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## Elastic solutions with arbitrary elastic inhomogeneity and anisotropy

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# Elastic solutions with arbitrary elastic inhomogeneity and anisotropy 

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#### Abstract

An efficient numerical algorithm is proposed to accurately compute the elastic fields in two-dimensional (2D) or three-dimensional (3D) microstructures with arbitrary elastic inhomogeneity and anisotropy. It combines the equivalent inclusion method of Eshelby, the microelasticity theory of Khachaturyan, and the spectral iterative perturbation method of Hu and Chen. Its efficiency is compared with those of existing approaches in the literature. The method can be conveniently implemented in phase-field modeling of stress-dependent microstructure evolution and/or of mass/ electrical transport.


Keywords: phase field microelasticity; equivalent inclusion method; spectral iterative perturbation; elasticity; simulation; mechanics

## 1. Introduction

Essentially, technologically important engineering materials are structurally inhomogeneous, containing defects such as voids and cracks, second-phase particles such as precipitates, compositional heterogeneities, or heterostructures of dissimilar materials. Very often, the inhomogeneous stress plays an important role in the microstructure evolution as well as the chemical and electrical transport processes. Therefore, our ability to efficiently compute the stress distribution is critical for accurately predicting the temporal stress-dependent three-dimensional (3D) microstructure evolution and transport processes.

A commonly used method for solving the elasticity equation is the finite element method (FEM) due to the availability of standard software packages as well as its ability to handle complicated boundary conditions. However, since the interfaces are moving during 3D microstructure evolution, FEM implementation requires constant re-meshing of the computational grid and hence is computationally intensive. Therefore, a number of numerical algorithms have been proposed for solving the mechanical equilibrium equation in structurally inhomogeneous solids [1-12].

[^0]For example, Leo et al. [13] and Zhu et al. [14] used the conjugate gradient method to solve the mechanical equilibrium equation for a solid with the elastic moduli varying linearly with composition field. Hu and Chen [11] developed a diffuse-interfacebased Fourier spectral iterative perturbation method (SIPM) in which the solutions to the mechanical equilibrium equation are computed to a desired accuracy by iterative refinements. It has been successfully applied to modeling spinodal decomposition [15], precipitate rafting [16], plastic deformation [17,18] and grain boundary migration in polycrystalline materials [19]. A similar method based on sharp-interface description was implemented by Moulinec and Suquet [5], Michel et al. [20] and Lebensohn [8], etc. Another approach is the phase-field microelasticity method [9,10] (PFMM) based on the equivalent eigenstrain concept introduced by Eshelby [1,21]. In this method, the strain energy of an elastically inhomogeneous solid is expressed as a functional of the equivalent eigenstrain field. The equivalent eigenstrain field is obtained by numerically solving the time-dependent GinzburgLandau equations. This method has been used to compute the stress distribution in solids containing voids and cracks and elastically inhomogeneous polycrystals.

In the present work, we propose a new method that combines the equivalent eigenstrain concept of Eshelby, the microelasticity theory of Khachaturyan, and the spectral iterative perturbation algorithm of Hu and Chen to solve the elasticity equation in elastically anisotropic and inhomogeneous systems. In particular, we first determine the displacement field and equivalent eigenstrain field by using the equivalent eigenstrain method and microelasticity theory and by assuming the equivalent eigenstrain is uniform within an inhomogeneity, or the uniform eigenstrain approximation (UEA). We then use obtained displacement field as the zeroth-order approximation for the spectral iterative perturbation method. We will simply name this new algorithm as SIPM + UEA. It should be noted that for a system containing a low volume fraction of ellipsoidal inhomogeneities, UEA solution is sufficient, and the proposed approach enjoys the same efficiency as elastically homogeneous systems.

In what follows, we outline a new procedure of calculating the displacement fields and equivalent eigenstrain fields directly using UEA and SIPM + UEA for arbitrary shaped inhomogeneities. Next, we compare the efficiencies and accuracies of SIPM, PFMM, and SIPM + UEA using simple examples and summarize our findings.

