Multi-Scale Modeling and Simulation of Adhesion, Nanotribology and Nanofluidics

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Engineering tools for designing macroscopic mechanical devices are well established, but break down as dimensions decrease to nanometer scales.[2] One reason is that interfacial effects become more important. Adhesion, capillary forces, and other factors can be ignored in most macroscopic machines, but often dominate behavior at nanometer scales. Indeed, undesired adhesion has been identified as the main cause of failure in microelectromechanical systems (MEMS).[2] Smaller length scales also lead to new physical effects. Flow boundary conditions change qualitatively as dimensions approach the mean free path, and packing effects and surface interactions can stabilize new phases with different structural, mechanical, chemical, and electrical properties.

Existing theoretical tools are adequate when there is a single relevant length scale, but in many processes there is an intimate interplay between phenomena at different scales. For example, atomic interactions in regions where surface separations are less than a few nanometers determine the global resistance to sliding and the strength of adhesive bonding. However, processes at larger scales control the conditions within these contact regions (mechanical loading and distribution of lubricant), as well as their number, size and geometry. Spanning the entire range of length scales with electronic structure calculations or molecular dynamics is both impractical and inefficient. The vast majority of atoms are in regions where deformations or flows are small and can be treated with continuum approaches. However, these approaches require constitutive relations and boundary conditions that are generally unknown.

Our goal is to develop hybrid algorithms that efficiently describe a wide range of length scales, and use these algorithms to study adhesion, tribology and fluid flow in geometries where some relevant dimensions are of nanometer scale. Both hierarchical and simultaneous approaches are being pursued. In the first, molecular dynamics (MD) simulations provide the required input for continuum approaches at larger scales. Results from continuum calculations are used in turn to identify the relevant conditions for further simulations. In the simultaneous approach, most of the system is described by continuum equations, but regions where conditions vary rapidly, such as interfaces, are described by MD simulations. Both approaches require improved algorithms for coupling information from different scales.

During the first year of funding we have concentrated on using hierarchical approaches with existing computational tools for each length scale, and on developing tools for simultaneous calculations. Research has fallen into two major areas that are outlined below. Each project has involved researchers from different departments and backgrounds, whose names are listed. The grant has provided full support and interdisciplinary training for two graduate students, Xiaobo Nie and Lin Pei, and two postdoctoral fellows, Sangil Hyun and Ramzi Kutteh.

Contact and lubrication of rough surfaces - Harrison, Hyun, Kutteh, Molinari, Pei, Robbins
Both molecular scale and continuum studies of contact have traditionally assumed uniform surface chemistry and simple geometries, such as atomically flat surfaces, spherical asperities, or sinusoidal modulations. Predictive models for adhesion in MEMS and other devices will require more realistic surface models. Many experimental surfaces have roughness over a wide range of scales that is characteristic of self-affine fractals.[3] We have developed algorithms for generating these and other surface geometries and calculating contact properties using finite-element and molecular dynamics simulations.

Finite-element studies have examined contact between non-adhesive, self-affine fractal surfaces. The Poisson ratio □, mesh size, roughness amplitude and roughness exponent have been varied. For elastic surfaces the total contact area A rises linearly[4] with the total force F (Fig. 1). The slope is weakly, and non-monotonically, dependent on □. The regions of contact and local stresses show power law spatial correlations. The local pressure has a long exponential tail (Fig. 1) that has a profound effect when plasticity is included within the finite elements. Very little analytic and almost no numerical work has been done on adhesive surfaces. Our short term goals are to extend our results to this case using cohesive elements, and examine the effect of roughness on the work of adhesion and friction. This will require information about the local adhesive and frictional forces between rough surfaces.

We have begun molecular dynamics calculations of contacts between amorphous solids with the same surface geometries as above. Results are qualitatively similar, but there is substantial plastic deformation at lower forces than would be expected from bulk models. Repeated contacts lead to work hardening and a greater range of elastic response. These results will be used to generate input needed for the planned studies of adhesive surfaces, and to test the assumptions of continuum models. Then hybrid models will be used for simultaneous calculations.

