Phase-field-based package for effective material properties of arbitrary three-dimensional microstructures

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Introduction
A phase-field-based package is developed to study effective material properties of three-dimensional (3D) microstructures. It allows computation of various properties including elastic modulus, diffusivity, heat conductivity, electric conductivity, dielectric permittivity, piezoelectric coefficient, magnetic permeability, piezomagnetic coefficient, and magnetoelectric coupling coefficient, etc., of any arbitrary complex microstructure with given constituent phases and their properties. These effective properties are calculated through modeling a set of material variables responsive to various applied external fields, wherein the microstructure response coupled with a series of equilibrium equations are numerically solved using a well-established phase-field functions library.

Such a simple yet versatile phase-field-based package is not only useful for predicting the effective material properties of a non-homogeneous medium, but also provides full 3D distributions of stress, electric, magnetic, temperature, and concentration fields, and thus is helpful in designing complex materials with improved properties.

User interface
The user interface is designed that allows the user to finish the whole process of simulation within the software, from parameters input and initial structures check to running the simulation, and to visualization of output data.

User friendly parameter input windows, along with a wide range of visualization methods for post process, such as heat plot, isosurface, streamline, superquarticar glyph, etc., is provided in the user interface.

Example 1: Elastic properties of composites
The elastic system is modeled by solving the elastic equilibrium equation \( \nabla \cdot \sigma = 0 \) using the iterative perturbation method based on Khachaturyan’s microelasticity theory.

Example 2: Magnetoelectric composites
A system with coupled elastic, electric and magnetic field which is described using the constitutive equations

and is modeled through iteratively solving the coupled elastic, electrostatic and magnetostatic equilibrium equations

using the Fourier spectral iterative perturbation method.

Phase-field modeling fortran function library
A fortran function library is established for solving various equations and calculating various functions in the phase-field modeling. The functions use the FORTRAN 2003 standard and are compatible with the Message Passing Interface (MPI) standard.

Some of the functions in the phase-field library are listed as following:
- Cahn-Hillard (diffusion) equation solver
- Allen-Cahn type equation solver
- Landau-Lifshitz-Gilbert equation solver
- Elastic equilibrium solver for bulk and thin film
- Elastic energy calculation
- Electrostatic equilibrium poisson equation solver
- Electrostatic energy calculation
- Driving force calculation for ferroelectrics
- Magnetostatic equilibrium solver
- Spatial derivative calculation

Real time console output

Customize working directory

The hard particles show a larger stress response yet a smaller deformation compared to the soft matrix.