( x_k \) onto \( \partial \Omega_\ell \) and sharing the same tangent plane with \( \partial \Omega_\ell \) at \( x_k^P \). The field \( \Phi_\ell \) then follows by analytical integration of the half-space as

\[
\Phi_\ell = \int_{\Omega_\ell} \beta_\ell \phi dv_\ell = \pi \beta_\ell \epsilon r_0^3 \left[ \frac{1}{45} \left( \frac{r_0}{r_k^P} \right)^9 - \frac{1}{3} \left( \frac{r_0}{r_k^P} \right)^3 \right] .
\]

Here, it is noted that \( \beta_\ell \) is assumed constant so that in can be pulled out of the integration. However, since \( \beta_\ell \) is the current density of \( \Omega_\ell \), the field \( \Phi_\ell \) still depends on the deformation of body \( \Omega_\ell \). We note that, in a more refined version of Method 3, we can include the principal curvatures of surface \( \partial \Omega_\ell \), for example by modelling \( \Omega_\ell \) as an ellipsoid. To evaluate (4.36) we need to determine the distance \( r_k^P \) between points \( x_k^P \) and \( x_k \). The projection of \( x_k \) onto
$x^P_k$ is shown in frame (b) for the case where $\partial \Omega_\ell$ is discretized by linear, two-node elements $\Gamma^e_\ell$ (e.g. for plane strain or axi-symmetry cases). For this particular case the projection point of $x_k$ is obtained as

$$x^P_k = N^a_\ell (\xi^P_k) x^a_k + N^b_\ell (\xi^P_k) x^b_k ,$$

(4.37)

where $N^a_\ell$ and $N^b_\ell$ are the two linear shape functions of nodes $x^a_\ell$ and $x^b_\ell$ of element $\Gamma^e_\ell$, and where $\xi^P_k$ is the location of $x^P_k$ along this element. It is given by

$$\xi^P_k = \frac{(x^b_\ell - x^a_\ell) \cdot (2x^P_k - x^a_\ell - x^b_\ell)}{(x^b_\ell - x^a_\ell) \cdot (x^b_\ell - x^a_\ell)} .$$

(4.38)

To derive the elemental FE force vector $f_C$ and its associated stiffness matrix, let us define two normalized vectors – along the projection and along the surface element – in the usual way, i.e.

$$\vec{r}^P_k = \frac{r^P_k}{r^P_k} , \quad r^P_k = x^P_k - x_k , \quad r^P_k = |r^P_k| ,$$

(4.39)

$$\vec{r}^{ab}_\ell = \frac{r^{ab}_\ell}{r^{ab}_\ell} , \quad r^{ab}_\ell = x^b_\ell - x^a_\ell , \quad r^{ab}_\ell = |r^{ab}_\ell| .$$

(4.40)

It is noted that we have $\vec{r}^P_k = -\mathbf{n}_\ell$ here. In view of definitions (4.39) we can rewrite eq. (4.35) as

$$b_k(x_k) = - \frac{\partial \Phi_\ell (r^P_k)}{\partial x_k} = - \frac{\partial \Phi_\ell}{\partial r^P_\ell} \frac{\partial r^P_\ell}{\partial x_k} = - F_\ell (r^P_k) \vec{r}^P_k .$$

(4.41)

where we have $\frac{\partial r^P_\ell}{\partial x_k} = - r^P_k$ and where the force $F_\ell := - \frac{\partial \Phi_\ell}{\partial r^P_\ell}$ follows readily from eq. (4.36). The contribution to the variation $\delta \Pi_C$, due to the body forces $b_k$ inside $\Omega_k$, is

$$\delta \Pi_{C,k} = - \int_{\Omega_k} \delta \varphi_k \cdot \beta_k b_k \, dv_k ,$$

(4.42)

according to formulation (3.16). Compared to eq. (3.16), we have thus reduced the double volume integration to a single volume integration, since $b_k$ is now given by the closed form expressions (4.40) and (4.36). As a further simplification we reduce the remaining volume integration over $\Omega_k$ to a surface integration over $\partial \Omega_k$ by writing

$$\int_{\Omega_k} \ldots \, dv_k = \int_{\partial \Omega_k} \int_{r^c_\ell} \ldots \, dr \, \cos \alpha_k \, da_k ,$$

(4.43)

where we have $\cos \alpha_k = \vec{r}^P_k \cdot \mathbf{n}_k = - \mathbf{n}_\ell \cdot \mathbf{n}_k$ according to figure 4.4 (a). Reduction (4.42) is somewhat similar to procedure (4.23) considered in Method 2. As in Method 2, we consider $\delta \varphi_k$ and $\beta_k$ constant along $\vec{r}^P_k$ so that eq. (4.42) becomes

$$\delta \Pi_{C,k} = \int_{\partial \Omega_k} \delta \varphi_k \cdot \beta_k F_S(r_S) \, \vec{r}^P_k \, \cos \alpha_k \, da_k ,$$

(4.43)

where

$$F_S(r_S) := \lim_{r_S \to -\infty} \int_{r_S}^{r^c_\ell} F_\ell(r) \, dr .$$

(4.44)
is the force function obtained by projecting \( F_\ell \) onto the surface \( \partial \Omega_k \). Here \( r_S \) denotes the distance between \( x_k^P \) and \( \partial \Omega_k \). In view of eq. (4.43) and FE interpolation (4.2), it becomes clear that the elemental force vector of surface element \( \Gamma_k^e \in \partial \Omega_k \) can be written as

\[
f_{C,k}^e = \int_{\Gamma_k^e} N_k^T \beta_k F_S(r_S) \hat{r}_k^P \cos \alpha_k \, da_k ,
\]

where \( N_k \) is the array of the FE shape functions of element \( \Gamma_k^e \). This array has the form of eq. (4.7). Eq. (4.44) can be evaluated analytically and we find

\[
F_S(r_S) = \Phi_\ell(r_S) = \pi \beta_\ell \epsilon r_0^3 \left[ \frac{1}{45} \left( \frac{r_0}{r_S} \right)^9 - \frac{1}{3} \left( \frac{r_0}{r_S} \right)^3 \right] ,
\]

since \( F_\ell(r) = \frac{\partial \Phi_\ell(r)}{\partial r} \). We note that operation (4.44) corresponds to the projection of the body forces \( b_k \), invoked within \( \Omega_k \), onto the surface \( \partial \Omega_k \). Such an approach is motivated by the fact that the region \( \Omega_k \) is usually very thin compared to the problem size. However, one may wish to circumvent this approximation and discretize eq. (4.41) directly. Using Nanson’s formula (4.30), integral (4.45) can be mapped back to the reference configuration giving

\[
f_{C,k}^e = \int_{\Gamma_k^e} N_k^T \beta_{k0} F_S(r_S) \hat{r}_k^P \cos \theta_k \, dA_k ,
\]

where \( \theta_k = \hat{r}_k^P \cdot F_k^{-T} N_k \). Note that \( F_S \) contains the current density \( \beta_\ell = \beta_{\ell0}/J_\ell \). To employ Newton’s method to solve (4.4), expression (4.47) needs to be linearized with respect to the degrees of freedom of surface elements \( \Gamma_k^e \) and \( \Gamma_\ell^e \). For now let us consider \( \theta_k \) and \( J_\ell \) as fixed. This is justifiable since the major change in \( f_{C,k}^e \) is caused by the force \( F_S \). The elemental stiffness matrices we thus obtain are

\[
k_{C,k,k}^e = \int_{\Gamma_k^e} N_k^T \beta_k \frac{\partial (F_S \hat{r}_k^P)}{\partial x_k} N_k \cos \alpha_k \, da_k ,
\]

\[
k_{C,k,\ell}^e = \int_{\Gamma_k^e} N_k^T \beta_k \left[ A \ N_\ell (\xi_k^P) + B \right] \cos \alpha_k \, da_k ,
\]

with

\[
\frac{\partial (F_S \hat{r}_k^P)}{\partial x_k} = -F_s^{\prime} \hat{r}_k^P \otimes \hat{r}_k^P ,
\]

\[
A := -\frac{\partial (F_S \hat{r}_k^P)}{\partial x_k} ,
\]

\[
B := \frac{F_S}{r_k^{ab}} \hat{r}_k^{ab} \otimes \hat{r}_k^P \left[ I , -I \right] ,
\]

and where the integration has been mapped back to the spatial configuration. Here \( I \) is the identity matrix in \( \mathbb{R}^2 \). We remark that the above procedure applies to all surface elements \( \Gamma_k^e \in \partial \Omega_1 \) and \( \Gamma_\ell^e \in \partial \Omega_2 \). From the general arrangement of the two surfaces \( \partial \Omega_1 \) and \( \partial \Omega_2 \), it becomes apparent that the projection points \( x_1^P \), of \( x_1 \) onto \( \partial \Omega_2 \), and \( x_2^P \), of \( x_2 \) onto \( \partial \Omega_1 \), are independent of each other. Therefore the assembled stiffness matrix \( K_C \) in general, will no longer be symmetric as was the case in Method 1 and Method 2. This asymmetry has also been noted in [105]. It can be observed numerically, however, that the stiffness contribution \( K_C \) (as well as the entire stiffness matrix \( K \)) becomes symmetric at
equilibrium, i.e. when Newton’s method has converged to zero residual \( f = 0 \).

Since Method 3 takes a similar approach as conventional macroscale computational contact mechanics, it provides a natural transition between the Coarse-Grained Contact Model and the former. We note that Method 3 is particularly easy to implement if one body is rigid and has simple geometry. Two such examples are the interaction with a rigid flat half-space, considered in sections 4.4 and 8.1, and the interaction with a rigid asperity, considered in section 8.3. We conclude Method 3 by noting that the expressions for \( \Phi(4.36) \), \( f_{C,k}^e (4.45) \) and \( F_S (4.44) \), are valid for general three-dimensional continua and are not restricted to plane strain or axi-symmetry. The formulas for \( x_k^P \), \( k_{C,kk}^e \) and \( k_{C,k,k'}^e \), however, are only valid for the 2-node surface element shown in figure 4.4 (b).

We summarize that we have developed three finite element formulations of the proposed nanoscale contact model: a volume interaction method, a surface interaction method, and finally, a point interaction method. The three methods are implemented in normalized form, which is discussed in appendix B. A numerical and conceptual comparison between the three integration methods is discussed in section 5. There, we also show a comparison with a molecular simulation. Finally, section 9 discusses a modification to Method 3 which enables it to be used for macroscale problems.

4.4 Regularized Potentials

In this section we shall discuss a few useful modifications to the two-point interaction potential \( \phi(r) \). It can be seen from the finite element formulation of the preceding sections that we only need the force function \( F(r) \) (e.g. eq. (3.7), (3.52), (4.29) or (4.46) depending on the formulation) and its derivative \( F' \) with respect to \( r \). The potential \( \phi \) is not needed computationally. Therefore we can directly consider modifications of the force function \( F(r) \). In the following we introduce three such modifications.

First, we can define a cutoff distance \( r_c \), beyond which the force \( F \) may be considered as negligible, i.e. we use the modified force function

\[
F_c(r) := \begin{cases} 
F(r) & r \leq r_c , \\
0 & r > r_c .
\end{cases}
\]  

(4.50)

We note that \( F_c(r) \) is non-differentiable at \( r = r_c \). This will not cause any problems computationally as long as we do not need to evaluate \( F' \) at \( r_c \), a case we can eliminate by placing \( r_c \) at a finite element interface.

Second, we propose a simple fix to a problem that can occur when the two bodies penetrate each other. Physically, we do not want to allow such penetration, however, it may still occur computationally. The force between two points \( \mathbf{x}_i \in \Omega_1 \) and \( \mathbf{x}_j \in \Omega_2 \) only depends on the distance between these points. Therefore the force function \( F(r) \) does not know if the bodies have penetrated each other. The situation is depicted in figure 4.5. For both cases, (a) and (b), the force between \( \mathbf{x}_i \) and \( \mathbf{x}_j \) may be repulsive. While this is desirable for case (a) it is clearly nonphysical for case (b). To alleviate this problem let us consider the modified force function

\[
F_m(r) := \begin{cases} 
F(r_m) + F'(r_m) (r - r_m) & r \leq r_m \\
F(r) & r > r_m ,
\end{cases}
\]  

(4.51)
where $r_m$ is a chosen distance, which satisfies $0 < r_m < r_0$. We further consider $F_m$ to be defined for all $r \in \mathbb{R}$, i.e. we extend the force relation to ‘negative’ distances $r$. Of course we now have to define a difference between negative and positive distances. In general the case displayed in figure 4.5 (a) should be associated with a positive distance, while the distance shown in figure 4.5 (b) should be negative. Figure 4.6 shows a plot of $F_m(r)$ for the choice $r_m = r_0/2$ (solid lines). For comparison the original function $F(r)$, given by eq. (3.7), is also shown (dashed line). Between frames (a) and (b) only the scaling of the vertical axis is different. By design $F_m$ is differentiable at $r = r_m$.

Let us illustrate the usefulness of using the modification $F_m$ by the following example. We consider a square, deformable block pushed against a flat, rigid obstacle as is shown in figure 4.7. The imposed displacement $u$ as well as the resulting load $P$ are considered as positive in the downward direction. The initial configuration of the block is shown in frame (a); the final configuration, together with the vertical stress component, is shown in frame (c). Using the unmodified force function $F$ we need at least 20 steps with step size $\Delta u = 0.05$ to reach the final state. The load-displacement curve and the gap-displacement curve obtained by
Figure 4.7: a. Initial configuration; b. Trial configuration after one step with $\Delta u = 1$; c. Final, converged configuration; d. Load-displacement curve; e. Gap-displacement curve

This calculation are shown by the red line in frames (d) and (e). It is noted that, due to the singularity of $F(r)$ at $r = 0$, large step sizes invoke large $F$ and thus cause ill-conditioning and poor convergence during the Newton iteration. In this example the step size $\Delta u = 0.05$ is already so large that the convergence is slow and non-quadratic. For larger step sizes Newton’s method does not converge at all. To attain quadratic convergence, the step size has to be reduced further to $\Delta u = 0.01$, thus requiring 100 steps for the present example. On the other hand if we use the modified force function $F_m$, we can solve the problem in only one step, i.e. $\Delta u = 1$, as is shown by the blue line in frames (d) and (e). For such a $\Delta u$, frame (b) shows the initial trial configuration used in Newton’s method. Furthermore, by using $F_m$ we obtain fast, quadratic convergence. Thus, using the proposed modification $F_m$, we can largely increase the efficiency (one step instead of 20) by maintaining the same accuracy (the final configurations from both computations are exactly the same). To achieve this accuracy, we note that the modified section of $F_m$ is only invoked to improve convergence, the final, converged solution, however, must lie in the unmodified part of $F_m$ where we have $F_m(r) = F(r)$. In this example the size of the box is $R_0 \times R_0$, and we have further chosen the parameters $\gamma_L = 5$, $\gamma_W = 100$, $\nu = 0.2$ and $r_m = 0.63r_0 = 0.802R_0$, where $r_m$ is only slightly smaller than the gap attained for the final configuration.
1. Estimate initial displacement field $u_0$
2. Estimate new region $\Omega_e(\Omega_e^k) \subset \Omega_e$ influencing element $\Omega_k^e$
3. Compute internal forces $f_{\text{int}}$ and stiffness matrix $K_{\text{int}}$
4. Compute interaction forces $f_C$, stiffness matrix $K_C$
   and update all influencing regions $\Omega_e(\Omega_k^e)$
5. Compute external forces $f_{\text{ext}}$
6. Apply displacement boundary conditions
7. Given $u_n$, solve for new displacement field $u_{n+1}$
8. Repeat from 3. until iteration has converged

Box 4.1: Newton iteration performed at each load step

problem is computed using Method 3.

The third and last modification we want to consider is to change $F$ such that the CGC model can be applied to macroscale problems. As the problem size becomes larger and larger, the functions $\phi$ and $F$ vary so fast that their behavior can no longer be resolved numerically and we must expect an ill-conditioned problem. For example consider the original force relation (dashed line) displayed in figure 4.6 (a). If two macroscopic bodies approach each other, they will not notice any interacting forces until suddenly the interaction force is near infinity. We cannot expect this to work well numerically. As the problem scales up, let us therefore consider replacing $F$ by an effective relation $F_e$. Such a modification is derived and studied in detail in section 9.

4.5 Implementation

In this section we briefly remark on the implementation of the three FE methods discussed earlier. A given problem is solved sequentially at subsequent time steps, or, under quasi-static conditions, at subsequent load steps. At each time or load step within the finite element simulation the solution is obtained from Newton’s method as derived in appendix B. Box 4.1 gives an overview of the algorithm for the quasi-static case. Some steps deserve further explanation:
First we need to determine an initial estimate of the unknown displacement field and the possible domains of interaction. These domains are $\bar{\Omega}_1$ and $\bar{\Omega}_2$ for Method 1, and $\partial \bar{\Omega}_1$ and $\partial \bar{\Omega}_2$ for Method 2 and 3. To keep the following discussion simple, let us, for now, use symbols $\Omega_1$ and $\Omega_2$ for all three methods. These interaction domains are dependent on the position and deformation of the interacting bodies and they thus evolve over time. Since the interaction decays with distance we only need an estimate of $\bar{\Omega}_1$ and $\bar{\Omega}_2$. In fact one can use the entire bodies $\Omega_1$ and $\Omega_2$ as interaction domains. While this is prohibitively expensive for Method 1, it becomes viable for Method 2 and in particular for Method 3. On the other hand, it is most efficient, if the interaction domains are assigned on an elemental basis. That is, every element $\Omega_i^e \in \bar{\Omega}_1$ is influenced by the region $\bar{\Omega}_2(\Omega_i^e)$ while every element $\Omega_j^e \in \bar{\Omega}_2$ is influenced by the region $\bar{\Omega}_1(\Omega_j^e)$. The entire region $\bar{\Omega}_1 \in \bar{\Omega}_1$ influencing the neighbor $\bar{\Omega}_2$ is then the union of all $\bar{\Omega}_1(\Omega_j^e)$. Likewise $\bar{\Omega}_2$ is the union of all $\bar{\Omega}_2(\Omega_i^e)$. In other words every
element has its own region it is influenced by. An illustration of this is given by figure 4.1 and figure 5.6, following in section 5.3. For every element we thus store a list containing its current influencing elements and then update this list at every iteration step, as is listed in box 4.1 (step 2 and 4). An efficient search algorithm is needed for this update, e.g. see [13]. The update at step 2 is based on the initial displacement $u_0$. The starting guess $u_0$ can, for instance, be taken as a simple translation of the converged solution of the preceding load step, as is done in the example displayed in figure 4.7.

Further, in step 3 through 5 the global force vector $f = f_{\text{int}} + f_C - f_{\text{ext}}$ and corresponding stiffness matrix $K = K_{\text{int}} + K_C$ need to be assembled from the elemental contributions. To assemble $f_{\text{int}}$ and $K_{\text{int}}$ a single loop over all finite elements is needed. To assemble $f_C$ and $K_C$ a further inner loop is required for a particular element $\Omega_k \in \Omega_k$ sampling over its influencing elements. (See appendix B for the assembly rules.) Before solving the system (step 7) the essential boundary conditions (3.1) must be enforced (step 6).

### 4.6 Comparison with Existing Contact Formulations

Closing section 4, we discuss how the three approaches presented above relate to some of the computational methods traditionally employed for macroscale contact mechanics problems, e.g. see [58], [100]. These are typically constructed as single surface integration formulations: on each body the traction arising from contact are integrated over the contact surface. The tractions are obtained as point-wise interaction as is shown in figure 4.1 (c). Since this is also the approach taken by Method 3, this formulation resembles the existing techniques most closely. In fact Method 3 can be seen as a so-called ‘Barrier Method’ [100], [53], where the barrier function is modelled upon an interatomic potential $\varphi$ and thus captures some of the physical aspects of atomic interaction. The modification $F_m$ (4.51) introduced in section 4.4 can be attributed to a class of methods known as ‘Cross-constrained Methods’ or ‘Interior/Exterior Penalty Methods’, which combine the penalty method approach (for penetrating bodies) with the barrier method approach (for separated, but interacting bodies). An example for such an approach is given in [104], which is similar to the force modification approach presented in (4.51).