## 2. Methods

According to Eshelby, for an infinite, elastically isotropic system containing an ellipsoidal inhomogeneity, the distribution of eigenstrain fields is uniform inside the inhomogeneity when it is subjected to a uniform applied stress [1,22]. Willis [23] and Kinoshita and Mura [21] later showed that Eshelby's conclusion is also valid in elastically anisotropic systems. Following Wang et al., we consider an elastically anisotropic and elastically inhomogeneous body that is also structurally inhomogeneous and is characterized by a shape function,

$$
\theta(\mathbf{r})= \begin{cases}1 & \text { inside the inhomogeneity }  \tag{1}\\ 0 & \text { outside the inhomogeneity. }\end{cases}
$$

The coordinate-dependent elastic stiffness, $C_{i j k l}(\mathbf{r})$, can always be presented as $C_{i j k l}(\mathbf{r})=C_{i j k l}^{0}-\Delta C_{i j k l}(\mathbf{r})$, where $C_{i j k l}^{0}$ is a reference elastic stiffness, and $\Delta C_{i j k l}(\mathbf{r})$ is the variation from the reference value. The structural inhomogeneities are described by fixed crystal lattice misfit strain (stress-free strain or eigenstrain), $\varepsilon_{i j}^{*}(\mathbf{r})$. The idea of Eshelby's equivalent eigenstrain theory is to replace the inhomogeneous system with an elastically homogeneous system containing an equivalent inclusion with eigenstrain $\varepsilon_{i j}^{0}(\mathbf{r})$, which is non-zero inside the inclusion and zero outside the inclusion. Thus, Hooke's law yields:

$$
\begin{equation*}
C_{i j k l}^{0}\left(\varepsilon_{k l}(\mathbf{r})-\varepsilon_{k l}^{0}(\mathbf{r})\right)=\left(C_{i j k l}^{0}-\Delta C_{i j k l}(\mathbf{r})\right)\left(\varepsilon_{k l}(\mathbf{r})-\varepsilon_{k l}^{*}(\mathbf{r})\right) . \tag{2}
\end{equation*}
$$

Following Khachaturyan's microelasticity theory [24,25], the total strain $\varepsilon_{i j}(\mathbf{r})$ can be described by the sum of homogeneous strain $\bar{\varepsilon}_{i j}$ and heterogeneous strain $\delta \varepsilon_{i j}(\mathbf{r})$ or the sum of elastic strain $e_{i j}(\mathbf{r})$ and eigenstrain $\varepsilon_{k l}^{*}(\mathbf{r})$ :

$$
\begin{equation*}
\varepsilon_{i j}(\mathbf{r})=\bar{\varepsilon}_{i j}+\delta \varepsilon_{i j}(\mathbf{r})=e_{i j}(\mathbf{r})+\varepsilon_{i j}^{*}(\mathbf{r}) . \tag{3}
\end{equation*}
$$

For a macroscopically homogeneous body, the homogeneous strain (or the macroscopic strain) $\bar{\varepsilon}_{i j}$ is determined by the mechanical boundary conditions. For example, the homogeneous strain is equal to the applied strain in constrained systems, and for systems under a constant stress, the homogeneous strain is given by

$$
\begin{equation*}
\bar{\varepsilon}_{i j}=S_{i j k l}^{0} \sigma_{k l}^{\mathrm{app}}+\overline{\varepsilon_{i j}^{0}(\mathbf{r})} \tag{4}
\end{equation*}
$$

where $S_{i j k l}^{0}$ is the elastic compliance of the homogeneous matrix, $\sigma_{k l}^{\text {app }}$ is the external applied stress, $\overline{\varepsilon_{i j}^{0}(\mathbf{r})}$ is the volume average of the equivalent eigenstrain. The inhomogeneous strain $\delta \varepsilon_{i j}(\mathbf{r})$ can be expressed [24-26]:

$$
\begin{equation*}
\delta \varepsilon_{i j}(\mathbf{r})=\frac{1}{2} \int_{\mathbf{q} \neq 0} \frac{\mathrm{~d}^{3} q}{(2 \pi)^{3}}\left[n_{i} \Omega_{j p}(\mathbf{n})+n_{j} \Omega_{i p}(\mathbf{n})\right] C_{p q s t}^{0} \tilde{s}_{s t}^{0}(\mathbf{q}) n_{q} e^{i \mathbf{q} \cdot \mathbf{r}}, \tag{5}
\end{equation*}
$$

where $\tilde{\varepsilon}_{i j}^{0}(\mathbf{q})$ is the Fourier transform of the field $\varepsilon_{i j}^{0}(\mathbf{r}), \tilde{\varepsilon}_{i j}^{0}(\mathbf{q})=\int_{V} \varepsilon_{i j}^{0}(\mathbf{r}) e^{-l \mathbf{q} \cdot \mathbf{r}} \mathrm{~d}^{3} r \Omega_{i j}(\mathbf{n})$ is the Green's function tensor defined by the inverse of $\Omega_{i k}^{-1}(\mathbf{n})=C_{i j k l}^{0} n_{j} n_{l}$ with $\mathbf{n}=\mathbf{q} /|\mathbf{q}|$, and $\iota=\sqrt{-1}$ is the imaginary unit.

