Challenges in computational nanoscale contact mechanics

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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 (Sauer, 2006). 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.

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 (Israelachvili, 1991; Persson, 2000) into the

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approaches of computational contact mechanics (Laursen, 2002; Wriggers, 2006). 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:

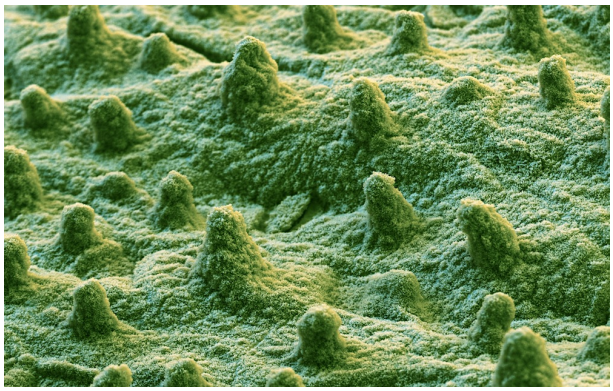
1. Computational contact mechanics: numerical accuracy, efficiency and stability, closest point projection onto discrete surfaces, friction algorithms, wear and lubrication modeling
2. Bridging the scales between atomistic and continuum description (see Sec. 3)
3. Efficient and accurate algorithms for nanoscale contact (see Sec. 3)
4. Complex surface microstructure at different length scales (see Fig. 1)
5. Physical instabilities caused by strong adhesion (see Sec. 4)
6. Peeling computations: numerical instabilities due to discretization error
7. Multiscale modeling and homogenization approaches (see Sec. 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 (Laursen, 2002; Wriggers, 2006). The challenges posed by complex microstructures are illustrated by the examples in Fig. 1. An efficient formulation for stable peeling computations is presented in Sauer (2011). 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

a.



b.

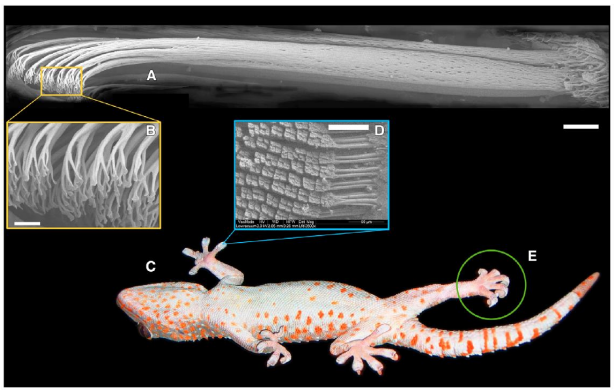


Fig. 1 a. Surface microstructure of the self-cleaning lotus leaf, adapted with permission from Eye of Science; b. Microstructure of the gecko adhesion mechanism (Autumn et al., 2006), adapted with permission from the Journal of Experimental Biology

$$\Pi = \Pi_{\text{int}} + \Pi_{\text{c}} - \Pi_{\text{ext}} \,, \tag{1}$$

where the individual contributions Π_{int}, Π_{ext} and Π_{c} denote the internal, external and contact energy. For macroscopic scales, contact between continua $\mathscr{B}_1$ and $\mathscr{B}_2$ is characterized by the the impenetrability constraint

$$g(\mathbf{x}_1, \mathbf{x}_2) \geq 0 \quad \forall\, \mathbf{x}_1 \in \partial\mathscr{B}_2,\ \mathbf{x}_1 \in \partial\mathscr{B}_2 \,, \tag{2}$$

which states that the gap g between arbitrary surface points must remain positive. The impenetrability causes the tractions $\mathbf{t}_{\text{c}}$ acting on the contact surface between the bodies (see Fig. 2). Utilizing the gap vector $\mathbf{g}$, the contact energy can be expressed as

$$\Pi_{\text{c}} = \int_{\partial\mathscr{B}_{\text{c}}} \mathbf{t}_{\text{c}} \cdot \mathbf{g} \, \mathrm{d}A \,. \tag{3}$$

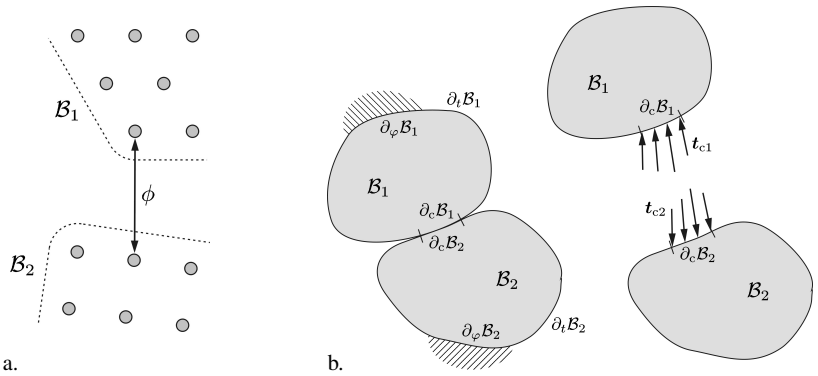


Fig. 2 Nanoscale (a.) versus macroscale (b.) contact description

On the other hand, at the nanometer scale and below, contact is resolved into the interactions of individual atomic particles (see Fig. 2). The interaction across the contact interface can be described by pair potentials like the Lennard-Jones potential