Compared to common contact approaches like the usual penalty, Lagrange multiplier or augmented Lagrangian methods, the three proposed methods offer some real advantages. First, the nodal force vector $f_{C,k}$ can be evaluated for all elements regardless of their distance to the neighboring body, thus avoiding the distinction between active and inactive constraints needed for the traditional approaches mentioned above. This is possible since $F(r)$ is a smooth, decaying function and not an on/off type constraint. (It is noted that from a practical standpoint, the elements are pre-sorted into possible interacting elements, as noted in section 4.5. In the traditional approaches these pre-sorted elements are then checked for actual contact, that is if the constraint is active or inactive. In Methods 1 through 3, all pre-sorted elements are considered as active.) Second, since the presented formulations are purely displacement based, one does not need to consider the LBB or inf-sup condition, characterizing numerical stability of mixed method approaches, e.g. see [10] and references therein. An important test to assess the consistency and accuracy of a given contact formulation is the contact patch test proposed by Taylor et al. [92] and later modified by Crisfield [24]. In section 6 it is verified that Method 3, proposed above, passes the patch test. On the other hand, in [26] the authors argue that some of the existing contact
algorithms, do not satisfy the LBB condition or the contact patch test. In summary, all methods proposed here need not be checked by the LBB condition and Method 3 further passes the contact patch test.
5 Numerical Analysis

This section serves as an illustration and discussion of the general behavior of the Coarse-Grained Contact Model introduced and derived in the preceding sections. To this end we have constructed a simple model problem, which, when normalized according to section 3.5, only depends on two parameters. A comparison between the three contact formulations and a comparison between molecular dynamics and the CGC model are shown.

5.1 A Model Problem

We consider the plane strain problem of a cylinder with radius $R_0$ located between two half-spaces, that are pushed together by a displacement $u$, as shown in figure 5.1 (a). Two finite element discretizations of the system, which exploit the symmetry of the problem, are shown in frames (b) and (c). At the boundary of the mesh, the short black bars indicate fixed dofs, the red bars indicate dofs where the displacement $u$ is prescribed and the two blue bars show the dofs we wish to record as functions of $u$. In particular we are interested in the gap $g$ between the two blue dofs. To solve the problem we have used the three methods described earlier. Both the cylinder and half-space are modelled by the same hyperelastic material based on the Cauchy-Born rule. We consider a fcc crystal where only nearest neighbors are interacting via the intrasolid potential $\psi$ given in eq. (3.40). The crystal unit cell of such a material is shown in figure 3.2 (b). We let this unit cell be aligned with the $x$, $y$ and $z$ (out of plane) axes of the model problem. The intersolid potential $\phi$ is chosen to be given by eq. (3.6), and we assume that the force $F(r) = -\frac{\partial \phi}{\partial r}$ is negligible beyond the cutoff radius $r_c$ as discussed in eq. (4.50). Fully normalized this model problem only depends on the two parameters $\gamma_L$ (3.53) and $\gamma_W$ (3.59) introduced in section 3.5. The length scale $\gamma_L$ is the ratio between the cylinder radius $R_0$ and the equilibrium spacing $r_0 = r_\phi$ of the potential $\phi$, while the energy scale $\gamma_W$ is proportional to the ratio of $\epsilon_\psi$ and $\epsilon_\phi$, the magnitudes of potentials $\psi$ and $\phi$. Since the Cauchy-Born rule is a local constitutive relation, we note that, upon normalization, the value of the equilibrium spacing $r_\psi$ of potential $\psi$ does not play any role in our model (see also appendix B). The spacing $r_\psi$ must only be assumed...
sufficiently small for the deformation to be homogeneous within the crystal unit cell. The
cutoff radius is selected such that the force $F$ drops below $1/1000$ of its maximum attraction
value. A detailed derivation of the normalized FE equations is given in appendix B.

Figure 5.2 (b) shows the rate of convergence of four successive meshes with largest element
diameters $h_1 = 5\sqrt{2}R_0/4$, $h_2 = 5\sqrt{2}R_0/8$, $h_3 = 5\sqrt{2}R_0/12$ and $h_4 = 5\sqrt{2}R_0/16$ for an
example using $\gamma_L = 10$ and $\gamma_W = 5$. Here we have defined the error in the potential energy
of the system as

$$e(h) := \frac{\Pi(h)}{\Pi(h_5)} - 1 ,$$

i.e. relative to a very fine mesh with $h_5 = 5\sqrt{2}R_0/20$. The deformed configuration and the
distribution of the stress $I_1 = \text{tr } \sigma$ of the finest mesh are shown in frame (a). Between the
two interacting bodies a large gap forms, which is characteristic of the CGC model. Note

Figure 5.2: a. Deformation and stress $I_1$; b. Convergence of the FE solution

that the stress $I_1$ has units $E_0/R_0^3$. The results are obtained by using the volume interaction
method (Method 1).

Next, we consider the example shown in figure 5.3, to illustrate the general behavior of the
model problem and to show a comparison of the three implementations denoted by Method
1 through Method 3. Here the model parameters are picked as $\gamma_L = 25$ and $\gamma_W = 5$. Frames
(c) and (d) show the deformation and stress field $I_1 = \text{tr } \sigma$ of the two contacting bodies.
The load-displacement curve $P(u)$ and the gap $g(u)$ between the two bodies, as obtained by
the three methods, are shown in frames (a) and (b). It can be seen that $P(u)$ and $g(u)$ are
practically equal for all three methods. A minor difference is observable in $P(u)$ between
Method 3 and the other two methods. For all methods the loading increment is initially
chosen as $\Delta u = 0.005R_0$ and then increased to $\Delta u = 0.01R_0$ after 40 steps. We have further
used $5 \times 5$ quadrature points for the volume integration of Method 1, $5$ quadrature points
per surface element of Method 2 and only $2$ quadrature points for the surface integration of
Method 3. We note that we cannot use fewer quadrature points in Method 1 and 2, since
this will make the simulation numerically unstable as is discussed in section 5.3. Effectively,
the quadrature points will be too far apart to ‘feel’ each other. Method 3 does not have
this drawback, and it runs stably for only two quadrature points per surface element. The
The enlarged (d) shows the distinct gap forming between the two solids. Interestingly, the gap \( g \) is approximately constant along the interface. This is due to the fact that the compressive stiffness of the gap, i.e. the stiffness associated with the intersolid potential \( \phi \), is very large compared to the elastic stiffness of the solids. Even though the gap is nearly constant the surface tractions can still vary considerably (as is illustrated by the results of section 8.2). Frame (b) further shows that, as the solid are pushed together and deform, the gap also remains nearly constant with \( u \). Again, this is due to the very large compressive stiffness of the interface. Considering that \( r_0 \) can be of the order of 0.5nm, \( R_0 \) becomes of the order of 10nm in this example.

### 5.2 Attractive Instability

In this section we illustrate that a physical instability can occur during interatomic attraction. Let us investigate what happens if we push two atoms together and then pull them apart again. Therefore let us consider the simple system displayed in figure 5.4 (a). Here \( r \) is the distance between the two atoms and \( \phi(r) \) is their interaction potential, which we...
assume to be given by eq. (3.6). The lower atom is considered fixed while we push the upper atom downwards with imposed displacement $u$, and required loading $P$. The spring, with stiffness $k$, models the stiffness of the loading device. For $r = r_0$ and $u = 0$, the force in the system is $P = 0$. The total potential energy of this system is then written as

$$\Pi(r) = \phi(r) + \frac{1}{2}k(u + (r - r_0))^2. \quad (5.2)$$

For a fixed displacement $u$, equilibrium is given by $\frac{\partial \Pi}{\partial r} = 0$ | $u=\text{fixed}$, from which we can find a relation between $r$ and $u$, namely

$$u = \frac{F(r)}{k} - r + r_0, \quad (5.3)$$

where the force $F(r) = -\frac{\partial \phi}{\partial r}$ is given by eq. (3.7). The inverse function $r = r(u)$, i.e. the atomic distance $r$ in dependence of $u$, is displayed in figure 5.4 (b) for three different values of $k$. We note that $r = r(u)$ cannot be written in closed form here. From eq. (5.3) the load-displacement curve follows as

$$P(u) = k(u + r(u) - r_0). \quad (5.4)$$

It is displayed in frame (c). From the two graphs we observe that, as $u$ becomes large, the repulsion between the atoms is so strong that the deformation is determined purely by the deformation of the spring. For large negative $u$, on the other hand, the attraction between the atoms is very weak so that $u \approx r_0 - r$ (dashed line), since the spring is barely deforming. The stability of the system can be investigated by examining $\frac{\partial^2 \Pi}{\partial r^2}$. It turns out that there is a critical spring stiffness

$$k_{cr} = 36\left(\frac{4}{13}\right)^{2/3} \frac{\epsilon}{r_0^2}. \quad (5.5)$$

For $k > k_{cr}$ the system will always be stable. However, if $k < k_{cr}$ the system develops an instability. The unstable section of the equilibrium path is shown in red in the graphs above. In this case, as we push the two atoms together their mutual attraction will suddenly overpower the spring and the atoms snap together into a new equilibrium position. Likewise, when pulling the atoms apart, they will suddenly snap free. In the literature this behavior is usually denoted as jump-to-contact and jump-off-contact [19].
We emphasize that this instability is physical, and it should therefore carry over into the numerical model. This is shown in figure 5.5. These results are obtained with Method 1 using the parameters $\gamma_L = 10/\sqrt{2}$ and $\gamma_W = 5$. The instability occurs during adhesion, and we can see from the load-displacement curve $P(u)$ and the gap $g(u)$ shown in frames (a) and (b), that the general behavior is essentially the same as for the 1D system shown in figure 5.4. The analogy is that $\phi$ in figure 5.4 represents the two body interaction potential $\Pi_C$, and the spring $k$ represents the stiffness associated with the internal energy $\Pi_{\text{int}}$. Contrary to the one-dimensional behavior for large positive $u$, the load $P(u)$ shown in frame (a) is not linear in $u$, but rather some power of $u$, which is in agreement with experimental indentation results [28], [38] and analytical models [48], [25]. For large negative $u$, i.e. great separation distances, the force $P$ between the bodies vanishes. The deformed configuration and the stress measure $I_1 = \text{tr}(\sigma)$ is shown in frames (c) and (d) for the values of $u$ and $P$ as specified in the figure. Here frame (c) shows the attraction as the bodies adhere, leading to strong tensile stresses, whereas frame (d) shows the repulsion during indentation, leading to large compressive stresses.

Similar to the 1D model discussed above, the occurrence of this instability is determined by the ratio between the contact stiffness, governed by the interaction energy $\Pi_C$, and the
elastic stiffness, governed by the internal energy $\Pi_{int}$. This ratio is controlled by parameter $\gamma_K$, defined in eq. (3.63): For small $\gamma_K$ the bodies are soft compared to the strength of adhesion and the system develops an instability, for large $\gamma_K$, on the other hand, the bodies are too stiff for the system to become unstable. The second parameter, $\gamma_L$, controls the size of the gap between the two bodies. The gap decreases for increasing $\gamma_L$, i.e. if the atomic equilibrium spacing $r_0$ becomes smaller compared to the problem size given by $R_0$. An extensive investigation of the behavior of the model in dependence of parameters $\gamma_L$ and $\gamma_W$ is discussed in section 7. It is noted that the unstable stretch of the load displacement curve of the problem displayed in 5.5 is traced quasi-statically by the arc-length continuation method. In practice there will be dynamic jump between the stable branches of $P(u)$.

### 5.3 Intersolid Interaction Zones

In the following we illustrate the interaction between the two bodies from the numerical point of view. Corresponding to figure 4.1 displayed in section 4, figure 5.6 below shows a discrete version of the interaction zones. Using Method 1, frame (a) shows the deformed FE mesh for the parameters $\gamma_L = 10$ and $\gamma_W = 5$. The region formed by the yellow elements is a discrete version of the interaction domains $\Omega_1$ and $\Omega_2$. In particular, the interaction domains of two elements are shown in pink: Element $\Omega^e_i$ interacts with the hemispherical region above, (also denoted by $\Omega_1(\Omega^e_j)$), while $\Omega^e_j$ interacts with the zone below ($\Omega_2(\Omega^e_i)$). It is shown that these domains can reach across the symmetry boundary, as has been argued in section 4.1. As is discussed in section 4.5, a search algorithm is implemented which computes the interacting region for each element $\Omega^e_k$, $k = 1, 2$. During subsequent loading these regions are updated. Figure 5.6 (a) can also be used to illustrate the interaction as implemented in Method 2. In this method the interacting domains $\partial \Omega_1$, $\partial \Omega_2$, $\partial \Omega_1(\Omega^e_j)$ and $\partial \Omega_2(\Omega^e_i)$ are formed by the outer surface of $\Omega_1$, $\Omega_2$, $\Omega_1(\Omega^e_j)$ and $\Omega_2(\Omega^e_i)$.

The interaction as derived in Method 3 is shown in frame (b) for the values $\gamma_L = 5$ and $\gamma_W = 5$. The quadrature points of surface elements $\Gamma^e_i$ and $\Gamma^e_j$ are projected onto the closest point on the neighboring surface as shown. Note that this projection is not always
perpendicular to the surface we are projecting onto. For example, as is seen for the first quadrature point of $\Gamma_1^c$, the closest projection point is a FE node.

As has been mentioned along with the example of figure 5.3, if two few quadrature points are used, a purely numerical instability can develop in Methods 1 and 2, and cause our FE simulation to blow up. As an example let us consider Method 2, where the interaction is restricted to the surfaces $\partial \Omega_1$ and $\partial \Omega_2$. Figure 5.7 (a) shows the deformed FE mesh of our model problem and the surface quadrature points used to evaluate the integrals for $f_C$ and $K_C$ numerically (eqs. (4.28) and (4.33)). During repulsion, the interaction is strongest between closest quadrature points. Essentially the interaction between three such points, as the ones shown in red, can behave as the snap-through of an arch, as is modelled in frame (b). The loading of the arch is caused by the imposed displacement $u$. The stiffness of the two rods is related to the intersolid potential $\phi$, whereas the stiffness of the springs is related to the intrasolid potential $\psi$. For some loading $u$, depending on the parameters $\gamma_L$, $\gamma_W$ and the geometry of the arch (which depends on the density of quadrature points), the arch becomes unstable and snaps-through. If this snap-through mechanism occurs, the bodies will intersect and we must discard the numerical solution even if it doesn’t blow up, which usually happens at this point. This problem is alleviated if we increase the density of quadrature points.

We note that this instability cannot occur for Method 3, since in this case each quadrature point only interacts with the closest projection point on the neighboring surface, as can be seen in figure 5.6 (b).

5.4 Comparison with Molecular Dynamics

The proposed contact model is motivated as an efficient alternative to molecular dynamics, which, depending on the problem size, can become prohibitively expensive. In this section we show that the CGC model can produce remarkably accurate predictions of molecular computations. As earlier we restrict ourselves to quasi-static motion. Under this restriction, molecular dynamics is also referred to as lattice statics. We consider the model problem introduced in section 5.1 with the parameters $\gamma_L = 5\sqrt{2}$ and $\gamma_W = \gamma_L^3 = 250\sqrt{2}$.

![Figure 5.7: a. Interacting quadrature points for Method 2; b. Simplified model](image)

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construct an atomic lattice we further need to specify the intra-atomic equilibrium spacing $r_\psi$ and a particular crystal structure. We chose a fcc crystal (see figure 3.2) with $r_\psi = \sqrt{2}R_0/20$, so that the Bravais lattice parameter becomes $a = R_0/20$. For the specified $\gamma_L$ and $\gamma_\psi$ we then have $r_\psi = 2r_\psi$ and $\epsilon_\psi = 4000\epsilon_\phi$. The atomic lattice and FE mesh chosen for this comparison are shown in figure 5.8 (a). They are displayed next to each other for comparison (there is no coupling considered between the two). The atomic lattice contains 2022 atoms corresponding to 4044 dofs, whereas the FE mesh contains only 57 elements, 77 nodes and 154 dofs. It is noted that the atoms shaded dark are located the distance $a$ below the light shaded atoms. Frame (b) shows the deformed configuration of lattice and

Figure 5.8: Comparison of molecular dynamics and the CGC model: a. Undeformed configuration; b. Deformed configuration; c. Superimposed deformation; d. Load-displacement curve;

FE mesh. Their agreement is very close. This is further illustrated in frame (c) which shows a superimposition of the the two configurations. It can be seen that the deformation on the surface does not match exactly, which is due to the different surface discretization of the two models. (See [62] for a discussion on the influence of the atomic surface roughness on mechanical contact.) The deformation further away from the zone of contact matches nicely. In particular, the deformation in the lower right corner of frame (c) confirms the
affine motion of the lattice according to the Cauchy-Born rule. The FE results shown are obtained from Method 2. A comparison of the load-displacement curves according to the three FE methods and the molecular computation is displayed in frame (d). As in the example of figure 5.3 the three FE formulations Method 1 through 3 compare well with each other. They further agree with the result obtained from the lattice statics computation. The agreement of the various methods should be regarded in conjunction with the gained efficiency displayed in table 5.1. For this we contrast the total number of intrasolid and

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<th>M1</th>
<th>M2</th>
<th>M3</th>
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<tr>
<td>Number of atoms / elements</td>
<td>2022</td>
<td>57</td>
<td>57</td>
<td>57</td>
</tr>
<tr>
<td>Number of intrasolid interactions</td>
<td>24264</td>
<td>1368</td>
<td>1368</td>
<td>1368</td>
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<tr>
<td>Number of intersolid interactions</td>
<td>7387</td>
<td>4832</td>
<td>270</td>
<td>46</td>
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<td>1.39s</td>
<td>0.34s</td>
<td>0.31s</td>
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Table 5.1: Computational efficiency of the Coarse-Grained Contact Model

intersolid interactions needed to solve the problem numerically. The intrasolid interaction is only based on nearest neighbor interaction. There are 12 neighbors surrounding each atom within the fcc lattice, so that for the molecular computation, we obtain 24264 interactions in total. For the CGCM, on the other hand, we only require 1368 such interactions: Using the Cauchy-Born rule we only need to evaluate 6 interactions at the 4 quadrature points of every element, i.e. $6 \times 4 \times 57 = 1368$. The intersolid interactions are included up to a cutoff radius of $r_c = 0.363 R_0$. They are counted within the codes and are obtained as listed in table 5.1. Using molecular dynamics we need to evaluate 7387 interatomic interactions. In Method 1 through 3 the intersolid interaction forces are obtained from evaluating integrals (4.6), (4.28) and (4.45) respectively. For this, here, 5 quadrature points are used in each dimension. We thus count 4832, 270 and 46 interactions for the three methods. Due to this significant decrease in intersolid and intrasolid interactions between the various methods, we observe the shown decrease in the CPU time (measured on an Intel P4 3.0 GHz CPU). It is noted that for the molecular computation, the interaction with out-of-plane atoms has to be accounted for. For Methods 1 through 3 this is done by analytical integration as described in section 3.3. In summary it can be seen that there is an increase in speed when going from molecular dynamics to Method 1, 2 and 3, due to the decrease in the dofs and in the number of interactions to evaluate. The computational cost to setup $\mathbf{f}_{\text{int}}$ and $\mathbf{f}_C$ scales linearly with the number of intrasolid and intersolid interactions. The solution time to solve the resulting equations of motion is controlled by the number of dofs.

As the problem size increases the savings become even more dramatic. This is shown in table 5.2 which lists the number of dofs and interactions for the example of figure 5.3. Here,

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<th>M3</th>
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<tr>
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</tr>
<tr>
<td>number of intrasolid interactions</td>
<td>$1.55 \cdot 10^6$</td>
<td>20,736</td>
<td>20,736</td>
<td>20,736</td>
</tr>
<tr>
<td>number of intersolid interactions</td>
<td>$5.0 \cdot 10^6$</td>
<td>231,875</td>
<td>2,025</td>
<td>96</td>
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</table>

Table 5.2: Computational efficiency of the example shown in figure 5.3
the values listed under ‘MD’ are estimates. It is emphasized that the comparison of tables 5.1 and 5.2 is by no means exhaustive, as it is restricted to reversible (i.e. elastic), quasi-static and temperature independent conditions.

It is noted that the savings in efficiency are inevitably linked to a loss of information. For instance, the coarse finite element description of the problem shown in figure 5.8 will not be able to accurately capture fracture or dislocation processes at the atomic scale.

5.5 Physical and Numerical Observations

Let us summarize some of the key findings of the study of the simple model problem depicted in figure 5.1. We first list the physical observations. In accordance with the discussion of section 3.5, these are:

1. Physically, the problem is only controlled by the two independent parameters $\gamma_L$ and $\gamma_W$. (We recall that we have fixed some further parameters by considering both bodies to be of the same anisotropic material, governed by the Cauchy-Born rule, with material axis aligned along $x$, $y$ and $z$.)

2. The parameter $\gamma_W$, introduced in eq. (3.59), is a material constant which represents the relative strength between the intrasolid interaction potential $\psi$ and the intersolid interaction potential $\phi$.

