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.

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:

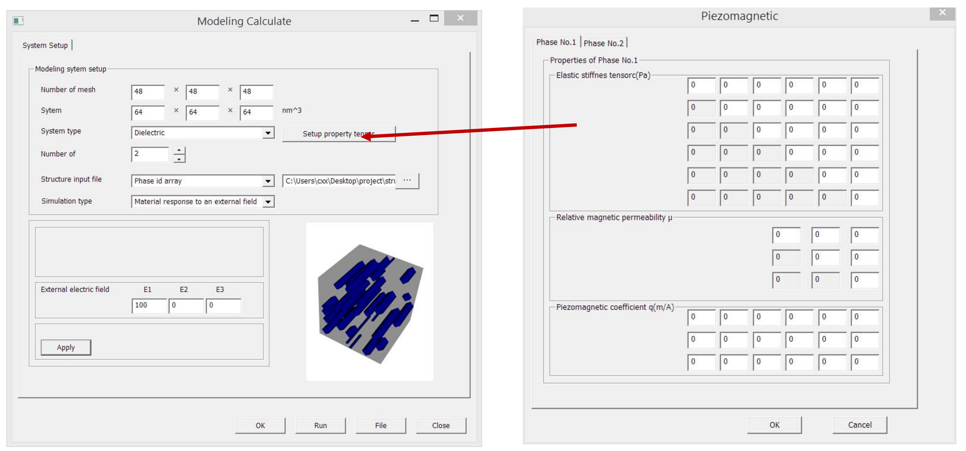
Cahn-Hillard (diffusion) equation solver
Allen-Cahn type equation solver
Landau-Lifshitz-Gilbert equation solver
Elastic equilibrium solver for bulk and thin film
Elastic energy calculation
Electrostatic equilibrium poisson equation solver
Driving force calculation for ferroelectrics
Magnetostatic equilibrium solver
Spatial derivative calculation

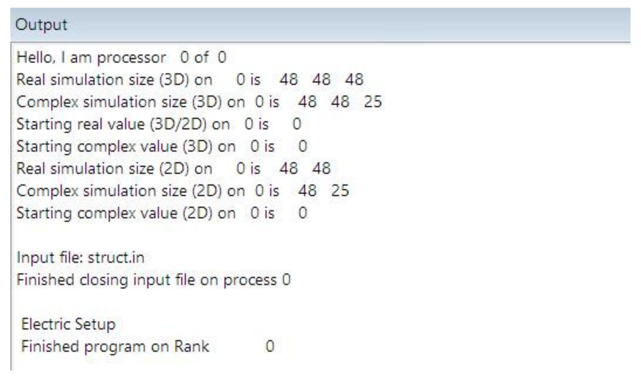
User interface

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.

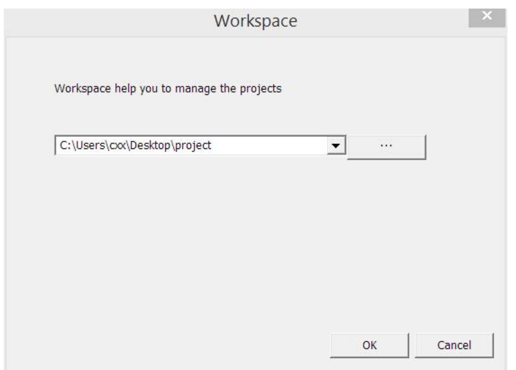
User friendly parameter input windows, along with a wide range of visualization methods for post process, such as heat plot, isosurface, streamline, superquaratic glyph, etc., is provided in the user interface.

