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Variational bounds for thermal fields in media with heterogeneous microstructure

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Abstract
This work develops a rigorous variational upper bound for the difference between thermal fields generated in uniform media and thermal fields generated in heterogeneous media, for the same external loading. The bound can be calculated in a simple manner, with knowledge only of the heterogeneous material properties and a relatively easy-to-compute thermal field associated with a uniform medium. In order to evaluate the bound, the difficult-to-compute thermal field, associated with the heterogeneous material, does not need to be calculated. Three-dimensional numerical examples are provided to illustrate the results.

Keywords
Heterogeneous media, thermal fields, variational bounds.

1. Introduction

New materials having complex microstructures and experiencing thermal loading are widespread, particularly due to the huge rise in photovoltaics, thermoelectric converters, thermal barrier coatings, and microelectronic devices. Many of these materials possess heterogeneous, unstructured microstructures, for example stemming from material processing impurities (such as precipitates) or due to intentional particulate-doping of a base medium in order to produce desired "functionalized" overall conductive properties. By mathematical construction, via homogenization methods, the overall properties are uniform. Usually, in macroscale analyses, the overall material properties are used, which leaves open questions on the behavior of true fields at microscale. In many cases, the microscopic fields generated in heterogeneous media dictate the start of material failure at macroscale. Analytical and semi-analytical methods have a long history and are invaluable in estimating the effective overall properties of media with a heterogeneous microstructure. See, for example, Maxwell [1, 2], Lord Rayleigh [3], Torquato [4], Jikov et al. [5], Hashin [6], Mura [7], Nemat-Nasser and Hori [8], and Huet [9, 10]. However, the objectives of those works are not the determination of the microscopic fields generated in heterogeneous media. In some cases, numerical methods, which attempt to spatially discretize the microstructure, for example using the Finite Element or Finite Difference methods, can capture the microscopic fields. However, it is at enormous computational expense. For overviews, see Ghosh [11], Ghosh and Dimiduk [12], Zohdi and Wriggers [13], and Zohdi [14].

The objective of this work is to develop a rigorous, easy-to-compute variational upper bound for the difference between the fields generated in uniform media and the fields generated in heterogeneous, unstructured media, for the same external loading. Importantly, the developed bound *avoids direct calculation of the fields*

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associated with the heterogeneous material and the huge associated computational effort. Numerical examples are given to illustrate the results.

2. The mathematical setting

2.1. Two representations of a material

We consider two realizations of a material (smooth and heterogeneous) used in the same boundary-value problem (BVP).

- A BVP using an idealized conductivity tensor $\mathbb{K}^0$ that is a constant, symmetric, bounded and positive-definite tensor-valued function:

$$\nabla \cdot (\mathbb{K}^0 \cdot \nabla \theta^0) + f = 0, \tag{1}$$

  with a boundary condition on the flux-specified portion of the boundary (Γ_f) being $\boldsymbol{Q}^0 = -\mathbb{K}^0 \cdot \nabla \theta^0 = \boldsymbol{Q}^*$ and a boundary condition on the temperature-specified portion of the boundary (Γ_θ) being $\theta = \theta^*$.
- A BVP using a conductivity tensor $\tilde{\mathbb{K}}$ that is a spatially varying symmetric bounded positive-definite tensor-valued function:

$$\nabla \cdot (\tilde{\mathbb{K}} \cdot \nabla \tilde{\theta}) + f = 0, \tag{2}$$

  with a boundary condition on the flux-specified portion of the boundary (Γ_f) being $\tilde{\boldsymbol{Q}} = -\tilde{\mathbb{K}} \cdot \nabla \tilde{\theta} = \boldsymbol{Q}^*$ and a boundary condition on the temperature-specified portion of the boundary (Γ_θ) being $\tilde{\theta} = \theta^*$.

