Modeling and simulation in tribology across scales: An overview

Micro/Nanoscale Models for Tribology: State-of-the-Art and Roadmap for Future Research

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Abstract
This review summarizes recent advances in the area of tribology based on a Lorentz Center workshop discussing the themes of rough surface representations, the breakdown of continuum theories at the nano- and microscales, as well as multiscale and multiphysics aspects for analytical and computational models, within the empirical context provided by experimental results. While the modeling community can adequately address elastic contact problems of great complexity at various scales, significant effort is still required to account for the effects of plasticity, adhesion, friction, wear, lubrication and surface chemistry in tribological models. Research directions for the future are proposed based on as yet unanswered fundamental questions and the perceived needs of the industry for comprehensive but simple and robust tribological models.

Keywords: tribology, multiscale modeling, multiphysics modeling, roughness, contact, friction, adhesion, wear, lubrication, surface chemistry

1. Introduction

The word tribology, which derives from the root tribo- (Greek τρίβος, meaning rubbing) and the suffix -logy (Greek -λογία, meaning the study of), was apparently coined by David Tabor and Peter Jost and was used in the famous Jost report of 1966 [1]. That report suggested that problems of lubrication in engineering needed an interdisciplinary approach –including chemistry and materials science, solid mechanics and physics. The famous calculation suggested that British industry could save £500 million a year "as a result of fewer breakdowns causing lost production; lower energy consumption; reduced maintenance costs; and longer machine life". Even today, friction losses are often evaluated as more than 1 per cent of GDP, and the discipline is therefore still flourishing.

More recently, new areas of tribology have emerged, including nanotribology (studying friction, wear and lubrication often with the Atomic force microscopy and MEMS/NEMS), biotribology (human joint prosthetics, dental materials, skin, etc), and ecological aspects of friction, lubrication and wear (tribology of clean energy sources, green lubricants, biomimetic tribology). Studies of the so-called "superlubricity" (the possible phenomenon of vanishing friction) have created great expectations of energy savings, and the recent creation of graphene is also greatly promising. (some ref. Here and there?)

Brief introduction of Lorentz workshop: structure, goals, participants (Table 1 in section 5); was it successful?

In this contribution, we do not expect to give a comprehensive state-of-the-art of this very wide topic, but we summarize some results evidenced from the participants of the Lorentz workshop held recently in Holland. There are fundamental open questions in the field, and for example, the community still debates if fractals in tribology as describing roughness have given answers to problems, or created questions of purely academic interest. A certain distance exists between different communities involved in tribology, in notation, language, how problems are posed, how solutions are presented. Analytical models are necessary to understand the behavior at the interface, otherwise numerical simulations may be pure black boxes.

One-paragraph general review of the types of modeling approaches used in tribology, discussed in detail in section 2.

Discussion of active research themes, discussed in detail in section 3.

Summary of fundamental/ open questions in the field and comments from industrial participants about the current needs for industry: give specific examples of applications, discussed in detail in section 4.

One of the key issues facing the tribology community is the apparent disparity between the fields of expertise relevant to such an interdisciplinary topic, which leads to a lack of communication between engineers, material scientists, applied physicists and chemists who work to solve similar tribological problems. Analytical models are necessary to understand the behavior at the interface, otherwise numerical simulations may be a black box (comment from B.N.J. Persson during the Lorentz workshop). Furthermore, physicists may be interested in a fundamental understanding of friction (a general law), while engineers need "numbers" that can be used for design, which may explain the extended utilization of numerical studies.

Difficulties are further compounded by divisions between modelers and experimentalists, as well as those working on analytical versus computational methods –and also between the proponents and users of different theories, computational methods and tools– and depending on the research applications. These issues are discussed in the paper as follows: various modeling methods and tools are discussed in section 2; research themes in tribology, including rough surface representations, scale effects and the breakdown of continuum theories at the nano- and microscales, material models and multiphysics aspects are addressed in section 3; a roadmap for future research is formulated in section 4; and, conclusions are given in section 5. Since increased visibility and cooperation between tribologists from different backgrounds will be necessary to improve on the state-of-the-art, the present review aims to provide a starting point for further collaboration and possible focal points for future research in tribology.

2. Tribological modeling methods

This section introduces the main modeling methods and tools currently used in tribological modeling, starting from analytical models and discussing methods inherently suitable for the micro- and nanoscales, as well as multiscale approaches.

2.1. Analytical models

2.1.1. Contact mechanics: where we stand

While a full review of contact mechanics is obviously an impossible task, K.L. Johnson's Contact Mechanics book [2] is still a very good starting point today. Later books and review papers, e.g. [3], have accounted for some of the progress made, but the field continues to expand across disciplines and is inherently hard to summarize. Nevertheless, one could take inspiration from Johnson's book chapters to attempt just that. For example, starting with the non-Hertzian normal contact of elastic bodies, one can identify some progress made in a number of areas such as the asymptotic singular stress field at wedge in sliding contact [4]. Similarly, there are certainly improvements made on anisotropic and layered plates and shells [ref?], but the biggest advances were probably made on adhesion; for example, the Johnson-Kendall-Roberts (JKR) model itself [5] has over 6,000 citations, while the body available in the literature is immense.

In the case of the normal contact of inelastic solids, significant technical developments in instrumented nanoindentation have been made (see, for example, the highly cited paper by Oliver & Pharr [6] with over 17,000 citations) since Johnson's core model of elasto-plastic indentation. Some progress was made on tangential loading and cyclic contact with the generalized solution of the Cattaneo problem [7] and developments (e.g. [8]). Fretting fatigue [9], crack analogues and notch analogues in fretting fatigue [10] have permitted some progress in understanding fretting, although the problem remains complicated

as there is contemporary presence of fatigue, surface damage, wear and stress gradients. There is not much work that is fundamentally new on the topic of rolling contact of elastic bodies, but a lot of computational work was performed for railways: examples aim to explain corrugation in rails [11-13], squeal (friction instabilities) [14], and rolling contact fatigue [15]. The rolling contact of inelastic bodies (shakedown, ratchetting, etc.), on the other hand, has seen limited development, e.g. [16], but is arguably difficult to model: ratchetting is very complicated and dependent on nonlinear kinematic hardening over millions of cycles makes that the problem ill-defined [17,18].

Calendering, referring to the elastic-plastic rolling of strips, and lubrication have also seen some developments with… [refs]; lubrication is discussed in more detail in section 3.8. On dynamic effects and impact, much work was published on the rate-and-state friction (RSF) law (discussed in section 3.6.2) and Adams' instability [19-21], while impact remains a separate and large area [22]. Following the classical contributions by J.R. Barber on, both, static and sliding contact reviewed in Johnson's book, new refined solutions and finite element formulations have appeared on thermoelastic contact (e.g. [23,24].

On the topic of rough surfaces, the most highly cited theory after GW is that of Majumdar and Bhushan [25], where Korcak's law was used to define a power law distribution of contact spots, a "bearing area" result very much in contrast with present understanding of contact area being formed by "resolution-dependent" contact spot sizes. This view of "magnification" dependent solution is not too different from the original Archard model [26] of spheres on spheres on spheres, where indeed the solution is obtained introducing at each step a sphere on a previous solution. Then, Ciavarella et al. [27] first obtained that the contact area decreases without limit as the resolution (or magnification) is increased, i.e. is in all respects a fractal, within the elastic assumption, a result which anticipates that of Persson, but obtained with a Weierstrass series as a fractal which, therefore, is less popular among tribologists. Persson's well known theory gives a clear approximation in the entire range of pressure [28], but a more precise estimate of a quantity which is hardly used in any quantitative model of tribology is certainly a great success mathematically, but is it in practice? The real physical problems remain unanswered: what is the real contact area? Is a "magnification dependent" quantity useful for any quantitative estimate? If so, the quantitative estimate requires plastic or other failure mechanisms, or adhesion at small scales, to converge to a well-defined value?

Too much emphasis is placed today on nominally flat stationary self-affine fractals, while very little work was performed on "shape" –particularly with adhesion–, where the basic contact problem of a rough sphere has not seen any real attempts of solution. One could argue that separation of length scales (if it exists) should be enough to study roughness at the relevant length scale and ignore shapes. Furthermore, if the roughness on the sphere –in this specific example– is not dominant, then the assumption of micro-contact holds and the problem could be solved analytically utilizing, for example, an extension of Guduru's solution to rough surfaces [29]. Otherwise, numerical calculations are necessary and could be used to separate the length scales within numerical methods. The topic of roughness is discussed extensively in section 3.1.

2.1.2. Multi-asperity models

Multi-asperity contact models are based on the approach introduced in the seminar Greenwood and Williamson paper of 1966 [30], where the probability density function (PDF) of summit heights and their curvatures allows one to calculate the normalized contact area and normal applied pressure. Later models, such as those of Bush-Gibson-Thomas (BGT) [31], Nayak-Thomas [32], Greenwood [33] and Carbone [34], built on the original GW and progressively relaxed a number of its assumptions. In the prediction of the area of contact as a function of the load, the Nayak parameter α is very important in

multi-asperity models: if α is high, linearity applies only to very small forces (and very large separations, e.g. 10 times the root-mean-square (RMS) roughness), in which case *one may wonder whether asymptotical linearity really is physically meaningful*. The prediction of the separation requires complex calculations, while, in the probability distribution, pressure goes to zero as per the Hertzian assumption [K4]. Unlike the original assumption of GW, asperity interaction is important as there is no lateral length beyond which interaction is zero for a finite nominal area of contact [35,36], but interaction becomes zero sufficiently far from a locally contacting asperity [37,38]; in fact, introducing asperity interaction gives better agreement for the proportionality coefficient κ [39]. But, what happens with coalescing asperities? While there is no self-consistency in multi-asperity theories (fitting is needed), introducing interaction in the elastic fields of contacting asperities and accounting for coalescing asperities gives a simpler (exponential) law for the pressure v. separation [K4].

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Example: I. Goryacheva:

- Macroscopic modelling approach: starting from a simple indentation model to develop a model that takes into account process parameters.
- Two-scale analysis: take into account the interaction of contact spots with elastic halfspace and include this into a macroscopic model.
- Refs: Appl Math and Mech, 1998; Contact mechanics in tribology, 1997.
- Three levels of asperity sizes considered; considered an adhesion zone outside the contact via a one-step Maugis-Dugdale model (and capillary adhesion via meniscus formation).
- …

M. Scaraggi: What happens if the local average pressure is larger than the full contact? Answer: this is asperity-level contact.

M. Toose: it's nice to have an analytical model. Can such a model be used in the study of friction as well? Answer: yes (this is the second part of the presentation, which was not discussed).

Additions (Irina Goryacheva):

Analytical macroscale models of the normal contact of the bodies with given macroshape and microgeometry parameters were developed based on two scales analysis and construction of additional displacement function which describes the surface roughness compliance taking into account the shape of asperities and elastic interaction between them (Irina Goryacheva. Contact mechanics in tribology (1997), Kluwer; Journal of Friction and Wear (1999), V.20 No 3; Tribology International (2006), V.39, pp.381-386). The models developed based on this approach also take into account

- height distribution of asperities (Irina Goryacheva.Contact mechanics in tribology, 1997, Kluwer; Tribology International (2006), V.39, pp.381-386),
- height distribution of asperities and the particular properties of the counterbody surface layer properties (the solution of the contact problem for the rigid body with given microgeometry and the two layered elastic half space was developed, see Torskaya, E. V. Modeling of frictional interaction of a rough indenter and a two-layer elastic half-space// Physical Mesomechanics, 2012, Volume: 15 Issue: 3-4 Pages: 245-250; E.V Torskaya Study of roughness effect on elastic indentation of coated bodies//Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science, Proc IMechE Part C: J Mechanical Engineering Science, 2016, Vol. 230(9), P. 1392–1397

- the microgeometry parameters and attractive stresses outside the contact zones due to molecular adhesion the solution is based on Maugis-Dagdale approximation of the Lennard_Jones potential) or capillary adhesion in the presence of menisci of fluid in the gap between the contacting surfaces (Yu.Makhovskaya, Mech. Solids. 2003. V. 38, No 2),

Macroscale models of the sliding contact of the rigid bodies with periodic microgeometry over the viscoelastic foundation were developed to study the dependence of the mechanical component of friction force (or friction coefficient) on sliding velocity, rheological properties of the viscoelastic foundation, microgeometry parameters, interface conditions, including

- adhesion effect in the gap between contacting bodies (I.Goryacheva,Yu.Makhovskaya, J. of Strain Analysis for Engineering Design, 2016. Vol.51 No 4),
- existence of the incompressible fluid in the gap between the contacting surfaces (I.Goryacheva, A.Shpenev Applied Math.&Mech, 2012, V.76, No.5)
- various shapes of asperities (B.Sheptunov, I.Goryacheva, M.Nozdrin, Friction&Wear, 2013 V. 34, No 2.)
- elastohydrodynamic lubrication in the gap between the rough cylinder and a viscoelastic foundation (I.Goryacheva, P.Usov, Applied Math.&Mech, 2012, V.76, No.5)

The effect of the viscoelastic interaction between two spherical asperities sliding over the viscoelastic half-space was analyzed by F.Stepanov (Applied Mech.&Tech Physics, 2015, V.56 No 6)

The effect of the adhesive friction at the contact spot on the mechanical component of friction force in sliding contact of the asperity over the viscoelastic half-space (3-D contact problem) was analyzed by Irina Goryacheva, Feodor Stepanov and Elena Torskaya (Applied Math.&Mech, 2015. V. 79. No 6).

