A virtual internal bond model for fracture dynamics

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Molecular dynamics (MD) model is used in simulating material fracture. Because the number of particles (atoms) is huge, in practice people often take a much smaller number of particles. A virtual internal bond (VIB) model was proposed recently and can be seen as a continuous MD model. The VIB model is a nonlinear conservation law of mixed type (hyperbolic or elliptic). We will use the VIB model as a framework to consider the relationship between the practical less-particle solution and the MD solution. There are infinitely many equilibrium solutions (configurations) corresponding to the model. The dynamical solution is also very difficult to analyze because of the type change from the hyperbolic to the elliptic. We find that some fracture cases can be simplified to a Riemann problem and its solution can be studied. We will consider a discretization of the model. A discrete equilibrium solution would be an approximation to a continuous equilibrium solution. The discrete dynamical solution is also demonstrated to approximate the constructed solution of the Riemann problem. Numerical simulation of one and two dimensional fracture examples based on this discretization will be presented as well. We will adopt Lennard-Jones potential for atomic interaction.