3. The geometrical parameter $\gamma_L$, introduced in eq. (3.53), controls the length scale of the problem. As is outlined in figure 2.1, the CGC model is designed for a certain range of parameters $\gamma_L$ and cannot be expected to do well beyond those. For $\gamma_L = \mathcal{O}(1)$ the problem is of nanoscale proportions and the number of numerical degrees of freedom (dofs) approaches the number of atomic dofs. For such cases there is little gain in efficiency in using the CGC model and it will thus make more sense to resort to the physically more accurate molecular model. On the other hand, as $\gamma_L$ increases, the bodies become larger and contain more and more atoms. The efficient approximations introduced by Method 2 and 3 will then become more and more accurate. However, if $\gamma_L$ becomes too large, the present formulation of the CGC model becomes ill-conditioned. In this case it will be more efficient to model contact by traditional means, i.e. not based on atomic interaction but rather based on a macroscopic impenetrability constraint. Alternatively, in section 9 we propose a simple modification of the CGC model, which renders it useful for macroscale problems.

4. The attractive instability, discussed in section 5.2, is controlled by the stiffness parameter $\gamma_K = \gamma_W/\gamma_L$, as defined by eq. (3.63). The instability occurs if $\gamma_K$ falls below a threshold value, that is when the two interacting bodies are soft compared to the strength of their mutual interaction. The likelihood to observe this instability thus increases if $\gamma_W$ decreases or when $\gamma_L$ increases. This is confirmed by the findings of section 7.

5. In eq. (3.60), we have further defined the parameter $\gamma_\Pi = \gamma_L\gamma_W$, which is a measure of how much of the system’s total energy is stored in the deformation of the two solids and how much is stored in the interaction energy of the bodies.
A numerical algorithm strives to capture the physical behavior accurately, while at the same time being efficient and stable. In the following we discuss the numerical findings, focusing in particular on numerical stability:

1. The main numerical parameters are the finite element mesh, the density of quadrature points, the time or load step and the cutoff radius $r_c$ of potential $\phi$.

2. We note that for our model to be algorithmically stable, there is a limit on the load step $\Delta u$ (or time step $\Delta t$ for dynamic problems). If this step become too large, Newton’s method will converge poorly or will fail to converge altogether. In the examples above to load step $\Delta u$ is chosen such that it is smaller than the gap between the bodies ($\Delta u < g$). Under this condition, the convergence of Newton’s method tends to be very good. In section 4.4 we have presented a modification of the potential $\phi$, which allows for stable computations with much larger load/time steps.

3. Method 1 and 2 are sensitive to the number of quadrature points used. Using too few quadrature points can lead to a failure mechanism of the method as is discussed in section 5.3. Method 3, on the other hand, is much more robust, since this failure mechanism cannot occur. Therefore, fewer quadrature are required to make Method 3 numerically stable.

4. The numerical stability of all methods deteriorates if the surface discretization of the interacting bodies is too coarse to capture the gap $g$ accurately. Therefore as $\gamma_L$ increases a finer and finer surface discretization is needed or else we risk ill-conditioning. Such a refinement will lead to an increase in the computational cost. On the other hand, in section 9 we show that by modifying the CGC model slightly, efficiency can be maintained without loosing accuracy or numerical stability.
6 The Contact Patch Test

In this section the consistency and accuracy of the contact formulations denoted as Method 2 and Method 3 are assessed by the so called contact patch test. Such a test was originally proposed in [92] and then later modified according to [24]. In its modified form the contact patch test consists of two blocks brought into normal contact by an imposed uniform displacement $u$, as is shown in figure 6.1 (a). As indicated, we consider the contacting surfaces to extend beyond the two modelled blocks. Such a contact condition is one of the predominant modes of two contacting solids. A possible finite element mesh of the problem is depicted in frame (b). For a general test of the numerical contact formulation the finite element nodes on the neighboring contact surfaces must be non-matching. If the blocks deform homogeneously, the problem can be solved analytically and we can thus assess the accuracy of the proposed contact formulations.

6.1 Analytical Patch Test Results

In the following we present two analytical patch test solutions, one for the contact as it is perceived at the macroscale and another for the contact as it is perceived at the nanoscale.

6.1.1 Macrocontact

We consider bringing two blocks together by an imposed displacement. As long as the blocks are separated they do not interact and thus move rigidly. In contact the blocks repel each other and deform as is illustrated in figure 6.2. According to this figure we define the stretches

$$\lambda_x := \frac{\ell_x}{L_x}, \quad \lambda_y := \frac{\ell_y}{L_y},$$

(6.1)

and the plane strain deformation gradient

$$F = \begin{bmatrix} \lambda_x & 0 & 0 \\ 0 & \lambda_y & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

(6.2)
with the Jacobian $J = \det \mathbf{F} = \lambda_x \lambda_y$. We consider $\lambda_y$ prescribed, i.e. we consider an imposed vertical deformation, as shown in figure 6.2. The problem is solved once $\lambda_x$ is found. Let us suppose the bodies are of identical material and governed by a Neo-Hookean constitutive model (see section 3.2.1) given by the stored energy

$$W_{\text{int}} = U(J) + \frac{\mu}{2}(I_1 - 3) - \mu \ln J, \quad U(J) = \Lambda/2(\ln J)^2,$$

where $I_1 = \text{tr} \mathbf{F} \mathbf{F}^T = \lambda_x^2 + \lambda_y^2 + 1$. From $W_{\text{int}}$ the Cauchy stress tensor $\mathbf{\sigma}$ follows as

$$\mathbf{\sigma} = U' \mathbf{I} + \frac{\mu}{J}(\mathbf{B} - \mathbf{I}), \quad U'(J) = \Lambda/J \ln J.$$

The principal stresses are aligned with the $\{x, y, z\}$ basis and are given by

$$\sigma_x = \frac{\Lambda}{J} \ln J + \frac{\mu}{J}(\lambda_x^2 - 1),$$
$$\sigma_y = \frac{\Lambda}{J} \ln J + \frac{\mu}{J}(\lambda_y^2 - 1),$$

$$\sigma_z = \frac{\Lambda}{J} \ln J.$$

For the homogenous deformation considered above the stress within the bodies is uniform. If the blocks are considered unconstrained in the $x$-direction, the stress component $\sigma_x$ must vanish, so that from the condition $\sigma_x = 0$ we find

$$\Lambda(\ln \lambda_x + \ln \lambda_y) + \mu(\lambda_x^2 - 1) = 0.$$

Given $\lambda_y$ this is a transcendental equation for $\lambda_x$ which can be solved numerically, e.g. using Newton’s method. Once $\lambda_x$ is found, the stress $\sigma_y$ can be evaluated. The internal energy stored in the system is given by $\Pi_{\text{int}} = W_{\text{int}}L_xL_yL_z$, which coincides with the total potential energy $\Pi$ here.

### 6.1.2 Nanocontact

At the nanoscale we have to take the gap between the two bodies into account. The deformation of the gap and the blocks is illustrated in figure 6.3. According to this figure...
we define the stretches

\[ \lambda_x := \frac{\ell_x}{L_x}, \quad \lambda_y := \frac{\ell_y}{L_y}, \quad \lambda_g := \frac{g}{G}, \quad \lambda_h := \frac{h}{H}, \]  

(6.7)

where \( L_y = 2H + G \) and \( \ell_y = 2h + g \). The two deformation gradients can then be written as

\[ F_h = \begin{bmatrix} \lambda_x & 0 & 0 \\ 0 & \lambda_h & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad F_g = \begin{bmatrix} \lambda_x & 0 & 0 \\ 0 & \lambda_g & 0 \\ 0 & 0 & 1 \end{bmatrix}, \]  

(6.8)

(assuming plane strain). Note that \( \lambda_h \) now plays the role of \( \lambda_y \) in the case of macrocontact.

The Jacobian of the deformation of the solids now follows as 

\[ J = \det F_h \lambda_x \lambda_h \].

Considering the conditions of Method 3, the traction acting on the current interface \( \partial \Omega_k \) is given by

\[ t_k(x_k) = \beta_k F_S(g) \mathbf{r}_k^P, \]  

(6.9)

where \( F_S \) is defined by eq. (4.46), where \( \mathbf{r}_k^P = [0 \ 1 \ 0] \) and where \( \beta_k = \beta_0 = \beta_0/J \). The only non-zero traction component of eq. (6.9) is the \( y \)-component

\[ t_y = \pi \frac{\beta_0^2}{J^2} r_0^3 \left[ \frac{1}{15} \left( \frac{r_0}{g} \right)^9 - \frac{1}{3} \left( \frac{r_0}{g} \right)^3 \right]. \]  

(6.10)

We note that the traction acting on the contact surface of the upper body is \( +t_y \), while the traction acting on the lower body is \( -t_y \). According to eq. (3.57) we can substitute \( W_{C,0} = \beta_0^2 c r_0^3 \) in the expression above. The reference configuration is considered to be stress free, so that the reference gap is given by

\[ G = g|_{t_y=0} = r_0/\sqrt[6]{15}. \]  

(6.11)

To solve the nanocontact problem we consider \( L_x, H, G, \mu, \Lambda \) given and prescribe the vertical deformation \( \lambda_y \). As before we suppose that the bodies are governed by a Neo-Hookean constitutive law and are unconstrained laterally. Through the equilibrium conditions \( \sigma_x = 0 \) and \( \sigma_y = t_y \) we thus find

\[ \Lambda (\ln \lambda_x + \ln \lambda_h) + \mu (\lambda_x^2 - 1) = 0, \]

\[ \Lambda (\ln \lambda_x + \ln \lambda_h) + \mu (\lambda_h^2 - 1) = -\pi \frac{W_{C,0}}{J} \left[ \frac{1}{15} \left( \frac{r_0}{g} \right)^9 - \frac{1}{3} \left( \frac{r_0}{g} \right)^3 \right]. \]  

(6.12)
Together with
\[ \lambda_y = \frac{2h + g}{2H + G}, \]  
we have three coupled nonlinear equations for the three unknowns \( \lambda_y, \lambda_h \) and \( \lambda_x \) (note \( g = \lambda_y G \) and \( h = \lambda_h H \)). It is convenient to normalize the lengths by \( R_0 \), i.e. \( \bar{g} = g/R_0 \) and so forth. We further choose \( L_x = R_0, \) \( L_y = R_0 \) and use the familiar definition \( \gamma_L := R_0/r_0 \) to get \( g/r_0 = \gamma_L \bar{g} \). The material constants are normalized as
\[ \bar{\mu} = \mu / E_Y = \frac{1}{2(1 + \nu)}, \quad \bar{\Lambda} = \Lambda / E_Y = \frac{2\bar{\mu} \nu}{1 - 2\nu}, \quad \gamma_W := \frac{E_Y}{W_{C,0}}, \] (6.14)
where \( E_Y \) is Young’s modulus and \( \gamma_W \) is the familiar energy parameter (see eq. (3.59)). Equation (6.12) is thus recast into
\[ \bar{\Lambda}(\ln \lambda_x + \ln \lambda_h) + \bar{\mu}(\lambda_x^2 - 1) = 0, \]
\[ \bar{\Lambda}(\ln \lambda_x + \ln \lambda_h) + \bar{\mu}(\lambda_h^2 - 1) = -\frac{\pi}{\gamma_W} \left[ \frac{1}{45} \left( \frac{1}{\gamma_L \bar{g}} \right)^9 - \frac{1}{3} \left( \frac{1}{\gamma_L \bar{g}} \right)^3 \right], \] (6.15)
which, together with eq. (6.13), is solved with the Newton-Raphson method.

It is further interesting to look at the energy stored within the system. The elastic energy stored within the solids is
\[ \Pi_{\text{int}} = W_{\text{int}} L_x 2H L_z, \] (6.16)
where the internal energy density \( W_{\text{int}} \) is given by eq. (6.3) replacing \( \lambda_y \) by \( \lambda_h \). The interaction energy can be obtained from the integration of the work of the contact traction over the contact surface, i.e.
\[ \Pi_C = \int_{\partial \Omega} \mathbf{t} \cdot d\mathbf{u}, \] (6.17)
In the current example this becomes
\[ \Pi_C(g) = \int_{g_0}^g \sigma_y \ell_x \, dg, \] (6.18)
which, notably, is not equal to \( \Pi_C \), initially defined by eq. (3.9), due to the approximation involved in Method 3. The total potential energy follows as \( \Pi = \Pi_{\text{int}} + \Pi_C \).

### 6.1.3 Comparison between Macrocontact and Nanocontact

We briefly examine the behavior of the simple analytical contact example, derived in the preceding two sections, as viewed from the macroscale and nanoscale. Figure 6.4 shows the behavior of the stretch \( \lambda_x \), the stress \( \sigma_y \) and the energy \( \Pi \) as functions of the prescribed stretch \( \lambda_y \). The problem parameters are as specified in the caption. Here the blue curves correspond to the nanocontact results, whereas the green curves show the behavior of macroscopic contact. The dashed green lines show the macroscopic behavior for the case where the two bodies remain perfectly bonded as they are pulled apart. In the case of nanocontact it is conclusive to look at the composition of the potential energy \( \Pi \), as shown in frame (d). It can be seen that for \( \lambda_y > 1 \), i.e. during adhesion, the energy \( \Pi \) is stored in \( \Pi_C \), whereas for \( \lambda_y < 1 \), i.e. during repulsion, most of the energy \( \Pi \) is stored in \( \Pi_{\text{int}} \).
6.2 Patch Test Results of Method 3

We now examine the contact formulation designated as Method 3 by using the contact patch test. Figure 6.5 shows a comparison of the analytical result of section 6.1.2 and the numerical results according to Method 3 of the CGC model. Shown is the behavior of stretches $\lambda_x$, $\lambda_y$, $\lambda_h$ and stress $\sigma_y$ over the range of prescribed vertical deformation $0.5 < \lambda_y < 2$. Frame (d) shows the deformed configuration at $\lambda_y = 0.5$, where we have $\lambda_h = 0.451$, $\lambda_g = 0.894$, $\lambda_x = 1.330$ and $\sigma_y = -1.004 E_0/R_0^3$. The finite element mesh considered for the shown results is the mesh given in figure 6.1 (b). To evaluate the contact integral (4.45) two quadrature points are used for each surface element $\Gamma_k^e$. It is illustrative to consider the relative stress error

$$e = \frac{\sigma_{y,\text{analyt}} - \sigma_{y,\text{FE}}}{\sigma_{y,\text{analyt}}},$$

between the analytical result and the finite element result. The error at $\lambda = 0.5$ is $e = 2.829 \cdot 10^{-6}$ uniformly across the mesh as depicted in frame (d). (The variation across the mesh is below machine precision here). Due to this very small error level we conclude...
that the contact implementation of Method 3 is consistent with its formulation. Thus the contact patch test is passed. It is remarked that mesh refinement has no influence on this remaining error which may be due to round off or some minor level of ill-conditioning.

As a final remark we note that frame (b) shows that for $\lambda_y > 1$ the overall deformation is composed solely of the deformation of the gap, whereas for $\lambda_y < 1$ the overall deformation is mainly accommodated by the deformation of the bodies. This is in accordance to the behavior of the potential energy $\Pi$, discussed in figure 6.4 (d).

6.3 Patch Test Results of Method 2

In contrast to Method 3, the numerical contact formulation designated as Method 2 is not consistent as is illustrated next. If a coarse mesh is chosen the results obtained from Method 2 can be quite poor as seen in figure 6.6 (a). Here the same error measure as defined by eq. (6.19) is shown. If the finite element mesh is refined the error decreases considerably as is seen in frame (b). For this mesh the maximum error is around 0.015, which is by the
order of $10^4$ larger than the error observed for Method 3 in the preceding section! Frame (b) also shows that the error is not evenly distributed, as is the case for Method 3. This distribution is caused by the non-matching meshes of the two blocks. As before, we choose two quadrature points per surface element. Increase of the number of quadrature points will also decrease the error. Frame (d) shows the decrease of error $e$ with decreasing finite element size $h$. As the contact formulation of Method 2 does not achieve a negligible error independent of the mesh refinement we conclude that this formulation is inconsistent and does not pass the contact patch test. The same conclusion follows for Method 1, due to the formal similarity of Methods 1 and 2, as displayed by eqs. (4.6) and (4.28). Even though Method 2 does not pass the patch test, it still achieves remarkably accurate results, as is shown by the stress comparison of frame (c) (obtained for the dense mesh shown in frame (b)). Here, the stress component $\sigma_y$ according to the CGC model, is taken as the average over the entire patch. The relative error in this average stress is only $1.10 \cdot 10^{-3}$ at $\lambda_h = 0.5$ (for the dense mesh shown in frame (b)). This level of accuracy also holds for the quantities $\lambda_h$, $\lambda_y$ and $\lambda_x$.

It is noted that, when using Method 2, the interaction along the extended surfaces of the
blocks, as indicated by figure 6.1 (a), has to be taken into account. This means that at both vertical boundaries a symmetry condition, as considered in section 4.1, has to be used for Method 2. Otherwise the presence of the edges will lead to spurious stresses there.
7 Scaling of the Coarse-Grained Contact Model

In this section we investigate how adhesive contact, as modelled by the CGCM, behaves for various parameters \( \gamma_L \) and \( \gamma_W \). For this we first fix \( \gamma_W \) to examine the behavior for increasing length scales \( \gamma_L \). Secondly, we fix \( \gamma_L \) and consider changing the energy ratio \( \gamma_W \). We conclude this section by a brief summary. To abridge the ensuing notation we introduce the equivalent parameters \( \tilde{\gamma}_L = \frac{\theta}{3/4} \gamma_L \) and \( \tilde{\gamma}_W = \sqrt{3} \gamma_W \). For this study we return to the problem shown in figure 5.1 (a), but now considered as an axi-symmetric problem instead of a plane strain problem. That is, we are looking at a sphere between two half-spaces. The radius of the sphere is chosen as the reference length \( R_0 \). As a further modification to the problem of section 5, we now use the empirical Neo-Hookean constitutive model (3.33) to describe the response of the two contacting solids. We assume identical material parameters \( E_Y := E_1 = E_2 \) and \( \nu := \nu_1 = \nu_2 \). We chose \( E_0 = E_Y R_0^3 \) as the reference energy of the system and use it, together with \( R_0 \), to normalize the system. Therefore \( R_0 \) and \( E_Y \) do not need to be specified. Poisson’s ratio is chosen as \( \nu = 0.2 \). The finite element meshes used to model this problem are depicted in figure 7.1. Mesh 1, shown in frame (a) and (b) contains 2528 nodes and 2400 elements, whereas mesh 2, displayed in frames (c) and (d) contains 1515 nodes and 1408 elements. It can be seen that the half-space is modelled by a block of size \( 8R_0 \times 8R_0 \), which is chosen this large to eliminate spurious boundary effects.

Scaling becomes important in many physical problems as soon as an intrinsic, characteristic length, such as \( r_0 \), is introduced into the problem. Examples include fracture mechanics [11], [12], turbulence [8] and gradient elasticity. The behavior of usual hyperelasticity is scale invariant, as it only depends on the deformation gradient \( F \), which is dimensionless.

7.1 Scaling of the Geometry

In this section we illustrate how the CGC model behaves for various length scales \( \gamma_L \). For this we consider the energy density ratio fixed at \( \tilde{\gamma}_W = 200 \) and compare the behavior for the eight cases \( \tilde{\gamma}_L \in \Gamma_L = \{2, 5, 10, 20, 50, 100, 200, 500\} \). It is important to note that the behavior of the system, as \( \gamma_L = R_0/r_0 \) changes, can be observed in two ways: First, we can consider \( R_0 \) as fixed, i.e. we adopt \( R_0 \) as our reference scale. So as \( \gamma_L \) increases we...
observe the system as \( r_0 \) decreases. One may say that our frame of reference is scaled by \( R_0 \). Second, we can consider \( r_0 \) fixed, and so as \( \gamma_L \) increases we are observing the system as \( R_0 \) increases. Our frame of reference is then scaled by \( r_0 \). From this second point of view an observer adopting the first viewpoint will appear increasing in size as \( \gamma_L \) increases, whereas the second observer will see the first observer decreasing. This distinction is important, since the system is observed differently from these two viewpoints. We denote the two points of views, or rather the two ‘scales of view’, as follows: When the geometry parameter \( R_0 \) is the length scale of the frame of reference, we shall speak of the geometrical scale of view, whereas when the material constant \( r_0 \) is the length scale of the frame of reference, we shall speak of the material scale of view. Alternatively, since \( R_0 \) is a macroscopic and \( r_0 \) a microscopic quantity, we will also refer to the first view as the macroscopic scale of view and to the second as the microscopic scale of view.

