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ADVANCED MATERIALS SIMULATION

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Numerical modelling of nanotribology : opportunities and challenges

Nanotechnology is a new frontier in research, and as with any new domain, new tools must be developed. As surface to volume ratios become large, engineering at the nanoscale will be dominated by surface science. While for a long time considered a traditional discipline of Mechanical Engineering, Contact Mechanics is prone to exciting developments. The study of Contact Mechanics at nanoscales, i.e. nanotribology, needs to fully account for adhesive forces, third body interactions and deformation mechanisms at contacting asperities. Understanding these factors as well as evolutions in the morphology of contact areas has the potential of explaining the origin of frictional forces and wear. This fundamental understanding is needed to guide us in the design of tailored-made lubricants and surface morphologies.

Be they at the macroscopic or nano scale, tribological problems are particularly difficult to comprehend. Different physical mechanisms (which include for instance environment, plastic deformation, third body interactions, phase transformations, recrystallisation) interact at disparate length scales. It is therefore not surprising that contact sciences have been primarily driven by careful experimental investigations. Nonetheless, as experiments go down in size and as computational power expands, numerical simulations become increasingly relevant to experimental work.

We begin the presentation with simulation results at the continuum scale. Finite-element calculations are conducted for normal and sliding contact of rough solids. The surfaces are modelled with self-affine fractals. In accordance to theory and experimental work, we observe a linear dependence between applied load and the real contact area, for both elastic and elasto-plastic solids. However, we contrast our results with prior theoretical models which do not explicitly take into account interactions between asperities. In the second part of the presentation, we review key atomistic (MD) simulations results from the literature. We highlight the limitations of a purely continuum approach and motivate the development of a multiscale framework, in which MD is directly coupled to finite elements. We present preliminary 3D simulation results of rough on rough sliding and give a road map for efficient parallel scaling of the simulation capability.