The analysis of the internal stresses inside the viscoelastic half-space under the moving asperity and its dependence on sliding velocity, contact density parameter , viscoelastic properties of the half-space was performed in F. I. Stepanov, E. V. Torskaya Study of stress state of viscoelastic half-space in sliding contact with smooth indenter // Journal of Friction and Wear, 2016, Volume 37, Issue 2, pp 101–106

The multiscale contact problem for a punch with fractal (Cantor–Borodich type) microgeometry sliding over Kelvin viscoelastic foundation was analyzed by I.A. Soldatenkov (Journal of Friction and Wear, 2015, Vol. 36, No. 3). The friction force was found by infinite summation of contributions of single asperities, each having the friction force determined via energy dissipation.

Effect of the punch macroscale geometry on friction was investigated by I.A. Soldatenkov in Journal of Friction and Wear. 2008, V. 29, No 1.

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2.1.3. Persson's theory

Another class of analytical models are based on Persson's theory [28], where the stress probability distribution is considered to be a function of the magnification ζ at which the rough surface is examined. In the absence of adhesion at the interface, the contact area is defined where the stress is positive at the interface; hence, the probability to have positive compressive pressure at the interface can be thought of as the fraction of the real to the nominal area of contact. Starting from full contact conditions where the problem is completely linear, one can move from the displacement to the stress distribution via a transfer function so that, if the surface height distribution is Gaussian, the resulting stress distribution will be Gaussian too. The RMS and variance of the slope depends on the high-frequency cutoff such that, at different magnifications, the variance of the PDF starts to increase as more length scales are added (the

issue of the multiscale nature of roughness is discussed in section 3.1); one can show (e.g. as in approach by Manners [40]) that this could be described via a diffusion equation, for which the correct boundary conditions, even for the non-adhesive case, are necessary. While this is tractable for the non- adhesive case (assuming vanishing PDF for vanishing pressure, as in Hertzian contacts), tackling adhesion at the interface is more complex. In this case, one can calculate the tractive stress by a condition similar to the Griffith condition for crack propagation, and introduce this into the boundary conditions. In all cases the initial condition of the diffusion equation is obtained by recalling that, at a magnification of one, the stress is equal to the nominal stress so the stress probability distribution is a Dirac delta function centered at the mean value of stress [K4].

While Persson's theory can give the real contact area at each magnification, some approximations are necessary, of which the most problematic is the assumption of full contact: the diffusivity function is obtained assuming full contact and no interaction between different scales (i.e. averaging at different scales are independent statistical processes). Very simple final formulas for the contact area can be derived from this model where no moments higher than m_2 are needed. In contrast, multi-asperity theories require spectral moments as high as m_4 for the Nayak parameter, while newer theories require up to m_6 [K4]; however, this is not a significant true effect, just that they become inaccurate at high Nayak band parameters (MAYBE HERE NEW PAPER OF VLAD YASTREBOV). At the same time, separation, which is needed, for example, to calculate the volume fraction of voids useful in percolation, is not easy to calculate with Persson's theory. Nevertheless, it can be calculated in the absence of adhesion by considering the following: when squeezing an elastic block against a rigid rough surface until a certain value of the contact area is reached, one need to do work which, at the end of the process, is completely "transformed" into elastic energy. Since the elastic energy at the interface can be calculated within the original Persson theory as a function of the nominal contact pressure, an ordinary differential equation can be derived that relates the change of separation to the change of nominal contact pressure, and which, therefore, allows the calculation of separation as a function of contact pressure [K4].

When comparing multi-asperity models and Persson's theory, one metric often used in the correct (linear) relation for the proportionality coefficient κ between the area and the applied load. Persson introduced terms in his theory to correct for this [K4]. When comparing to experiments (using a PDMS block as the elastic solid with $E = 2.3\ MPa$, versus asphalt and concrete surfaces), Persson's theory matches the experiments –unlike the BGT model– in the linear behavior of the log-linear plot at relatively high loads, when there is a sufficiently large number of contact spots; this points to an exponential dependence [K4]. None of the original (GW or Persson) theories can say something about the local gaps, although Persson's theory can be also used to calculate the PDF of the local gap distribution. A different way to calculate local gaps if is via numerical modelling; this is discussed in the summary of the recent contact-mechanics challenge (see section 3.4). The proportionality coefficient for two- and one-dimensional contacts is predicted to be ~ 2.51 by BGT and ~ 1.60 by Persson's theory, while the "real" value is ~ 2 [K4].

After many studies, it has become apparent that the difference in the area-load coefficient only becomes important at intermediate pressures and large Nayak bandwidth parameters. But, once again, the correct contact area is not used much in any tribology model. Perhaps a more important quantity is the load-separation relationship. Here, Persson developed some semi-analytical reasoning, which seem to include empirical fitting parameters [41], which would require some better examination. Persson's theory seems to suggest complete "disagreement" over asperity models. We can show here quickly that this is over-statement.

2.2. Finite and Boundary Element Methods

The finite element method (FEM) is…

Pending content from J. Lengiewicz…

What is referred to here as a boundary element method (BEM) is a method that solves the complementarity problem

$$h \cdot p = 0, \;\; h \geq 0, \;\; p \geq 0, \tag{1}$$

where h is the deformed gap between the surfaces and p is the contact pressure. In the purely linear elastic case,

$$h = \delta + g + u_e, \tag{2}$$

where δ is (related to) the rigid body separation, g is the (initial) gap between the undeformed upper g_u and lower surfaces g_l, i.e., $g = g_u - g_l$ and u_e is the elastic deformation. For an elastic half-space, the elastic deformation is given by the Boussinesq-Cerruti integral equation:

$$u(x,y) = \int_{-\infty}^{\infty} K(x-x')p(x')dx', \tag{3}$$

where

$$K(x-x') = -\frac{2}{\pi E^*}\ln|x-x'| \tag{4}$$

in 2D and

$$K(x-x') = \frac{1}{\pi E^*}\frac{1}{\sqrt{(x-x')^2+(y-y')^2}} \tag{5}$$

in 3D. The composite elastic modulus is given by

$$\frac{1}{E^*} = \frac{\left(1-\nu_1^2\right)}{E_1} + \frac{\left(1-\nu_2^2\right)}{E_2} = \frac{2}{E'}. \tag{6}$$

An efficient way of obtaining a solution satisfying the LCP in (1) is to formulate and minimize total complementary potential energy V^*. This type of approach is well-described in the paper by Tian and Bhushan [42], which incorporates a linear elastic-perfectly plastic material model where the hardness H (of the softer surface) governs the plastic deformation. The total complementary potential energy V^* can in this case be formulated as

$$V^*(p) = \frac{1}{2}\iint_{\Omega} p u_e dA - \iint_{\Omega} p\left(\delta + g - \frac{1}{2}\Delta u_p\right)dA, \tag{7}$$

where Δu_p is the incremental plastic formation. The solution to the corresponding complementarity problem

$$h_p \cdot p = 0, \;\; 0 \leq h_p, \;\; 0 \leq p \leq H, \tag{8}$$

can then be found by minimization subject to the constraint $0 \leq p \leq H$, i.e.,

$$\min_{0 \le p \le H} V^*(p), \tag{9}$$

In the two-part paper by Sahlin et al. [43,44], a linear elastic-perfectly plastic BEM based on the model in [42], with the solution procedure adapted from Stanley and Kato [45] and accelerated by means of the DC-FFT technique presented by Wang et al. in [46] is detailed. This particular BEM has been rigorously justified by means of comparison to the experimental results for bi-sinusoidal surfaces presented by Johnson, Greenwood, and Higginson [47] and verified against other computational contact mechanics methods in Almqvist et al. [48]. From the analysis in the latter work, it was concluded that the BEM is applicable for the whole range from initial to complete contact. In this particular BEM, convergence is reached when all (only elastically deformed) contact points, for which $0 \le p < H$, lie within a specified maximum deviance from *the contact plane*, where $h_p = 0$. It should be noted that this max norm-based convergence criterion is drastically different from the Euclidian norm based one, which is applied in so called greedy Conjugate Gradient Methods (CGM). In the paper by Bemporad and Paggi [49], which presents a detailed analysis of BEM solution algorithms, a counterexample is given which shows that the greedy CGM fails in getting the correct solution. This wouldn't be the case if the algorithm detailed in [43,44] was used instead. More results obtained by using the BEM including elastoplastic deformation can be found in [50-57].

FT-BVM stands out for efficient computation (rigorous treatment of measured profiles feasible) [K1].

Long-range correlation relevant for fractal versus bearing area methods (Slide 36, and RT7) [K3].

Note: you must re-introduce some content into BEM (linear elastic contact); there is no fractal characterization of the surface. *lots of discussion generated* [K3].

FEM/ BEM needs very fine mesh to achieve high resolution; MD or mixed MD-FEM or MD-BEM techniques can treat a relatively small number of DOFs [K4].

The advantage of BEM compared to FEM is that rough interfaces can be easily modeled [RT14].

If you want to include 3 orders of magnitude of roughness, the required discretization is very high. Idea: discretize only contact spots via a non-uniform meshing to capture the effect of singularities in the distribution due to the presence of roughness. Use a "comb" of Dirac delta functions spaced by the wavelength to study periodic contacts and alleviate the limitations of using the Flamant solution. Contact areas are determined by minimizing the total energy for a fixed separation. Adhesion results in geometric nonlinearities: hence, you must follow a slow loading process and to the minimization at each step (e.g. doing loading v. unloading –with the same model– you end up with hysteresis) [K4]. Result: Original Persson's theory predicts 50% smaller contact area in 1D+1D contacts, during loading; this difference becomes much smaller (20%) if you look at 3d contact as Persson's theory is a sort of mean field theory, the latter being more accurate as the dimensionality is increased (issue with dimensionality and its relation to mean-field theories). For separation, the agreement with Persson's model is good except at high separations. The tails of the stress PDF are Gaussian. Caveat: you have to be sure the discretization is such that the numerically calculated stress PD goes to zero when the stress goes to zero: a wrong stress PD prevents the right estimation of the coefficient kappa.

2.3. Crystal plasticity and Discrete Dislocation Dynamics

A variety of plasticity models exist at different scales: MD, dislocation dynamics, crystal plasticity, J2-theory [RT14]…

Pending content from S. Stupkiewicz…

Discrete dislocation dynamics is a modeling technique to study plasticity at the microscale [58-63]. Plasticity is described by the collective motion of discrete dislocations on their crystallographic slip systems. The solid is modeled as a linear elastic continuum, and the dislocations by means of their linear elastic fields, which are accurate outside of the dislocation core. Atomistic aspects are included by means of constitutive rules that govern dislocation nucleation, glide, and interaction with obstacles. Given that both the dislocations and the solid are described using linear elasticity, it is possible to solve boundary value problems relying on the principle of superposition. The solution to the boundary value problem is given at each time increment and at every material point as the sum of the dislocation fields and their image fields. The image fields can be calculated using finite elements, although for contact problems, where rough surfaces need to be described using a fine discretization, it is computationally more efficient to use other techniques, such as for instance Green's function molecular dynamics [64].

Three-dimensional dislocation dynamics simulations have been performed to study nanoindentation, e.g., [65] or compression of micro-pillars, e.g., [63], and consistently showed limited dislocation plasticity in agreement with experimental work.

Contact between bodies with simple geometry was instead studied using plane strain two-dimensional dislocation dynamics, where edge dislocations glide on three sets of slip systems. Wei Siang Ng et al. [66] modeled Dislocation dynamics simulations of contact between a crystal with sinusoidal profile and a rigid flat, which resulted surface result in highly fragmented contact areas due to the exit of dislocations from free surfaces. This lead to and a peaky contact pressure profiles, with high localized pressure, very different from what a continuum model would be predicted by continuum models. A comparison between contact pressure profiles obtained using dislocation dynamics and crystal plasticity is presented in [67]. There, it is also shown that when plasticity is described by dislocation dynamics the motion of dislocations gives rise to a stronger interaction between plastic zones underneath the asperities than what would be predicted by crystal plasticity. As a consequence, asperities are more difficult to be flattened.

Komvopoulos et al. [68] modeled indentation of a flat crystal by means of a rigid rough surface with multi-scale roughness. Surface asperities were treated as a collection of Hertzian contacts and dislocations could glide only on a single crystallographic slip system. An interesting outcome of this study is that, as the load increases, asperity interactions emerge at different length scale, so do interactions between plastic zones.

In relation to plastic zones, large positive stress concentrations were found in the subsurface region in correspondence of dislocation pile-ups by Polonsky and Keer [69] and by Nicola et al. [70]. It is important to capture the presence of tensile stress states since they can promote crack nucleation.

When both bodies in contact can deform by dislocation plasticity [66], the contact pressure between a sinusoidal and flat bodies is independent of how plasticity is apportioned, i.e., whether dislocation sources are all in one body, all in the other, or equally shared between them.

The onset of static friction for a flat contact was presented by Deshpande et al. [Deshpande: missing ref.]. Decohesion between surfaces was modeled by means of a cohesive zone, which would open when the interfacial tractions would reach a critical value. This work points to the competition between plastic deformation (dominant for larger contact areas) and loss of adhesion (dominant when the contact is so small, that plasticity is limited).