With this distinction we now examine the behavior of the system for changing \( \gamma_L \). Figure 7.2 shows the load-displacement curve \( P(u) \) and the development of the gap \( g(u) \) as the two bodies are coming into contact. Here we have adopted the macroscopic scale of view,

![Figure 7.2: 'Macroscopic scale of view' of a. load \( P(u) \) and b. gap \( g(u) \), both for \( \tilde{\gamma}_W = 200 \)](image)

where \( P \), \( g \) and \( u \) are normalized by the macroscopic parameters \( R_0 \) and \( E_0 = E_Y R_0^3 \). The seven curves shown in each frame correspond to the parameter list \( \Gamma_L \) except for \( \tilde{\gamma}_L = 500 \), which is hardly distinguishable from \( \tilde{\gamma}_L = 200 \). (The curves are computed with Method 3 using the mesh shown in figure 7.1 (c) and using sufficiently small displacement increments \( \Delta u \) for the curves to appear smooth.) The dependance of the load \( P \) and the gap \( g \) on the displacement \( u \) is characterized by three phases. We term the first phase the rigid phase, since the two bodies approach each other rigidly, without yet interacting. During this phase the force between the two bodies is zero; The gap decreases linearly. The second phase, termed the adhesion phase, is characterized by an attractive (here negative) force \( P \). During this phase the slope of \( g(u) \) becomes steeper, i.e. the rate of change of the gap increases. The third phase is characterized by a large repulsive force \( P \); Now, the gap \( g \) only decreases slightly with \( u \) since the interface, or contact, stiffness is much larger than the elastic stiffness of the two solids. This last phase is termed the contact phase.
Let us now analyze the behavior of $P$ and $g$ as $\gamma_L$ changes. Figure 7.2 shows the self-similarity of $P(u)$ and $g(u)$ across the geometrical scaling. In particular let us consider the minimum $P_{\text{min}}$ of $P$, where the adhesion is strongest, and the contact gap at $u = 0.2R_0$, denoted by $g_c$. As the length scale $\gamma_L$ increases, it can be observed that both $g_c$ and $P_{\text{min}}$ decrease, and the location of $P_{\text{min}}$, as well as the boundaries between the three phases, move to the right. Further, let us look at the slope $P'(u)$, which represents the overall stiffness of the system. During the contact phase (i.e. for large positive $P(u)$) the stiffness $P'(u)$ is independent of $\gamma_L$. The reason for this behavior is that during the contact phase the mutual approach of the two bodies does not result in the decreasing of the gap but is rather accommodated by the deformation of the bodies themselves. Their stiffness is characterized by $K_{\text{int}}(3.61)$, which is independent of $\gamma_L$. During the adhesion phase, on the other hand, changes in the approach are accommodated by changes of $g$, rather than by the deformation of the solids. The stiffness of the gap is characterized by $K_C(3.62)$, which is dependent on $\gamma_L$.

In summary it is seen that $\gamma_L$ determines the boundaries of the three phases, the magnitude of the extremum $P_{\text{min}}$ and the size of the contact gap $g_c$. It can be found that $P_{\text{min}} \sim \gamma_L^{-1}$ and $g_c \sim \gamma_L^{-1}$ (see section 7.3). The slope $P'(u) =: k_c$ during contact, on the other hand, is hardly affected by $\gamma_L$.

Let us now examine the behavior of the problem from the microscopic scale of view, where forces and lengths are normalized by the material constants $r_0$ and $e_0 := E\gamma r_0^3$. This is shown in figure 7.3 for the same parameter list $\Gamma_L$ except for $\gamma_L = 2$ which is indistinguishable from $\gamma_L = 5$. As can be seen from frame (a), at this scale of view, the maximum adhesive force $P_{\text{min}}$ now increases with increasing $\gamma_L$. This is exactly opposite to the trend observed in figure 7.2 (a). From the macroscopic scale of view adhesion plays less of a role as $\gamma_L$ increases, whereas from the microscopic scale of view adhesion plays a stronger role as $\gamma_L$ increases. A further difference between the two scales of view is displayed in the behavior of the stiffness $k_c = P'(u)$ during the contact phase. From the macroscopic scale of view this stiffness is observed as independent of $\gamma_L$, whereas form the microscopic scale of view the contact stiffness increases along with $\gamma_L$. (Recall that we have fixed $\gamma_W$). Further, the perceived behavior of the gap, also changes between the two scales of view: During the

![Figure 7.3: 'Microscopic scale of view' of a. load $P(u)$ and b. gap $g(u)$, both for $\bar{\gamma}_W = 200$](image-url)
contact phase, the contact gap \( g_c \) (e.g. taken at \( u = 0.2R_0 \)) depends strongly on \( \gamma_L \) from the macroscopic scale of view, while \( g_c \) (e.g. at \( u = r_0 \)) hardly depends on \( \gamma_L \) from the microscopic scale of view.

In closing, we again emphasize that the behavior of the considered quantities, i.e. load, stiffness and gap, depend on the scale of observation, as is illustrated by the differences of figures 7.2 and 7.3.

### 7.2 Scaling of the Energy

Let us now assess the behavior of loading, stiffness and the gap between the two bodies as the energy density ratio \( \gamma_W \) changes. For this we fix the length scale at \( \delta L = 50 \) and look at the seven cases \( \delta W \in \Gamma_W = \{20, 50, 100, 200, 500, 1000, 2000\} \). Figure 7.4 shows the behavior of \( P(u) \) and \( g(u) \) for the considered \( \gamma_W \). It can be observed that the maximum adhesion \( P_{\min} \) decreases as \( \gamma_W \) increases, whereas the contact stiffness \( k_c \) and contact gap \( g_c \) are practically independent of \( \gamma_W \). Furthermore, it can be observed, that below a threshold value of \( \gamma_W \) the adhesive approach turns unstable, as happens for the cases \( \delta W = 50 \) and \( \delta W = 20 \). The unstable equilibrium path is marked as a dashed line in figure 7.4. The appearance of this physical instability, which has been noted in section 5.2 before, can be explained by the parameter \( \gamma_K \) (3.63): As \( \gamma_K \) decreases (due to the decreasing of \( \gamma_W \)) the strength of adhesion, characterized by the stiffness \( K_{C,0} \), increases with respect to the internal stiffness \( K_{\text{int},0} \).

Note that the load-displacement curve shown for \( \delta W = 20 \), is not smooth but slightly oscillating. This is due to a discretizational error: For small \( \gamma_W \) the surface deformation becomes very large, due to the strong adhesion, such that further mesh refinement is needed to improve the results. The case \( \delta L = 50, \delta = 200 \) and the case \( \delta L = 50, \delta = 20 \) are further examined in the examples of section 8.2.

We further note that for fixed \( \gamma_L \), as is considered here, there is no difference between the macroscopic and microscopic scales of view, as the two become fixed to one another by the

![Figure 7.4: a. Load \( P(u) \) and b. Gap \( g(u) \), both for \( \delta L = 50 \)](image-url)
ratio $\gamma_L$. Figure 7.4 shows the macroscopic scale of view. The microscopic scale of view is obtained by stretching the lengths $u$ and $g$ by $\gamma_L$ and stretching the forces $P$ by $\gamma_L^2$.

### 7.3 Summary

Let us summarize the key observations of the discussion above together with some of the findings of section 3.5 and 5.5:

1. The interaction modelled by the CGC model occurs in three stages: the rigid phase, the adhesion phase and the contact phase. Adhesion is marked by $P_{\text{min}}$; the contact phase is marked by the contact stiffness $k_c$ and the contact gap $g_c$.

2. As $\gamma_L$ changes we have to distinguish between observing the system from the microscopic or macroscopic scales of view as they affect the perceived behavior.

3. As $\gamma_L$ increases the force $P_{\text{min}}$ decreases from the macroscale perspective and increases from the microscale perspective.

4. As $\gamma_L$ increases the contact stiffness $k_c$ at the macroscale is unchanged while the contact stiffness at the microscale increases.

5. From the macroscopic scale of view the contact gap $g_c$ decreases significantly as $\gamma_L$ increases, whereas it only changes slightly from the microscopic scale of view.

6. As $\gamma_W$ decreases the adhesive peak force $P_{\text{min}}$ increases.

7. The contact stiffness $k_c$ and contact gap $g_c$ remain mostly unchanged as $\gamma_W$ changes.

8. The occurrence of unstable behavior during adhesion is characterized by small values of parameter $\gamma_K = \gamma_W / \gamma_L$. The tendency for instability is thus increased for growing $\gamma_L$ and decreasing $\gamma_W$.

Figure 7.5 below quantifies how the changes in $\gamma_L$ and $\gamma_W$ affect the adhesive peak force $P_{\text{min}}$. This quantity is often referred to the ‘pull-off’ force in the literature, since it equals the maximum tensile force required to pull the two adhering bodies apart. Frame (a) shows that, from the macroscopic scale of view, $P_{\text{min}}$ increases approximately linearly with $1/\gamma_L$. The behavior of the force between the two scales of view is

$$\frac{P}{(e_0/r_0)} = \gamma_L^2 \frac{P}{(E_0/R_0)}.$$  \hspace{1cm} (7.1)

It thus follows that, from the microscopic scale of view, $P_{\text{min}}$ increases linearly with $\gamma_L$. Frame (b) shows that for fixed $\gamma_L$ and varying $\gamma_W$ the pull-off force increases linearly with $1/\gamma_W$. Figure 7.6 shows the influence of $\gamma_L$ and $\gamma_W$ on the contact gap $g_c$. The contact gap is not a constant quantity - it changes slightly during the compression of the two bodies. We therefore arbitrarily measure $g_c$ at some common displacement $u$ (which is $u = 0.2R_0$ for (a) and $u = 0.1R_0$ for (b)). Frame (a) shows that $g_c$ increases linearly with the inverse of $\gamma_L$. On the other hand, frame (b) shows that $g_c$ decreases as $\gamma_W$ increases. This relation, however, is neither constant or linear with respect to $\gamma_W$ nor is it linear with respect to
We note that all the results of figures 7.2–7.6 are obtained from a finite element computation using the mesh displayed in figure 7.1 (c).

Let us finally remark on the limits of parameters $\gamma_L$ and $\gamma_W$. If $\gamma_L \to 1$, the sphere contains only few atoms and it will be physically more appropriate to use molecular dynamics. As $\gamma_L$ becomes very large, more and more finite elements are required to resolve the surface interaction and the current formulation becomes inefficient. To regain efficiency for large $\gamma_L$ (say $\gamma_L > 200$) the method can be slightly modified as is discussed in section 9. If $\gamma_W \to 0$, the bodies deform hugely and behave more like fluids instead of solids. The current finite element formulations will become inappropriate and other methods are called for. If $\gamma_W \to \infty$, the bodies become rigid. Then the geometry remains fixed during contact and analytical contact models can be used to describe the problem, such as are discussed in the following section.
8 Applications of the CGC Model

In this section we discuss several applications of the Coarse-Grained Contact Model. We first examine the deformation of a carbon nanotube cross section. The main part of this section is spend on the second example, a comparison of the CGC model with analytical contact theories. The third and last example considers the case of frictionless sliding.

8.1 Carbon Nanotubes

As a first application, we consider the deformation of a (40,40) carbon nanotube (CNT) cross section under plane strain conditions. A review of the mechanical behavior of CNT’s is given in [73]; for a CNT image see figure 1.1 (a). The (40,40) tube consists of a hexagonal graphene structure with 160 carbon atoms around the circumference. The intersolid potential parameters are chosen as $r_\phi = 0.383\text{nm}$ and $\epsilon_\phi = 2.39\text{meV}$. The tube is modelled linear elastically with Young’s modulus $E_Y = 5.0\text{TPa}$, Poisson’s ratio $\nu = 0.19$ and wall thickness $t = 0.075\text{nm}$. See [68] for a proposed range of material parameters. Figure 8.1 shows the undeformed tube (a), its interaction with a rigid graphite substrate (b), with neighboring tubes in a bundle (d) and with itself as it collapses (c). All configurations shown are stable and drawn to scale. The tube is modelled by 40 geometrically exact 2-node beam elements, e.g. see [76], [84], [85] and also [99]. The dots shown in the figures indicate the FE nodes. Using 40 element, the atomic density becomes 4 atoms per element corresponding to a reduction in the dofs by about 2.7 compared to a full molecular simulation. The results shown in fig. 8.1 are in agreement with experimental and computational results from the literature. A MD solution of case (b), the adhesion of the CNT to a rigid substrate can be found in [43] and [44]. Molecular simulation of the collapsing CNT have been obtained by [31] and [91], a finite element solution can be found in [68] and [107]. Experimental data showing the interaction of two CNT’s are found in [79]. We note that, using simplifying assumptions on the geometry, the CNT self-collapse can also be studied by analytical means, e.g. see [35], [91]. We finally note that figure 8.1 (a)

![Figure 8.1: a. Undefomed (40,40) CNT; b. Adhesion of the CNT to a rigid substrate; c. Self-Collapse of the CNT; d. Adhesion of three CNTs](image-url)
and (c) show that the ring itself has two stable equilibrium positions, i.e. the potential energy $\Pi$ has at least two local minima. In principle if we consider a very stiff ring, there will only be one stable configuration, namely the undeformed ring. As the stiffness of the ring becomes softer more local minima of $\Pi$ will appear. For extremely small ring stiffness one can imagine that there are many ‘collapsed’ configurations.

We note that the complex, three dimensional behavior of interacting CNTs, as is for example observed in [72], has been studied in much greater detail by the works of [2], [3], [74], and [75]. The mechanical properties of carbon nanotubes can also be strongly influenced by atomic defects in the graphene structure [106].

8.2 Adhesive Contact of Spheres

In this section we give a comparison between the Coarse-Grained Contact model and prominent analytical contact theories. The earliest treatment of the subject goes back to the contact model obtained by Hertz in 1882, e.g. see [49]. His theory, however, does not account for adhesion between the contacting bodies. In the 1970’s the Hertzian model was extended by the JKR [48] and DMT [25] theories to include adhesion. A controversy ensued on which of the two theories was correct, since they both predict different behavior of the contacting bodies. Only later it was realized that the two models apply to different situations: The JKR model applies to the limit case $\gamma_W \to 0$, when the contacting bodies are very soft, whereas the DMT model applies to $\gamma_W \to \infty$ when the bodies are comparably stiff. In the nineties, Maugis developed a model, based on cohesive fracture, that reconciles the JKR and DMT models: They become special cases of his model, usually referred to as the Maugis-Dugdale (M-D) model. Since these analytical models have been experimentally verified, e.g. see [48], [56], they are used in the following to validate the CGC model. We note that the analytical theories mentioned above are restricted to infinitesimal deformations, linear elasticity and simple geometry, such as the contact between two spheres – limitations that do not restrict the CGC model.

8.2.1 Analytical Contact Models

Figure 8.2 (a) shows a description of spherical contact. Here $E_1$, $E_2$, $\nu_1$ and $\nu_2$ denote the Young’s moduli and Poisson’s ratios of the two contacting, elastic bodies. Their radii are given by $R_1$ and $R_2$. Note that $R_2 = \infty$ corresponds to an infinite half-space. The force pressing the two bodies together is denoted by $P$. It is commonly considered as positive in compression. Due to the elastic deformation of the solids, the two spheres approach each other under compression. In the far-field this approach is denoted by $\delta$. For isotropic spheres the contact surface is a circle with diameter $2a$. The normalized contact pressure $p$ between the two contacting bodies is displayed in figure 8.2 (b). It illustrates the differences of the four analytical contact models. According to the Hertz and the DMT model the pressure distribution is elliptical and positive (i.e. compressive) throughout the contact zone. In case of the JKR model the contact pressure turns negative (i.e adhesive) at the fringe of the contact zone. At $r = a$, the pressure is singular, indicating a drawback of the JKR model. According to the M-D model the pressure extends beyond the contact zone, $a$, taking the constant value $p = -\lambda$ for $a \leq r \leq ma$, where $m > 1$ is a parameter of this model.
In the following we outline the Hertz, JKR, DMT and M-D theories, e.g. see [64], [51]. We start by defining the combined elastic modulus
\[ E := \left( \frac{1 - \nu_1^2}{E_1} + \frac{1 - \nu_2^2}{E_2} \right)^{-1}, \] (8.1)
and the reduced radius
\[ R := \left( \frac{1}{R_1} + \frac{1}{R_2} \right)^{-1}. \] (8.2)
Further we consider the normalization of the force \( P \), the contact radius \( a \), the approach \( \pm \) and the pressure \( p \) as
\[ \bar{P} := \frac{P}{\pi w R}, \quad \bar{a}^3 := a^3 \frac{4E}{3\pi w R^2}, \quad \bar{\delta}^3 := \delta^3 \frac{16E^2}{9\pi^2 w^2 R}, \quad \bar{p}^3 := p^3 \frac{9R}{2\pi w E^2}, \] (8.3)
where \( w \) is the work of adhesion which is measured in units of energy per surface area. It is defined as the work required to separate two bodies adhering over a unit area from their equilibrium position to infinity [46]. It is similar to the surface energy, which is defined as the work necessary to increase the surface area of a body, and which can be viewed as the work required to separate two bonded parts of the body.

According to the Hertz theory we have
\[ \bar{P}(\bar{a}) = \bar{a}^3, \quad \bar{\delta}(\bar{a}) = \bar{a}^2, \] (8.4)
i.e. the force increases cubically, while the approach increases quadratically with increasing contact radius \( a \). Combining these two expressions one arrives at the load displacement curve \( \bar{P} = \bar{P}(\bar{\delta}) \). By substituting (8.3) into (8.4) it can be noted that the work of adhesion \( w \) has no influence on the model. For the Hertz model the pressure distribution within the contact area is given by
\[ \bar{p}(r) = \frac{3\bar{a}}{\pi} \sqrt{1 - \left( \frac{r}{\bar{a}} \right)^2}, \quad \text{for} \quad r \leq a. \] (8.5)
Outside the contact area, i.e. for \( r > a \), the pressure is zero.

For the JKR theory we have the two relations
\[ \bar{P}(\bar{a}) = \bar{a}^3 - \sqrt{6\bar{a}^3}, \quad \bar{\delta}(\bar{a}) = \bar{a}^2 - \frac{2}{3} \sqrt{6\bar{a}}, \] (8.6)
which depend on the work of adhesion since \( w \) does not cancel as it does for the Hertz formula.

For the DMT model the corresponding relations between force \( P \), approach \( \delta \) and contact radius \( a \) are

\[
P(\bar{a}) = \bar{a}^3 - 2, \quad \delta(\bar{a}) = \bar{a}^2,
\]

(8.7)

which also depend on \( w \).

To state the M-D model we require the transition parameter

\[
\lambda := \sigma_0 \sqrt{\frac{3R}{2\pi wE^2}}.
\]

(8.8)

It is dimensionless and corresponds to the normalization of \( \sigma_0 \), which is the constant value of the adhesive stress within \( a \leq r \leq ma \). Letting \( \lambda \to \infty \) yields the JKR model, while \( \lambda \to 0 \) gives the DMT case. Given \( \lambda \) and the contact radius \( \bar{a} \), one can solve the transcendental equation

\[
\frac{\lambda \bar{a}^2}{2} \left( \sqrt{m^2 - 1} + (m^2 - 2) \arctan \left( \frac{\sqrt{m^2 - 1}}{m} \right) \right) + 4\lambda \bar{a} \left( \sqrt{m^2 - 1} \arctan \left( \frac{\sqrt{m^2 - 1}}{m - 1} \right) - m + 1 \right) = 1,
\]

(8.9)

for the parameter \( m \). This parameter corresponds to the ratio of the Hertzian contact radius \( a \) and the contact radius \( ma \) of the M-D model, as is illustrated in figure 8.2 (b). The JKR model is obtained from \( m \to 1 \) while \( m \to \infty \) corresponds to the DMT model. For the M-D model the relation between force, approach and contact radius are, for a given \( \lambda \),

\[
P(\bar{a}) = \bar{a}^3 - \lambda \bar{a}^2 \left( \sqrt{m^2 - 1} + m^2 \arctan \left( \frac{\sqrt{m^2 - 1}}{m^2 - 1} \right) \right),
\]

\[
\delta(\bar{a}) = \bar{a}^2 - \frac{4}{3} \bar{a} \lambda \sqrt{m^2 - 1}.
\]

(8.10)

Further, for a given parameter \( \lambda \) and contact radius \( \bar{a} \), the radial pressure distribution is

\[
\bar{p}(r) = \frac{3\bar{a}}{\pi} \sqrt{1 - \left( \frac{r}{\bar{a}} \right)^2} - \frac{2\lambda}{\pi} \arctan \sqrt{\frac{m^2 - 1}{1 - \left( \frac{r}{\bar{a}} \right)^2}}, \quad \text{for } r < \bar{a},
\]

\[
\bar{p}(r) = -\lambda, \quad \text{for } a \leq r \leq ma.
\]

(8.11)

The load displacement curves \( \bar{P} = \bar{P}(\delta) \), described implicitly by eqs. (8.4), (8.6), (8.7) and (8.10) for the four models, are displayed in figure 8.3 (a). It can be observed that for the Hertz model \( \bar{P} \geq 0 \), since no adhesion occurs. It can further be seen that the M-D model poses a transition between the JKR and DMT models. The pressure distribution \( \bar{p}(r) \) according to eqs. (8.5) and (8.11) is displayed in figure 8.2 (b). As a further distinction, the four models – Hertz, JKR, DMT and M-D – can be arranged in a so-called ‘adhesion map’ [51], which identifies the appropriate model in dependence of the normalized contact load \( \bar{P} \) and the strength of adhesion represented by parameter \( \lambda \).