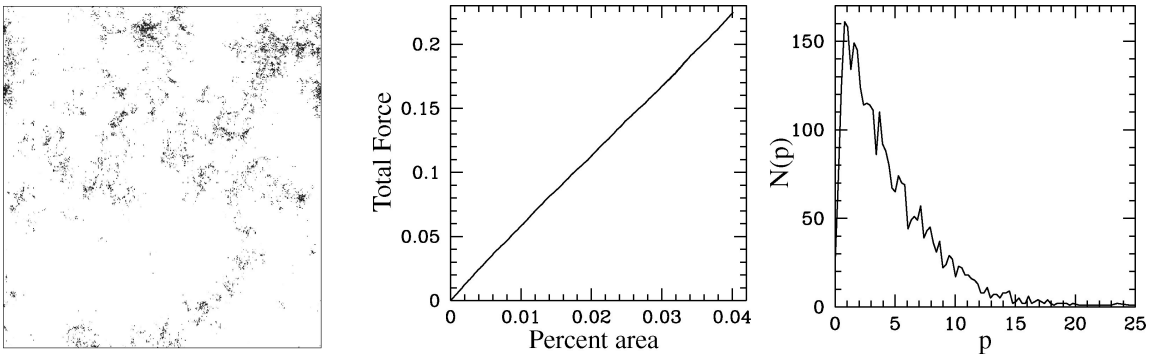

Figure 1. Left: Contact area (black) between self-affine surface (512x512 surface nodes) and flat. Middle: Fraction of area in contact vs. total force. Right: Distribution of local pressures p.

Surface roughness has a profound effect on the flow and distribution of lubricants between surfaces. Normal stresses produced by flow lead in turn to deformation of the surfaces that change the flow. At the macroscopic scale this coupling is called elastohydrodynamics, and is crucial for the function of both engines and joint cartilage. We have begun MD calculations that include long-range elastic deformation for the first time. The amount of deformation is strongly dependent on the roughness, lubricant thickness, sliding velocity, and pressure.

Multi-scale algorithms – Bernstein, Chen, Kutteh, Nie, Robbins

Our goal is to develop an algorithm that describes most regions of space with continuum equations, but treats interfacial and high stress regions with classical or tight-binding molecular dynamics. Most previously proposed methods have limits that make them poorly suited to the scientific problems of interest. We have chosen to build on an algorithm that can be used for finite temperature, non-equilibrium dynamics and allows flux of atoms between continuum and atomic regions due to fluid or plastic flow.[5] The interface between continuum and atomic regions is divided into three layers. In the layer closest to the atomic region, MD results for stress and flux (or strain) provide boundary conditions for the continuum region. In the layer closest to the continuum region, the continuum solution defines the ensemble for the MD simulation. The middle layer allows the two solutions to relax independently. The original algorithm was susceptible to drift of the layers, leading to an unacceptable thinning of the MD region. This difficulty was overcome by determining the boundary condition for the MD region from continuum velocities instead of pressures. A simpler version of the algorithm for elastic solids is currently being tested.

Figure 2 compares flow fields from MD, hybrid and pure continuum calculations of flow past a bump. The full MD and hybrid results are in excellent agreement and the hybrid algorithm has no difficulty in treating steady state flows in and out of the continuum region. The full continuum calculation differs from the other results because of inadequate boundary conditions. The MD parameters were chosen so that a no-slip condition was appropriate on flat surfaces, and this condition was assumed in the continuum calculation. However, the sharp corners of the bump cause changes in the local boundary condition that affect the flow over the entire system. Resolving this discrepancy by a complex, spatially varying boundary condition may be possible, but is neither desirable nor practical. Hybrid methods naturally resolve such difficulties, providing accurate, time-dependent boundary conditions for the continuum regions.

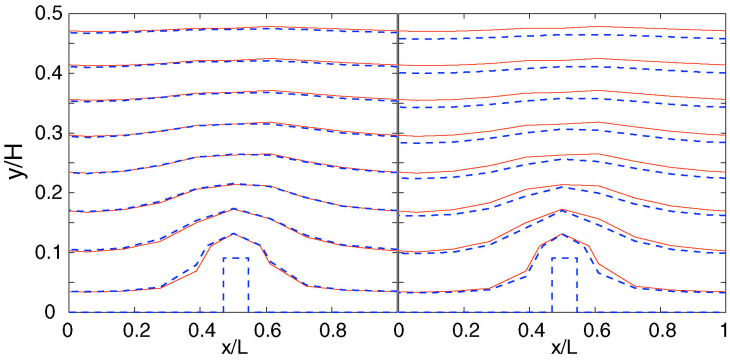

Fig. 2. Streamlines for flow in channel with bump on wall. Left panel compares MD (dashed) and hybrid (solid) results. Right panel compares continuum (dashed) and hybrid (solid) results.

References

[1] For further information about this project link to <http://www.pha.jhu.edu/groups/multi/> or email mr@jhu.edu.
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