While all dislocation dynamics simulations show that plasticity in contact problems is less than what would be predicted by continuum models, results are limited to small deformations, and often to two-dimensional simple problems.

A way to incorporate microscale size-dependent plasticity into contact models would be to fit the dislocation dynamics results for the deformation of a non-local plasticity theory, such as strain gradient plasticity or even include such effects in a statistical model. The advantage of statistical models, like the one recently developed by Song et al. [71], is their extremely low computational cost, which would make them attractive for use by the industry; however, a statistical approach based on the GW model, for example, would suffer from the same limiting assumptions discussed earlier (see section 2.1) and may not be directly applicable to realistic representations of roughness (see section 3.1), while incorporating dislocation dynamics results into Persson's theory may be a prohibitively complex exercise. Furthermore, the results of the statistical approach compared with a full SGP finite element simulation are found to give a harder response; clearly, there is room for improvement with the incorporation of plastic interactions, or the consideration of three-dimensional asperities in dislocation dynamics simulations.

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2.4. Classical and ab initio Molecular Dynamics

Classical molecular dynamics (MD) has been used…

When modeling tribochemistry, discussed in more detail in section 3.9, MD techniques [72-74] or quantum calculations (DFT) [75] are used to study atom motion during friction or chemical reactivity, respectively. To combine both types of information, reactive force-field MD [76], ab initio MD techniques [77] or tight binding coupled with MD [78] techniques have also been used to extract in-situ information of interfacial material behavior.

The atomic description of friction is usually provided in terms of the atom arrangement forming the sliding surfaces and the lubricant in between them; Newtonian (or Langevin) equations of motion are solved in the presence of an external load and a drift force pulling the sliding surfaces. In this way, it is possible to sample the evolution of the geometry of the system in order to obtain information on friction, adhesion, and wear [79]. A deeper insight of the local electronic and geometric characteristics is required to capture subtleties that a molecular mechanic description cannot represent; indeed, quantum mechanical approaches have been used to this aim [80] focusing on the theoretical modeling of a specific stoichiometry and chemical composition. The selection of the proper chemical composition, stoichiometry, and geometry determining the observed friction coefficient is usually based on experimental data, while theoretical works have the role to model the selected material to uncover peculiar properties.

A broader and more general theoretical framework of the microscopic friction would, indeed, help researchers to focus the experimental exploration on only those materials that are promising candidates with enhanced frictional properties. The term microscopic friction refers to the friction generated by the relative motion of few adjacent atom layers; it is the result of the local electronic and structural features of the material at the atomic level, originating from the atomic type and the geometric arrangement of the atoms. When microscopic friction involves only atomic layers of the bulk structure with no structural irregularities (dislocations, layer truncations etc.), we can name it as intrinsic friction, since it can be considered as a property peculiar of the pure compound without imperfections [81]. In consequence, all tribological properties originating from intrinsic friction, are referred as intrinsic of the considered system. The knowledge of intrinsic tribological properties is nowadays becoming mandatory with the

advance of the experimental techniques, now capable to micromanipulate free-standing atomic layers [82].

Recent ab initio studies on intrinsic friction [81,83,84] focused on the characterization of the atomic motions that produce a global slide of adjacent layers and how the atomic types determine such motions. In this framework, all the possible sliding directions are represented as suitable linear combinations of vibrational (phonon) modes and no assumption is done on the layer drift direction. By proper tuning of the related vibrational frequencies, it is possible to tune the intrinsic frictional response. This can be understood in terms of the classical picture. Each phonon mode represents a periodic atomic motion about an equilibrium position due to a harmonic restoring force with associated frequency ω, such that $\omega = \sqrt{k_f/m}$, where k_f is the force constant and m is the reduced mass of the atoms involved in the motion. The lower is the frequency ω, the weaker is the restoring force to which k_f is associated, and the higher is the amplitude of the corresponding atomic displacement at a fixed system energy. Wider atomic displacements, representing a global shift of one atomic layer with respect to its adjacent ones, correspond to facile layer sliding. The selection of proper atomic types facilitating atomic layer sliding can be done by combining electro-structural descriptors such as cophonicity, covalency and group-theoretical geometric distortion decomposition [83,85-87].

2.5. Multiscale models: concurrent and hierarchical schemes

Contact mechanics of rough surfaces is by definition a multiscale problem due to the multiscale features of surface roughness. The solution of the contact problem is strongly dependent on the number of wavelengths of roughness taken into account in the topology of the surface, as pioneeringly pointed out by Archard in 1953 [88] in his model of roughness conceived as a hierarchical assembly of asperities upon asperities whose size is dependent on the considered scale of observation. Although it is an idealized model, it has been suitably generalized by many authors and has inspired theoretical and computational studies aiming at understanding the role of roughness at the different scales of observation, see e.g. [26,27,89-91] among many others. Recently, the topic is becoming again of interest with the increased potentiality of molecular dynamics in studying nanoscale contact problems [92-95] that unveil interesting mechanisms of contact interactions occurring at the nanoscale. At the same time, the advent of molecular dynamics simulations opens new challenges due to the still limited time and size scales of the simulations that can be performed with the aid supercomputers. As proposed in fracture mechanics (see e.g. Budarapu et al. [96] for some recent progress on this matter and a wide overview of existing methods), coupling of discrete models based on molecular statics or dynamics and continuum models could be a solution strategy to overcome the previous issues. In this regard, coupling can be pursued via a top-down or a bottom-up approach. In the former, coarser models of roughness are solved first, and the displacement field is passed as a boundary condition to the finer scale models of roughness, in a hierarchical way. In the latter, fine scale models are solved first, and the contact response can be up-scaled as a constitutive traction-separation relation to be used in the contact models at the upper scales. In both scenarios, the solution scheme can be hierarchical with a one way passing of information, or concurrent, with a two-way feedback interaction between the models at the different scales. Clearly, concurrent solution schemes are computationally much more expensive than hierarchical ones, and the choice of one over the other should depend on the physics of the problem at hand. Therefore, further research on scale separation in contact interactions is deemed to be required to guide the choice of the most appropriate computational method preserving the accuracy of the description of the physical problem considering also the effect of the inherent uncertainties.

3. Research themes in tribology

This section introduces active topics for research in tribology, while different theories, techniques and models used to investigate these were reviewed in section 2. As the global forces acting on an interface are integral quantities along the interface (for example, the friction force is the integral of the shear stress over the contact area), various models can predict rather similar forces using different assumptions. Comparisons of models to experiments are therefore necessary, not only in terms of global forces but also in terms of local measurements, for instance, of temperature, strains or the real area of contact. Examples of such validation studies include MEMS-based stress measurements of the static or steadily sliding contact of a rigid indenter on a finite-thickness elastic coating captured by FEM [97] and analytical [98] models, and near-surface temperature fields in fretting contacts measured with infrared thermography, which were found in good agreement with FEM calculations involving frictional heat flux and thermos-elasticity [99]. Local measurements become increasingly accessible due to the miniaturization of local probes and the development of full-field evaluation techniques like digital image correlation (DIC) [100] or infrared imaging [101]. Imaging techniques are especially interesting for performing local measurements at a contact interface in a non-invasive way, but the choice of possible materials is limited as they must be transparent to the radiation used (e.g. visible or infrared light). Where relevant, reviews of experimental results are summarized to augment our understanding of tribological phenomena.

The problem of normal contact between rough surfaces has been studied extensively –for example, the reader is referred to a recent paper on the contact-mechanics challenge [K1] whose results are summarized in section 3.4– and can be considered to be well understood, but almost all other issues in tribology remain open for future research, as summarized below, starting from the nature of surface roughness itself.

3.1. Surface roughness

3.1.1. The nature of surface roughness

One of the fundamental issues in the modeling of contact between rough surfaces is the realistic representation of roughness. As the roughness of real engineering surfaces spans multiple length scales –whether measured experimentally or created using numerical methods (e.g. via simulations of sandblasting and shot peening [102], or through surface randomization algorithms [103,104])–, the question is essentially *which length scales are relevant in tribological modeling* and, alternatively, *should one bother to implement accurate roughness representations in tribological models*?

From an engineering perspective, the answer appears to be straightforward: accounting for roughness or not should be decided based on the application being modeled. Roughness is used for quality control in manufacturing and is very often an input for contact mechanics. At first glance, application-specific considerations correspond to distinct length scales: contact and friction between tectonic plates occurs along fault lines of the order of kilometers, while contact at the head-disk interface of hard disk drives can be of nanometer level. Upon closer examination, however, contact occurs over multiple length scales even in such “extreme” cases: macroscale sliding during earthquakes can be described via microscopic slip mechanisms at the level of micro-junctions [K2], while, in addition to nanoscale contact at the head-disk interface, the longer wavelength waviness of the disk surface plays a role in the dynamic excitation where it manifests as dynamic microwaviness and may result in catastrophic head crashes [105-107]. Hence, the engineering response could be adapted as follows: *the application should dictate the length scales at which modeling roughness is relevant*.

The wealth of parameters used in roughness characterization –amplitude (S_a, S_q, S_{sk}, S_{ku}), spatial (S_{al}, S_{tr}, S_{td}) and hybrid parameters (S_{dq}, S_{dr}), or Abbott-Firestone (bearing area) curve-based parameters (S_k, S_{pk}, S_{vk}, material ratios, and volume parameters for 3D measurements) [K3]– demonstrate the complexity of arriving at a universal description of surface roughness, since most models utilize only parameters deemed necessary to described specific functions: for example, S_a, S_k, S_{pk} and S_{vk} alone are important in the determination of contact stiffness [K3]. Moving away from statistical descriptions of roughness, fractal representations based on concepts of self-affinity and isotropy of properties were introduced to tribology much more recently, even though Archard first introduced a concept of fractals already in 1957 [108], much before Mandelbrot, with his model of spheres upon larger spheres upon larger spheres applied to contact and friction. More "realistic" fractals first came into tribology when Whitehouse and Archard [109] introduced the autocorrelation function (ACF) and discovered that their ground surface had an exponential one. The implication of their result, with their theoretical predictions matching their experimental measurements, was that between one-third and one-quarter of all their sample points would be a peak, regardless of the sampling interval they chose (!), while the mean peak curvature depended strongly on the sampling interval. They did note that the Fourier transform of an exponential ACF was a power law at large wavevectors, like Sayles and Thomas [110] will later confirm for a number of surfaces. It is useful to read today the Sayles and Thomas Nature paper abstract: "Topography is often considered as a narrow bandwidth of features covering the form or shape of the surface. After detailed study of many measurements we consider that as well as the possibility of a dominant range of features there is always an underlying random structure where undulations in surface height continue over as broad a bandwidth as the surface size will allow. We consider this a result of many physical effects each confined to a specific waveband but no band being dominant. We invoke the central limit theorem and show through Gaussian statistics that the variance of the height distribution of such a structure is linearly related to the length of sample involved. In another form, the power spectral density, this relationship is shown to agree well with measurements of structures taken over many scales of size, and from throughout the physical universe."

The lower wavevector dependence on RMS amplitude of roughness and the non-stationarity of surface roughness are two concepts much neglected in later literature, since we now concentrate on the wild effect of the upper wavevector truncation, which affects violently the contact area, the rubber friction dissipation, and many other physical properties.

A very interesting finding of Whitehouse and Archard came when they measure the profile of a rough surface along the same track, before and after a single passage of a lubricated slider. They found that, while the main scale roughness was still present, all the fine scale roughness had been removed [109]. Keeping in mind the limited metrology of the time, *one could ask whether we should measure or worry about the initial roughness at all*.

Following the introduction of fractal roughness, numerical models began to utilize the power spectral density (PSD) to fully define surface roughness. Due to thermodynamic considerations, the PSD does not necessarily lead to a well-defined "unique" response: different manifestations of surfaces in the real space are possible for the same PSD. While the effect of non-Gaussianity or scatter within a nominally identical Gaussian surface generator has limited effect in some quantities, it is clear that this is not generally true. Imperfect tails of Gaussian surfaces as easily provoked by low fractal dimensions since the PSD involves essentially a Fourier series with terms whose size decreases significantly with frequency and, hence, the central limit theorem does not apply (it would work for slopes and curvatures). For example, even small deviations from the ideal Gaussian random roughness case seem to lead to dramatic increase in adhesion for rough surfaces due to a finite number of asperities or a finite tail in the

height distribution [111,112]. This result will need accurate verification with more precise numerical models. Furthermore, as modern fractal parameters do not have a correspondence to traditional ones such as skewness, there might be an advantage in using traditional characterizations, perhaps to augment fractal ones for non-Gaussian surfaces [K3],[113].