We are further interested in the stress field inside the elastic half-space due to the surface pressure \( p(r) \). It can be obtained by integrating the known solution for a point load acting on a half-space. As an example, the vertical stress component \( \sigma_z \) at point \( Y \) (see figure 8.3 (b)), due to a concentrated point load \( P' \) at point \( X \) \((r = 0, \ z = 0)\), is given (in cylindrical coordinates \( \{r, \varphi, z\} \)) by

\[
\sigma_z(r, z) = \frac{3P' z^3}{2\pi \rho^5},
\]

(8.12)
where \( \rho^2 := r^2 + z^2 \), e.g. see [95] or [49]. The stress field has a singularity beneath the applied point load, which vanishes in the following integration. Integrating the stress field (8.12) for all point loads \( P' = p(s) dA \), with \( dA = s d\varphi ds \) and \( p(s) \) from eq. (8.11), yields

\[
\sigma_z(r, z) = \int_A \sigma_z' = -\frac{3}{\pi} \int_0^c s \, p(s) \int_0^{\pi} \frac{z^3}{\rho^5} \, d\varphi \, ds ,
\]

where \( \rho^2 = r'^2 + z^2 \) and \( r'^2 = r^2 - 2rs \cos \varphi + s^2 \) according to figure 8.3 (b). Due to the complexity of the integrand, eq. (8.13) is evaluated numerically. It may be noted that at the surface \( (z = 0) \) we must have \( \sigma_z(r, 0) = -p(r) \), so that we can avoid evaluating the integrand at the surface, where it turns singular.

### 8.2.2 Formal relation between the M-D and CGC Models

In order to relate the two models we have to identify the work of adhesion \( w \) in the CGC model. Recall that \( w \) is defined as the work per unit surface area required to separate two adhering bodies from their equilibrium position to infinity. In the derivation of Method 3 in section 4.3 we obtained the force \( F_S \) (4.46). It corresponds to the force exerted upon the surface element \( da_k \) of body \( \Omega_k \) due to the presence of the neighboring body \( \Omega_{\ell} \). The work of adhesion is thus defined as

\[
w := -\beta_k \int_{rS,0}^{\infty} F_S(r) \, dr ,
\]

where \( rS,0 \) is the equilibrium distance of the two neighboring bodies which follows from the condition \( F_S = 0 \) as \( rS,0 = r_0 / \sqrt{15} \). It is sensible to consider the reference configuration in eq. (8.14) so that we use \( \beta_{10} \) and \( \beta_{20} \) instead of \( \beta_1 \) and \( \beta_2 \) in the definition above. Without this approximation the work of adhesion becomes dependent on the local deformation and we cannot associate \( w \) with a material constant anymore, as is usually considered. For the case \( \beta_{10} = \beta_{20} = \beta_0 \) equation (8.14) is evaluated as

\[
w = f_w \beta_0^2 \epsilon \, r_0^4 ,
\]
where we have introduced the constant \( f_w := \frac{\pi}{8} \sqrt{15} \). In view of definition (3.58) we thus have the identity

\[
w R_0^2 = f_w \Pi_{C,0} ,
\] (8.16)
i.e. the interaction energy \( \Pi_C \) is proportional to the work of adhesion \( w \) multiplied by the area \( R_0^2 \).

Further, we need to establish a link between the normalization of the CGC model, as discussed in section 3.5, and the normalization of the M-D model defined by eq. (8.3). For this we consider the specific problem displayed in figure 8.2 and particularized by \( E_Y := E_1 = E_2, \nu := \nu_1 = \nu_2, R_1 = R_0, R_2 = \infty \) and \( \beta_0 := \beta_{10} = \beta_{20} \). According to eqs. (8.1) and (8.2) we thus have \( E = f_E E_1 \), for \( f_E := \frac{1}{2(1-\nu_1^2)} \), and \( R = R_0 \). As derived in section 3.5 the CGC model is normalized by the parameters \( \bar{R}_0 \) and \( \bar{E}_0 := \int_0 \bar{E} \bar{R}^3 \), so that the normalization of a force \( F \) becomes \( \bar{F}_C = \bar{R}_0 / \bar{E}_0 F \), where the bar and subscript \( C \) are used to indicated the normalization scheme of the CGCM. The normalized force \( \bar{F}_{MD} \), as used by the Maugis-Dugdale and related models, is given by eq. (8.3). From eqs. (8.16) and (3.60) it thus follows that

\[
\bar{F}_C = f_F \bar{F}_{MD} , \quad f_F := \frac{\pi f_w}{\gamma w \gamma L} ,
\] (8.17)
i.e. we have established the factor \( f_F \) relating the two normalization schemes. Likewise we treat the normalization of a length, given by \( \bar{L}_C = L / \bar{R}_0 \) for the CGCM and given by eqs. (8.3) and (8.3) for the contact radius \( a \) and approach \( \delta \) within the M-D model. Now by using eqs. (8.16), (3.60) and the definition of \( f_F \) we establish the relation between the normalization of the contact width

\[
\bar{a}_C = f_a \bar{a}_{MD} , \quad f_a := \frac{3}{2} f_F f_E ,
\] (8.18)
and the relation between the normalization of the approach

\[
\bar{\delta}_C = f_\delta \bar{\delta}_{MD} , \quad f_\delta := f_a^2 .
\] (8.19)

Finally the relation between the stress normalization is obtained as

\[
\bar{\sigma}_C = f_\sigma \bar{\sigma}_{MD} , \quad f_\sigma := \frac{3}{2} \sqrt{\frac{2}{5}} f_F f_E^2 ,
\] (8.20)
where \( \bar{\sigma}_C = \sigma \bar{R}_0^3 / \bar{E}_0 \) is the stress normalization within the CGCM and where \( \bar{\sigma}_{MD} \) is the normalized stress of the M-D model, given by eq. (8.3).

With equations (8.17)-(8.20) we have established the formal relation between the two models, the analytical M-D model (which contains the JKR and DMT models as special cases) and the computational CGC model. Before comparing these, let us summarize their key features:

The M-D model only contains one free parameter, namely the transition parameter \( \lambda \). Physically it corresponds to a normalization of the peak attractive surface stress \( \sigma_0 \), a quantity that may be difficult to assess experimentally. Further, the parameter \( \lambda \) is assumed fixed for a given material, a restriction which breaks down during the adhesion phase when the peak adhesion has not yet been attained. The analytical contact theories are only defined as long as an area of contact, represented by the contact radii \( a \) and \( c = ma \), is given. As
such a concept breaks down during separation of the bodies, the analytical contact theories can’t capture the adhesive interaction of separated bodies. The load-displacement curves of the Hertz, JKR, DMT and M-D theories, shown in figure 8.3 (a), all terminate even though, the interaction continues to act weakly over much larger distances, as is indicated by the following computational result obtained from the CGC Model. For these reasons, the analytical models cannot be expected to be very accurate during the adhesion phase. These models are further restricted to linear elasticity and infinitesimal deformations, so that we cannot expect them to perform well as the deformation becomes large.

The Coarse-Grained Contact Model, on the other hand, is a large deformation model which accurately captures the long-range interaction during the adhesion phase. Fully normalized, it depends on two parameters, the length scale $\gamma_L$ and the energy density ratio $\gamma_W$, which give the model greater flexibility in modelling adhesive contact. It is further emphasized that the CGCM is a model formulated for arbitrary geometry, whereas the M-D model applies only to particular cases like the spherical contact considered above.

### 8.2.3 Comparison between the M-D and CGC Models

Let us now compare the behavior of the analytical M-D model, discussed above, and the Coarse-Grained Contact Model. The M-D model is linear elastic, for the CGC model we choose the Neo-Hookean relation discussed in section 3.2.1. Poison’s ratio is chosen as $\nu = 0.2$.

As a first example we pick the parameters $\gamma_L = 50$ and $\gamma_W = 200$, a case which has also been studied in sections 7.1 and 7.2. The results for this case are displayed in figure 8.4. Frame (a) shows the load-displacement curve $P(u)$ of the computational and the four analytical models, the Hertz, JKR, DMT and M-D theories. The agreement between the CGC and M-D models is excellent over a wide range of displacements. As the approach grows large the M-D model loses its accuracy since the small deformation assumption is violated. As has been mentioned earlier the M-D model is not defined for large separations, so that for this situation ($u < 0$) only the computational CGCM result exists. As the bodies are pulled apart their interaction decays smoothly but, in principle, remains non-zero for arbitrary large distances, an effect which is failed to be captured by the M-D model. Frame (b) shows the normal pressure distribution $p(r)$ acting on the surface of the two opposing bodies. It is taken from the state $u \approx 0.043R_0$ and $P \approx 5.8 \cdot 10^{-3}E_0/R_0$, shown as a red dot on the $P(u)$ curve. This state corresponds to a contact radius of $a \approx 0.23R_0$ in the M-D model. In the compressive ($p > 0$) regime we observe excellent agreement between the two models. In the tensile regime ($p < 0$), it is seen that the pressure distribution of the CGCM is continuous and decays smoothly to zero, whereas the pressure distribution of the M-D model is discontinuous and drops to zero abruptly. In all results presented on this first example, the parameter $\lambda$ of the M-D model, which corresponds to the tensile stress level, is chosen on a best fit basis as $\lambda = 0.25$.

Frame (c) and (d) show the vertical stress component $\sigma_z$ of the two models, which are also in excellent agreement, even quantitatively. The same state $\{P, u\}$ as above is chosen. For the chosen parameters $\gamma_L$, $\gamma_W$ the tensile, adhesive stresses, which are present at the fringe of the contact zone, are small compared to the compressive stresses. The CGCM result is obtained form a finite element solution with the mesh shown in figure 7.1 (a), the M-D result is obtained from the numerical evaluation of eq. (8.13).
As a second example we pick $\bar{\gamma}_L = 50$ and $\bar{\gamma}_W = 20$, that is the bodies are now softer than in the first example. For this second case a physical instability exhibits itself during contact, as has been discussed before in sections 5.2 and 7.2. The results for this case are displayed in figure 8.5. In frame (a) the load-displacement curves $P(u)$, as obtained by the two models, are compared. Their overall agreement is very good. The physical instability displays the characteristic looping behavior, where for a given displacement $u$ we have three possible loads $P$. As has been remarked earlier the analytical contact theory cannot capture the adhesive phase accurately. Therefore differences between the analytical and computational results are inevitable. The path of $P(u)$, as obtained by the CGCM, is also supported by the numerical results reported in [39], which are based on infinitesimal theory. Frame (b) shows the normal pressure distribution $p(r)$ acting on the surface of the two opposing bodies. Again we observe excellent agreement. Now, the adhesive pressure is much larger than for the first example. Its magnitude dominates over the compressive pressure. The pressure is taken at the state $u \approx 0.042R_0$ and $P \approx 0$, indicated by the red dot on the $P(u)$ curve. The M-D results are obtained for the choice $a \approx 0.33R_0$. Since $P = 0$ the
vertical component of the shown pressure distribution integrates to zero. In all the results
presented on the second example, the parameter $\lambda$ of the M-D model is chosen on a best
fit basis as $\lambda = 1.3$. Frames (c) and (d) show the excellent agreement of the vertical stress
component $\sigma_z$ of the two models. Note the large local, adhesive stress peak developing
between the two contacting bodies. To capture this stress peak and the associated strong
deformation, a highly resolved FE mesh is needed. The mesh used in this computation is
displayed in figure 7.1 (c) and (d). The stress distribution $\sigma_z$ is computed at the same state
$\{P, u\}$ considered for the pressure distribution of frame (b). It is noted that for $\gamma_W = 20$
the bodies are so soft that their adhesion leads to a strong bulging deformation of the two
opposing surfaces, as can be seen in frame (d). This follows from the fact that the stiffness
ratio $\gamma_K$ (measuring the softness of the contacting solids) decreases along with $\gamma_W$. For low
$\gamma_W$ the behavior of the M-D comes very close to the behavior of the JKR model.
For the example of figure 8.5, the evolution of the deformation and stress distribution $\sigma_z$ of
the two contacting bodies is shown in figure 8.6. The five states displayed in frames (b)–(f)
correspond to the red dots shown on the load-displacement curve shown in frame (a). In

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Figure 8.6: a. Load-displacement curve for $\bar{\gamma}_L = 50$, $\bar{\gamma}_E = 20$; b.-f. Deformation and stress field $\sigma_z$ during adhesive contact at the states shown as red dots in (a).

particular, note that for the state in frame (e), the net force acting between the two bodies is zero. In other words the surface traction acting on the two opposing surfaces integrate to zero exactly. For state (f) the net force is compressive whereas for states (b), (c) and (d) the net force is tensile. The largest tensile force occurs at state (d).

8.3 Frictionless Sliding

The last example considered, demonstrates that Method 3 does not invoke tangential forces along the contact surface, so that any occurring sliding along the interface is frictionless and thus an energy conserving process. We consider the sliding contact of two parabola-shaped bodies as shown in figure 8.7. Such a contact mechanism can occur between the surface asperities of two sliding, rough bodies. In this example, the upper asperity is considered rigid. In this case the contact formulation of Method 3, chosen here, is comparably easy to implement. Frames (a)–(c) show the deformation and vertical stress component $\sigma_y$ within the lower asperity. The lower body is pushed at its base by an imposed displacement $u$. The resultant horizontal reaction at this boundary, $P$, as a function of $u$ is shown in frame (d). The open circles correspond to the three configurations shown in frames (a)–(c). The lower asperity is moved from left to right and it is undeformed and stress free at the beginning and the end of this process. The work required to move the asperity is given by the area
The problem is considered as a plane strain problem with the chosen parameters $\gamma_L = 20$, $\gamma_W = 100$ and $\nu = 0.3$. The bottom asperity is modelled elastically by the Neo-Hookean constitutive relation (3.33).

If dissipative processes are considered, e.g. through an inelastic material response, the total energy of this sliding example is not conserved. One may thus model global sliding friction, even when no sliding friction occurs locally.

under $P(u)$. It can be confirmed numerically that the total work for this process is identical to zero, i.e. the considered process, and thus the contact formulation of Method 3, is energy conserving. Five quadrature points per surface element are used to integrate $f_{C,k}$ (4.45).
9 Going from Nanocontact to Macrocontact

Initially, the Coarse-Grained Contact Model has been developed to investigate contact at the nanoscale, (i.e. nm-scale), and we have, so far, focused on this case exclusively. In this section we study the application of the proposed model to the contact at larger scales, like the μm- and mm-scale. It is argued below, that for increasing length scales, the CGCM becomes either inefficient or ill-conditioned. In this section we propose a simple modification of the CGC Model for increasing scales, which avoids ill-conditioning while maintaining efficiency and accuracy.

9.1 Effective Force Function

It has been argued that as the length scale increases the direct formulation of Method 1 should be replaced by the approximations of Methods 2 and 3. In Method 3 the interaction between neighboring bodies is formed by the interaction of the neighboring surfaces. As this formulation is best suited for larger scales we will base the modification on Method 3. The idea of this modification is very simple: instead of using the original force function \( F_S \) (4.46) to compute the contact integral \( f_{c,k} \) (4.45), we will use a modified, effective force function \( F_e \). By this modification we introduce an approximation, whose accuracy can be quantified as is shown later. The reason for introducing such a modification can be illustrated by figure 9.1. Frame (a) shows the original force function \( F_S \) versus \( r/r_0 \) as a well behaved smooth function. As \( r_0 \) is usually of the order of nanometers, we are looking at a nanoscale picture of \( F_S \). Frame (b) on the other hand shows \( F_S \) from a much larger scale at which \( F_S \) appears highly irregular and non-differentiable: as \( r \) decreases \( F_S \) is mostly zero until it suddenly explodes at \( r = 0 \). We are thus faced with a dilemma for computations at larger scales: We either need a very fine FE mesh and small time step \( \Delta t \) to resolve \( F_S \), which will make the solution very costly, or, using a coarse mesh and large step size \( \Delta t \) for efficiency, we run into ill-conditioning and loss of convergence of the numerical solution procedure. We therefore introduce a smoother, effective force function \( F_e \), as it is shown in frame (b), so that the simulation retains efficiency without becoming ill-conditioned.

We obtain \( F_e \) by a ‘coarse-graining’ of \( F_S \), similar to the coarse-graining procedure initially used to derive the CGC model from molecular dynamics (see appendix A). Since \( F_S \) is only defined for \( r \geq 0 \) we perform the coarse-graining at the \( \ln(r) \) scale. Hence, we introduce the variable

\[
\hat{r} := \ln \frac{r}{r_0}, \quad (9.1)
\]

and use it to define the coarse-graining operation of a function \( f(\hat{r}) \) as (see also eq. (A.9))

\[
f_e(\hat{r}) := \int_{\hat{r}}^{\infty} \delta_\eta(\hat{y}) f(\hat{x}) \, d\hat{x}, \quad (9.2)
\]

where \( \hat{y} = \hat{x} - \hat{r} \) and where the Gaussian distribution

\[
\delta_\eta = \frac{1}{\sqrt{\pi} \eta} \exp \left( - \frac{\hat{y}^2}{\eta^2} \right), \quad (9.3)
\]

is the chosen coarse-graining function. For a discussion on definition (9.2) and its dependence on the coarse-graining parameter \( \eta \) see section A.2 and figure A.1. A graph of \( \delta_\eta \) for
\( \eta = 1.75 \) is shown in figure 9.1 (a). Given \( \hat{r} \), the force function of Method 3,

\[
F_S(r) = \pi \beta_3 r^3 \left[ \frac{1}{45} \left( \frac{r_0}{r} \right)^9 - \frac{1}{3} \left( \frac{r_0}{r} \right)^3 \right],
\]

(9.4)
can be written as

\[
\tilde{F}_S(\hat{r}) = F_0 \left[ \frac{1}{45} e^{-9\hat{r}} - \frac{1}{3} e^{-3\hat{r}} \right],
\]

(9.5)

with \( F_0 = \pi \beta_3 r_0^3 \). (In the last equation we have introduced the tilde to distinguish the functions \( F_S(r) \) and \( \tilde{F}_S(\hat{r}) \).) According to eq. (9.2) we thus obtain the effective force as

\[
\tilde{F}_e(\hat{r}) := \int_{\infty}^{-\infty} \delta_\eta(\hat{y}) \tilde{F}_S(\hat{x}) \, d\hat{x}
\]

(9.6)

\[
= \frac{F_0}{45} \int_{\infty}^{-\infty} \delta_\eta(\hat{y}) e^{-9\hat{y}} \, d\hat{x} - \frac{F_0}{3} \int_{\infty}^{-\infty} \delta_\eta(\hat{y}) e^{-3\hat{y}} \, d\hat{x}.
\]

It can be shown (see remark below) that

\[
\int_{-\infty}^{\infty} \delta_\eta(\hat{y}) e^{\alpha \hat{y}} \, d\hat{y} = c \, e^{\alpha \hat{r}},
\]

(9.7)

with the constant \( c = e^{a^2 \eta^2 / 4} \), so that we find

\[
F_e(r) = F_0 \left[ \frac{1}{45} \left( e^{\frac{9\eta^2}{4} \frac{r_0}{r}} \right)^9 - \frac{1}{3} \left( e^{\frac{3\eta^2}{4} \frac{r_0}{r}} \right)^3 \right].
\]

(9.8)

It is noted that when \( \eta \to 0 \) we have \( F_e \to F_S \), i.e. the effective force contains \( F_S \) as a limit case. Figures 9.1 (b) and (d) show the effective force function \( F_e \) for the four cases \( \eta = \{1.75, 1.86, 1.94, 2.02\} \), i.e \( \exp(9/4 \eta^2) = \{1000, 2500, 5000, 10000\} \). It is seen that for increasing \( \eta \), the function \( F_e \) is shifted to the right. This offset will lead to an increase in the gap \( g \) between the two contacting bodies, as is discussed in the following section. To formally compare the original function \( F_S \) with the modified function \( F_e \) let us consider the equilibrium distance of \( F_e \)

\[
r_{e,0} = \frac{e^{3\eta^2}}{\sqrt[15]{5}} r_0,
\]

(9.9)

for which \( F_e = 0 \), the work of adhesion

\[
w = -\beta_k \int_{r_{e,0}}^{\infty} F_e(r) \, dr = F_0 \beta_k r_0 \frac{\sqrt[15]{5}}{8} e^{-\frac{15}{4} \eta^2},
\]

(9.10)

according to eq. (8.14), and the absolute minimum of \( F_e \) given by

\[
F_{e,\min} = \frac{-2\sqrt[5]{5}}{9} F_0 e^{-\frac{27}{4} \eta^2}.
\]

(9.11)

It can be seen that for increasing \( \eta \), both \( w \to 0 \) and \( F_{e,\min} \to 0 \), while \( r_{e,0} \to \infty \). In other words the adhesive contribution to \( F_e \) completely vanishes as \( \eta \) increases. This is confirmed by the four curves of \( F_e \) shown in frame (b): the attractive part of \( F_e \) has become insignificant compared to the level of attraction present in \( F_S \). While the attractive part
vanishes the repulsive parts of $F_S$ and $F_e$ display an interesting similarity at different scales. For example if $\eta = \sqrt{4/3 \ln 10} = 1.752$, i.e. $\exp(9/4\eta^2) = 1000$, then the force function $F_e$ viewed at the scale $1000r$ is similar to $F_S$ viewed at the scale $r$. This case is shown in frame (c). Formally, this similarity can be expressed as

$$F_{e,R}(cr) = F_{S,R}(r) \quad c = e^{\frac{9}{4}\eta^2},$$  \hspace{1cm} (9.12)

where

$$F_{S,R}(r) = \frac{F_0}{45} \left( \frac{\tau_0}{r} \right)^9, \quad F_{e,R}(r) = \frac{F_0}{45} \left( e^{\frac{9}{4}\eta^2} \frac{\tau_0}{r} \right)^9,$$  \hspace{1cm} (9.13)

denote the repulsive parts of $F_S$ and $F_e$. Eq. (9.12) states that the modified system experiences the same force at $cr$ than the original system experiences at $r$. From eq. (9.12) we can further deduce that the change $\Delta F_{e,R}$ at $cr$ within the increment $c \Delta r$ is equal to the change $\Delta F_{S,R}$ at $r$ within the increment $\Delta r$.