Parameter input window

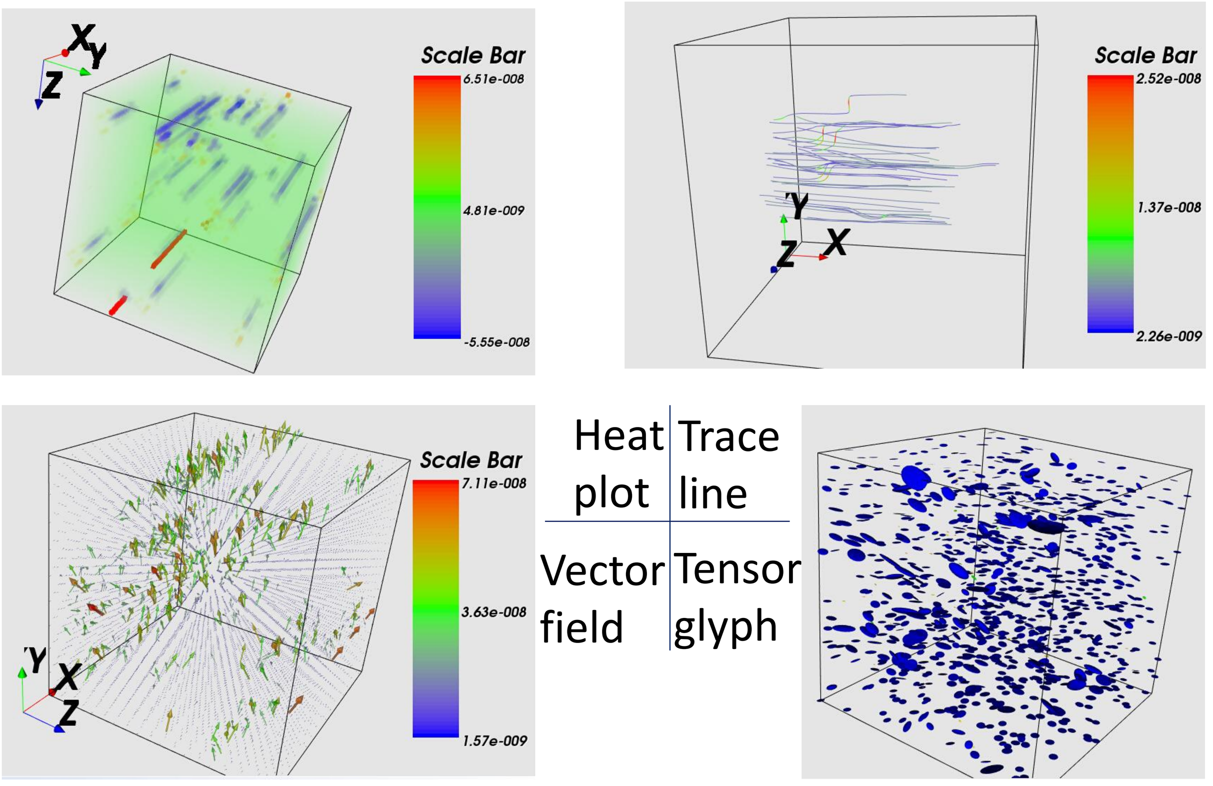




Real time console output

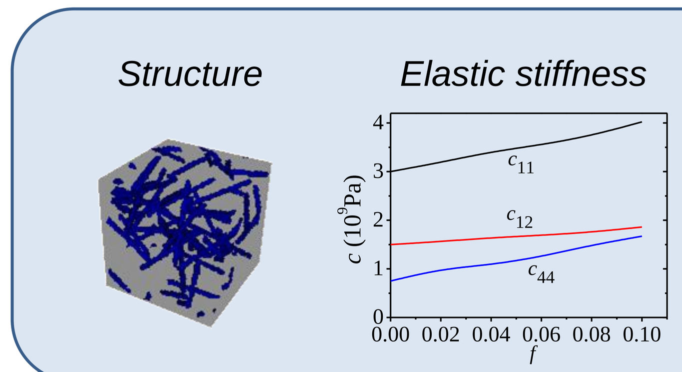


Customize working directory



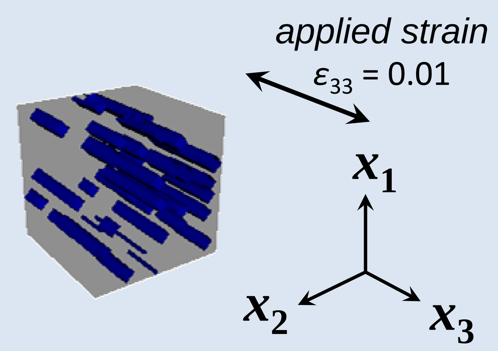
Example 1: Elastic properties of composites