The perceived universality of the PSD in fully describing surface roughness was demonstrated by Persson who showed that a 1D line scan, a 2D AFM scan and a 2D STM scan all lie on the same PSD plot for a grinded steel surface with the fractal dimension being $D_f = 2.15 \pm 0.15$ for many engineering surfaces [102]. At the same time, however, and in the absence of random phases, a profile PSD with a slope of -2 (as in the work of Whitehouse and Archard) does not necessarily represent a rough surface, but can also be a square wave (that has all phases equal to zero), while a slope of -3 may well correspond to semi-circles nestling together (demonstration by J.A. Greenwood during the Lorentz workshop) [RT3]. Having a Gaussian distribution of heights does not automatically suggest uncorrelated spectra. Higher order autocorrelation functions may be needed but the topic of non-Gaussian fractal surfaces is not very developed at present. A further consideration on the use of the PSD is the definition of the low- and high-frequency cutoff values, with the former corresponding to the slopes, but with the role of the latter resulting in serious discrepancy for Hurst exponents smaller than 0.5 [RT3]. Indeed, despite the progress in multiscale methods and the large literature that has emerged, the big problem remains with physical quantities that depend on slopes or curvatures, as the latter remain fundamentally arbitrary for a fractal due to their dependence on the truncation based on a high-frequency cutoff. In consequence, the real contact area, local pressure, and most of the local quantities are ill defined; however, one does not always need to worry about the high-frequency cutoff, as some macroscopic quantities, such as stiffness, electrical and thermal conductance, are well known to depend only on the RMS amplitude of roughness. This was known already in multi-asperity models and was also demonstrated by Barber [114]. Nevertheless, at the limit of atomistic roughness, one could argue that adding small wavelengths below the repulsive distance would result in constant roughness and contact properties: perhaps the high-frequency cutoff is related to the atomistic nature of the contact [RT3],[115].

The Nayak parameter [RT7]…

…

3.1.2. Measuring roughness

The metrology of surface roughness measurements plays a crucial role in our understanding of roughness as well [K3]. Abbott and Firestone measured surface roughness by using a pen-recorder to draw an amplified version of the motion of a “stylus” (a broken razor blade) over a surface [116]. Since then, a multitude of techniques have been developed or adapted for measuring roughness: tactile and optical profilometers, stripe projection scanners, scanning probe microscopes (SPM), transmission electron microscopes (TEM), etc. These techniques, whether contacting (stylus-based) or non-contacting, have a number of limitations that should be taken into account when interpreting the data. It is well known, for example, that the stylus tip geometry filters the measured signal, while high contact stresses at the stylus tip can lead to significant deformations [117]. Furthermore, the lateral measurement resolution affects the measurements in part due to longer measurement times leading to low frequency noise while, when measuring atomistic roughness, the smaller lateral resolution (relative to the vertical one) results in missing data between measurement points. Post-processing is also critical in extracting roughness information from raw data with a number of aspects –shape removal (tilt), the restoration of missing data (“perforated” surface data) using built-in triangulation or grid-fit routines, and the filter type and cut-off length (Gaussian versus robust, regressive-type RGRF filters) [K3]– affecting the end result. Furthermore, artefacts may occur due to diffraction effects around sharp edges caused by

calibration grid height steps; in this case, high magnification and high numerical aperture yield low noise. In certain cases, results differ across measurement methods: comparisons of contacting and non-contacting measurement techniques show large differences in predicted bearing curves, for example, with confocal microscopy yielding three-times higher roughness values than atomic force microscopy [K3]. In contrast, when comparing measurements and predictions of leakage volume as a function of time in sealing applications, roughness measurements with contacting and non-contacting methods do not result in large difference in flow factors (with proper filtering), unlike the large differences observed with artificial calibration surfaces [K3].

It appears that functional parameters such as the real area of contact, contact stiffness, flow factors, etc. are needed in addition to "traditional" roughness parameters [K3]; however, robust definitions of such functional parameters –as in the case of the real area of contact discussed previously– are lacking or are highly dependent on computational and experimental methods. Currently, only the repulsive contact area is clearly defined in computations and remains, both, physically meaningful and experimentally measurable at lower resolutions; the real adhesive contact area remains elusive and cannot be measured experimentally, while further complications arise when higher resolutions are required [K1]. Perhaps, proper characterization of the initial roughness prior to contact, as has been done extensively for normal contacts (see also section 3.4), may be unnecessary, especially when studying friction: "when things are moving, things are changing" (comment by J.A. Greenwood during Lorentz Center workshop). Similarly, it may be argued that high fidelity in representations of the spectral content of roughness is unnecessary: for example, when investigating the effect of filtering of the spectral content on functional parameters such as the real contact area, acceptable accuracy is achieved in the calculation of S_a and A_r already for ¼ of the total spectral content [K3]; however, caution is necessary when truncating the spectrum as this changes the RMS gradient (by a factor of $\sqrt{10}$ [why?]) [K3]. While high fidelity in the representation of the roughness spectral content may be unnecessary for certain applications –in fact, a number of models assume that only the low wavelength information of surface slopes is necessary [Persson; K3], whereas examples such as the Wenzel roughness parameter quantifying the wettability of surfaces relates to RMS slope [K4]–, the multiscale nature of roughness (including, for example, the waviness of a cylinder lining's honing grooves) must be accounted for in complex phenomena such as elastohydrodynamic lubrication (EHL), where it greatly affects flow factors and permeability [50], [RT1]. Hence, *it can be argued that functional parameters –and not roughness itself– are the only "trustworthy" tribological parameters*.

References needed for the following review:

SPM-based roughness: very high lateral and normal resolutions (side-walls of the tip determine the lateral resolution).

TEM-based experiments (R. Carpick's group): atomic-scale roughness strongly influences the pull-off force; agreement with simulations by I. Szlufarska; effects of atomic-scale roughness by Luan and Robbins.

Optical methods: larger areas, 3d data, fast acquisition; issues with artefacts.

Multi-scale topography tribometer (M. Dienwiebel's group): topography, as well as dynamic friction experiments. Can you resolve which part of the friction comes from where in the tabor friction law).

From measurements to model: Pastewka's work to generate PSDs from experimental data including the effects of filtering.

1d v. 2d plus averaging of PSD plays a role (Patewka's group): OK for isotropic surfaces.

Beware of artefacts: For instance, controversy in fracture mechanics (fractal nature): two different exponents, corresponding to two different physical mechanisms. Turns out, this was merely an artefact of the measurements.

J. Frenken: AFMs are not calibrated and have hysteresis. If you do a large scan, the motion is not linear and many people do not correct for this. There is a lot of bogus data because of this.

…

3.2. Scale effects and the breakdown of continuum theories

Contact between two bodies –perceived as continua– is well-defined and occurs when the distance between them is zero. Applying the same reasoning to the atomistic scale would imply that contact occurs when the distance between two atoms is also zero; but, is this a valid statement? Luan and Robbins studied the contact between a flat surface and nanoscale indenters of different structures (spherical crystalline, amorphous and stepped crystalline) and showed that the details of the atomic structure matter in the contact pressure distribution in adhesive versus non-adhesive contact conditions [92,118]. Subsequent work by other research groups showed that the accurate calculation of the contact area at a given length scale could yield reliable results [119-121], but this requires the careful post-processing and interpretation of atomistic results with appropriate definitions of criteria for contacting atoms and the "area of contact for an atom." For the latter, one method of calculation involves the assumption that the real contact area is the sum of the contact areas of each atom determined to be in contact [119,122]. *But is the concept of contact area meaningful at all for atomistic models?* Similarly to the notion of contact itself, the contact area is a well-defined quantity at low magnifications (comment by B.N.J. Persson during the Lorentz workshop), i.e. at scales where the discrete nature of atoms is not relevant. Perhaps better alternatives to using the concept of contact area would be, instead, to measure a physically meaningful functional property such as friction or electrical resistance, or extracting the pressure distribution over the interface by looking at the distribution of forces. A further point for consideration is that contact area is also difficult to measure experimentally: illumination of the interface or imaging can be used (possibly involving transparent materials) but there still exists a limiting value for the dimension of each pixel that, upon interpretation, may yield errors in the real area of contact of the order of 10% error [ref. Julien].

The concept of contacting distance is similarly ill-defined at the atomic scale. To begin with, the thermal fluctuations of atoms play a role in the estimated contact area; this can be accounted for in atomistic simulations, for example, by averaging contacting atoms over time [93]. Even with averaging, the distance between atoms at which contact "occurs" is also not straightforward to calculate. Researchers have used various methods in atomistic simulations using idealized materials, such as introducing potential energy- or distance-based cutoffs for specific crystal or amorphous material structures (see [122] for examples), but the situation is far from clear when real materials with multiple elements or alloys, inhomogeneities, impurities, etc. are considered. It is interesting to note that, even in the ideal case where a Lennard-Jones-type potential can be used to define repulsion and adhesion between two particles (or atoms), *contact and friction can actually occur at nonzero separations* (comment by J.A. Greenwood during the Lorentz workshop).

Mapping roughness parameters from continuum theories is also challenging for the atomic scale. For example, given a continuum function of position, one can calculate the mean contact slope used, for example, in Persson's theory (see review in section 2.1.3), but how should one proceed when the surface is discrete? One possibility would be to take the step height over the terrace width to calculate a slope

that would presumably match the continuum RMS slope [ref. Lars?], but is this universally true? Furthermore, system behavior at the atomic scale depends on the specific realizations of the system under study which holds, for example, for simulations of the adhesive contact of rough nano-spheres [123]. Questions then arise as to which extent such effects might affect the macroscopic picture. They seem to be relevant already at the microscale for percolation problems, while statistical fluctuations seem to be important in cyclic loading (hysteresis) [ref. Marco Paggi?]. Are they relevant for MEMS/NEMS? *A sampling strategy is required to model representative rough surfaces at the various scales as well as a proper way to map quantities from one scale to another.*

The breakdown of continuum at the atomistic scale can also be observed in other phenomena. When referring to density functional theory (DFT), for example, the work function of transition metals (TM) becomes non-scalable when particle clusters decrease in size, and the continuum model by Smalley [124] (is this the correct reference?) breaks down. The transition between the scalable and non-scalable regimes is at around 100 atoms in the case of gold. An anti-correlation is found between the binding energy and the vertical detachment energy, which may have important implications in relation to catalysis: e.g. while bulk gold is inert, small gold clusters are reactive [125]. *The question that arises is whether rough metal surfaces are more reactive than atomically smooth surfaces and, also, whether amorphous surfaces are more reactive than crystalline surfaces*, given that they contain more imperfections. To tackle these questions there is a need for accurate tight-binding and/or empirical models at the atomistic scale. Additionally, it is important to have a good sampling strategy for rough as well as amorphous surfaces.

Continuum models remain predictive to very small scales, even when there are topological instabilities: one needs simply to enhance models with additional terms that take care of the fluctuating thermodynamics (Landau-Lifshitz equation). The continuum description (Washburn's law) for nanoscale quantities of liquids is extremely robust and can be modified to capture the finite-size-effects that are captured by coarse-grained MD simulations: properties of a pre-wetting monolayer, a related Navier-slip, nanoscopic contact angles and wall-induced oscillatory pressure fluctuations [126]. In the case of fluid lubricants, the breakdown of continuum is related to an increase in viscosity and a transition towards a solid-like state, accompanied by stick-slip behavior. The increased viscosity is non-scalable: when the lubricant film thickness decreases down to a few nanometers, i.e. the size of the lubricant molecules, there is a deviation from typical bulk behavior as was observed in surface force apparatus (SFA) studies [127-129]. This transition from ultra-thin lubrication to dry friction under high pressure and shear has been studied using molecular dynamics [130]. The presence of nanoscale roughness frustrates the ordering of the fluid molecules, leading to high friction states. Experimentally measured viscosities were reported, for example, for perfluoropolyethelene (PFPE) molecularly thin films deposited on the atomically rough substrates used in hard disk drives [131,132] and used in subsequent analytical models to predict the tribological behavior at the head-disk interface [133,134]. In the case of SFA-type experiments, analytical expressions for the normal (e.g. Kapitza's solution [135]) and shear forces acting on a spherical probe moving parallel to a substrate within a fluid film [136] appear to hold up to the point where a fluid film can be defined as being continuous and are indeed used to interpret the experimental data to extract the complex viscosity from amplitude and phase information of the probe vibrations [137]; however, this description does not hold between the breakdown of the lubricant film and the initiation of solid contact [133]. The same consideration holds for the case of heat conduction, when the mean free path of the electrons becomes comparable to the asperity size. *How can we model such transition regimes (where relevant)?*

Scale effects are also observed in simulations of sliding of a circular disk on the atomic surface of a large substrate [138], where two regimes can be distinguished in the static friction normalized to the

shear strength: one limit corresponds to the elastic limit, the other to the rigid limit. The transition takes place when the radius of the disc exceeds the length of the core radius of interfacial dislocations. Looking at material constitutive laws, a breakdown of isotropic plasticity is observed in the ploughing of an unconstrained micro or nano-crystalline surface, where the material bulges until it folds. Folds similar to those observed experimentally can also be found in MD simulations [139]. The effect is caused by dislocation plasticity being active on specific slip directions in the various crystals. While this cannot be captured by isotropic plasticity or visco-plastic regularization, a crystal plasticity model that includes a hardening law which can capture localized plasticity should be able to account for this behavior. Size-dependent plasticity is discussed in more detail in section 3.3.