We summarize that by coarse-graining $F_S$ according to operation (9.6), we have obtained the effective force function $F_e$. Physically, this modification is motivated by the notion that a coarser description of the problem (e.g. coarser FE mesh) should also ‘feel’ a coarser
interface force $F_e$. This coarsening is useful for problems at large scales, when it is inefficient to refine the description of the problem such that $F_S$ can be resolved. As the scale of a problem increases we simply use the effective function $F_e$ with increasing $\eta$. In doing so the repulsive behavior of the interface force is retained while the attractive part is gradually lost, which is in agreement with common experience.

**Remark**: Proof of eq. (9.7).
It is first noted that the Gaussian distribution $\delta_\eta$ satisfies the normalization property

$$1 = \int_{-\infty}^{\infty} \delta_\eta(\hat{y}) \, d\hat{y} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\xi^2} \, d\xi,$$

where we have substituted $\xi = \hat{y}/\eta$. We thus have

$$\int_{-\infty}^{\infty} \delta_\eta(\hat{y}) \, e^{a \hat{x}} \, d\hat{x} = e^{a \hat{r}} \frac{1}{\sqrt{\pi \eta}} \int_{-\infty}^{\infty} e^{-\hat{y}^2/\eta^2} \, e^{a \hat{y}} \, d\hat{y}$$

$$= e^{a^2 \eta^2/4} \, e^{a \hat{r}} \frac{1}{\sqrt{\pi \eta}} \int_{-\infty}^{\infty} e^{-(\hat{y}/\eta - a\eta/2)^2} \, d\hat{y}$$

$$= e^{a^2 \eta^2/4} \, e^{a \hat{r}} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-z^2} \, dz = e^{a^2 \eta^2/4} \, e^{a \hat{r}},$$

where we have substituted $z = \hat{y}/\eta - a\eta/2$ and used eq. (9.14) in the last line. □

### 9.2 Numerical Comparison

In the following we show that using the effective force function $F_e$ instead of $F_S$ can greatly increase the FE efficiency while maintaining excellent accuracy. We consider the contact between sphere and half-space (as considered in sections 7 and 8.2) with the parameters $\gamma_L = 200$, $\gamma_W = 200$ and $\nu = 0.2$. The results are displayed in figure 9.2. We first consider the case of using the original force function $F_S$ as given by eq. (9.4). Frames (a) and (c) show the deformation and stress invariant $I_1$ of the two contacting bodies. The red curve in frames (d), (e) and (f) shows the load $P(u)$ and the gap $g(u)$ in dependence of $u$. Enlargement (c) shows that the gap between the two bodies is very small: it is of the order $O(1000)$ times smaller than the sphere radius $R_0$. (As the gap is usually nanoscale in proportions the problem size is now on the order of $\mu$m.) Due to the tiny size of the gap, a highly refined FE mesh and very small load increments $\Delta u$ are required computationally, as is shown in table 9.1. Secondly, we consider the case of using the modified, effective

<table>
<thead>
<tr>
<th></th>
<th>original $F_S$</th>
<th>modified $F_e$</th>
</tr>
</thead>
<tbody>
<tr>
<td>number of elements</td>
<td>1408</td>
<td>728</td>
</tr>
<tr>
<td>max. step size $\Delta u$</td>
<td>0.005</td>
<td>0.05</td>
</tr>
<tr>
<td>CPU time</td>
<td>735s</td>
<td>21s</td>
</tr>
</tbody>
</table>

Table 9.1: Efficiency gain from using the effective force function $F_e$.

For this we pick $\eta = \sqrt{4/9\ln 10}$, such that $\exp(9/4\eta^2) = 10$, i.e. the
proportionality constant in eq. (9.12) is \( c = 10 \). As the gap \( g \) is determined by the repulsive interface forces, it can thus be expected that the gap also increases by a factor of 10. This is confirmed by the results of frame (b), which shows the deformation and stress \( I_1 \) for the second case. Due to the increase in \( g \) a coarser mesh and much larger steps \( \Delta u \) can be used, as is listed in table 9.1. The agreement observed in frames (a) and (b) between the two cases is excellent. The load-displacement and gap-displacement curves for the modified case are displayed in blue in frames (d)-(f). The agreement between the red and blue curves is remarkably good, in particular for large indentation depths. Frame (e) shows an enlargement of \( P(u) \) for the adhesion phase. It can be seen that the modified method captures the behavior of the original \( P(u) \) up to a tolerance of about 0.005\( R_0 \). Due to this tolerance, the attractive hump shown in frame (e) is lost, however the overall behavior, shown in frame (d), is excellent. The tolerance in the gap is even lower. It is noted that the blue curve in frame (f) has been divided by the factor of 10 for comparison. Further in frame (d), the blue curve is offset horizontally by 9/10 of the gap. Since the factor of 10 is known a priori by the choice of \( \eta \), the modified solution can be used to predict the behavior of the original solution up to the noted tolerance.

By the above comparison we have demonstrated that the modified force function \( F_e \) can be used to efficiently and accurately obtain the behavior of the original problem up to a certain tolerance. This tolerance depends on the parameter \( \eta \), so that by choosing \( \eta \), a given problem can be computed efficiently up to any desired accuracy \( \eta \rightarrow 0 \) yields the original, exact scheme. For truly macroscopic problems (e.g. \( \gamma_L > 1000 \)) the increase in efficiency will be even more dramatic. A reason why the presented modification works so well is the fact that the spatial distribution of the gap \( g \) between the two contacting bodies is nearly constant, even though the contact tractions vary strongly. The modification can then be viewed as the removal of a thin, constant slice of the surface of the two contacting bodies and attributing it to the newly expanded gap.
Figure 9.2: Deformation and stress $I_1$ for: a. the original method; and b. the modified method; c. Enlargement of (a.); d. Load $P(u)$; e. Enlargement of (d.) ; f. Gap $g(u)$ ;
10 Conclusion

10.1 Review

In this work we have presented, derived and studied a large deformation, computational, quasi-continuum contact approach, which is based on interatomic interactions. These are modelled by two potentials: the intersolid potential $\phi$, governing the interaction of atoms of two distinct bodies, and the intrasolid interaction potential $\psi$, governing the interaction of particles within each body. The interatomic interactions are homogenized, or coarse-grained to obtain an effective hyperelastic continuum contact description, and the model is thus termed the Coarse-Grained Contact Model.

As outlined in section 2, the proposed model takes its place between the common molecular dynamics and the continuum mechanics approaches, and therefore its governing equations can be derived from both these descriptions, as is discussed in section 3 and appendix A. In both cases it is shown that the CGC model can be formulated as a variational principle governing a conservative system. The model is formulated for three-dimensional, hyperelastic solids of arbitrary geometry. Two types of constitutive relations are considered, the Cauchy-Born rule, based on the atomic structure of the solids, and the empirically motivated Neo-Hookean model.

In section 4 the implementation of the model within the finite element formulation is discussed. To treat the contact interaction forces, three implementations are presented: Method 1, a volume interaction formulation, Method 2, a surface interaction formulation, and Method 3, a point interaction formulation. Compared to a molecular description, the three formulations are marked by increasing efficiency, while at the same time being remarkably accurate. A comparison and efficiency assessment of the three methods and a molecular simulation is shown in section 5. This section also illustrates the general behavior of the CGC model and addresses physical and numerical instabilities that can arise. Further, in section 6, the accuracy and consistency of the proposed contact formulation is investigated by means of a contact patch test. It is shown that Method 3 is an accurate and consistent nanoscale contact formulation.

Fully normalized, the behavior of the CGC model is governed by two parameters: $\gamma_L$, which describes the overall problem size, and $\gamma_W$, which is a relative measure between the amount of energy stored in the deformation of the solids and the amount of energy stored in the contact interface. Section 7 presents an extensive investigation of the behavior of the CGC model over a wide range of parameters $\gamma_L$ and $\gamma_W$. It is shown that some of the characteristics of the CGC model, like the strength of adhesion, are scale dependant, while other characteristics, like the macroscopic contact stiffness, are not.

In section 8 several applications of the CGC model are considered: we illustrate the deformation and interaction between carbon nanotubes, we discuss a comparison of the CGCM with several analytical adhesive contact theories, like the JKR and Maugis-Dugdale models, and we consider a simple frictionless sliding example. These results are in agreement with experimental and numerical findings reported in the literature, thus validating the proposed CGC model.

In section 9 we show that the CGC model, which is originally designed to describe the interaction of nanoscale bodies, can be applied to macroscale contact problems. This is achieved by introducing a simple modification of the CGC model, which effectively cor-
responds to a second level of homogenizing, or coarse-graining, of the atomic interaction forces. With this modification the proposed model becomes applicable to large deformation contact/interaction problem over a wide range of length scales: at the nanometer scale the model presents an efficient alternative to molecular simulations, while at the macroscale the model presents a physically motivated alternative to currently used contact models.

10.2 Outlook

While we have shown that the CGC model is an efficient and accurate alternative to model contact/interaction problems over a wide range of length scales, it can nevertheless be improved in multiple ways.

First, the physical modelling can be extended both on the constitutive (i.e. intrasolid) and on the interaction (i.e. intersolid) level. Examples for the former include the study of inelastic processes, like viscoelasticity or plasticity, e.g. through the homogenization of dislocations, or the study of fracturing, due to atomic debonding. An example for the latter case, is the study of contact friction at small scales, e.g. see [50], [70], [86]. An important contribution to the overall friction force is the interlocking, deformation and abrasion of surface asperities, which can be studied by the CGC model. A preliminary result displaying the interaction of surface asperities is considered in section 8.3. Another extension is the inclusion of thermal effects. Also, one may wish to use other potentials than the Lennard-Jones one, such as are listed in section 2.2.

Second, the computational modelling can be extended. So far, the surface approximation technique of Method 2 has been formulated for plane strain conditions, whereas a general three dimensional description is still lacking. Further, the surface projection currently formulated in Method 3 is restricted to a linear surface discretization. This can cause problems when large sliding motion occurs in the interface for the case that the surface elements are large compared to the contact gap. A smoother surface discretization can be expected to improve matters.

Thirdly, a further study of the modified CGC model, outlined in section 9 is useful. In particular, it will be important to identify parameters $\eta$ which achieve a good balance between efficiency and accuracy. In this respect a comparison between the modified CGCM and some common macroscale contact models will be useful.

Finally, the CGC model constitutes a suitable tool for the study of several further applications, in particular for problems where the intersolid interaction leads to large deformations. This is the case for soft materials or structures such as are found in many bio-mechanical applications, like the adhesion of individual cells [23] and the adhesion used by the Gecko [6]. This latter example is particularly interesting due to the hierarchical mechanical structure found on the gecko’s toes [32] and its inspiration for synthetic adhesives [87]. Other interesting examples are the modelling of sintering, i.e. the bonding of contacting solids, the investigation of friction, e.g. due to the interaction of asperities, as mentioned above, and the study of tribology at small scales [18].
A Coarse-Graining

In this appendix we describe the derivation of the Coarse-Grained Contact Model from the governing equations of molecular dynamics. Our approach is motivated by obtaining a continuum description from coarsening, or homogenizing, an underlying discrete, e.g. atomic, system. This is in contrast to other approaches commonly taken, which consider coarsening a fine discrete system into a coarse discrete system. An example is the coarse-graining technique presented by Rudd et al. [77], [78]. A similar approach to the one discussed here, is taken by Goldhirsch and coworkers [36], [34]. We start by presenting the equations governing molecular dynamics.

A.1 Molecular Dynamics

Consider the model problem of two interacting bodies as is shown in figures 2.1 and 3.1. For now the two bodies are considered as a discrete assembly of atoms. Their current configurations $\hat{\Omega}_1$ and $\hat{\Omega}_2$ are comprised of $n_1$ and $n_2$ discrete atoms or molecules. These configurations are not continua, and we use the hat on $\hat{\Omega}_1$ and $\hat{\Omega}_2$ to indicate this. The location of all atoms within $\hat{\Omega}_1$ is described by the position $z_i \in \hat{\Omega}_1$ for $i \in I_1$, where $I_1$ is the set of $n_1$ subscripts denoting the $n_1$ number of atoms within body 1. Further $z_j \in \hat{\Omega}_2$ for $j \in I_2$ describes the position of the $n_2$ atoms within body 2. For such a discrete assembly of atoms the potential energy is given by

$$\hat{\Pi}(\hat{\Omega}) = \hat{\Pi}_{\text{int}}(\hat{\Omega}) - \hat{\Pi}_{\text{ext}}(\hat{\Omega}), \quad (A.1)$$

where the hat is used to emphasize that this is the energy of a discrete system and where the set $\hat{\Omega} = \{z_i, z_j\}$ denotes the collection of all $n_1 + n_2$ atomic positions.

In principle each atom interacts with all other atoms. For this derivation let us only consider pairwise interaction between atoms, and disregard interactions involving 3 or more atoms. We further assume the additivity of the interactions [46]. Then the internal energy can be written as

$$\hat{\Pi}_{\text{int}}(\hat{\Omega}) = \sum_{k=1}^{b_1} \psi_1(r_k) + \sum_{k=1}^{b_2} \psi_2(r_k) + \sum_{k=1}^{b_{12}} \phi(r_k), \quad (A.2)$$

where the first sum is over all two-atom bonds $b_1$ of body $\hat{\Omega}_1$, the second sum is over all $b_2$ bonds of body $\hat{\Omega}_2$, and the last contribution is the sum over all $b_{12}$ bonds involving one atom of each body. Further, $\psi_1$, $\psi_2$ and $\phi$ are the interaction potentials of the three cases, which are considered to be different, since the two bodies may be comprised of atoms belonging to different elements. These pair-potentials only depend on the distance between atoms, i.e. the length of bond $k$, denoted by $r_k$. We recall that $\psi$ is termed the intrasolid potential, since it governs the interaction of atoms within the solid, and $\phi$ is termed the intersolid potential since it governs the interaction of atoms belonging to two distinct solids. (As a further generalization, $\psi$ may also be viewed as the interaction energy of atoms belonging to a close neighborhood, as found in covalent, ionic or metallic bonds, whereas $\phi$ is seen as the interaction of remote atoms, as is the case in van der Waals attraction.) Now, let us rewrite the internal energy (A.2) as

$$\hat{\Pi}_{\text{int}}(\hat{\Omega}) = \hat{\Pi}_{\text{int},1}(\hat{\Omega}_1) + \hat{\Pi}_{\text{int},2}(\hat{\Omega}_2) + \hat{\Pi}_{\text{int},12}(\hat{\Omega}), \quad (A.3)$$
where \( Z_1 = \{ z_i \}, i \in \mathcal{I}_1 \) and \( Z_2 = \{ z_j \}, j \in \mathcal{I}_2 \) is the collection of atomic positions in body 1 and 2. The sum over the bonds can be converted into a double sum over the atoms, so that the three contributions can be written as

\[
\begin{align*}
\hat{\Pi}_{\text{int},1} &:= \sum_{k=1}^{b_1} \psi_1(r_k) = \frac{1}{2} \sum_{i \in \mathcal{I}_1} \sum_{k \in \mathcal{I}_1} \psi_1(r_{ik}), \quad r_{ik} := |z_i - z_k|, \\
\hat{\Pi}_{\text{int},2} &:= \sum_{k=1}^{b_2} \psi_2(r_k) = \frac{1}{2} \sum_{j \in \mathcal{I}_2} \sum_{k \in \mathcal{I}_2} \psi_2(r_{jk}), \quad r_{jk} := |z_j - z_k|, \\
\hat{\Pi}_{\text{int},12} &:= \sum_{k=1}^{b_{12}} \phi(r_k) = \sum_{i \in \mathcal{I}_1} \sum_{j \in \mathcal{I}_2} \phi(r_{ij}), \quad r_{ij} := |z_i - z_j|,
\end{align*}
\]

Note that a factor of \( 1/2 \) is required in the first two equations, since each bond is counted twice in the double summation. This does not occur in the third equation, since the sets \( \mathcal{I}_1 \) and \( \mathcal{I}_2 \) are disjoint, hence no factor of \( 1/2 \) is needed. In the equations above \( \hat{\Pi}_{\text{int},1} \) and \( \hat{\Pi}_{\text{int},2} \) denote the internal energy of bodies 1 and 2, and \( \hat{\Pi}_{\text{int},12} \) denotes the interaction energy between the two bodies, (which can be seen as an internal energy contribution of the entire system). It is convenient to replace the second sum in \( \hat{\Pi}_{\text{int},I}, I = 1, 2 \) by a new function \( \Psi_I \) such that the internal energy for the two bodies can be written as

\[
\hat{\Pi}_{\text{int},I} = \sum_{i \in \mathcal{I}_1} \Psi_I(z_i), \quad \Psi_I(z_i) := \frac{1}{2} \sum_{k \in \mathcal{I}_I} \psi_I(r_{ik}), \quad r_{ik} := |z_i - z_k|, \quad I = 1, 2.
\]

In the case of the external potential let us look at its variation, which is written as

\[
\delta \hat{\Pi}_{\text{ext}} = \sum_{i \in \mathcal{I}_1} \delta z_i \cdot f_i + \sum_{j \in \mathcal{I}_2} \delta z_j \cdot f_j,
\]

where \( f_i \) and \( f_j \) are the external forces acting on the atoms of body 1 and 2, and where \( \delta z_i \) and \( \delta z_j \) are the variations in the atomic positions. The kinetic energy of the discrete system is expressed as

\[
\hat{K} = \frac{1}{2} \sum_{i \in \mathcal{I}_1} m_i |z_i|^2 + \frac{1}{2} \sum_{j \in \mathcal{I}_2} m_j |z_j|^2,
\]

given the atomic masses \( m_i, m_j \) and velocities \( \dot{z}_i, \dot{z}_j \). With the energies (A.1), (A.3), (A.6) and (A.7) defined above, the \( n_1 + n_2 \) equilibrium equations of the discrete system follows from

\[
\frac{d}{dt} \left( \frac{\partial \hat{L}}{\partial \dot{z}_k} \right) - \frac{\partial \hat{L}}{\partial z_k} = 0, \quad k \in \mathcal{I}_1 \cup \mathcal{I}_2,
\]

where \( \hat{L} = \hat{K} - \hat{\Pi} \) is the Lagrangian of the discrete system.