In order to obtain an analytical solution for $\varepsilon_{i j}^{0}(\mathbf{r})$, we assume it is uniform inside and zero outside the inclusions or

$$
\begin{equation*}
\varepsilon_{i j}^{0}(\mathbf{r})=\varepsilon_{i j}^{00} \theta(\mathbf{r}) \tag{6}
\end{equation*}
$$

where $\varepsilon_{i j}^{00}$ is a position-independent constant tensor. The Fourier transform of the eigenstrain $\varepsilon_{i j}^{0}(\mathbf{r})$ is given as

$$
\begin{equation*}
\tilde{\varepsilon}_{i j}^{0}(\mathbf{q})=\varepsilon_{i j}^{00} \int_{V} \theta(\mathbf{r}) e^{-\tau \mathbf{q} \cdot \mathbf{r}} d^{3} r=\varepsilon_{i j}^{00} \tilde{\theta}(\mathbf{q}) \tag{7}
\end{equation*}
$$

Substituting Equations (3)-(7) into Equation (2), and rearranging the terms yield

$$
\begin{equation*}
A_{i j s t} \varepsilon_{s t}^{00}=b_{i j}, \tag{8}
\end{equation*}
$$

where

$$
\begin{align*}
A_{i j s t} & =\Delta C_{i j k l}(\mathbf{r})\left(I_{k l s t} \overline{\theta(\mathbf{r})}+\frac{1}{2} C_{p q s t}^{0} \int_{\mathbf{q} \neq 0} \frac{\mathrm{~d}^{3} q}{(2 \pi)^{3}}\left[n_{k} \Omega_{l p}(\mathbf{n})+n_{l} \Omega_{k p}(\mathbf{n})\right] n_{q} \tilde{\theta}(\mathbf{q}) e^{\iota \mathbf{q} \cdot \mathbf{r}}\right)-C_{i j s t}^{0} \theta(\mathbf{r}), \\
b_{i j} & =\Delta C_{i j k l}(\mathbf{r})\left(\varepsilon_{k l}^{*}(\mathbf{r})-S_{k l m n}^{0} \sigma_{m n}^{\mathrm{app}}\right)-C_{i j k l}^{0} \varepsilon_{k l}^{*}(\mathbf{r}), \tag{9}
\end{align*}
$$

$I_{i j k l}$ is a fourth rank unit tensor, and $\overline{\theta(\mathbf{r})}$ is the volume averaged shape function representing the volume fraction of the inhomogeneities. Therefore, $\varepsilon_{s t}^{00}$ can be analytically obtained as $A_{i j s t}^{-1} b_{i j}$ where $A_{i j s t}^{-1}$ is the inverse of $A_{i j s t}$. For $\varepsilon_{s t}^{00}$ to be independent of position, $A_{i j s t}$ and $b_{i j}$ should be position independent within the inclusion. When the volume fraction of inhomogeneity is small and the shape of the inhomogeneity is ellipsoidal, $A_{i j s t}$ and $b_{i j}$ are independent of position within the inclusion provided the eigenstrain from structural inhomogeneity $\varepsilon_{k l}^{*}(\mathbf{r})$ is uniform within the inclusion. In this case, Equation (8) gives the exact solution to the mechanical equilibrium equation.

For arbitrary shaped inhomogeneities with large volume fraction, we propose to combine UEA and SIPM, i.e., using the uniform equivalent eigenstrain field $\varepsilon_{i j}^{0}(\mathbf{r})\left(=\varepsilon_{i j}^{00} \theta(\mathbf{r})\right)$ to obtain the zeroth-order displacement field for SIPM [24,25]:

$$
\begin{equation*}
\tilde{u}_{k}^{0}(\mathbf{q})=-\frac{\iota}{|\mathbf{q}|^{2}} \Omega_{i k}(\mathbf{n}) q_{j} \tilde{\sigma}_{i j}^{0}(\mathbf{q}) \tag{10}
\end{equation*}
$$

where $\sigma_{i j}^{0}(\mathbf{r})=C_{i j k l}^{0} \varepsilon_{k l l}^{0}(\mathbf{r}), \tilde{\sigma}_{i j}^{0}(\mathbf{q})$ is the Fourier transform of $\sigma_{i j}^{0}(\mathbf{r})$, and $C_{i j k l}^{0}$ is the elastic stiffness tensor of the homogeneous reference medium. SIPM is then used to iterate the displacement fields to obtain an accurate solution.