$$\phi(r) := \varepsilon\left(\frac{r_0}{r}\right)^{12} - 2\varepsilon\left(\frac{r_0}{r}\right)^{6} , \tag{4}$$

which, for example, is suitable to describe van-der-Waals adhesion between the bodies. Here r is the distance between the two particles, and r_0 and ε are material constants characterizing the interaction. Given the pair potential ϕ, the contact energy of the discrete particle system follows from the sum

$$\Pi_{\mathrm{c}} = \sum_{i}^{n_1}\sum_{j}^{n_2} \phi(\mathbf{x}_i - \mathbf{x}_j) , \tag{5}$$

which is taken over all interacting particles of the two bodies.

A seamless transition between both approaches can be generated if the discrete sum in eq (5) is replaced by the continuous integral (Sauer and Li, 2007b)

$$\Pi_{\mathrm{c}} = \int_{\mathscr{B}_1}\int_{\mathscr{B}_2} \beta_1\,\beta_2\,\phi(\mathbf{x}_1 - \mathbf{x}_2)\,\mathrm{d}v_2\,\mathrm{d}v_1 , \tag{6}$$

where β_1 and β_2 denote the molecular densities of the bodies. According to this formulation the contact forces between the bodies follow as gradients of potential ϕ. This approach yields accurate results down to length scales of a few nanometers (Sauer and Li, 2008; Sauer and Wriggers, 2009). At large scales this formulation resembles phenomenological constitutive adhesion and cohesion models (Raous et al., 1999; Xu and Needleman, 1994) that are enforced computationally by barrier or cross-constrained methods (Wriggers, 2006; Zavarise et al., 1998). This transition, as well as further computational details and efficient contact algorithms, are discussed in Sauer and Li (2007b, 2008); Sauer and Wriggers (2009); Sauer (2011).

4 Adhesion Instability

During strong adhesion of soft bodies an instability can occur: The adhesive forces can become so strong that they overpower the internal forces of the solids. This phenomenon can be illustrated by the simple 1D example shown in Fig. 3.a (Sauer, 2006): Two particles are considered that interact with the Lennard-Jones potential (4). The internal deformation of the solids is modeled by a spring with constant stiffness k. The lower particle is considered fixed, while the upper particle is pushed

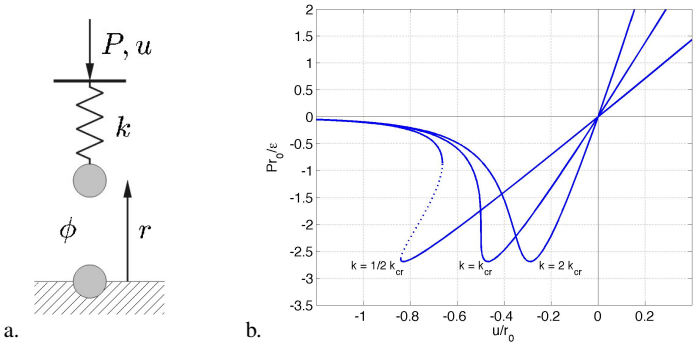


Fig. 3 a. Adhesive contact example; b. Load-displacement curve.

downward by an imposed displacement u that requires the force P. For $r = r_0$ and $u = 0$, the force in the system is $P = 0$. The total potential energy of this system is then given by

$$\Pi(r) = \phi(r) + \frac{1}{2}k\big(u + (r - r_0)\big)^2 \,. \tag{7}$$

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

$$u(r) = \frac{F(r)}{k} - r + r_0 \,, \tag{8}$$

where $F(r) := -\frac{\partial \phi}{\partial r}$ is the interaction force of the Lennard-Jones potential. From eq. (8) the load-displacement curve follows as

$$P(u) = k\big(u + r(u) - r_0\big) \,. \tag{9}$$

It can be displayed as $P(r)$ vs. $u(r)$ as is shown in figure 3.b. This graph shows that, as u becomes large, the repulsion between the particles 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 particles is very weak so that $P \to 0$ and $u \to r_0 - r$, since the spring is barely deforming.