### A.2 Spatial Coarse-Graining

The purpose of the following discussion is to motivate the step from molecular dynamics towards the continuum and to characterize how the two descriptions are related to each
other. The transition is accomplished by a method called coarse-graining.

The continuous system may contain the same amount of information as the discrete system, however for several reasons, like computational efficiency, it is more useful to let it contain less information as the underlying discrete system. Coarse-graining furnishes a procedure to reduce the amount of information from one description to another. Compared to the initial refined system it provides a coarser system. Here coarse-graining can also be used to coarsen a discrete system into an effective discrete system or to coarsen a continuum into an effective continuum. An example for the first case is the common application of coarsening a molecular dynamics system into a coarser, effective system containing fewer degrees-of-freedom (dofs).

We begin by presenting the coarse-graining in the spatial domain. We consider two continua with current configurations $\Omega_1$ and $\Omega_2$ corresponding to the discrete bodies $\tilde{\Omega}_1$ and $\tilde{\Omega}_2$. We define two coordinates $x_1 \in \Omega_1$ and $x_2 \in \Omega_2$, which are considered continuous functions within these domains. At atom $i$ of body 1 we have $x_1 = z_i$, however $x_1$ is also defined at locations within body 1 where no atom is present, whereas $z_1 = \{z_i\}$ is not defined at such a point. In the ensuing discussion, when no distinction between the two bodies is necessary, we can drop the subscripts and also write $z_i \in \Omega, i \in \mathcal{I}$, and $x_i \in \Omega$.

Consider a function $\hat{f}(x)$ defined in unbounded, $d$-dimensional space $x \in \mathbb{R}^d$, e.g. $d = 3$. We define the spatial coarse-graining of the function $\hat{f}$ by the operation

$$f(x) := \int_{\mathbb{R}^d} \delta_h(x - y) \hat{f}(y) \, dv_y, \quad (A.9)$$

where $dv_y$ denotes the ($d$-dimensional) volume element associated with coordinate $y$. Thus a new, effective function $f(x)$ is obtained, which is an approximation to $\hat{f}(x)$. The accuracy of this approximation depends on the coarse-graining function $\delta_h$, which for example, can be chosen as the Gaussian distribution

$$\delta_h(y) := \frac{1}{(\sqrt{\pi}h)^d} \exp\left(-\frac{y \cdot y}{h^2}\right), \quad (A.10)$$

where $h$ is the coarse-graining parameter. As $h \to 0$, $\delta_h(y)$ approaches the Dirac delta function $\delta(y)$ and the function values of $\hat{f}$ and $\hat{f}$ become equal. The Gaussian distribution (A.10) integrates to unity over $\mathbb{R}^d$, that is

$$\int_{\mathbb{R}^d} \delta_h(y) \, dv_y = 1, \quad (A.11)$$

so that eq. (A.10) is normalized. Therefore a constant function $\hat{f}(x_i) = c$ reproduces the same constant function $f(x) = c$, i.e. a constant function is invariant under the coarse-graining operation (A.9).

As an example, let us consider the current particle density $\hat{\beta}(x)$ of a discrete assembly of particles $\Omega$, given by

$$\hat{\beta}(x) := \sum_{i \in \mathcal{I}} \delta(x - z_i) \quad (A.12)$$

It is a continuously defined function taking singular values at the particle location $x = z_i$. Applying the coarse-graining operation (A.9) to $\hat{\beta}$, we obtain the current coarse-grained
density $\beta(\mathbf{x})$ as

$$
\beta(\mathbf{x}) := \int_{\mathbb{R}^d} \delta_h(\mathbf{x} - \mathbf{y}) \sum_{i \in \mathcal{I}} \delta(\mathbf{y} - \mathbf{z}_i) \, dv_y = \sum_{i \in \mathcal{I}} \delta_h(\mathbf{x} - \mathbf{z}_i) ,
$$

(A.13)

which is a smooth approximation to $\hat{\beta}$. Here the last equality follows from the integrating property of the delta function

$$
g(\mathbf{x}) = \int_{\Omega} \delta(\mathbf{y} - \mathbf{x}) \, g(\mathbf{y}) \, dv_y ,
$$

(A.14)

for all $\mathbf{x} \in \Omega \subset \mathbb{R}^d$ and where $g(\mathbf{x})$ is a bounded function. Similar to the particle density $\hat{\beta}$, the current mass density $\hat{\rho}(\mathbf{x})$ is given by

$$
\hat{\rho}(\mathbf{x}) := \sum_{i \in \mathcal{I}} \delta(\mathbf{x} - \mathbf{z}_i) \, m_i ,
$$

(A.15)

where $m_i$ is the mass of particle $i$. By the use of eq. (A.9) the coarsened, current mass density follows as

$$
\rho(\mathbf{x}) := \sum_{i \in \mathcal{I}} \delta_h(\mathbf{x} - \mathbf{z}_i) \, m_i .
$$

(A.16)

The physical meaning of the coarse-graining operation (A.9) is the weighted averaging of $\hat{f}$ over the support space $\mathcal{S}(\mathbf{x}) = \{ \mathbf{y} \mid |\mathbf{x} - \mathbf{y}| \leq h \}$. The former function $\hat{f}$ is thus approximated by the coarse-grained function $f$. Clearly, as $h \to 0$ approximation (A.9) becomes exact. Eq. (A.9) is also exact, for all $h$, if $g(\mathbf{x})$ is a constant or even linear function in $\mathbf{x}$, due to the symmetry of $\delta_h$. Therefore, if $h$ is chosen such that $\hat{f}$ is approximately linear within the support space $\mathcal{S}$, the accuracy of equation (A.9) will be very good. In fact, according to this criteria, approximation (A.9) can be made arbitrarily accurate, thus enabling a seamless transition between molecular dynamics and the CGCM.

In the following we consider a simple 1D coarse-graining example. Figure A.1 (a) and (b) shows the coarse-grained function

$$
g(x) = \int_{-\infty}^{\infty} \delta_h(x - y) \, f(y) \, dy ,
$$

(A.17)

according to eq. (A.9), of the fine scale function $f(x) = \frac{1}{5} \cos x$ using $\delta_h$ from eq. (A.10) with $h = 0.5$ and $h = 5$. Let us define the ‘error’ between $g(x)$ and $f(x)$ as

$$
e(x) := \frac{f(x) - g(x)}{f(x)} .
$$

(A.18)

The error $e$ at $x = 0$ in dependence of $h$ is shown in frame (c). It can be seen that the error vanishes for $h \to 0$ whereas for large $h$ we have $e = 1$, i.e. all information is lost by the coarse-graining procedure. The two open circles at $h = 0.5$ and $h = 5$ indicate the error in the two examples of frames (a) and (b). Finally frame (d) shows the coarse-graining of the multiscale function

$$f(x) = \frac{1}{10} \cos(10x) - \frac{1}{5} \cos x ,
$$

(A.19)

which is constructed of a fine scale and a coarse scale contribution. It is seen that the fine scale part is entire lost in operation (A.17), whereas the coarse scale part is retained.
The example above shows that coarse-graining is an averaging scheme dependant on a parameter, $h$, regulating which kind of fine scale information is lost and which is retained. It characterizes the degree of resolution of the coarse-grained function $g$. In solving a given problem one must also decide on a tolerance in the accuracy. The resolution $h$ should then be chosen based on this tolerance.

Note that the spatial coarse-graining scheme (A.9) is also used in section 9 to construct a second level of coarsening of the CGC model.

**A.3 Applying Spatial Coarse-Graining to Molecular Dynamics**

Let us now use the coarse-graining operation introduced in the previous section to derive the continuum equations from the underlying molecular system. We first consider the coarsening of the potential energy $\Pi$ (A.1) of the discrete system. To this end we consider the summation of a function $\delta f(z_i)$ over all atomic sites $z_i \in \Omega$, $i \in I$. Due to property
(A.14) we have

\[ \sum_{i \in I} \hat{f}(z_i) = \int_{\Omega} \sum_{i \in I} \delta(x - z_i) \hat{f}(x) \, dv_x = \int_{\Omega} \hat{\beta}(x) \hat{f}(x) \, dv_x , \number{(A.20)} \]

where we have used the definition of the particle density \( \hat{\beta} \) (A.12) in the second identity. Approximating \( \delta(x) \) by \( \delta_h(x) \), i.e. approximating \( \hat{\beta}(x) \) by \( \beta(x) \), we arrive at

\[ \sum_{i \in I} \hat{f}(z_i) \approx \int_{\Omega} \beta(x) \, \hat{f}(x) \, dv_x . \number{(A.21)} \]

So by using the coarse-graining scheme defined in the preceding section the discrete summation is approximated by a continuous integral. As has been noted before, the accuracy of this approximation becomes exact for all \( h \), if \( \hat{\beta}(x) \) is a linear function. In other words the accuracy of eq. (A.21) will be very good, if \( h \) is adjusted such that \( \hat{\beta} \) is close to a linear function within the support space of the coarse-graining function \( \delta_h \).

In view of eq. (A.21) the internal energy \( \hat{\Pi}_{\text{int},I} \) (A.5) of the discrete body \( \hat{\Omega}_I, I = 1, 2 \), is coarse-grained as

\[ \hat{\Pi}_{\text{int},I} \approx \Pi_{\text{int},I} := \int_{\Omega_I} \beta_I(x) \Psi_I(x) \, dv , \number{(A.22)} \]

where

\[ \Psi_I(x) = \frac{1}{2} \sum_{k \neq i} \psi_I(r_k) , \quad r_k = |x - z_k| , \quad z_k \neq x , \number{(A.23)} \]

is the continuous counterpart of the discrete function \( \Psi_I(z_i) \) given in eq. (A.5). We thus have obtained the continuum potential \( \Pi_{\text{int},I} \) from the coarsening of the corresponding discrete potential \( \hat{\Pi}_{\text{int},I} \). We note that for a deforming solid, the current interatomic distance \( r_k \) depends on the deformation gradient \( F_I \), so that we can write \( \Psi_I = \Psi_I(F_I) \). In view of the usual expression of the internal energy \( \Pi_{\text{int},I} \) for a hyperelastic continuum (3.12), the function \( \Psi_I(F_I) \) can thus be associated with the strain energy density \( W_I \). The energy density per current volume and the energy density per reference volume follow as

\[ w_I(F_I) = \beta_I \Psi_I(F_I) , \quad W_I(F_I) = \beta_{I0} \Psi_I(F_I) , \number{(A.24)} \]

where \( \beta_{I0} = \beta_I/J_I \) denotes the atomic density of the reference configuration and where \( J_I = \det F_I \) is the Jacobian of the deformation. Eqs. (A.24) and (A.23) immediately take us to expression (3.41), the starting point of the Cauchy-Born rule discussed in section 3.2.2.

By applying eq. (A.21) twice, the double summation of the discrete interaction energy \( \hat{\Pi}_{\text{int},12} \), given in eq. (A.4), is coarse-grained by the double integration

\[ \hat{\Pi}_{\text{int},12} \approx \Pi_C := \int_{\Omega_1} \int_{\Omega_2} \beta_1(x) \beta_2(r) \phi(r) \, dv_2 \, dv_1 , \quad r = |x_1 - x_2| . \number{(A.25)} \]

Here \( \Pi_C \) denotes the interaction energy of the continuum and \( \phi \) denotes the intersolid interaction function as introduced in section A.1 and earlier in section 2.1.
In a similar manner the continuum approximation $\delta \Pi_{\text{ext},I} (I = 1, 2)$ to the discrete external energy variation $\delta \Pi_{\text{ext},I}$ (A.6) is obtained. Through the use of eq. (A.21) we find

$$\delta \Pi_{\text{ext},I} \approx \delta \Pi_{\text{ext},I} := \int_{\Omega_I} \delta x_I \cdot \vec{b}_I \ dv_I + \int_{\Gamma_{I,I}} \delta x_I \cdot \vec{t}_I \ da_I ,$$  
(A.26)

where the external forces $f_I$ have been identified with either applied body forces $\vec{b}_I$ (per unit volume) acting on $\Omega_I$ or applied tractions $\vec{t}_I$ acting on $\Gamma_{I,I} \subset \partial \Omega_I$, the traction specified part of the boundary of $\Omega_I$.

Finally, we need to derive the coarse-graining of the discrete kinetic energy (A.7). Consider a representative body denote by $^\Omega$, when discrete, or $\Omega$, when continuous. According to the integrating property (A.14) of the delta function we have the identity

$$\varphi(Z_i) = \int_{\Omega_0} \delta(X - Z_i) \varphi(X) \ dV_X ,$$  
(A.27)

where the integration is carried out over the reference configuration $\Omega_0$, and where $Z_i \in \Omega_0$ is the reference position of atom $i$ currently located at $z_i \in \Omega$. The function $\varphi$ is considered as the motion mapping points from the reference configuration to the current configuration, i.e. $x = \varphi(X)$, so that we further have

$$z_i = \int_{\Omega_0} \delta(X - Z_i) \ x \ dV_X .$$  
(A.28)

On the other hand, property (A.14) can also be applied to the current configuration $\Omega$. It thus follows that

$$z_i = \int_{\Omega} \delta(x - z_i) \ x \ dv_x = \int_{\Omega_0} \delta(X - Z_i) \ x \ dV_X ,$$  
(A.29)

which establishes a relation between the integration over the two configurations $\Omega_0$ and $\Omega$. Applying the material time derivative $\frac{\partial(...)}{\partial t}|_{X \ \text{fixed}}$ to eq. (A.28) we obtain

$$\dot{z}_i = \int_{\Omega_0} \delta(X - Z_i) \ \dot{x} \ dV_X ,$$  
(A.30)

and further, mapping the integral back to the current configuration according to eq. (A.29), we get

$$\dot{z}_i = \int_{\Omega} \delta(x - z_i) \ \dot{x} \ dv_x ,$$  
(A.31)

where $\dot{z}_i$ and $\dot{x}$ are the velocities associated with $z_i$ and $x$. Next we note that the delta function satisfies the following property

$$\delta(x - z_i) \ \delta(y - z_i) = \delta(x - z_i) \ \delta(y - x) .$$  
(A.32)

Using eqs. (A.31) and (A.32) the kinetic energy of particle $i$ can thus be written as

$$\frac{m_i}{2} \dot{z}_i \cdot \dot{z}_i = \frac{m_i}{2} \int_{\Omega} \delta(x - z_i) \ \dot{x} \ dv_x \cdot \int_{\Omega} \delta(y - z_i) \ \dot{y} \ dv_y$$

$$= \frac{m_i}{2} \int_{\Omega} \delta(x - z_i) \ \dot{x} \cdot \int_{\Omega} \delta(y - x) \ \dot{y} \ dv_y \ dv_x$$

$$= \frac{m_i}{2} \int_{\Omega} \delta(x - z_i) \ \dot{x} \cdot \dot{x} \ dv_x .$$  
(A.33)
The total kinetic energy $\hat{K}$ of the discrete assembly of particles is thus given by

$$\hat{K} = \frac{1}{2} \sum_{i \in I} m_i \dot{z}_i \cdot \dot{z}_i = \frac{1}{2} \int_{\Omega} \sum_{i \in I} \delta(x - z_i) m_i \dot{x} \cdot \dot{x} \; dv_x , \quad (A.34)$$

which, in view of the definition of the mass density $\hat{\rho}$ (A.15), becomes

$$\hat{K} = \frac{1}{2} \sum_{i \in I} m_i \dot{z}_i \cdot \dot{z}_i = \frac{1}{2} \int_{\Omega} \hat{\rho}(x) \dot{x} \cdot \dot{x} \; dv_x . \quad (A.35)$$

Approximating $\delta(y)$ by $\delta_h(y)$, i.e. $\hat{\rho}(x) \approx \rho(x)$, we finally arrive at the coarse-grained kinetic energy, $K \approx \hat{K}$, of the continuum, given by

$$K := \frac{1}{2} \int_{\Omega} \rho(x) \dot{x} \cdot \dot{x} \; dv_x . \quad (A.36)$$

The derivation of the coarse-grained kinetic energy above is valid for both bodies and one may simply attach the subscript $I = 1, 2$ to eq. (A.36) above.

Through equations (A.22), (A.25), (A.26) and (A.36) we have thus transformed the molecular system, derived in section A.1, into a coarsened continuum description, termed the Coarse-Grained Contact Model. The Lagrangian of the continuum description is defined as $L = K - \Pi$, which can be expanded into

$$L = \sum_{I=1}^{2} [K_I - \Pi_{\text{int},I} + \Pi_{\text{ext},I}] - \Pi_C , \quad (A.37)$$

for the two-body interaction. The equations of motion of the two interacting continua can now be obtained from the stationary value of the action

$$A = \int_{t_1}^{t_2} L \; dt , \quad (A.38)$$

as has been derived in section 3.1.

### A.4 Temporal and Spatial Coarse-Graining

The spatial coarse-graining scheme presented in the preceding sections can by extended by the temporal component. Since time is continuous, temporal coarse-graining of a time dependent function $\hat{f}(t)$ can be defined, analogously to the spatial counterpart (A.9), by the integral

$$f(t) := \int_T \delta_t(t - s) \; \hat{f}(s) \; ds , \quad (A.39)$$

where $T$ denotes the temporal domain and $\delta_t(t - s)$ denotes the temporal coarse-graining function. It may not be useful to consider the Gaussian distribution as a candidate for $\delta_t$, as it looks into the future. It seems preferable to coarse-grain time using only past information. Both spatial and temporal coarse-graining can be combined. As an example let us consider
a continuous function \( \hat{f}(x, t) \). Combining eqs. (A.39) and (A.9) then yields the space-time coarse-graining operation of \( \hat{f} \) as

\[
f(x, t) := \int_{\Omega} \delta_t(t - s) \int_{\mathcal{T}} \delta_h(x - y) \hat{f}(y, s) \, dy \, ds .
\]  

(A.40)

Note that in general the position \( x \) is time dependent, i.e. \( x = x(t) \). Ideally, operation (A.40) should be invariant under the spatial and temporal coarse-graining ordering, so that the integration over \( \Omega \) and \( \mathcal{T} \) is exchangeable. Instead of coarse-graining space-time one may alternatively work in phase-space, that is coarse-graining positions and velocities. Such an approach is taken in the works of [77], [78]. The steps of the previous section can now be retraced to derive the space-time coarse-grained continuum from molecular dynamics.

Concluding we remark that we have considered a simple coarse-graining technique based on the Gaussian distribution. This approach can be generalized considering other coarse-graining functions or by refining the physical picture, e.g. by including thermal effects. In this regard we are essentially touching on the field of statistical mechanics, e.g. see [21], [98]. One may also consider an approach which distinguishes between the internal energy of surface and bulk atoms. This is not studied here, however, the framework of the Coarse-Grained Contact Model can accommodate such an approach.
B Normalized FE Equations

Appendix B lists the normalized finite element equations as they are implemented. The normalization scheme is motivated by the reduction of the physical parameters \( E, Y, r_0 \), \( r_{\phi} \) and \( \gamma_{\psi} \) to the two characterizing model parameters \( \gamma_L \) and \( \gamma_W \), as has been discussed in section 3.5. According to that section we define the length scale \( \gamma_L \) and the energy scale \( \gamma_W \) as

\[
\gamma_L := \frac{R_0}{r_0}, \quad \gamma_W := \frac{W_{\text{int},0}}{W_{C,0}},
\]

where

\[
W_{\text{int},0} := \frac{E_0}{R_0^3}, \quad W_{C,0} := \frac{\beta_0^2 \epsilon_\phi}{R_0^3 / \gamma_L^2}.
\]

For simplicity it is supposed that both bodies have the same material (i.e. \( E_{Y,1} = E_{Y,2}, \nu_1 = \nu_2, \beta_1 = \beta_2, r_{\phi,1} = r_{\phi,2} \) and \( \gamma_{\psi,1} = \gamma_{\psi,2} \)). From the computational point of view, all numerical quantities are treated as dimensionless. To normalize a quasi-static problem the reference length \( R_0 \) and reference energy \( E_0 \) are introduced, from which follow reference quantities for force, \( E_0 / R_0 \), and stiffness, \( E_0 / R_0^3 \). Any physical length \( L \), energy \( E \), force \( F \) and stiffness \( K \) can thus be normalized as

\[
\hat{L} := \frac{L}{R_0}, \quad \hat{E} := \frac{E}{E_0}, \quad \hat{F} := \frac{R_0}{E_0} F, \quad \hat{K} := \frac{R_0^2}{E_0} K,
\]

where the bar is used to denote a dimensionless quantity.

