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Methods and numerical aspects of nanoscopic contact area estimation in atomistic tribological simulations

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ABSTRACT

We show how data obtained from molecular dynamics (MD) simulations of nanoscale friction should be treated for producing constitutive system parameters with a proper error estimation. A visualisation scheme for discrete atomistic geometries based on the smooth particle method (SPM) was parametrised and validated to yield an accurate and computationally robust estimation of the contact area between two touching nanoscopic asperities. We present some thoughts on the error estimation of the contact forces occurring due to the load and the shearing motion. The variance in the friction force constitutes the main source of error for the fitting of the constitutive system parameters. The dependence of the constitutive system parameters on the number of available data points was also studied. It was shown that an equal spacing (by load) of the data points can result in better values for the system parameters than the convergence trend suggests.

1. Introduction

By post-processing molecular dynamics (MD) data based on the smooth particle method (SPM) [1], the authors have previously shown that a three-term kinetic friction law [2]

$$F(L) = F_0 + \tau A_{\mathrm{asp}}(L) + \mu L \tag{1}$$

holds for both mixed- and boundary-lubricated nanotribological systems. Here $F(L)$ is the load-dependent friction force, whereas the load independent Derjaguin-offset F_0 [3] together with the shear strength τ and the kinetic coefficient of friction (CoF) μ form the unique set of constitutive system parameters which characterises the nanoscopic systems of interest from a tribological point of view. The Bowden–Tabor term $\tau A_{\mathrm{asp}}(L)$ in Eq. (1) is ascribed to the adhesion-controlled friction [4] and, in addition to the constant Derjaguin-offset F_0, accounts for the irregular departure of the friction-versus-load behaviour $F(L)$ from the well-known Amontons–Coulomb law μL [5,6] via the load-dependent asperity contact area $A_{\mathrm{asp}}(L)$.

There are several methods known in the literature to estimate $A_{\mathrm{asp}}(L)$ at the atomic length scale, especially when dealing with single-asperity contact situations [7]. In a wide class of approaches, the contact pressure distribution, e.g., the radial one, is used to estimate the contact radius and hence $A_{\mathrm{asp}}(L)$ [8,9]. In another group of approximations, the number of atoms within the contact zone is determined, and by multiplying this by an estimate for the atomic contact area, $A_{\mathrm{asp}}(L)$ is obtained [10,11]. In our MD + SPM scheme, a material density is constructed around the atomic positions that lie within the solid regions of the investigated nanotribological system, such that when solid–solid contact occurs during sliding, the corresponding asperity contact area is considered as the minimal cross-section of the solid bridge [2]. The authors have previously shown that the thus-defined quantity $A_{\mathrm{asp}}(L)$ does not vary linearly with the load L, but is proportional to the number of contact atoms [1].

In this work we will discuss methods which are applied to analyse the output of MD shear simulations. First we will briefly review the post-processing tool by the authors [1,2], which can be used for mapping discrete MD data to the continuum as well as for defining and determining the asperity–asperity contact area in a mixed-lubrication simulation. Furthermore, the theoretical concepts and numerical methods required for calculating contact forces in MD shear simulations will be discussed. Finally, we will show that these forces and the contact area provide a proper basis for obtaining all relevant tribological system parameters, namely the Derjaguin-offset F_0, the shear strength τ, and the kinetic CoF μ.

2. Setup of nanosystems

All theoretical and computational aspects covered in this work will be exemplified with data obtained from MD shear simulations of three nanotribological systems which were carried out using

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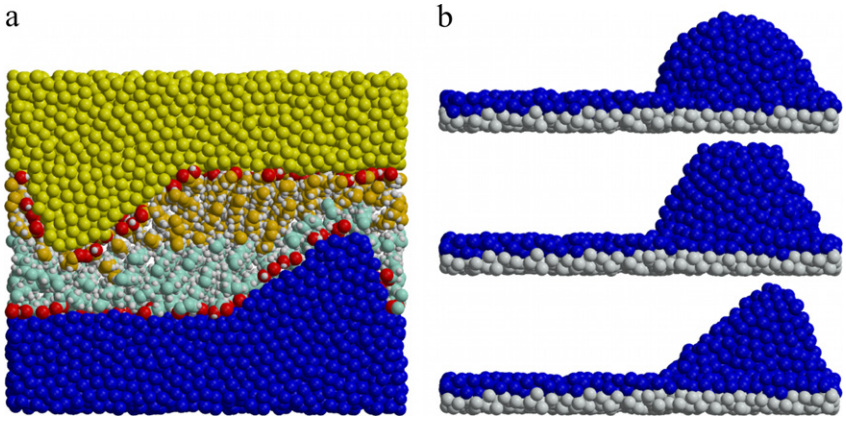

