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An atomic interaction-based continuum model for computational multiscale contact mechanics

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A computational multiscale contact mechanics model is presented which describes the interaction between deformable solids based on the interaction of individual atoms or molecules. The contact model is formulated in the framework of large deformation continuum mechanics and combines the approaches of molecular modelling [1] and continuum contact mechanics [2]. In the following a brief overview of the contact model is given. Further details can be found in [3], [4] and [5].

1 Model Formulation

Consider two deformable bodies in their current configuration, denoted by $\mathcal{B}_1$ and $\mathcal{B}_2$. The interaction between two atoms located at the points $\boldsymbol{x}_1 \in \mathcal{B}_1$ and $\boldsymbol{x}_2 \in \mathcal{B}_2$ is modelled by the Lennard-Jones potential

$$\phi(r) = \epsilon\Big(\frac{r_0}{r}\Big)^{12} - 2\epsilon\Big(\frac{r_0}{r}\Big)^{6} , \tag{1}$$

where $r = |\boldsymbol{x}_1 - \boldsymbol{x}_2|$ denotes the distance of the atoms and where r_0 and ϵ are material parameters characterizing the atomic interaction. The corresponding force between the atoms results from changes of the distance r, i.e. $F(r) = -\frac{\partial \phi}{\partial r}$. A positive force F indicates repulsion, e.g. during contact, while negative F indicate attraction, e.g. during adhesion of the bodies. The interaction between the atoms thus invokes the force pair $F\bar{\boldsymbol{r}}_1$ and $F\bar{\boldsymbol{r}}_2$, where the unit vectors $\bar{\boldsymbol{r}}_1 = (\boldsymbol{x}_1 - \boldsymbol{x}_2)/r$ and $\bar{\boldsymbol{r}}_2 = (\boldsymbol{x}_2 - \boldsymbol{x}_1)/r$ mark the direction of the forces as is shown in figure 1. In general body $\mathcal{B}_1$ is influenced by all atoms of

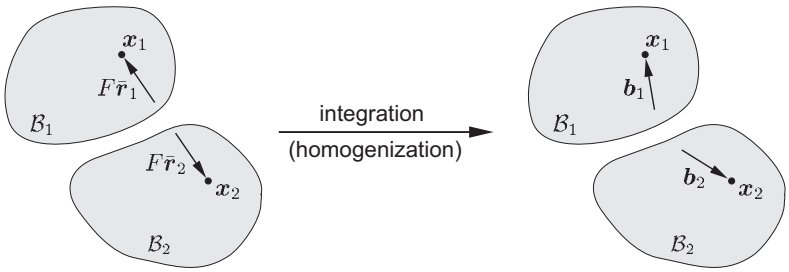

Fig. 1 Homogenization of the interaction of two nanoscale bodies $\mathcal{B}_1$ and $\mathcal{B}_2$

body $\mathcal{B}_2$ while body $\mathcal{B}_2$ is influenced by all atoms of body $\mathcal{B}_1$. Thus a body force is generated in each body which is given by the integration

$$\boldsymbol{b}_1(\boldsymbol{x}_1) = \int_{\mathcal{B}_2} \beta_2\, F(r)\, \bar{\boldsymbol{r}}_1 \,\mathrm{d}v_2 \;, \qquad \boldsymbol{b}_2(\boldsymbol{x}_2) = \int_{\mathcal{B}_1} \beta_1\, F(r)\, \bar{\boldsymbol{r}}_2 \,\mathrm{d}v_1 \;, \tag{2}$$

(see figure 1). Here β_I denotes the atomic density of body $\mathcal{B}_I$. The equilibrium equation of both bodies ($I = 1, 2$) reads

$$\operatorname{div} \boldsymbol{\sigma}_I + \beta_I\, \boldsymbol{b}_I = \boldsymbol{0} \;, \tag{3}$$

where $\boldsymbol{\sigma}_I$ is the Cauchy stress inside body $\mathcal{B}_I$. Multiplying these equations with the test functions $\delta\boldsymbol{\varphi}_1$ and $\delta\boldsymbol{\varphi}_2$ and integrating over the bodies yields

$$\int_{\mathcal{B}_1} \delta\boldsymbol{\varphi}_1 \cdot \big(\operatorname{div} \boldsymbol{\sigma}_1 + \beta_1\, \boldsymbol{b}_1\big)\,\mathrm{d}v_1 + \int_{\mathcal{B}_2} \delta\boldsymbol{\varphi}_2 \cdot \big(\operatorname{div} \boldsymbol{\sigma}_2 + \beta_2\, \boldsymbol{b}_2\big)\,\mathrm{d}v_2 = 0 \;, \quad \forall\, \delta\boldsymbol{\varphi}_I \;. \tag{4}$$