## 3. Results and discussion

To test the accuracy of the proposed new algorithm, we performed two-dimensional simulations in elastically inhomogeneous systems containing a cavity. In this case the elastic contrast is infinite since the elastic modulus of a cavity is zero. A computational domain containing $1024 \times 1024$ grid points is chosen. Periodic boundary conditions are imposed along $x$ - and $y$-directions. Plane strain assumption is used for the 2D simulations. We initially consider a particular elliptical inhomogeneity with eccentricity zero embedded in a square domain subjected to a specified uniaxial stress along the $y$-axis (Figure 1a). The faces perpendicular to the $x$-axis are stress free. In order to compare with analytical solutions, we assume the surrounding domain to be elastically isotropic with a Poisson's ratio of 0.3.

To alleviate Gibbs effect in Fourier transforms in the spectral method arising from a sharp interface, we introduced a diffuse-interface shape function in the following form:

$$
\begin{equation*}
\theta(\mathbf{r})=\frac{1}{2}\left\{1.0-\tanh \left[\beta\left(d(\mathbf{r})-d_{0}(\mathbf{r})\right)\right]\right\}, \tag{11}
\end{equation*}
$$

where $d(\mathbf{r})$ is the distance of any point $(x, y)$ from the center of the ellipse, $d_{0}(\mathbf{r})$ denotes the length of the line segment drawn from the center to the surface, $\beta$ is a positive parameter controlling the width of the surface.


Figure 1. (a) Schematic of a 2D domain containing a circular cavity subjected to uniaxial applied stress along the $y$-axis. The faces perpendicular to $x$-axis are stress free. $R$ is the radius of the circular cavity. (b) Displacement error and iteration steps curves calculated from SIPM and PFMM methods. Normalized stress distributions along (c) A-A and (d) B-B sections calculated from PFMM, SIPM, and UEA comparing with ANA.

We first compare the efficiencies of two existing techniques: SIPM and PFMM. Figure 1b shows the number of iterations required for a particular relative displacement error in SIPM and PFMM for the case of a circular cavity. The relative displacement error was calculated using the following definition:

$$
\begin{equation*}
\text { Relative error } \zeta=\frac{\sum_{\mathbf{r}} \sqrt{\left(u_{x}^{n}(\mathbf{r})-u_{x}^{\mathrm{accu}}(\mathbf{r})\right)^{2}+\left(u_{y}^{n}(\mathbf{r})-u_{y}^{\mathrm{accu}}(\mathbf{r})\right)^{2}+\left(u_{z}^{n}(\mathbf{r})-u_{z}^{\mathrm{accu}}(\mathbf{r})\right)^{2}}}{\sum_{\mathbf{r}} \sqrt{\left(u_{x}^{\mathrm{accu}}(\mathbf{r})\right)^{2}+\left(u_{y}^{\mathrm{accu}(\mathbf{r}))^{2}+\left(u_{z}^{\mathrm{accu}}(\mathbf{r})\right)^{2}}\right.}, \text {, }, \text {, }, \text {. }{ }^{2}} \tag{12}
\end{equation*}
$$

where $u_{i}^{n}$ is the displacement solution of the $n$th iteration, and $u_{i}^{\text {accu }}$ is the achievable most "accurate" displacement solution for a particular technique. Theoretically, the


Figure 2. (a) Schematic of a 2D domain containing a square cavity subjected to uniaxial applied stress along the $y$-axis. The faces perpendicular to $x$-axis are stress free. $2 a$ is the side length of the square cavity. (b) Displacement error and iteration steps curves calculated from SIPM, UEA + SIPM, PFMM, and UEA + PFMM methods. (c), (d) Normalized stress distributions along A-A and B-B sections calculated from UEA + PFMM and UEA + SIPM.
final converged results for PFMM and SIPM should be the same, but they converge to slightly different final displacement distributions. Therefore, for each method, we use its own final converged solution as the reference to calculate the displacement error. In order to remove the effect of iterative time interval $\Delta t$ in PFMM on the comparison result, the maximal $\Delta t$ was used to promise the convergence. In our simulation, the computational times of each iterative step for PFMM and SIPM are nearly the same, thus the number of iterative steps to a given relative error reflects the convergent speed. It is shown that SIPM converges faster than PFMM in Figure $1 \mathrm{~b}-\mathrm{d}$ show the computed normalized elastic stress distribution along the A-A and B-B sections. The computed stress fields by SIPM, PFMM, and UEA are compared with the analytical solution (ANA). One can see that the computed profiles from SIPM, PFMM, and UEA method show excellent agreement among each other and are slightly different from the analytical solution. The difference between the numerical solutions and the analytical solution stems from the fact that