Fig. 1. Molecular dynamics system setup. (a) Section through the system with one slanted pyramid asperity per slider. Colours: Fe (top)—yellow, Fe (bottom)—blue, C (top)—orange, C (bottom)—light blue, H—white, O—red. Different colours for Fe and C in the top and bottom halves of the system only serve to better show the sliding interface. (b) Semi-spherical (top), truncated cone (centre), and slanted pyramid asperity (bottom). The grey atoms give an idea of the number of atoms which are kept rigid throughout the simulation. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

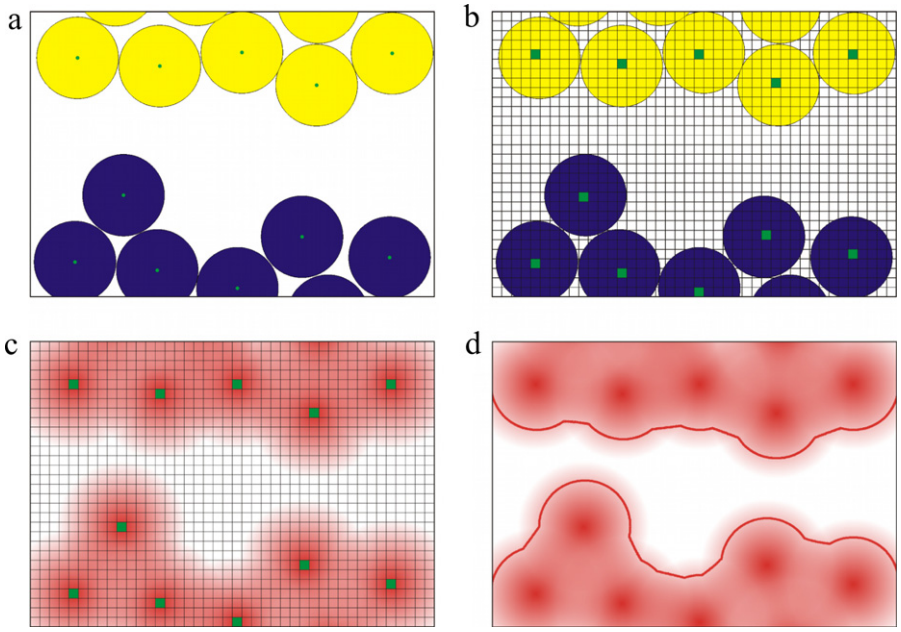

Fig. 2. From MD to continuum with SPM, illustrated in 2D for identical surface atoms. (a) Discrete representation of MD nanosystem. (b) Meshing of the simulation box; the green squares are the atomic centre elements. (c) Convolution of the centre element distribution with the kernel function yields a quasi-continuous material density distribution. (d) Surface visualisation as an iso-surface at a given density threshold ρ_0 (bold red line). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

LAMMPS [12]. The system geometries are identical to those discussed in the first part of Ref. [2], and were chosen to study the impact of load- and shape-dependent asperity contact on the friction force.

The thickness of the amorphous Fe substrates, which are modelled with a Finnis–Sinclair potential with the parameters taken from Ref. [13], is 1.96 nm. This is equivalent to 4050 atoms or ∼12 monolayers of bcc Fe(100) per substrate. Stearic acid molecules, interacting via the OPLS-AA force field [14], are physisorbed to the substrates and act as a boundary lubricant. The lubricant coverage of 66 molecules per slider (corresponding to an available substrate area per headgroup of roughly 42 Å^2) is the same for all three asperity types (semi-spherical, truncated cone and slanted pyramid). A snapshot of the system with the slanted pyramid asperity can be seen in Fig. 1(a), while Fig. 1(b) shows the three different asperity shapes. A Langevin thermostat acting only in the direction normal to the load and shear keeps the substrate temperature at 300 K. The 62 applied loads L range from 2.07 to 44 nN in steps of 0.69 nN, corresponding to nominal pressures between 75 MPa and 1.6 GPa in steps of 25 MPa. Our simulations are therefore effectively carried out in an *NPT* ensemble, with a constant number of atoms, constant pressure and constant temperature. Sliding along the horizontal (x-)direction took place at a velocity of 4 m/s for a duration of 2.5 ns including a dynamic equilibration period of 500 ps which does not contribute to the analysed dataset.

3. Smooth particle visualisation

Depending on the asperity shape and the applied load, the two asperities may engage in contact during shear. The calculation or even the definition of the asperity contact area is awkward in the discrete MD representation. So in order to transform an atomistic nanosystem, where the coordinates of the atoms' centre positions as well as the atom radii are known, see Fig. 2(a), to its smooth particle representation, a mesh of size d (e.g., equal to 40 pm for the amorphous Fe substrates introduced in Section 2) is laid over the