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Using the divergence theorem eq. (4) can be rewritten as

$$\sum_{I=1}^{2}\left[\int_{\mathcal{B}_I}\operatorname{grad}(\delta\boldsymbol{\varphi}_I):\boldsymbol{\sigma}_I\,\mathrm{d}v_I-\int_{\mathcal{B}_I}\delta\boldsymbol{\varphi}_I\cdot\beta_I\,\boldsymbol{b}_I\,\mathrm{d}v_I\right]=0\,,\quad\forall\,\delta\boldsymbol{\varphi}_I\,, \tag{5}$$

which is the weak form of the proposed contact-interaction model. The first term describes the internal virtual work, due to the deformation of the solids, while the second term denotes the virtual work due to contact. If externally applied body forces $\bar{\boldsymbol{b}}_I$ in $\mathcal{B}_I$ and surface tractions $\bar{\boldsymbol{t}}_I$ on $\partial_t\mathcal{B}_I$ are considered, the weak form (5) must be extended by the external virtual work contribution $\delta\Pi_{\mathrm{ext}}$ [3]. It is noted that the weak form (5) can also be derived from a variational principle considering the potential energy $\Pi=\Pi_{\mathrm{int}}+\Pi_{\mathrm{C}}-\Pi_{\mathrm{ext}}$ where

$$\Pi_{\mathrm{C}}:=\int_{\mathcal{B}_1}\int_{\mathcal{B}_2}\beta_1\,\beta_2\,\phi(r)\,\mathrm{d}v_2\,\mathrm{d}v_1\,, \tag{6}$$

describes the interaction energy between the two bodies. We remark that the integration can be significantly simplified, if a cutoff radius of the atomic interaction potential ϕ is considered. This leads to numerically highly efficient implementation methods. Details are discussed [3] and [5].

2 Numerical Example

As a numerical example we consider the nanoindentation of a stiff Vickers indenter ($\mathcal{B}_1$) into a soft substrate ($\mathcal{B}_2$). The weak form (5) is discretized by a nonlinear finite element approach. The problem setup is displayed in figure 2a. The bodies are

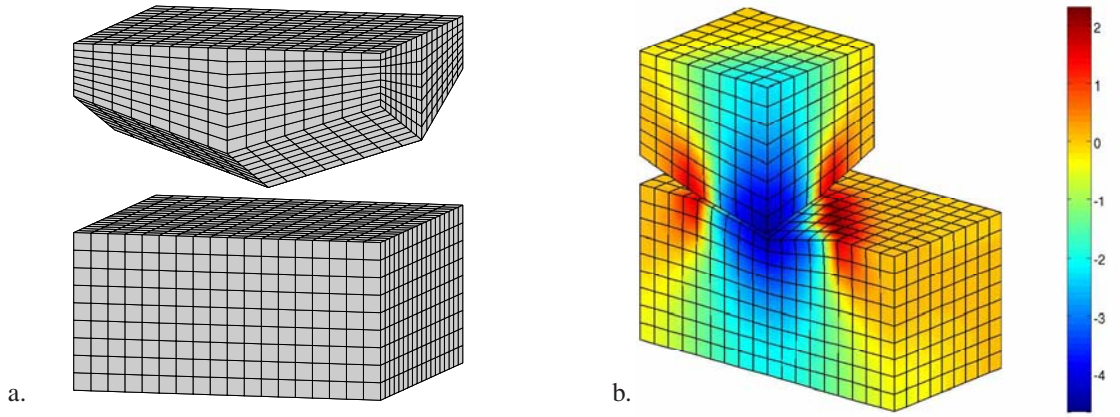

Fig. 2 a. Nanoindentation model; b. Deformation and stress σ_{33} during indentation

modelled by a Neo-Hookean material law with the Poisson's ratio $\nu_1=\nu_2=0.2$ and Young's modulus $E_1=3E_2$. Figure 2b show the vertical normal stress component σ_{33} scaled by

$$\operatorname{arsinh}\left(\frac{\alpha\,\sigma_{33}}{\max\left(\sigma_{33}\right)}\right)\,, \tag{7}$$

where α is a scaling factor chosen as $\alpha=5$ and where $\max\left(\sigma_{33}\right)$ denotes the maximum of σ_{33}. As is indicated by figure 2b large, compressive (i.e. negative) stresses appear at the center of contact due to the atomic repulsion modelled by ϕ (1). At the fringe of the contact zone, on the other hand, tensile (i.e. positive) stresses appear due to the attractive part in ϕ.

The generality of the proposed contact model allows the study of a large class of contact-interaction problems. In [3] the interaction between carbon nanotubes is investigated, while in [4] a comparison with the JKR model [6] is shown. The presented contact model allows the study of contact over a wide range of length scales as is shown in [5]. Currently under investigation are the adhesion mechanisms occurring in some biomechanical systems.

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