Analysis and Simulation of a Nonlinear Wave Equation of Mixed Type for Fracture Dynamics

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Abstract

Modeling and simulation of material motion play an important role in understanding and predicting material behaviors. such as dislocation and dynamic fracture. Most of the problems in this area are very challenging to analysts and many of them have not been well studied. Modeling, theoretical analysis and explanation of various phenomena observed are far from complete. We shall consider a virtual internal bond (VIB) model with randomized cohesive interactions between material particles in the literature of material science. It differs from an atomic model in that a phenomenological "cohesive force law" is assumed to act between "material particles" which are not necessarily atoms. It also differs from a cohesive surface model in that, rather than imposing a cohesive law along a prescribed set of discrete surfaces, a randomized network of cohesive bonds is statistically incorporated into the constitutive law of the material and the macroscopic collective behavior of this random bond network is obtained through the so-called Cauchy-Born rule, i.e. by equating the strain energy function on the continuum level to the potential energy stored in the cohesive bonds due to an imposed deformation. The VIB model is intended to integrate the macroscopic view of cohesive surfaces dispersed in a continuum background with the "atomistic" view of interatomic bonding. One application we are concerned of is the fracture dynamics, where near the crack tip we generally need to consider the atomistic interaction or scale. As an example we shall adopt the 6-12 Lennard-Jones atomic interacting potential which is a reasonable approximation to atomic interaction of a number of real materials. The model is a nonlinear wave equation of mixed type. There is instability in the elliptic region and usual numerical methods might not work. We examine the artificial viscosity method for the model and apply central type schemes directly to the corresponding viscous system. We provide a formal justification of convergence of the scheme despite the difficulty of the type change. The exact solution of a Riemann problem is constructed to justify the numerical simulation for the one-dimensional case. We then generalize the method to a two-dimensional material with a triangular or hexagonal lattice structure. Computational results for the two-dimensional example are provided.