…

3.3. Material models and plasticity

It has been demonstrated experimentally and numerically that, both, the material hardness H [140-142] and the yield strength Y [143-145] are size-dependent quantities: they are not material constants but depend on the size of the plastically deforming material. Experiments show, for instance, that the strength of pillars under compression increases with decreasing diameter [143,144], and that a flat metal surface is harder to micro-indent or nano-indent than to indent with macroscale indenter [140,141]. Both phenomena occur because the availability of dislocations at the small scale is limited, given that the spacing between dislocation sources becomes comparable to the size of the loaded area. Therefore, even a very high local pressure, will not induce sufficient dislocation nucleation. Contact between rough surfaces has similarities with, both, multiple indentation as well as the flattening of multiple short pillars. The analogy is closer to the latter case, since surface asperities are not freestanding but connected to a substrate that can deform both elastically and plastically. If size-dependent plasticity is indeed affecting the response of rough, then continuum plasticity models for contact and friction would break down, since they miss a length scale capable of capturing size dependence. Neglecting the size-dependence of plasticity would lead to the prediction of an earlier onset of plastic deformation and underestimate the amount of work hardening during plastic deformation. This would have consequences in the estimate of the evolution of the contact area.

The matter becomes even more complicated when high strain and high strain rates are involved. Then, plasticity can also appear in the form of grain boundary sliding [ref].

During the dry sliding of copper, a transition from micro- to nano-crystalline structure has been observed [ref?], while similar observations have been made for various types of materials and various applications [refs?]. The transformation occurring in the microstructure is driven by the high strain rates, when the worn surfaces become a mixture of particles in an amorphous matrix. As an example, tungsten carbide (WC) in frictional contact with tungsten (W) causes the crystalline W structure to turn into amorphous W with a dispersion of nano-diamonds [ref?]. Melting does not seem to be occurring, also given that the local speeds involved are small. There is evidence, however, of WC melting during hard rock drilling [ref Vlad: Tkalich, Wear, 2017]. Amorphization is a phenomenon that has also been shown in MD simulations [ref Moseler? RT12], while other mechanisms can affect the internal microstructure of contacting bodies such as plasticity by grain boundary sliding, which leads to weakening of the material and phase transformation [RT12].

Material inhomogeneities…

Composites…

Non-uniform temperature distribution always occurs at the interface; adding such temperature (energy dissipation) effects makes the systems nonlinear [K4]…

The contact mechanics and tribology of soft matter can be studied via the BEM, which has significant advantages over the FEM in that rough surfaces can be easily modeled (see section 2.2). In general, viscoelasticity causes shrinkage of the contact area for increasing speed [RT14]. For example, the contact behavior of a rigid sphere in reciprocating sliding contact with a viscoelastic half-space ranges from the steady-state viscoelastic solution, with traction forces always opposing the direction of the sliding rigid punch, to a multi-peaked pressure distribution with tangential forces in the direction of the sliding punch. This behavior is controlled by the size of the contact, the frequency and amplitude of the reciprocating motion, and the relaxation time of the viscoelastic body [146].

…

3.4. Normal contact between rough surfaces

The recent contact-mechanics challenge compares various modeling approaches in their ability to properly solve a well-defined normal contact problem [Mueser, Tribol Lett, 2017]. A surface height spectrum was generated [102] featuring a roll-off and self-affine region, as was a manifestation of this randomly rough surface in real space. The following approximations were made: small surface slopes, linear elasticity, short-range adhesion, periodic boundary conditions, and a hard-wall constraint. As a result, the ratio of the true to the apparent contact area was expected to be $\cong 2p/E^*/\bar{g}$, where p is the contact pressure, E^* is the contact modulus, and $\bar{g}$ is the RMS-gradient of surface heights. This information was made available to researchers who were asked to compute any function or functional for purposes of comparison. Specific metrics used in the subsequent analysis included the gap and stress along a reference line; stress and contact patch histograms; and relative contact area and mean gap values. Submitted solution methods could be categorized into brute-force computing, where errors could come from the discretization, and models mapping onto simpler equations using uncontrolled approximations. More specifically, results utilized exact (boundary-value) methods, Persson theory without adhesion, multi-asperity models that assume local constitutive relations without interaction between contact patches (“bearing models”), as well as all-atom MD simulations, where the surface size was scaled down by a factor of 100, and experiments, where the surface size was scaled up by a factor of 1000. The reference solution was calculated using GFMD (see section 2 for a review of computational methods and models).

Good agreement with the reference solution was found for, both, experiments and all-atom MD; when comparing the gap across the reference line, the effect of removing the small-slope approximation gave excellent agreement for all-atom MD. Multi-asperity models were found to overestimate the gap, while exact methods agreed almost exactly at the greatest magnification; however, results of the stress across the reference line (local zoom-in) showed great scatter. When looking at the stress distribution histogram, which was almost Gaussian, multi-asperity models were found to overestimate the stress, while in the presence of adhesion, when small patches become unlikely, these models produced very similar trends for the patch-size distribution. All solutions showed reasonable agreement for the contact area as a function of load, as well as for the mean gap as a function of load with the exception (for the latter) of all-atom MD, where inherently accounting for plasticity results in deviating results for larger pressures.

In summary, very close agreement was observed between all systematic approaches with differences becoming visible when quantities required high resolution. At the same time, these approaches showed good agreement with experiments and all-atom MD, suggesting that common approximations might be

less problematic than believed. Reasonable agreement was found between the reference solution and the non-adhesive Persson theory on all reported properties, while multi-asperity methods agreed with each other but deviated from the reference solution (even though newer models accounting, for example, for asperity interaction were not compared in this study). It could therefore be argued that the suitability of modeling methods and tools can be determined based on the properties one would need to extract: for example, *predicting contact area versus load or mean gap versus load seems to be consistent across methods* and, arguably, *the most suitable model would be the simplest one*. On the other hand, extracting local quantities at higher resolution would require numerical methods able to achieve sufficient discretization. Beyond the simple case of normal contact, the situation becomes more complex very fast.

3.5. Adhesion

Only short-range adhesion was included in the contact-mechanics challenge discussed in section 3.4, based on the value of the local Tabor parameter $\mu_T = 3$ which was close to the JKR limit. The model setup was such that adhesive hysteresis was insignificant up to moderate contact pressures [Mueser, Tribol Lett, 2017].

While asperity theories predicted a strong influence of RMS amplitude, Pastewka and Robbins [147] formulated a criterion for "stickiness" by numerical observation of the slope of the (repulsive) area-load, which appears to be independent of the RMS amplitude. This work has generated some discussion (see, for example, [111,112,148]) and its conclusions are still debated. Another incongruence comes from the recent paper by Joe et al. [149] which suggests that the adhesive contact problem converges to a limit result when the spectrum is increased in fine detail; hence, there cannot be a strict dependence on RMS slopes and curvature as Pastewka and Robbins found numerically.

For very soft rubber (almost liquid), the work of adhesion is about twice as large on a rough surface; this effect may be due to the effect of increasing the contact area. However, the last word is still not out on adhesion and surface energy since this postulate is not always verified in experiments and theories [111,112]. All present theories of rough adhesion are approximate in partial contact, and using particularly very elaborate theories constructed around one parameter such as the RMS slope which may not be known with accuracy is problematic; however, theories may change depending on experimental evidence emerges (discussion between M. Ciavarella and B.N.J. Persson during the Lorentz workshop).

Daniele: Adhesion of a rough sphere with a plane. Can we model hysteresis in adhesion contact with analytical models? At the moment we don't have an analytical solution.

Persson: adhesion is just a small part of the problem you have dissipation at the "crack tip". The problem is very complicated

Ciavarella: we should use an effective work of adhesion in the JKR regime. This is the problem that is still open. We can use simulations because at the moment we are not able to estimate the "effective" work of adhesion.

Pending additional content from D. Dini…

…

3.6. Friction

Past research has suggested that surfaces do not slide but, instead, create wear particles at the interface [150], resulting essentially in a turning process for the scraped material in a manner analogous to rubber friction [RT3]. *Therefore, the successful modeling of friction may well depend on incremental advances from investigations of wear, lubrication and tribochemistry*. Nevertheless, a number of advances were

made in the understanding of friction, grouped in the next sections into the onset of sliding, friction laws and rubber friction.

3.6.1. The onset of sliding

Apart from identifying new and understand specific mechanisms occurring at or close to the contact interface, tribological models can be used as quantitative tools to reproduce and interpret experimental observations: this is especially true for friction. Since most contact and friction measurements are made at the system-size level (e.g. total normal and friction forces), models predicting system-size quantities could be denoted as "macroscale models", irrespective of the actual length scale considered. As a provocative example, *a model of atomic force microscopy experiments is a macroscale model if its aim is to predict the total friction force that the tip experiences*. But what are the properties of models actually enabling such quantitative comparison?

It is clear that *friction is intrinsically a multiscale problem, so that no current model can couple all length scales from the atomic level to the system size*. Because macroscale models must include and capture information up to the system scale, they will be limited at lower scales, relying on assumptions about the behavior law of the system at the smallest scale included. Since this smallest scale describes the collective behavior of a large number of underlying units (micro-contacts, grains, molecules and so on), the small-scale behavior law is intrinsically a statistical law. For instance, the Amontons-Coulomb friction law which is often assumed at a contact interface in analytical, FEM or BEM models actually summarizes in one scalar value (the friction coefficient) the fact that the area of real contact is roughly proportional to the local pressure. Since the model of Greenwood and Williamson [30], we know that the latter relationship results from statistical averaging over many micro-contacts between asperities having randomly distributed heights. Similarly, the critical displacement D_c involved in the rate-and-state friction law is commonly interpreted as the average slip distance required to renew the population of micro-contacts within a multi-contact interface [151-153].

A frictional interface can be modeled using a homogeneously loaded contact between elastic half-spaces only in very specific instances; instead, most real contacts have complex geometries, boundary conditions, and loading configurations leading to unavoidable pressure and shear stress heterogeneities along the contact interface. Since friction laws need to couple both the normal and shear stresses to predict where and when slip will occur, the stress distribution along the interface needs to be accurately modeled. This is why, in order to offer quantitative predictions of the tribological behavior of an interface, macroscale models need to account for the elasto-dynamics of the bodies in contact: *the incorporation of temporal phenomena, together with realistic boundary conditions, into frictional models is essential*.

As a practical example, let us consider how macroscale models were progressively improved to reproduce some aspects of the experimental results reported by the group of Fineberg about the onset of sliding of extended interfaces [154-159]. Their main observation is that the transition from static to kinetic friction is mediated by the dynamic propagation of micro-slip fronts along the interface: ahead of the front, the interface is still in its stuck state, while it is already slipping behind it. Macroscopic sliding only occurs when the front has spanned the whole interface [154]. In this context, not all fronts lead to macroscopic sliding. Precursors to sliding are sometimes observed, which correspond to fronts spanning only a fraction of the contact interface. These precursors manifest themselves at macroscale as a series of dents in the loading curve, indicating partial load relaxation [155]. The first models for the length of precursors were 1D [160-164]. Although the ad-hoc introduction of an initial shear stress field was improving the results [163], none of these models could be compared quantitatively with Fineberg's experiments, in which the height of the slider was not negligible. Only with 2D models based on spring-

block or FEM representations of the elasto-dynamics of the slider [165-167] could the predictions match quantitatively the observations. Those models were based on Amontons-Coulomb's description of the frictional interactions at the interface, with static and kinetic friction coefficients. Recently, a fracture-based description provided equally good predictions of the precursor length [168,169], strengthening the idea of an equivalence between the friction and fracture descriptions of the onset of sliding, often used in earthquake science [170]. In particular, the fracture-like stress field around the tip of micro-slip fronts, measured through an array of miniature strain gauges was captured by analytical [158] and FEM models [159].

Although a velocity-independent Amontons-Coulomb friction is sufficient to predict the precursor length and the fact that fronts speed depends on the local pressure to shear stress ratio [156], it fails to explain the unexpectedly large range of front speeds observed [165,171]. While the fastest fronts, propagating at about the sound speed in the contacting materials, were expected from standard shear fracture theory, abnormally slow fronts, orders of magnitude slower, were observed but unexplained. A single front could alternate between both types in a single event [154]. Note that slow fronts here are distinct from quasi-static fronts, the propagation speed of which is proportional to the external driving velocity, like those involved in the onset of sliding of sphere-on-plane contacts [2,172,173]. Dynamic slow fronts have been predicted theoretically within a 1-dimensional model of the interface using an improved state-and-rate friction law featuring a velocity-weakening-then-strengthening behavior. In this model, the slow front speed is related to the velocity at which the steady-state friction coefficient is minimum [174,175], which is supported by observations of slow rock friction [176].

Unfortunately, this approach did not explain the possible transition from fast to slow front regimes observed within a single event. This was achieved using a multi-scale model [177,178] with the following ingredients: the 2D model of [165] is complemented by a micro-junction based description of the interface [179] in which the loading/breaking/reformation cycle of each junction is controlled by a time scale. This time-scale is inspired by the time scale identified experimentally in [157], and observed to control the transition from fast slip to slow slip when the interface starts to slide. It was argued to correspond to the cooling time of the interface after the rapid heat deposition as the micro-junctions break upon front passage. Such heating is presumably responsible for local melting of the interface, a phenomenon which is also clearly involved in seismology where rock melts and reforms leaving fault veins. The main implication of this time scale is that, after a slip phase, the interface does not re-stick perfectly, but transiently allows for some further, slow slipping. Thus, slow fronts are fronts that would arrest in the absence of this slow slip mechanism, but can continue to propagate, much more slowly, due to the slow slipping occurring in the broken part of the interface. It was also found that the selection of the front type (fast or slow) is not only dependent on the shear to normal stress ratio, but also on the local disorder in shear forces sustained by the micro-junctions [177]. As a result, local static friction is history-dependent, with potentially a factor of two in the variation of the coefficient of static friction due to the rupture history of the interface [179]. All these results suggest that friction features multiscale aspects, both, in the spatial and time domains, that must be accounted for in models.