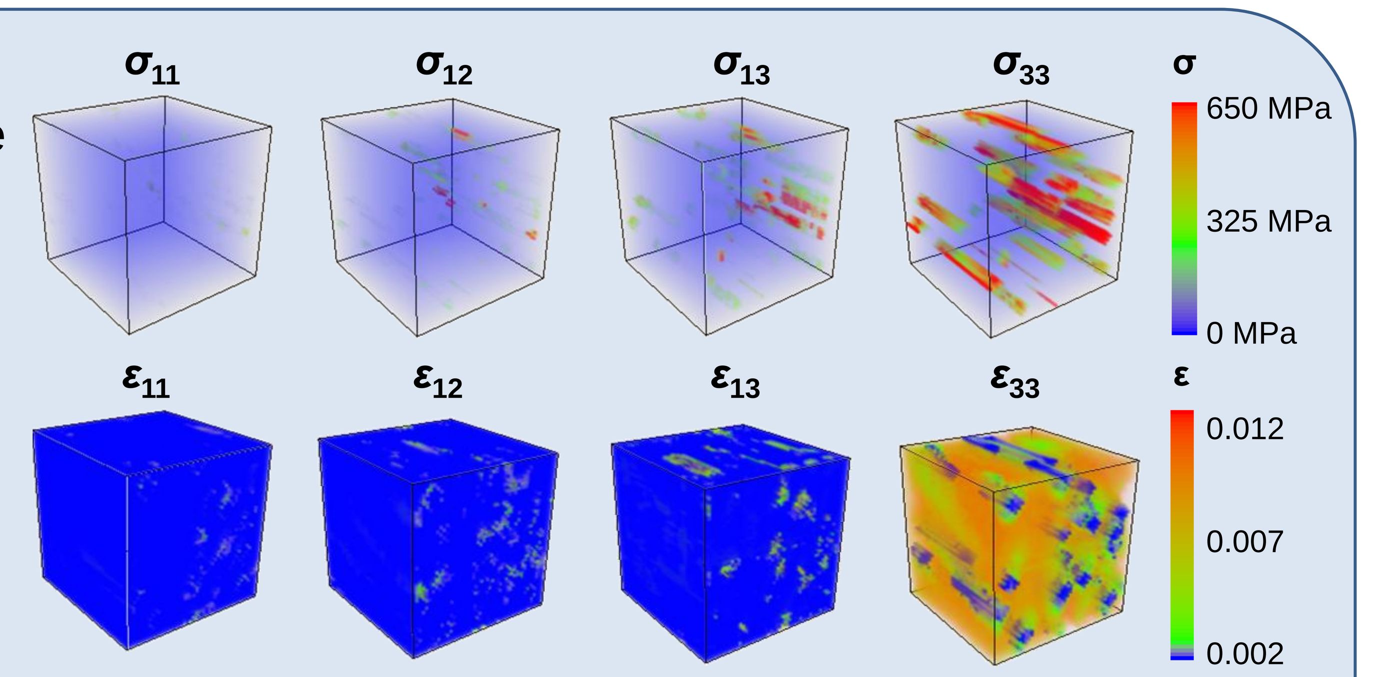
The elastic system is modeled by solving the elastic equilibrium equation $\nabla \cdot \boldsymbol{\sigma} = 0$ using the iterative perturbation method based on Khachaturyan's microelasticity theory.



Elastic stiffness of a composite with a soft matrix and hard secondary-phase particles with increasing volume fractions *f*.

Stress and strain distributions in a composite with an arbitrary structure where cylindrical hard particles are embedded in a soft matrix, upon applying a strain $\varepsilon = 0.01$





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

Example 2: Magnetoelectric composites

A system with coupled elastic, electric and magnetic field which is described using the constutive equations

$$\begin{pmatrix} \boldsymbol{\varepsilon} \\ \mathbf{D} \\ \mathbf{B} \end{pmatrix} = \begin{pmatrix} \mathbf{c}^{-1} & \mathbf{d}^T & \mathbf{q}^T \\ \mathbf{d} & \varepsilon_0 \boldsymbol{\kappa}_r & \boldsymbol{\alpha} \\ \mathbf{q} & \boldsymbol{\alpha}^T & \mu_0 \boldsymbol{\mu}_r \end{pmatrix} \begin{pmatrix} \boldsymbol{\sigma} \\ \mathbf{E} \\ \mathbf{H} \end{pmatrix}$$

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

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma} = 0, & \boldsymbol{\sigma} = \mathbf{c}\left(\boldsymbol{\varepsilon} - \left(\mathbf{d}^T \mathbf{E} + \mathbf{q}^T \mathbf{H}\right)\right) \\ \nabla \cdot \mathbf{D} = 0, & \mathbf{D} = \varepsilon_0 \boldsymbol{\kappa}_r \mathbf{E} + \mathbf{d}\boldsymbol{\sigma} + \boldsymbol{\alpha}\mathbf{E} \\ \nabla \cdot \mathbf{B} = 0, & \mathbf{B} = \mu_0 \boldsymbol{\mu}_r \mathbf{H} + \mathbf{q}\boldsymbol{\sigma} + \boldsymbol{\alpha}^T \mathbf{H} \end{cases}$$

using the Fourier spectral iterative perturbation method.

The influence of aspect ratios *r* of secondary-phase particles on the effective properties of a composite with 20vol% cylindrical secondary-phase $CoFe_2O_4$ magnetic particles embedded in a piezoelectric PZT matrix