To normalize the finite element formulation derived in section 4, let us consider two volume elements \( \Omega_i^e \in \Omega_1 \) and \( \Omega_j^e \in \Omega_2 \) as shown in figure 4.2 (a). According to eq. (3.9), the interaction energy between these two elements is given by

\[
\Pi_{C,ij} := \int_{\Omega_i^e} \int_{\Omega_j^e} \beta_i \beta_j \phi \, dv_j \, dv_j = \int_{\Omega_i^e} \int_{\Omega_j^e} \beta_0^2 \phi \, dV_j \, dV_j,
\]

where \( \phi(r) \) is the interaction potential given by (3.6). The second identity is obtained by pulling the integration back to the reference configuration \( \Omega_{i0}^e \) and \( \Omega_{j0}^e \) of the two elements. The reference configuration is normalized as \( \Omega_{i0} := \Omega_i^e / R_0^3 \), \( d\hat{V} := dV / R_0^3 \), so that the normalized interaction energy is written as

\[
\hat{\Pi}_{C,ij} := \frac{\Pi_{C,ij}}{E_0} = \int_{\Omega_{i0}^e} \int_{\Omega_{j0}^e} \bar{\phi} \, dV_j \, dV_j , \quad \bar{\phi} := \frac{\beta_0^2 \phi(r) R_0^6}{E_0} = \frac{\gamma_L^3}{\gamma_W} \left[ \frac{1}{(\gamma_L r)^{12}} - \frac{2}{(\gamma_L r)^6} \right],
\]

according to eqs. (B.3)\(_1\) and (B.3)\(_2\). In the definition of the normalized potential \( \bar{\phi} \) we have made use of eqs. (B.1) and (B.2). It is noted that when \( \gamma_L \) becomes large, i.e. when the problem becomes macroscopic in size, the normalized distance \( \hat{r} \) becomes small, so that the product \( \gamma_L \hat{r} \) remains of the order of unity at equilibrium (where \( \hat{F} = 0 \)) and thus the formulation for \( \bar{\phi} \) is well-conditioned there. Let us now consider the finite element implementation ‘Method 1’ discussed in section 4.1. The elemental force vector \( f_{C,i} \) (4.6)\(_1\)
and it is therefore normalized according to eq. (B.3) as
\[ \bar{f}_{C,i} := \frac{f_{C,i} R_0^2}{E_0} = - \int_{\Omega_{e,i}} \int_{\Omega_{e,j}} \mathbf{N}_i^T \mathbf{F} \mathbf{\bar{r}} d\mathbf{V}_j d\mathbf{V}_i, \]
\[ \bar{F}(\mathbf{\bar{r}}) := \beta_0 \frac{F(r) R_0}{E_0} = \frac{12 \gamma_L^4}{\gamma W} \left[ \frac{1}{(\gamma_L \mathbf{\bar{r}})^{13}} - \frac{1}{(\gamma_L \mathbf{\bar{r}})^7} \right]. \]  
(B.6)

A similar expression is obtained for the normalized force vector \( \bar{f}_{C,j} \) (4.6)_2 acting on element \( \Omega_{f}^e \). The stiffness contributions listed in eq. (4.11) and (4.12) are normalized according to eq. (B.3). For example we obtain
\[ \bar{k}_{C,ij} := \frac{k_{C,ij} R_0^2}{E_0} = - \int_{\Omega_{e,i}} \int_{\Omega_{e,j}} \mathbf{N}_i^T \frac{\partial (\mathbf{F} \mathbf{\bar{r}})}{\partial \mathbf{x}_j} \mathbf{N}_j d\mathbf{V}_j d\mathbf{V}_i = \bar{k}_{C,ij}^T, \]
\[ \frac{\partial (\mathbf{F}(\mathbf{\bar{r}}))}{\partial \mathbf{x}_j} = \frac{\mathbf{F}}{\mathbf{\bar{r}}} I + \left[ \frac{\partial \mathbf{F}}{\partial \mathbf{\bar{r}}} - \frac{\mathbf{F}}{\mathbf{\bar{r}}} \right] \mathbf{\bar{r}} \otimes \mathbf{\bar{r}}, \]  
(B.7)

and corresponding expressions for \( \bar{k}_{C,ii}, \bar{k}_{C,j} \). If we consider solving a plane strain problem the element domains \( \Omega_{e}^e \) and \( \Omega_{f}^e \) are two-dimensional and are normalized as \( \Omega^e = \Omega^e / R_0^2 \), \( d\mathbf{V} = d\mathbf{V} / R_0^2 \). The integration in eq. (4.6) then yields the nodal force vector \( \mathbf{f}_{C,i} \) in units of force per length, and it is thus normalized by
\[ \bar{f}_{C,i} := \frac{f_{C,i} R_0^2}{E_0} = - \int_{\Gamma_{e,i}} \int_{\Gamma_{e,j}} \mathbf{N}_i^T \mathbf{\bar{F}} \mathbf{\bar{r}} d\mathbf{V}_j d\mathbf{V}_i, \]
\[ \mathbf{\bar{F}}(\mathbf{\bar{r}}) := \beta_0^2 \frac{\bar{F}(r)}{E_0} = \frac{\pi \gamma_L^3}{\gamma W} \left[ 693 - 1 - \frac{15}{4} \frac{1}{(\gamma_L \mathbf{\bar{r}})^6} \right]. \]  
(B.8)

where \( \bar{F} \) (3.52) is the force function for plane strain (see section 3.3). Similar expressions follow for the stiffness matrices. Next, consider the implementation ‘Method 2’, discussed in section 4.2. The nodal force vector listed in eq. (4.31) is derived for plane strain conditions and it is therefore normalized as
\[ \bar{f}_{C,i} := \frac{f_{C,i} R_0^2}{E_0} = - \int_{\Gamma_{e,i}} \int_{\Gamma_{e,j}} \mathbf{N}_i^T \mathbf{F}_s \mathbf{\bar{r}}_s \theta_i \theta_j d\mathbf{\bar{A}}_j d\mathbf{\bar{A}}_i, \]
\[ \mathbf{\bar{F}}_s(\mathbf{\bar{r}}) := \beta_0^2 \frac{F_s(r)}{E_0} = \frac{\pi \gamma_L}{\gamma W} \frac{77}{2560} \frac{1}{(\gamma_L \mathbf{\bar{r}})^{10}} - \frac{5}{16} \frac{1}{(\gamma_L \mathbf{\bar{r}})^4}, \]  
(B.9)

where \( \theta_i \) and \( \theta_j \) (see (4.32)) are dimensionless and where the force \( F_s \) is given by eq. (4.27). Finally, if Method 3 is used in plane strain problems, the nodal force vector \( \mathbf{f}_{C,k} \) (4.45), is normalized as
\[ \bar{f}_{C,k} := \frac{f_{C,k} R_0^2}{E_0} = \int_{\Gamma_{e,k}} \mathbf{N}_k^T \mathbf{F}_s \mathbf{\bar{r}}^P \theta_k d\mathbf{A}_k, \]
\[ \mathbf{\bar{F}}_s(\mathbf{\bar{r}}) := \beta_0 F_s(r) \frac{R_0^3}{E_0} = \frac{\pi}{J_r \gamma W} \left[ \frac{1}{45} \frac{1}{(\gamma_L \mathbf{\bar{r}})^{9}} - \frac{1}{3} \frac{1}{(\gamma_L \mathbf{\bar{r}})^{3}} \right]. \]  
(B.10)

Note that the force function \( F_s(r) \), defined in eq. (4.44) contains the density \( \beta_\ell = \beta_0 / J_\ell \). Next, we discuss the normalization of the internal forces represented by the vector \( \mathbf{f}_{\text{int}} \). In
view of eq. (B.3) the internal energy $\Pi^e_{\text{int}}$ (see (3.12)) of an element $\Omega^e$ is normalized as

$$\bar{\Pi}^e_{\text{int}} := \frac{\Pi^e_{\text{int}}}{E_0} = \int_{\Omega^e} \frac{1}{J} \bar{W} \, d\bar{v}, \quad (B.11)$$

where we have

$$\bar{W} = \frac{W R_0^3}{E_0} = \frac{W}{E_Y} = \frac{\Lambda}{2} (\ln J)^2 + \frac{\mu}{2} (I_1 - 3) - \bar{\mu} \ln J, \quad \bar{\Lambda} = \frac{\Lambda}{E_Y}, \quad \bar{\mu} = \frac{\mu}{E_Y}, \quad (B.12)$$

for the Neo-Hookean model discussed in section 3.2.1 or

$$\bar{W} = \frac{W}{E_Y} = \frac{W}{\beta_0 \epsilon_{\psi}} \frac{1}{2} \sum_{k \in S_c} \left[ \frac{1}{\bar{r}^2_k} - \frac{2}{\bar{r}^6_k} \right], \quad (B.13)$$

for the Cauchy-Born model discussed in section 3.2.2. Note that the definition of $E_0$ and $E_Y$ are such that $E_0 / R_0^3 = E_Y = \beta_0 \epsilon_{\psi}$ as introduced in section 3.5. Here we have defined $\bar{r}_k := r_k / r_{\psi}$ as the distance within the normalized unit cell $S_c$. Due to the locality assumption of the Cauchy-Born rule $r_k$ can be normalized by $r_{\psi}$ instead of using $R_0$. Hence the length $r_{\psi}$ can be eliminated from the model and does not play any further role. This will not be possible if a nonlocal formulation is chosen. In this case $r_{\psi}$ appears as an intrinsic length scale of the model. The internal force vector acting on element $\Omega^e$ due to energy $\Pi^e_{\text{int}}$ is given as

$$f^e_{\text{int}} = \int_{\Omega^e} \mathbf{B}^T_{UL} \sigma \, dv, \quad \mathbf{B}_{UL} = \left[ \mathbf{B}^1_{UL} \mathbf{B}^2_{UL} ... \mathbf{B}^n_{UL} \right], \quad (B.14)$$

e.g. see [9]. Here $\mathbf{B}^A_{UL}$, is the B-Matrix for node $A = 1, ..., n$ of element $\Omega^e$ according to the updated Lagrangian formulation [14]. For plane strain problems it is

$$\mathbf{B}^A_{UL} = \begin{bmatrix} N_{A,1} & 0 \\ 0 & N_{A,2} \\ N_{A,2} & N_{A,1} \end{bmatrix}, \quad (B.15)$$

where $N_{A,1}$ and $N_{A,2}$ are the components of the spatial gradient grad $N_A = \frac{\partial N_A}{\partial x}$ of the shape function of node $A$. Note that $\mathbf{B}_{UL}$ has units of $1/\text{length}$, and so the normalization of $f^e_{\text{int}}$ follows as

$$\bar{f}^e_{\text{int}} := \frac{f^e_{\text{int}} R_0}{E_0} = \int_{\Omega^e} \bar{\mathbf{B}}^T_{UL} \bar{\sigma} \, d\bar{v}, \quad \bar{\mathbf{B}}_{UL} = R_0 \mathbf{B}_{UL}, \quad (B.16)$$

where the normalized stress tensor is given by

$$\bar{\sigma} = \frac{\sigma R_0^3}{E_0} = \frac{\bar{\Lambda}}{J} \ln J \, I + \frac{\bar{\mu}}{J} (\mathbf{B} - I), \quad (B.17)$$

for the Neo-Hookean model (3.36) and

$$\sigma = \frac{\sigma R_0^3}{E_0} = \frac{6}{J} \sum_{k \in S_c} \left[ -\frac{1}{\bar{r}^2_k} + \frac{1}{\bar{r}^6_k} \right] \bar{r}_k \otimes \bar{r}_k, \quad (B.18)$$
for the Cauchy-Born rule (3.44). Here we have defined the unit direction \( \hat{r}_k := r_k / r_k \) according to eq. (3.44). The elemental stiffness matrix corresponding to \( \mathbf{f}_{\text{int},i} \) is given by

\[
\mathbf{k}^e_{\text{int}} = \mathbf{k}^e_{\text{mat}} + \mathbf{k}^e_{\text{geo}},
\]

where

\[
\mathbf{k}^e_{\text{mat}} = \int_{\Omega^e} \mathbf{B}^T_{\text{UL}} \mathbf{a} \mathbf{B}_{\text{UL}} \, dv,
\]

is the material stiffness contribution and

\[
\mathbf{k}^e_{\text{geo}} = \begin{bmatrix}
\mathbf{k}^{11}_{\text{geo}} & \mathbf{k}^{12}_{\text{geo}} & \cdots & \mathbf{k}^{1n}_{\text{geo}} \\
\mathbf{k}^{21}_{\text{geo}} & \mathbf{k}^{22}_{\text{geo}} & \cdots & \mathbf{k}^{2n}_{\text{geo}} \\
\vdots & \vdots & \ddots & \vdots \\
\mathbf{k}^{n1}_{\text{geo}} & \mathbf{k}^{n2}_{\text{geo}} & \cdots & \mathbf{k}^{nn}_{\text{geo}}
\end{bmatrix},
\]

is the geometrical stiffness contribution. Here \( n \) is the number of nodes of element \( \Omega^e \) and \( \mathbf{I} \) is the identity matrix in \( d \)-dimensional space \( \mathbb{R}^d \). In the expression for \( \mathbf{k}^{AB}_{\text{geo}} \) \( i \) and \( j \) are dummy indices which are summed over. The normalized material stiffness is

\[
\mathbf{k}^e_{\text{mat}} = \frac{\mathbf{k}^{e}_{\text{mat}} R_0^2}{E_0} = \int_{\Omega^e} \mathbf{B}^T_{\text{UL}} \bar{\mathbf{a}} \mathbf{B}_{\text{UL}} \, d\bar{v},
\]

with

\[
\bar{\mathbf{a}} := \frac{\mathbf{a} R_0^3}{E_0} = \frac{\bar{\lambda}}{J} \mathbf{I} \otimes \mathbf{I} + \frac{2}{J} (\bar{\mu} - \bar{\lambda} \ln J) \mathbf{I},
\]

for the Neo-Hookean model (3.38) and

\[
\bar{\mathbf{a}} := \frac{\mathbf{a} R_0^3}{E_0} = \frac{6}{J} \sum_{k \in S} \left[ \frac{14}{r_k^{12}} - \frac{8}{r_k^6} \right] \hat{r}_k \otimes \hat{r}_k \otimes \hat{r}_k \otimes \hat{r}_k
\]

for the Cauchy-Born rule (3.46). The normalization of the geometrical stiffness block \( \mathbf{k}^{AB}_{\text{geo}} \) follows as

\[
\bar{\mathbf{k}}^{AB}_{\text{geo}} = \frac{\mathbf{k}^{AB}_{\text{geo}} R_0^2}{E_0} = \int_{\Omega^e} \bar{N}_{A,i} \bar{\sigma}_{ij} \bar{N}_{B,j} \, d\bar{v},
\]

with \( \bar{N}_{A,i} = R_0 N_{A,i} \) and where \( \bar{\sigma} \) is given by eq. (B.17) or (B.18), depending on the model. The external force follows according to (3.14) as

\[
\mathbf{f}^e_{\text{ext}} = \int_{\Omega^e} \mathbf{N}^T_{\Omega} \rho \mathbf{b} \, dv + \int_{\Gamma^e} \mathbf{N}^T_{\Gamma} \mathbf{t} \, da,
\]

and it is normalized according to eq. (B.3).

Let us now briefly discuss the assembly of the global FE arrays from the elemental FE arrays listed above. In accordance with figure 4.1 we let \( \mathcal{I} \) and \( \mathcal{J} \) be the set of elements \( \Omega_i^1 \in \Omega_1 \) and \( \Omega_j^2 \in \Omega_2 \), we let \( \mathcal{I} \) and \( \mathcal{J} \) be the set of elements \( \Omega_i^1 \in \Omega_1 \) and \( \Omega_j^2 \in \Omega_2 \), we let \( \mathcal{I} \) and \( \mathcal{J} \) be the set of elements \( \Omega_i^1 = \Omega_1(\Omega_j^2) \) (i.e. which influence element \( \Omega_j^2 \)), and let \( \mathcal{J} \) be the set of elements \( \Omega_j^2 = \Omega_2(\Omega_i^1) \) (i.e. which influence element \( \Omega_i^1 \)). Whenever Methods 2 or 3 is addressed this notation actually refers to surface domains and surface elements. The internal forces (B.16) are assembled by looping over all finite elements and
assigning them into the appropriate slots. We denote this assembly operation for body \( \Omega_1 \) and \( \Omega_2 \) as

\[
\begin{align*}
\bar{f}_{\text{int},1} &= \bigwedge_{i \in I} \bar{f}^e_{\text{int},i}, & \bar{f}_{\text{int},2} &= \bigwedge_{j \in J} \bar{f}^e_{\text{int},j}.
\end{align*}
\]  
(B.27)

Analogously we have

\[
\begin{align*}
\bar{K}_{\text{int},1} &= \bigwedge_{i \in I} \bar{k}^e_{\text{int},i}, & \bar{K}_{\text{int},2} &= \bigwedge_{j \in J} \bar{k}^e_{\text{int},j},
\end{align*}
\]  
(B.28)

for the assembly of the elemental stiffness matrices \( k^e_{\text{int}} \) (B.19). The assembly of the interaction forces \( \bar{f}^e_{C,k} \) according to the three methods follows similarly as

\[
\begin{align*}
\bar{f}_{C,1} &= \bigwedge_{i \in I} \bar{f}^e_{C,i}, & \bar{f}_{C,2} &= \bigwedge_{j \in J} \bar{f}^e_{C,j},
\end{align*}
\]  
(B.29)

For Method 3 the elemental contributions \( \bar{f}^e_{C,k} \) is given by (B.10). For Methods 1 and 2 they first have to be obtained by

\[
\begin{align*}
\bar{f}^e_{C,i} &= \sum_{j \in J} \bar{f}^e_{C,i} , & \bar{f}^e_{C,j} &= \sum_{i \in I} \bar{f}^e_{C,j},
\end{align*}
\]  
(B.30)

the summation of contributions (B.6), (B.8) or (B.9) according to eq. (4.10). The stiffness assembly follow similarly as

\[
\begin{align*}
\bar{K}_{C,11} &= \bigwedge_{i \in I} \bigwedge_{j \in J} \bar{k}_{C,ii}, & \bar{K}_{C,12} &= \bigwedge_{i \in I} \bigwedge_{j \in J} \bar{k}_{C,ij}, \\
\bar{K}_{C,21} &= \bigwedge_{j \in J} \bigwedge_{i \in I} \bar{k}_{C,ji}, & \bar{K}_{C,22} &= \bigwedge_{j \in J} \bigwedge_{i \in I} \bar{k}_{C,jj}.
\end{align*}
\]  
(B.31)

As in eqs. (B.29), (B.30) the summation in \( \bar{K}_{C,11} \) and \( \bar{K}_{C,22} \), and the second assembly in \( \bar{K}_{C,12} \) and \( \bar{K}_{C,21} \) are only required for Methods 1 and 2 but not for Method 3.

Now, quasi-static equilibrium is obtained by enforcing

\[
\begin{align*}
\bar{f}(u) = \begin{bmatrix} \bar{f}_{\text{int},1} + \bar{f}_{C,1} - \bar{f}_{\text{ext},1} \\ \bar{f}_{\text{int},2} + \bar{f}_{C,2} - \bar{f}_{\text{ext},2} \end{bmatrix} = 0,
\end{align*}
\]  
(B.32)

which is solved by Newton’s method. We therefore expand \( \bar{f}(\bar{u}) \) at \( \bar{u}_{n+1} \) into the Taylor series

\[
\bar{f}(\bar{u}_{n+1}) = \bar{f}(\bar{u}_n) + \left. \frac{\partial \bar{f}}{\partial \bar{u}} \right|_{\bar{u}_n} (\bar{u}_{n+1} - \bar{u}_n) + \ldots.
\]  
(B.33)

Setting \( f(u_{n+1}) = 0 \) we obtain

\[
\bar{f}(\bar{u}_n) + \bar{K}(\bar{u}_n) \Delta \bar{u}_n = 0,
\]  
(B.34)

which can be solved for the increment \( \Delta \bar{u}_n := \bar{u}_{n+1} - \bar{u}_n \) given \( u_n \) and the global stiffness matrix

\[
\bar{K} = \frac{\partial \bar{f}}{\partial \bar{u}} = \begin{bmatrix} \bar{K}_{\text{int},1} & 0 \\ 0 & \bar{K}_{\text{int},2} \end{bmatrix} + \begin{bmatrix} \bar{K}_{C,11} & \bar{K}_{C,12} \\ \bar{K}_{C,21} & \bar{K}_{C,22} \end{bmatrix}.
\]  
(B.35)
References


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