



Mechanical and Civil Engineering Thesis Defense

Wednesday, June 24, 2015

10:30a.m. in 101 Guggenheim (Lees-Kubota Hall)

“A fully-nonlocal energy-based formulation and high-performance realization of the quasicontinuum method”

Jeffrey Amelang

Graduate Student, Mechanical Engineering

•**Abstract** The quasicontinuum (QC) method was introduced to coarse-grain crystalline atomic ensembles in order to bridge the scales from individual atoms to the micro- and mesoscales. Though many QC formulations have been proposed with varying characteristics and capabilities, a crucial cornerstone of all QC techniques is the concept of summation rules which attempt to efficiently approximate the total Hamiltonian of a crystalline atomic ensemble by a weighted sum over a small subset of atoms. In this work we propose a novel, fully-nonlocal, energy-based formulation of the QC method with support for legacy and new summation rules through a general energy-sampling scheme. Our formulation does not conceptually differentiate between atomistic and coarse-grained regions and thus allows for seamless bridging without domain-coupling interfaces. Within this structure, we introduce a new class of summation rules which leverage the affine kinematics of this QC formulation to most accurately integrate thermodynamic quantities of interest. By comparing this new class of summation rules to commonly-employed rules through analysis of energy and spurious force errors, we find that the new rules produce no residual or spurious force artifacts in the large-element limit under arbitrary affine deformation, while allowing us to seamlessly bridge to full atomistics. We verify that the new summation rules exhibit significantly smaller force artifacts and energy approximation errors than all comparable previous summation rules through a comprehensive suite of examples with spatially non-uniform QC discretizations in two and three dimensions. Due to the unique structure of these summation rules, we also use the new formulation to study scenarios with large regions of free surface, a class of problems previously out of reach of the QC method. Lastly, we present the key components of a high-performance, distributed-memory realization of the new method, including a novel algorithm for supporting unparalleled levels of deformation. Overall, this new formulation and implementation allows us to efficiently perform simulations containing an unprecedented number of degrees of freedom with minimal approximation error.

