An augmented phase-field model with viscous stresses for defect dynamics

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Abstract

This work begins by applying phase-field modeling to predict 1-d interface motion with inertia in an elastic solid with a non-monotone stress-strain response. In classical nonlinear elasticity, it is known that subsonic interfaces require a kinetic law, in addition to momentum balance, to obtain unique solutions; in contrast, for supersonic interfaces, momentum balance alone is sufficient to provide unique solutions. However, conventional phase-field models coupled to elastodynamics are unable to model, even qualitatively, the supersonic motion of interfaces. This work identifies the shortcomings in the physics of standard phase-field models to be: (1) the absence of higher-order stress to balance unphysical stress singularities, and (2) the ability of the model to access unphysical regions of the energy landscape.

This work then proposes an augmented phase-field model to introduce the missing physics. The augmented model adds: (1) a viscous stress to the momentum balance, in addition to the dissipative phase-field evolution, to regularize singularities; and (2) an augmented driving force that models the physical mechanism that keeps the system out of unphysical regions of the energy landscape. When coupled to elastodynamics, the augmented model correctly describes both subsonic and supersonic interface motion. This augmented model was then used for fracture simulations.

1. Introduction

Current phase-field models are largely unsuitable for phenomena in which inertial effects – rather than energy minimization alone – play a significant role. To model the general setting without inertia, it is typical to minimize the total energy with respect to the strain field and use steepest-descent dynamics for the evolution of ϕ. When inertia is present, energy minimization is not relevant, and the kinetic energy has an important contribution. The material can then explore parts of the energy landscape far from the minimizing curve; however, the energy landscape away from the minimizing curve has no physical connection to the original classical elasticity energy. We see in our numerical calculations that the material does explore nonphysical regions of the energy landscape — particularly at large interface velocities. This is a central reason for phase-field models to fail in correctly modeling supersonic interfaces.

The second problem is the appearance of an unphysical singularity that forces the stress and strain to go to infinity at a point for a supersonic interface in the standard phase-field formulation. We also find that a regularization of the momentum equation – in addition to the usual regularization of phase-field models – resolves this singularity. While it possible to use various regularizing stresses, we choose to use a viscous stress because this is the simplest, has a clear physical interpretation, and is readily compatible with standard numerical methods, e.g. FEM with C^0 continuity. We note that all real materials have some level of dissipation, and even in materials in which dissipation is generally small, it can be very important in problems of shocks that are near sonic or supersonic. Therefore, it is not surprising that it plays an important role in phase-field models that aim to be valid when inertial effects are significant.

2. Results

To address the issues identified in the introduction, we propose an augmented phase-field model that has these 2 extra terms:

1. A local dynamical term that moves the system – along the ϕ direction only, to avoid disrupting momentum balance – away from unphysical regions in the energy landscape. This term corresponds to

accounting for the missing physics of a driving force that would drive the evolution away from high/ infinite energy forbidden regions.

2. A viscous dissipative stress that regularizes the singularities mentioned in the introduction and accounts for the missing physics of dissipative mechanisms that are always active and particularly important at defects and singularities.

A comparison of initial-value problems for standard phase-field model with supersonic interfaces when performed without (Fig.1) and with the augmentations (Fig.2) shows us that while the interfaces in ϕ and strain used to decouple, they are now propagating together with the addition of the two terms.

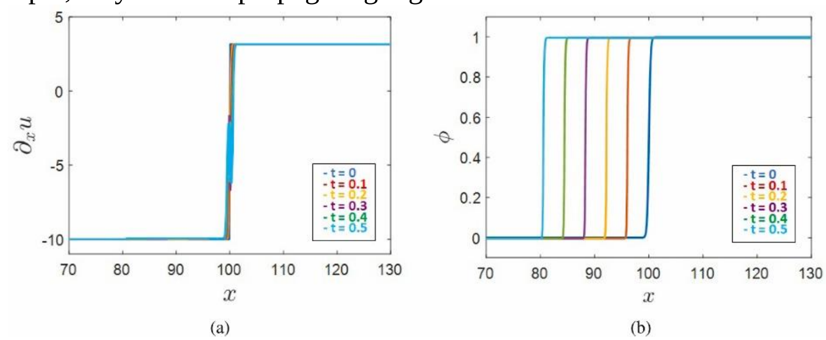

Fig.1 – Initial-value problems for the standard phase-field model with supersonic interfaces. The strain interface (a) has barely moved and is subsonic while the ϕ interface (b) is moving at supersonic speeds.

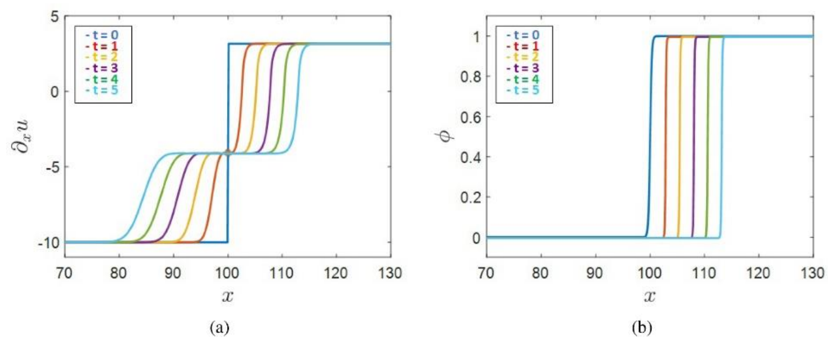

Fig.2 – Initial-value problems for the standard phase-field model with supersonic interfaces, using both the augmented driving force and viscous stresses. The evolution is precisely as we desire, in that the strain and ϕ interfaces move together supersonically with no undesirable oscillations.

3. Conclusions

A key shortcoming of existing phase-field models that is discussed in this work is that the energy landscape is expanded by introducing the phase-field, and this expanded energy landscape has numerous unphysical regions. For equilibrium problems, the system is governed by energy minimization, and hence it does not explore these unphysical regions. However, in dynamic problems with inertia, the potential energy is balanced against the kinetic energy. Therefore, energy-minimization formulations of the energy are found to be inadequate to avoid the unphysical regions, and we require additional physics to prevent the system from exploring the unphysical regions. In short, if new equations and variables are introduced, we require additional physics to ensure that they behave appropriately in all regimes of application. Our proposed augmentation of phase-field models includes this additional physics in the form of an additional driving force.

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