The stability of the system can be investigated by examining $\frac{\partial^2 \Pi}{\partial r^2}|_{u=\text{fixed}}$. Setting this derivative equal to zero, we can identify the critical spring stiffness

$$k_{\text{cr}} = 36\Big(\frac{4}{13}\Big)^{4/3} \frac{\varepsilon}{r_0^2} \,. \tag{10}$$

For $k > k_{\text{cr}}$ the system will always be stable. However, if $k < k_{\text{cr}}$ the system develops an instability. The unstable section of the equilibrium path is shown as a dashed line in the figure above. In this case, as we push the two particles together their mutual attraction will suddenly overpower the spring and the particles snap together into a new equilibrium position. Likewise, when pulling the particles apart, they will suddenly snap free. This behavior carries over to continuous systems (Crisfield and Alfano, 2002; Sauer and Li, 2007a).

5 Multiscale contact modeling

Even though computational power has increased immensely in the past, it remains impossible to resolve even micrometer-scale problems at full atomic resolution. Therefore multiscale methods are needed that combine different modeling levels into one holistic model. To find appropriate multiscale models one must decide which details and effects to include at the various levels. To a large degree this presumes the knowledge of the characteristics that are emphasized and the characteristics that are lost between the scales and it thus become necessary to validate and refine chosen models. The demand for multiscale modeling lies both in the development of theoretical formulations, that unify different descriptions at various length scales, and in the development of efficient computational formulations, that achieve to span a large range of length scales. Helpful modeling components are coarse-graining techniques, reduced order modeling, adaptive model refinement and FE^2 strategies.

The selection of an appropriate multiscale approach for contact depends on the specific problem at hand. An example is the adhesion mechanism of the gecko shown in Fig. 4. To model the adhesion mechanism of the gecko toes, five modeling levels are considered: A directional lamella model, at the millimeter scale, a seta model at the 10 μm scale, a spatula model at the 100 nm scale, an effective contact model at the nanometer scale, and a molecular interaction model at the Ångstrom scale. Advances in this direction have appeared in Sauer (2009, 2010).

6 Conclusion

This paper discusses some of the challenges encountered in nanoscale contact mechanics. Some of these have been addressed and partly resolved satisfactory by re-

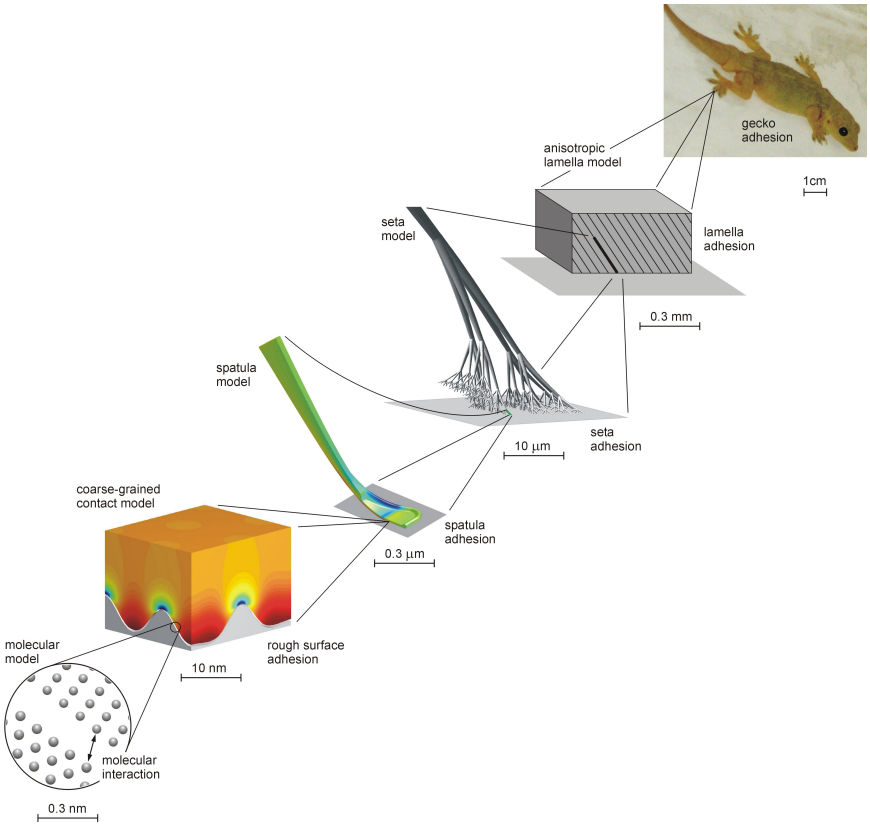


Fig. 4 Multiscale modeling hierarchy of the adhesion mechanism used by the gecko

cent research activity. Other challenges are still open topics that call for further theoretical, experimental and computational research. Among those are multiscale methods, time integration algorithms, nanoscale friction modeling, multifield methods and nanoscale material modeling.

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