Chapter 5
Challenges in Computational Nanoscale Contact Mechanics

Roger A. Sauer

I have known Peter Wriggers since summer 2005 when he came to visit Berkeley and we discussed my doctoral research on computational nanoscale contact mechanics [7]. After graduation I took the opportunity to work with him at the Leibniz University Hannover. There I had the chance to teach the graduate courses ‘continuum mechanics’ and ‘contact mechanics’, coordinate various research projects, and, perhaps most challenging, get familiar with the German academic system. Since January 2010 I work at the Graduate School AICES in Aachen. I wish Peter Wriggers all the best for the future (R.A. Sauer).

Abstract. This paper outlines the differences between nanoscale and macroscale contact descriptions and gives an overview of the challenges encountered at the nanoscale. The adhesive instability, common to nanoscale contact, is illustrated by a simple example. Further emphasis is placed on multiscale approaches for contact.

1 Introduction

Nanoscale contact mechanisms are essential for many applications, like adhesives, small scale surface characterization and machining, MEMS and NEMS (Micro- and Nano-electro-mechanical systems), self-cleaning surfaces, gecko adhesion, cohesive fracture and peeling problems. At this scale it becomes necessary to integrate the fundamental physical phenomena [3, 5] into the approaches of computational contact mechanics [4, 15]. The challenges encountered in this are discussed in the following sections.

2 Nanoscale Contact Challenges

At small length scales several physical and numerical challenges present themselves that need to be accounted for in a computational framework. These challenges are:
1. Computational contact mechanics: numerical accuracy, efficiency and stability, closest point projection onto discrete surfaces, friction algorithms, wear and lubrication modeling
2. Bridging the scales between atomistic and continuum description (see Sect. 3)
3. Efficient and accurate algorithms for nanoscale contact (see Sect. 3)
4. Complex surface microstructure at different length scales (see Fig. 1)
5. Physical instabilities caused by strong adhesion (see Sect. 4)
6. Peeling computations: numerical instabilities due to discretization error
7. Multiscale modeling and homogenization approaches (see Sect. 5)
8. Nanoscale contact dynamics: efficient and accurate integration algorithms
9. Interaction between nanoscale friction and adhesion
10. Multifield contact problems, e.g. thermal equilibrium and chemical reactions at nanoscale interfaces
11. Nanoscale material models for specific applications: soft adhesives, liquids, granular media
12. Parameter identification and determination

Substantial work has been done to address the first challenge \[4, 15\]. The challenges posed by complex microstructures are illustrated by the examples in Fig. 1. An efficient formulation for stable peeling computations is presented in \[12\]. Challenges 2, 3, 5 and 7 are addressed in the following sections. Challenges 8–12 are mostly open research topics that call for further theoretical, experimental and computational research. Contact models that successfully describe various contact aspects need to be integrated into holistic top-down and bottom-up approaches. Such approaches attempt to find a unified description of various phenomena across different length scales and thus try to link macroscopic and microscopic model parameters. A helpful modeling framework for this is the bottom-up contact model outlined in the following section.

### 3 Nanoscale versus Macroscale Contact

In this section the different descriptions commonly used for nanoscale and macroscale contact are contrasted. Considering conservative systems in both cases, the total potential energy can be written as

\[
Π = Π_{\text{int}} + Π_{\text{c}} - Π_{\text{ext}}
\]

where the individual contributions \(Π_{\text{int}}, Π_{\text{ext}}\) and \(Π_{\text{c}}\) denote the internal, external and contact energy. For macroscopic scales, contact between continua \(B_1\) and \(B_2\) is characterized by the the impenetrability constraint

\[
g(x_1, x_2) ≥ 0 \quad ∀ \ x_1 ∈ ∂B_2, \ x_2 ∈ ∂B_2
\]

which states that the gap \(g\) between arbitrary surface points must remain positive. The impenetrability causes the tractions \(t_c\) acting on the contact surface between the