3.6.2. Friction laws

As soon as some motion is involved at the interface, models need to incorporate a friction law. The most classical and widely known friction law is the one of Amontons-Coulomb (AC), which states that no sliding occurs as long as the ratio of the shear force Q to the normal load P remains below a certain threshold defined as the static friction coefficient μ_s. Maintaining a constant sliding speed requires the application of a kinetic friction force $F_k = \mu_k P$, with μ_k usually being smaller than μ_s. The AC law, which has been defined here from the global forces acting on the interface, is commonly used locally along extended interfaces. In those cases, the friction coefficients are to be compared to the local ratio

of shear to normal stress $q(x)/p(x)$. Practically, a fundamental question arises about the value to be used for the local friction coefficients: *should one use the values of the corresponding global coefficients or should these be different at the local contacts?*

Whereas the global and local kinetic friction coefficients are expected to be equal, the situation is very different for static friction coefficients. It has been shown experimentally that the static friction coefficient depends on the stress distribution at the interface prior to the onset of sliding [180], and that $q(x)/p(x)$ can exceed the macroscopic friction coefficient by a factor of two [157]; these results have been reproduced in models of heterogeneous frictional interfaces [162,181]. The fundamental reason behind this behavior is the following: *the global and local static friction coefficients are equal only if all points at the interface reach their slipping threshold at the very same instant*. This situation corresponds, for instance, to an ideally homogeneous interface submitted to homogeneous loading. In practice, this never happens: when slip at the interface becomes unstable, a large portion of the interface is loaded below its threshold, so that the total tangential load born by the interface is smaller than its theoretical maximum value. The consequence is that, in general, the global static friction coefficient is smaller than its local counterpart [177,182], and it is thus challenging to infer a local static friction coefficient from macroscopic measurements.

Although practically useful and rather easy to implement in models, AC's friction law cannot capture a series of effects repeatedly observed in rough contacts (see [153] or [152] for reviews). First, the static friction coefficient, μ_s, slowly increases with the time the interface spent at rest. This effect is interpreted as an increase of the area of real contact over time, through asperity creep, an effect denoted as geometrical aging. Depending on the material creep can be of plastic [183] or viscoelastic [184]. Another cause of increase of μ_s is due to the strengthening of the contact with time, presumably due to relaxation of the glass-like material forming the very interface, an effect denoted as structural aging. Second, the kinetic sliding friction coefficient in steady sliding is velocity-dependent, typically with a logarithmic velocity-weakening. This effect is partly due to an intrinsic velocity-dependence of the interface's shear strength, and partly to the time-dependence of the area of real contact: slower sliding gives more time to the micro-contacts to grow in size before they break and are replaced by fresh, smaller micro-contacts. Those effects are taken into account in the so-called rate-and-state friction law [19], which is widely used in various fields related to friction, in particular earthquake and landslide science.

Despite its many successes, the rate-and-state friction law must also be used with caution. The logarithmic velocity-weakening is based on observations at low-velocity, smaller than about 100µm/s. At higher slip rates, a velocity strengthening regime due to viscous effects is also expected, and is indeed generically observed beyond some crossover velocity [185]. At even higher velocities, in the range typical to unstable slip, up to a few m/s, sliding is accompanied by significant temperature rise, possibly several hundred degrees. Such heating can induce transient phase changes [157], in the vicinity of the contact interface. In these conditions, friction may not be controlled only by a critical length scale (the average micro-contact size) but also by time scales [157,177]. Heat can also favor chemical reactions, in particular in tectonic faults with fluids and high pressure. Such reactions tend to self-lubricate the interface, with low friction resistance at the highest slipping rates [186]. Such systems are challenging to model, due to the strong multi-physics coupling required to capture the most salient controlling phenomena.

3.6.3. Rubber friction: Some open issues from mesoscale experiments on elastomers

Rubber friction is a very interesting topic, because it shows a rich behaviour, but where some progress has been made. Persson's 2001 multiscale theory of contact was developed originally for this application [187]. As friction is macroscopic it should be more easily measurable than contact area, on which we

have discussed that the “magnification” dependence makes the idea of a “value” quite ill-defined. However, it turns out that the “magnification” dependence also translates and applies to macroscopic friction in this case, and in these respects, the introduction of “multiscale” ingredients in Persson 2001 does not change much the picture in Persson in 1998 and similarly by Popov in his 2010 book [188]: the friction coefficient is essentially defined at the smallest asperities in contact --- like the “real” contact area, this depends violently on the RMS slope of the surface, and the way we decide to measure it.

As Persson 1998 and Popov 2010, we can reason at asperity scale with a given typical size of contact, and the result does not change: we seem to return to the need to do “functional filtering” concept, and therefore truncate the spectrum. Indeed, quite surprisingly, Lorenz et al. [189] seem to suggest the truncation of the spectrum of the surface should be such that the rms slope is fixed to h’rms=1.3! As agreed by Bo Persson at the Lorentz meeting, this may not be a “universal number”, and may not pass the test of time. Incidentally, Lorenz et al. refer to some unpublished data to propose this universal finding, and we do not find this much useful for scientific discussion of this critical point.

In these respects, the multiscale nature of surfaces which seems to have played a large role in the Literature in recent years, it really has a much less profound role than we expected, and the sophisticated model really introduces a fitting equation similar to engineering equations.

…

In section 3.6.1, we argued that new insights into friction can be reached by comparing model predictions to experimental measurements made not only at the system-sized scale (macroscopic loads) but also at local scales (ideally full field evaluations). In several aspects, elastomers are good model materials to perform such comparisons. Due to their low elastic modulus, the amplitude of the interfacial displacements under tribological solicitations is typically large enough to be easily monitored optically, using contact imaging techniques (see e.g. [190,191] for tire rubber). In particular, polydimethylsiloxane (PDMS) is increasingly used for in situ measurements of displacement fields (see e.g. [172,173,192-194]). PDMS has the further advantages to have a low loss modulus, and to fracture at extremely high strains, well beyond those associated with frictional solicitations. Thus, its behavior can be compared to elastic models, sometimes incorporating non-linear elasticity at high strains [195].

Access to local displacement and stress at such rubber interfaces allowed to identify some phenomena that are not yet satisfactorily incorporated in friction models. As a first example, rough interfaces have finite normal and shear stiffness due to the compliance of each individual micro-contact. Although those stiffness values affect the behavior of contact interfaces (see e.g. [196] for the role of the normal stiffness and [173] for the role of the tangential stiffness on rough sphere-on-plane contacts), most model consider, for the sake of simplicity, perfectly smooth interfaces. Such models could be improved by including the effect of roughness through effective boundary conditions on smooth interfaces (as done, for example, in [197,198]). As a second example, the contact mechanics and frictional properties of elastomer contacts are found to be affected by the value of a pre-stretching applied to the rubber (see, e.g., [199,200]), due to a stretching-induced anisotropy of the interface. Keeping in mind that any contact loading leads to a non-vanishing field of in-plane tensile strain, in particular near the contact edges, stretching effects are expected to be involved in virtually all tribological situations. Improved friction models should aim at incorporating those effects.

3.7. Wear

Martin Dienwiebel reported on experiments of sliding in the presence of third bodies (debris) and the use of tribofilms. The process parameters are of paramount importance in both friction and wear experiments [RT12].

Pending content from J.-F. Molinari…

…

3.8. Lubrication

Hydrodynamic lubrication…

Elastohydrodynamic lubrication (EHL)…

An interesting application coupling EHL and viscoelasticity is for… [ref Putignano; RT14]. Film thickness changes dramatically when the viscoelasticity inside the material is activated; viscoelastic effects grow with increasing speed, yielding film thicknesses that differ from the classical description with a peak that moves from the outlet to the inlet of the fluid. Similar effects can be observed when examining the pressure distribution and can explain experiments where the film breaks at the inlet of the contact and not the outlet [ref?]. In short, *viscoelasticity couples with the viscosity of the fluid*.

Solid lubricants…

Pending content from C. Putignano (and maybe A. Almqvist?)…

…

3.9. Tribochemistry

The control of friction and wear in a tribological contact is known to be related to several parameters such as the nature of rubbing surfaces (roughness, physico-chemical composition, mechanical properties), contact conditions (pressure, shear stress), temperature, environment, etc. In particular cases, chemical reactions occurring during sliding will strongly influence the tribological behavior of the interface through the generation of new compounds. These phenomena are studied in the field of tribochemistry and are often observed in boundary lubricated contacts [201]: a characteristic example is molybdenum dialkyldithiocarbamate (MoDTC) which is a well-known friction modifier additive used in engine oil that is able to significantly reduce friction through the generation of molybdenum disulfide (MoS_2) lamellar flakes in the contact [202,203]. The classical approach to study such phenomena is to characterize surfaces by identifying new compounds after tribological tests (post-mortem characterization). The thickness of the tribofilms usually ranges from few to several hundreds of nanometers. Surface-sensitive tools are so needed to physico-chemically characterize surfaces with depth analyses of few nanometers. The analyzed area should also be as small as possible in order to describe nanoscale features. Recently, more and more in-situ experimental tools, coupling friction testing and in-situ characterization, have been used to gain access into interfacial material modifications during rubbing [204-208]. Alternatively, tribochemistry is studied with MD and quantum calculation tools, as discussed in section 2.4.

The activation of tribochemical reactions cannot be described with a universal mechanism but depends on conditions at the interface. During severe contact, for example, a "new" (nascent) surface is revealed, which reacts differently with the additives or the chemical environment from the initial one [209]. In the presence of insulating materials –mostly under dry conditions–, studies suggest that electrons and particles are emitted during sliding that could influence tribochemical reactions [210,211]. Under high-speed contact, the increase of temperature could be important with the thermal energy pushing through the energy barriers of chemical reactions. In such a case, the tribochemical reaction mainly occurs because of thermal energy generated in the contact [212]. Furthermore, in some cases, normal and shear stresses applied on the "interfacial material" could promote a tribochemical reaction [205,213,214]. In this case, tribochemical reactions are promoted by the mechanical energy, which helps decrease the

energy barriers of the chemical reaction pathway. Relevant models have been reviewed by Spikes and Tysoe [215].

In general, the interface is at thermodynamical equilibrium when the temperature stays constant in the contact, either, at very low sliding speeds when no significant increase of temperature is found, or at high sliding speeds when the melting point of the contacting material has been reached. In all other cases, the interface is not at thermodynamical equilibrium and its behavior becomes significantly more complex [212].

3.10. Biotribology

3.10.1. Cellular interactions

Contact mechanics has significantly contributed to biotribology for the understanding and simulation of wear in hip joint prostheses and related applications [216]. In the last few years, new perspectives for contact mechanics research in biotribology are emerging as far as the problem of contact interactions between biological cells is concerned; see, for example, a wide overview in [217-221]. In addition to classical mechanical interactions between cells in compression and tension, including friction and adhesion, the microscopic characterization of biological contacts is complicated by the need of modeling additional fields responsible for the mechano-transduction of biological cells, vital for the simulation of biological phenomena. For instance, abnormal mechano-transduction in the cardiac tissue related to the conversion of a mechanical signal into a change in cell growth or remodeling is expected to be a source for a variety of diseases [222]. Therefore, modelling and simulation of contact interactions between multiple cells, accounting also for their deformability, is a problem considered of paramount importance towards the understanding of emergent collective behaviors [222].

In cardiac dynamics, myocytes, which are the fundamental cells composing the cardiac tissue, interact among each other in a very complex way across their boundaries, transferring physiological quantities, electric current, and also mechanical tractions. Moreover, as an additional source of complexity, their boundaries evolve in time, as a result of growth, remodeling and aging effects [222]. From the mathematical point of view, the complex myocyte dynamics and its electrophysiological behavior can be described by a set of reaction-diffusion partial differential equations for the diffusive membrane voltage and for the local electrophysiological gating fields [223,224]. The anelastic myocyte stretching is induced by the local fiber activation field, which depends on the electrophysiological quantities and in particular on Calcium dynamics. The nonlinear coupling between electrophysiology and the hyperelastic material response induced by the excitation-contraction mechanisms is typically modelled via the multiplicative decomposition of the deformation gradient into elastic and anelastic parts; see, for example, [225-227] for more details on theoretical and computational aspects related to this modeling strategy. Specifically, the anelastic active deformation gradient can be provided by the subcellular calcium/voltage dynamics, while the elastic deformation gradient is computed as customary [225].

Complementing these continuum mechanics formulations with suitable interface constitutive relations to address the problem of myocyte-myocyte interaction is an open problem, whose preliminary attempts to solve it have been proposed in [228]. Mechanical interactions should account for adhesion and contact tractions dependent on the local cell-cell separation, to reproduce the experimental evidence. Finally, as a further model improvement, roughness of cell-cell interfaces should be accounted for, leading to a distribution of partially insulated conductive spots rather than a fully conductive interface. In this regard, the fundamental discoveries in the field of electric and thermal contact problems in the presence of roughness are expected to be applicable and extendable also to myocyte contacts. As proposed in [228], the myocyte interface can be modeled as an imperfect zero-thickness boundary layer, whose response

can be governed by nonlinear constitutive relations generalizing the popular cohesive zone models used in fracture mechanics for pure mechanical interactions; see, for example, [229] for thermo-mechanics. The mechanical field has to be coupled with the other fields to be transferred across the interface, such as the electric field. Notably, as regards the relation between electric current and voltage, the results established in [114,230] are expected to play an important role.

