Bridging Scales in Boundary Lubrication: Atomistic-Continuum Coupling Enabled by Machine Learning

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Abstract

Friction and lubrication are inherent multiscale problems, particularly when the gap between contacting bodies is on the order of molecular interaction length scales. These conditions occur predominantly in the so-called boundary lubrication regime under high normal loads, low sliding speeds or with low viscosity lubricants. Continuum descriptions of the interfacial flow problem can be augmented with atomistic simulations to account for various nonlinear effects, such as fluid-wall slip. However, modeling lubrication across scales beyond purely sequential approaches has so far remained elusive.
In this talk, I will present a reformulation of the classical lubrication equations that allows straightforward concurrent coupling between continuum and molecular models. Instead of using fixed-form constitutive expressions that are parametrized a priori using atomistic methods, we build surrogate models for the interfacial shear stress and normal pressure on-the-fly.

Concurrent coupling is achieved by an active learning scheme based on Gaussian process regression, which allows for a data-efficient interpolation of the microscopic stresses obtained from molecular dynamics simulations in a high-dimensional parameter space. Furthermore, the Gaussian process posterior variance enables quantifying the uncertainty of pressure and shear stress distributions within the gap.
We validate the proposed method for nanoscale flow of simple fluids around single and multi asperity topographies, which paves the way for accurate simulations of boundary lubrication on experimental length and time scales.

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