The Quasi-continuum Approximation And Virtual Internal Bond Model For Material Dynamics

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In many applications materials are modeled by a large number of particles (or atoms) where any particle interacting with any other through a pair potential energy. The equillibrium configuration of the material is the minimizer of the total energy of the system. The computational cost is high since the number of atoms is huge. Recently much attention has been paid to a so-called quasicontinuum (QC) approximation which is a mixed atomistic/continuum model. In the talk I will briefly introduce results for the convergence analysis of the method in the steady state case and comment on when the method may fail. I will then focus more on a simple generalization of the idea to a dynamical case and numerically study the convergence of the method in a time-average sense assuming the nearest neighbor interaction. We will relate the discrete model to continuous virtual internal bond model, which is a nonlinear wave equation of mixed type. We can construct the solution of its Riemann problem assuming certain admissible condition and use the solution to justify or guide our study of approximation methods. We will also give numerical examples which indicate that when such model is used for simulation of fracture dynamics it may only be reliable for the early stage of the fracture.