Further research in envisaged as far as the computational techniques are concerned. The anisotropic nonlinear elastic material response of cardiac myocytes, along with the coupling with the diffusive and reactive fields, naturally requires the use of the finite element method rather than the boundary element method, which is however very effective for contact problems involving roughness [49]. Hence, the possibility to address nonlinear multi-field contact problems within the finite element method urges the development of computationally efficient numerical schemes for microscopic roughness. Finally, for the solution of multi-field problems, fractional time stepping techniques are very promising, since they may be conveniently used to split the different field dynamics [231].

3.10.2. Contact scale issues in experimental biotribology

Nanotribological experimental approaches have been employed for contact mechanics and tribological studies of biological tissues that have long been studied with macroscale experimental tools too. Thus, comparison across different contact scales became readily available. A prime example is synovial joint system, including cartilage tissues as well as synovial fluids. Application of AFM to cartilage as nanoindentor was particularly fruitful thanks to its high spatial resolution that was unprecedented by conventional indenters. Examples include (1) detection of different elasticity/stiffness on the proximal vs. distal areas of cartilage [232,233], (2) detection of different elasticity/stiffness on varying vertical zones of cartilage [234], (3) identification of more compliant characteristics of pericellular matrix than territorial/interterritorial matrices of cartilage [235], and (4) distinction of healthy area from enzymatically defected area of cartilage exclusively with very sharp (nanometer-sized) AFM probes [236], which led to the development of AFM-based arthroscopy [237], etc. Further studies have been carried out to characterize the frictional/lubricating properties of cartilage tissues by means of AFM [238-240]. A common observation is that excellent lubricating capabilities of cartilage tissues, which have reported from many macroscale experimental studies [241], were not reproduced on small scale. Ateshian et al. attributed it to the inability to activate biphasic lubrication mechanism, i.e. contribution of both solid and fluid phases in cartilage matrix to smooth gliding for cartilage interfaces, when cartilage was slid against a sharp AFM tip [238]; too small contact area achieved by AFM probe on cartilage surface inhibits the activation of interstitial fluid pressurization. This may indicate an intrinsic hurdle or, alternatively, a fundamental challenge in usage of AFM for nanotribological studies of cartilage. Instead, nanoscale tribological researches have more focused on model thin films prepared with individual constituents of cartilage and/or synovial fluids, such as lubricin [242,243], hyaluronic acid [243,244], or glycosaminoglycans (GAGs) [245,246]. Despite various new information gained from these thin films, excellent lubricating performance that is expected from articular joint system was not observed either. Typically, this behavior is linked to the lack of synergistic operation between constituents of cartilage and/or synovial fluids [247]. While this analysis is certainly valid, it is worth considering other possibilities, for example, instrumental artefact in AFM and/or its intrinsic challenges that were addressed as mentioned above. Moreover, when it comes to frictional properties on both cartilage tissues and model thin films on small scale contact, contact mechanical modelling studies have been relatively scarce to date.

3.10.3. Skin tribology

Besides the brain, no other organ of the human body is so prevalent in our every-day biological and social life than the skin. It is the first line of defense of our body against the external environment and,

as a result, this complex biophysical interface is endowed with multiple physiological functions which extend from protection, through thermoregulation and multiphysics sensing to cellular processes and biochemical synthesis [248,249]. The skin controls many types of exchanges between our inner and outside worlds which take the form of mechanical, thermal, biological, chemical and electromagnetic processes. These processes concurrently operate as parts of a very dynamic system featuring highly non-linear feedback mechanisms [248,250,251] where mechanics is pivotal. As mounting evidence suggests, the skin microstructure can play a critical role in how macroscopic deformations are modulated at the microscopic level [252]. These structural mechanisms are also at the heart of skin tribology by being part of, and conditioning mechanical load transmission [250,253-255]. Skin biotribology is fundamental to many industrial sectors from biomedical devices, personal care and cosmetic products to vehicle safety, textile, sport equipment, wearable electronics and tactile surfaces.

It is widely accepted that skin friction is made of a deformation-induced and adhesion components [253,256-259] but, up to now [250], adhesion-induced friction has been deemed to be the dominant contributor to macroscopic friction. Applying a computational homogenization procedure to a 2D anatomically-based finite element multi-layer model of the skin, Leyva-Mendivil et al. [250] recently showed that deformation-induced friction can be significant when the skin surface is subjected to the action a single rigid indenter of sub-millimeter size. It was shown that the macroscopic coefficient of friction between the skin and a rigid slider moving across its surface is noticeably higher that the local coefficient of friction applied as an input parameter to the finite element analyses [250] (Figure 1). Similar observations were reported by Stupkiewicz et al. [260] in a similar 3D computational contact homogenization study: geometrical effects alone can have a significant impact on macroscopic frictional response of elastic contacts. These results support the idea that accounting for the microstructure of biological tissues and the heterogeneous nature of their mechanical properties could be critical in determining their biotribological properties.

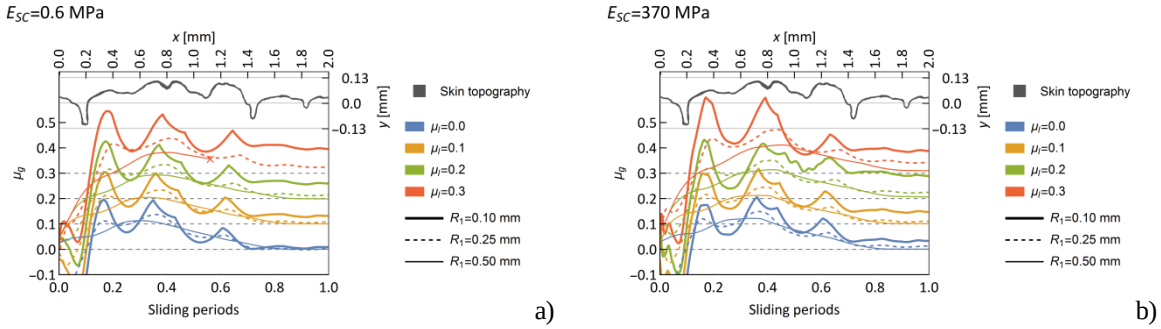

Figure X. Evolution of the cumulative global coefficient of friction along the sliding path as the indenter (of radius R1, R2 and R3) slides over the skin surface (one sliding period). The geometry of the skin surface is layered over this plot to relate evolution of global friction and geometric features of skin micro-relief. a) High relative humidity environment (Young's modulus of stratum corneum ESC = 0.6 MPa); b) Low relative humidity environment (ESC = 370 MPa). Adapted from [250].

To date, despite much experimental and modelling studies investigating shear stress at the surface of the skin in relation to skin injuries and pressure ulcers [261-263], very little efforts have been devoted to develop methodologies to gain a more quantitative and mechanistic understanding of how shear stresses are induced at the level of skin micro-relief asperities, and how they propagate from the skin surface to the deeper layers where they are likely to mechanically stress living cells.

Ultimately, excessive stress or strain can lead to cell damage and death, which, at a meso/macroscopic level translates into tissue damage and loss of biological structural integrity. The biophysical response of cells under direct mechanical loading and short-range electromagnetic interactions is therefore central to the multiscale nature of skin biophysics and biotribology. If one considers that, non-withstanding the strong sensitivity of the skin to fluctuations in environmental conditions, (finite strain) mechanics is

typically coupled to biochemistry and other physical processes such as thermal transfer, it is clear that the formulation of any type of sufficiently descriptive contact theory of the skin is going to require substantial integrative efforts. Due to the fibrous nature of their cytoskeleton, cells also features strongly anisotropic properties, which, combined to their extreme deformability, calls for new contact theories of biological soft matter. This presents numerous challenges at a theoretical, computational and experimental level but also provides outstanding opportunities to establish an ambitious research road map to push further the boundaries of our current knowledge and capabilities, in biotribology and biological soft matter in general, and in skin tribology in particular.

The skin is a heterogeneous, living and adaptive structure which features a strong intra- and inter-individual variability in its structural and biophysical properties. These properties vary according to body location, health status and history, diet, age, lifestyle, external environmental conditions (e.g. temperature, humidity, pollution level, water quality, sun exposure, contact with external surfaces) and internal environmental conditions (e.g. hormones, pregnancy, water and glucose levels, tension lines) [264,265]. Sex and ethnicity are notable sources of inter-individual variability. There are therefore formidable challenges in representatively characterizing the skin ultrastructure as well as its biophysical and tribological properties. It is our opinion, that, as a matter of reason and practicability, the inherent extreme complexity of biological soft tissues that stems from their living, adaptive, structural, multiphasic, multiscale and multiphysics nature, will, naturally and progressively, shift research efforts from "traditional analytical" biotribological models of contact to data-rich computational models exploiting data mining and machine learning techniques [266]. These techniques are likely to play an increasing role in the future to make sense of large and complex heterogeneous data sets, whether they originate from physical or computer experiments, or expert knowledge. Multi-variate and multiscale data-based and/or physics-based statistical models of the skin built from the results of machine learning (i.e. meta-models) could then replace computationally expensive physics-based finite element models, and be used to predict a variety of scenarios and outcomes. Image-based computational contact homogenization procedures will be pivotal in enabling these knowledge-generating techniques. Through this type of approach, a more fundamental and mechanistic understanding of the multi-factorial nature of skin biotribology [267,268] will be established [250]. Computational multiscale methods combining atomistic, molecular and continuum techniques [269-271] are likely to play an increasingly important role in the modeling of skin biotribology in the forthcoming decades.

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D. Veeregowda:

Teaser: tribological experiments on the cornea of a pig's eye.

Ocular tribology: "barbaric experiments" friction of cornea and contact lens; mimic variable sliding velocity; velocity of the closing eye lid larger than that of opening (pressure, velocity, size).

Similarly to ocular: oral tribology, dental tribology, hip and knee joint tribology.

Skin tribology is the largest percentage of biotribology publications (In-Science Direct 2013-2016).

Hardly any modeling work.

Pain due to high friction (Sjogrend syndrome): chronic disease affecting 0.5 to 2% of world population.

Example: saliva: proteins formed/ combined from different glands. Surface textures are different across the locations where the proteins are produced. Saliva coated on glass and put in a tribotester: coefficient

of friction is the same at the nano- and macroscale (0.041 +/- 0.18). What should we do to examine the origin of friction? Mechanism: mucins hold water and create low friction films (100 nm for un-stimulated saliva).

Solution: in situ tribology (couple friction to film thickness, roughness, corrosion and surface chemistry) (e.g. Hou and Veerwgowda, J Royal Soc Interface, 2016). Put saliva between PDMS and germanium and examine friction coefficient (~0.02). As a function of time, the glycosylated proteins show elastic response however there is a non-elastic changes in the bound water state.

Is it the case that modeling is not necessary here?

J. Scheibert: is there any engineering analogue to synovial fluid with similar tribological properties? Answer: these are abundant, e.g. surface-adsorbing, brush-like polymers have shown promising results. But this is the case under low pressure conditions only.

D. Veeregowda: ionic brushes seemed promising. Problems: biocompatibility and discrepancy in the pressures these structures can withstand.

B. Persson: in nature you have cartilage v. cartilage; is it supposed to operate in other environments? Answer: this is relevant, for example, in implants where non-biological materials come into the interface.

D. Veeregowda: company wants to understand the adhesive and frictional behavior of single bacterial cells; models would be necessary to eventually predict the infection rate in implants. Many studies exist for single bacteria; however, behavior is different for bacterial colonies. Surface topography would be very important (M. Scaraggi).

4. Roadmap for future research

4.1. Fundamental research questions

Building on the contact-mechanics challenge [K1]:

- Why not compare the cases with real differences such as plasticity, long-range adhesion, etc. (Paggi)? It is hard to introduce an exact reference solution to plasticity, for example, using FEM (Mueser). It might be interesting to also look at adhesion pull-off force in a future challenges (Ciavarella).
- How difficult would it be to remove the periodic BC in the simulations for comparison with experiments (Chateauminois)? It was less of an issue that would have been expected; need to take a multi-grid computational approach (FT-BVM) (Mueser).
- Currently, the real adhesive contact area cannot be measured experimentally, while only the repulsive contact area is clearly defined in computations (e.g. exact DFT calculations). How can we change this (Mueser in response to comment by Scheibert)?

Friction [K2]:

- Can the parameter of the statistical distribution be calculated from the results of Fineberg (Paggi)?
- Heterogeneous material would be interesting. How can this be modeled (Molinari)? There is a melted film at the interface (Malthe-Sorenssen).

- How can these results be related to the real contact area (Molinari)? This depends on how the real contact area is measured (Malthe-Sorenssen).
- How about the propagation of stress singularity in Fineberg's papers? New experiments of Fineberg with lubrication are surprising (Ciavarella).
- Is there experimental evidence of the existence of slow fronts (and not something else) (Yastrebov)? The results are not quasi-statically driven in the model (Malthe-Sorenssen).

