Abstract

Continuum mechanics has been remarkably successful in explaining the macroscopic behavior of materials. However, almost every mechanical process of interest at the continuum scale traces its origins to the phenomena occurring at the atomistic scales, be it fatigue, fracture, yielding, plasticity, etc. A typical challenge that researchers face is understanding how such atomic-scale phenomena determine macroscopic behavior. Although theoretically, it is possible to simulate an atomically complex system that is large enough to approach the continuum limit, the hard limit posed by the availability of computational resources has rendered it possible to simulate a system only as large as trillion atoms. In comparison, a mole of any substance has 10^{23} particles. The concept of multiscale modeling has emerged to tackle this situation – one can understand the continuum-scale behaviour of a material by modeling it at the continuum scale while simultaneously utilizing the information obtained at the atomic scales without requiring a high fidelity atomic-scale model.

In this thesis, we develop a sequential multiscale framework for studying the problem of liquid droplet erosion (LDE). In LDE, the repetitive impact of liquid droplets on a solid surface result in fatigue. The problem of LDE is a multiscale-multiphysics problem – what we observe as fatigue damage due to LDE at the continuum scale arises due to defect formation and bond breakage at the atomic scale over a long period. These defects coalesce, and finally manifest at the continuum scale where the different domains of mechanics – classical mechanics, hydrodynamics, shock wave propagation, fracture mechanics, and non-equilibrium thermodynamics – are intertwined and determine the material response. Complicating the matter is the fact that a continuum-treatment of the problem needs to account for fluid-structure interaction, surface tension, etc. as the liquid droplet impacts the solid surface. Given this, we propose a multiscale model, where one need not model the liquid droplet at all in the continuum scale. This is achieved by coupling the continuum scale smooth particle hydrodynamics (SPH) with the atomic-scale molecular dynamics (MD) simulations through proper constitutive modeling across the two length scales. Our model relies on computing the material (elastic and fracture) properties of a hypothetical material at the atomic scale, and use them in the SPH simulations directly. The liquid droplets at the continuum scale are replaced with the equivalent boundary stresses obtained from the atomic scale MD simulations, thereby simplifying the modeling process.

Naturally, two questions arise – (i) whether the methods (MD and SPH), occurring at completely different length scales and solving completely different differential equations, provide equivalent results, and (ii) how correct it is to replace the liquid droplet at the continuum scale with the equivalent boundary stresses obtained from the atomic scale simulations. To answer the first question, we systematically compare the traditional Eulerian SPH, the Total Lagrangian SPH, and the MD simulations for five commonly encountered problems – (i) a solid projectile impacting a target, (ii) uniaxial tensile testing of a beam, (iii) unidirectional stretching a pre-notched rectangular plate, (iv) elastic collision between two rubber-like rings, and (v) impact loading on the free end of a cantilever beam, and show that the continuum scale methods provide results that are in good quantitative agreement with the MD simulations. However, modeling the contact is a bottleneck in problems involving impact. To answer the second question, we show that there is a good qualitative agreement between the MD simulations and the previously published finite element results if one looks at the stress developed in the solid

substrate and the liquid droplet, as the latter impinges on the former. Due to this, in the continuum SPH model, one can omit the modeling of the liquid droplets, and replace them with equivalent boundary stresses.

To study fatigue damage due to LDE, we propose pseudo-spring based SPH frameworks, where the loading and the material properties are taken directly from the MD simulations. The proposed frameworks can determine the mode-I and the mode-II stress intensity factors reasonably well for a variety of loading modes and specimen geometry. The utility of the frameworks is demonstrated for studying fatigue damage due to liquid droplet impingement, wherein we show that the fatigue crack propagation is accurately captured. As the Paris law constants determined from the MD simulations are assumed to be mode-independent, we observe the fatigue life to first increase as the shear load is increased. The situation can be tackled by calculating the mode-dependent Paris law constants for different types of loading – shear, normal and both.

Keywords: Multiscale modeling, Smooth Particle Hydrodynamics, Molecular Dynamics, Fatigue, Liquid Droplet Impact