Figure 3. (a) Elastic strain energy calculation for the circular cavity, including the total energy by SIPM and PFMM, the elastic energy in the cavity domain $E^{\mathrm{el}}\left(\mathbf{r}_{\mathrm{D}}\right)$ by PFMM. (b) Energy calculation for the square cavity, including the total energy by SIPM, UEA + SIPM, PFMM and UEA + PFMM, the elastic energy in the cavity domain $E^{\mathrm{el}}\left(\mathbf{r}_{\mathrm{D}}\right)$ by PFMM and UEA + PFMM.
all the numerical solutions were obtained with periodic boundary conditions with a diffuse-interface description for the cavity surface while the analytical solution is for ideally circular cavity in an infinite matrix with a sharp-interface description.

The excellent agreement between SIPM and UEA or PFMM and UEA implies that UEA provides an excellent solution for systems containing ellipsoidal inhomogeneities. When the geometry of the inhomogeneity is non-ellipsoidal, we argue that the UEA solution can be a good initial guess for SIPM and PFMM.

We compare the computational efficiencies of (UEA + SIPM) and (UEA + PFMM) algorithms with those of the existing PFMM and SIPM techniques for the case of the system containing a square cavity as an example. The iteration time required for convergence is plotted for each method as a function of accuracy of the solutions in Figure 2b. It is obvious that both the computational efficiencies are improved by employing the displacement solution and equivalent eigenstrain from UEA method as zeroth order displacement field in SIPM and initial eigenstrain field in PFMM, respectively. The improvement is obvious when the relative error is lower than $1 \%$, which is sufficient for a good approximation. It should be noted that the most efficient method for this particular case is (UEA + SIPM), and it is followed by SIPM, UEA + PFMM, and PFMM. Figure 2c and d show the computed normalized elastic stress distribution along the A-A and B-B sections. The stress fields from (UEA + SIPM ) and (UEA + PFMM) agree extremely well with each other.

In order to further elucidate the convergence of our developed methods, the elastic strain energy changes as a function of iterations are calculated using both methods for the systems discussed above. We use $\Delta E=E^{n}-E^{\infty}$ to show the energy convergence, where $E^{n}$ denotes the total elastic strain energy of the system in $n$th iteration and $E^{\infty}$ means the total energy of the final iteration. Figure 3a shows that SIPM converges faster than PFMM for total energy calculation. Also the elastic strain energy in the inhomogeneous domain calculated by PFMM decreases and becomes stable with iteration increasing because for inhomogeneity of cavity the equivalent eigenstrain field is evolved by minimizing the elastic energy only in the inhomogeneous domain [27,28]. In addition, the iterations converge faster when the solutions from UEA are employed as zeroth-order displacement field and initial eigenstrain field in SIPM and PFMM, respectively, as shown in Figure 3b.

## 4. Summary

In summary, we developed a new UEA algorithm based on Khachaturyan's microelasticity theory to analytically obtain the elastic solution for system containing ellipsoidal inhomogeneities of small volume fraction. By combining UEA with SIPM or PFMM, the computational efficiency is greatly improved for solving the mechanical equilibrium equation in elastically inhomogeneous systems containing arbitrary shaped inhomogeneities of arbitrary volume fractions. By comparing the efficiencies of SIPM, PFMM, (UEA + SIPM), and (UEA + PFMM), we found that $($ UEA + SIPM $)$ is the most efficient way to compute the elastic solution in elastically inhomogeneous systems. Even if the methods have been applied to two-dimensional (2D) systems in this work, the methods can be generally applied to three-dimensional (3D) systems. Since UEA is an analytical procedure to calculate the initial guess for the displacement fields, subsequent iterations in SIPM do not depend on the choice of the homogeneous reference medium.

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