Roughness [K3]:

- The "influence" of magnification: what is the limiting magnification for this fractal repetition? At which magnification will the contact pressure be enough to cause yield (Almqvist)?
- M. Moseler: can we look into the contact? You can get percolation functions with a synchrotron, but it has not yet been done (J. Frenken).
- Higher order autocorrelation functions may be needed but the topic of non-Gaussian fractal surfaces is not very developed at present.

Nanoscale behavior:

- Are rough surfaces more reactive than atomically flat surfaces?
- Are amorphous surfaces more reactive than crystalline surfaces?
- Can we formulate a modified continuum description that extends hydrodynamics to smaller scales? Extended continuum descriptions require additional material parameters. How can we get them?
- How does heat conduction change when the mean free path of electrons becomes of the same size as the asperities?

Plasticity and material models:

- How does plastic deformation affect surface topography and friction?
- What is the effect of including large deformation in the description of plastic flow?
- Is size-dependent plasticity relevant for real rough surfaces? To which extent does it affect contact and friction?
- Does the importance of plasticity fade with increasing the number of loading cycles ?
- What is the role of surface steps during contact, are they sources for additional dislocations?
- Is plasticity important only for large deformations?
- To which extend does plastic interaction between asperities affect the contact response of rough surfaces?
- Would viscoplasticity couple with the viscosity of the lubricant?
- What type of size effects would occur in soft materials? What about nano-scale dynamic heterogeneities with characteristic times spanning different orders of magnitude?

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4.2. Tribological solutions for the industry

Controlling friction in steel-making processes is necessary to improve the quality of deep-drawn and rolled products and increase the production rate. A very undesirable phenomenon closely related to friction is adhesive wear, responsible for flaking and galling after a few hundred pieces are produced. In practice, the industry uses primarily experimental studies to understand the frictional response of steel at different moments during the deep-drawing process. The drawback of this approach is that different friction coefficients are measured in different experiments: draw-bead tests, U-bead tests, flat die tests

with shaped specimens or flat die tests with bending. Consequently, it is very challenging to extract useful information by comparing empirical results and any understanding is complicated by lack of reproducibility, since different batches of pieces contain inhomogeneities and defects, while tools are also characterized by inhomogeneous roughness and dimensions.

Experiments show that the morphology of electro-galvanized and hot dip-galvanized steel has significant impact on tribological properties (presentation by M. Toose of TATA Steel during the Lorentz workshop). The industry currently uses tribological models that are based on continuum theories and incorporate limited microscale aspects and simplified roughness representations, or phenomenological models that strongly rely on experience: e.g. the friction coefficient is varied within a known range to predict process parameters (presentation by M. Veldhuis of Philips Drachten during the Lorentz workshop). Correspondingly, a loss of productivity in the industry (estimated to 25% of the theoretical productivity) is thought to occur due to the inability to control temperature-dependent tribological effects: for example, plastic deformation results in a temperature-induced increase in friction at start-up, for which products are thrown away for the first 30 minutes of production. Philips currently uses a micromechanics-based numerical models to predict friction coefficients that vary with local pressure, strain and temperature, e.g. [272]. Such models calculate the load-carrying capacity of lubricant-filled cavities, where the Young's modulus and flow stress are modelled as temperature-dependent, and are validated with experimental measurements. At the same time, however, numerical models need to satisfy certain criteria: they require computationally-efficient simulation strategies, should be usable in automated control systems to allow in-line adjustment of process settings based on (meta)data, and they should be robust across various processes and demonstrators at both ends of the dimensional range. Hence, there is need for simple (perhaps, even, analytical) but comprehensive predictive models of friction as well as system-level simulations that can incorporate tribological aspects into the modeling of multi-stage deformation processes. Some open questions are related to the aspects discussed elsewhere in this review paper: what scales are relevant in friction modeling (section 3.1)? How relevant is the effect of plasticity on friction (sections 3.3 and 3.6)? What is the role of bulk and thin film lubricants (section 3.8)?

While unanswered questions remain and improved models are needed in the "classical" manufacturing world, tribological issues persist also for semiconductor companies such as ASML that use fast extreme ultraviolet (EUV) lithography on large tens-of-micrometers-thick wafers to manufacture integrated circuits with positioning accuracies of the order of nanometers. Physics and chemistry questions are relevant for such processes, focusing on EUV source, scanner, metrology and process attributes. Current positioning methods involve electrostatic forces used to fix the wafers onto burls on the substrate; improving and optimizing positioning accuracy requires multiphysics modeling across scales since wafer-support forces lead to wafer distortions and, in turn, to overlay and height (out of focus) errors. Adhesion and friction play an important role in wafer support as does the contact and clamping history: the order in which contact with individual burls is established is different every time. Furthermore, positioning is a dynamical contact phenomenon that, at such small scales, results in accelerations of 50g [RT12]. The "ultimate dream" for the industry is to realize switchable friction without wear (presentation by J. Frenken of ARCNL during the Lorentz workshop).

Hence, there is more to friction than roughness, with the microstructure and its evolution playing an important role that needs to be included in numerical models, but there is also much more to tribology than friction. The industry is interested in, both, robust system-level models that include multiscale phenomena and cutting-edge nanoscale understanding of multiphysical phenomena. The following is a collection of questions that the industry requires tribological solutions for:

- How does plastic deformation affect surface topography and friction?
- Under which condition do adhesive and abrasive wear occur?
- How do coatings improve wear resistance?
- Under which circumstances is debris incorporated in the contacting material?
- What is the mechanism of galling and when does it take place?
- How can we achieve switchable friction at the micro- and nanoscales?
    - What is the role of adhesion and friction on wafer support during EUV lithography?
    - How does contact and clamping history affect EUV lithography wafer distortions and positioning accuracy?
    - Will it beneficial to introduce special coatings (graphene, diamond-like carbon, etc.) or structures (micro- and nanopillars) at the wafer-substrate burl interface?

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- SKF technology platforms: bearings and units, seals, services, lubrication systems, mechatronics.

The core business of SKF is the production of roller bearings, a product that is conceptually rather simple: two concentrically rings separated by a set of rolling elements used to reduce friction. Despite its simplicity, throughout the service life of a roller bearing, several phenomena that are not currently fully understood take place. Among these, the friction and contact between the different moving parts play a major roll, because, at the end, they will govern the duration of the useful life of the bearing. This is why there is a commercially-driven need to better understand, even at the atomic scale, all these tribological phenomena.

- Example: two iron surfaces with lubricant studied with non-equilibrium MD. Surface roughness and surface coverage was varied in these studies: friction increases with roughness and decreases with surface coverage.

As a proof-of-concept, and as a first step towards realistic MD simulations of the operating conditions of roller bearings, nonequilibrium molecular dynamics simulations of stearic acid adsorbed on iron surfaces with nanoscale roughness were performed [273]. Although it is not yet possible to make a one-to one quantitative comparison of MD simulations and experiments, interesting conclusions regarding the governing tribological mechanisms where obtained:

First, the stearic acid films were able to maintain separation of asperities on opposing surfaces for all the systems simulated, due to strong adsorption of the head groups. Second, on surfaces with nanoscale roughness, systems with a higher coverage of stearic acid generally yielded lower the friction coefficients and Derjaguin offsets. Last, although an increase in the surface roughness generates more disordered stearic acid films, the friction coefficients and Derjaguin offsets are only slightly increased.

- Tribolayer formation and the effect of run-in at the piston-cylinder interface?
- How about the changes in the coefficient of friction in tribo-tests?
- Atomistic v. experiments:
    - Comment on iron oxide: how can we properly model oxides at the interface?
    - Friction coefficients v. sliding velocity: comparison of all-atom, united-atom and experiments). The choice of potential greatly affects the results; how trustable is the information?

Although there has recently been an increased interest on the simulation of tribological contacts [130,273-275], which, together with the ever-growing available computational power, has resulted in the development of more realistic atomistic models, a number of fundamental issues still remain. These issues can be classified in two main categories: those that are intrinsic to the method and those that are not.

The problems or limitations intrinsic to the method are mostly related to the time and length-scales that can be reached, and are usually considered to be among the most difficult to solve. Nevertheless, since they are recurrent issues for a wide range of applications, they appeal to a larger audience and, naturally, a more important effort is being put into solving them.

One possible way to deal with the time and length scale problem is to link atomistic with larger scale methods in order to reduce the complexity of the problem and have access to information at larger scales. Good examples of this type of approach are the quasi-continuum method [276], which is able to couple continuum and atomistic approaches for simulating the mechanical response of polycrystalline materials, and the CPL library [277], a communications and topology management system for coupling continuum fluid dynamics to molecular dynamics.

Other possible methods to reach longer timescales, while retaining full atomistic details, have been derived from transition state theory. The main idea of these methods is to accelerate molecular dynamics simulations of infrequent-event processes in order to reach simulation times several orders of magnitude longer than direct molecular dynamics [278]. The most common methods are: parallel replica dynamics, hyper-dynamics, temperature- accelerated dynamics, and on-the-fly kinetic Monte Carlo.

…

- Computer difficulties for Molecular Dynamics:
    - Simply based on the number of degrees of freedom, you cannot scale to quantities of relevance to the engineering scales.
    - Examples:
        - Evolution of grains (M. Moseler): what is the effect of BCs?
        - Multiscale modeling of 2d contacts (work of Molinari and Robbins).
        - Connection with higher scales (CPL library; Imperial College work).
        - Quasi-continuum simulations.
- Example: In the case of plastic deformations, for instance occurring during sliding motion between two metallic surfaces, many dislocations are nucleated at the surfaces and under maintained load may travel long distances. In a MD simulation, the small size of the domain will artificially trap them and create artificial hardening, that should occur in very thin coatings. In order to address this issue, advanced concurrent coupling strategies are being developed where dislocations can be passed to a continuum representation [279,280]. In 3D, dislocations are lineic networks, so that a dislocation may cross the coupling interface. Such hybrid dislocations should behave as single dislocation structures. This requires reciprocal BCs (Curtin's and Molinari's groups; CADD3d project since 2013). "This has been a gigantic effort".
- Thermostat problem: residual kinetic energy v. sliding distance shows differences between full MD (used as the reference), reduced, coupled, and reduced + coupling methods. How can you make temperature time-dependent?

G. Anciaux: we have two options

1. We can go for very complex and comprehensive simulations, something that is technically possible but very effort and time consuming to implement.
2. We do MD as we do now. However, The BCs matter a lot (also emphasized by L. Nicola). Would it make sense to get a probability density function from continuum theories in order to relevant boundary conditions to the MD models ? Can we asses if the set of simulations that were conducted in the past are comprehensive enough to gain knowledge for the engineering scale ?

J-F Molinari: depending on the type of problem of interest, perhaps the PDF (averaging all details) might be sufficient.

J. Scheibert: is there no time issue with MD (e.g. even 1 m/s would be very high)? Answer: yes. What are the relevant situations to be computed at the atomic scale?

G. Vorlaufer: anything that you simulate with MD will be essentially flat contact.

V.A. Yastrebov: the oxide layer would probably play a role as well.

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4.3. Collaborative platforms for tribologists

Considering the state-of-the-art presented at the workshop, a need for collaborative platforms for tribologists has emerged. A shared platform, organized via a dedicated web-site, could include the following sections: (i) a collaborative platform with open source software provided by research groups, useful also for dissemination purposes; (ii) a collection of contact problem results reporting, for each case study, the surface topology used as input for the simulation/experiment, the material parameters and the constitutive model, and a description of the assumptions of the computational model used to obtain the contact response; (iii) a list of simulation and testing facilities of research groups working on contact mechanics, with links to their websites and laboratories, listed according to the major problems of industrial interest. This collaborative platform is envisages to have an important impact on the community to foster novel round robin campaigns, provide material useful for benchmark tests, and increase the awareness of companies in the applicability of contact mechanics research to solve problems of industrial interest.

Identification of reference systems for benchmarking and model/experiment comparison…

J. Frenken: what would be the ideal experiment to be used by modelers/ theoreticians? (e.g. 3d printed surface, or sinusoidal surface.) Answer: before considering these very complex fractal surfaces, it could be interesting to go back to simple topographies in the spirit of GW where we can play by-design with the statistical features within a limited range of length-scales (A. Chateauminois). Won't you always have roughness (A.I. Vakis)? There are techniques that would let you select in a controlled way the relevant roughness content (A. Chateauminois).

Note: BEM code made available to calculate contact pressure or pressure distribution at contact.enigineering or tribo.iam-cms.kit.edu/contactapp

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5. Conclusions

One of the main outcomes of the workshop was the realization that, despite the modeling community's ability to address elastic problems of great complexity at various scales, significant effort is still required to account for the effects of plasticity, adhesion, friction, wear, lubrication and surface chemistry in tribological models. Weak, strong and monolithic coupling schemes between different physical phenomena at small scales, which are critical for tribological behavior at the system scale, were considered during respective round-table and key-note lectures. Numerical methods were also discussed relative to their inherent length scales: finite element and boundary element methods versus discrete dislocation dynamics for the microscale, and classical versus ab initio molecular dynamics and density functional theory for the nanoscale. Emphasis was placed on the advantages and disadvantages of employing concurrent or hierarchical multiscale schemes coupling these methods, while the need to develop improved tools requiring less computational effort and time was put forth by industrial participants who would like to use such tools to optimize and control their processes and products. All these issues constitute future areas for tribological research and have been made visible to participants who expressed their interest in pursuing this further in an inter-disciplinary manner.

Table 1. List of participants and their affiliations.

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