2.2. Bounding objective

It should be clear that the field associated with the uniform material is relatively easy to compute and the field associated with the heterogeneous material is virtually impossible to compute analytically and extremely difficult to compute numerically, since one needs a spatial mesh resolution that is extremely fine in order to capture the material heterogeneities and the associated thermal field. The objective is to develop a normalized bound, denoted Λ, only in terms of the easy-to-compute temperature field associated with the uniform medium:

$$\frac{||\tilde{\theta} - \theta^0||}{||\theta^0||} \leq \Lambda(\theta^0). \tag{3}$$

The mathematical tools will involve variational methods, next.

3. Variational (weak) formulations

The solution to the uniform, constant-coefficient problem, denoted θ^0, is characterized by the following weak formulation of equation (1):

$$\boxed{\begin{array}{l} \text{Find } \theta^0 \in H^1(\Omega), \theta^0|_{\Gamma_\theta} = \theta^*, \quad \text{such that} \\ \displaystyle\int_\Omega \nabla v \cdot \boldsymbol{Q}^0 \, d\Omega = \int_\Omega f \cdot v \, d\Omega + \int_{\Gamma_f} \boldsymbol{Q}^* \cdot \boldsymbol{n} v \, dA \qquad \forall v \in H^1(\Omega), v|_{\Gamma_\theta} = 0, \end{array}} \tag{4}$$

where v is a test function and $H^1(\Omega)$ is a standard Hilbert space.

The solution corresponding to the nonconstant, heterogeneous coefficient problem, denoted $\tilde{\theta}$, is characterized by the following weak formulation of equation (2):

$$
\boxed{\begin{array}{l}\text{Find } \tilde{\theta} \in H^1(\Omega), \tilde{\theta}|_{\Gamma_\theta} = \theta^*, \quad \text{such that} \\ \displaystyle\int_\Omega \nabla v \cdot \tilde{\boldsymbol{Q}}\, d\Omega = \int_\Omega fv\, d\Omega + \int_{\Gamma_f} \boldsymbol{Q}^* \cdot \boldsymbol{n} v\, dA \qquad \forall v \in H^1(\Omega), v|_{\Gamma_\theta} = 0.\end{array}} \tag{5}
$$

4. Variational bounds

We have, for any admissible function, $w \in H^1(\Omega)$ and $w = \theta^*$ on Γ_θ, a definition of the primal energy norm

$$
0 \leq ||\theta - w||^2_{K(\Omega)} = \int_\Omega (\nabla\theta - \nabla w) \cdot \tilde{\mathbb{K}} \cdot (\nabla\theta - \nabla w)\, d\Omega. \tag{6}
$$

From equations (4) and (5), we have

$$
\int_\Omega \nabla v \cdot \tilde{\mathbb{K}} \cdot \nabla\tilde{\theta}\, d\Omega = \int_\Omega \nabla v \cdot \mathbb{K}^0 \cdot \nabla\theta^0\, d\Omega = \int_\Omega fv\, d\Omega + \int_{\Gamma_f} \tilde{\boldsymbol{Q}} \cdot \boldsymbol{n} v\, dA. \tag{7}
$$

Subtracting $\int_\Omega \nabla v \cdot \tilde{\mathbb{K}} \cdot \nabla\theta^0\, d\Omega$ from both sides yields

$$
\int_\Omega \nabla v \cdot \tilde{\mathbb{K}} \cdot \nabla(\tilde{\theta} - \theta^0)\, d\Omega = \int_\Omega \nabla v \cdot (\mathbb{K}^0 \cdot \nabla\theta^0 - \tilde{\mathbb{K}} \cdot \nabla\theta^0)\; d\Omega. \tag{8}
$$

Since v is an arbitrary virtual temperature field , we may set $v = \tilde{\theta} - \theta^0$ to yield

$$
\begin{aligned}
||\tilde{\theta} - \theta^0||^2_{K(\Omega)} &= \int_\Omega \nabla(\tilde{\theta} - \theta^0) \cdot (\mathbb{K}^0 \cdot \nabla\theta^0 - \tilde{\mathbb{K}} \cdot \nabla\theta^0)\; d\Omega \\
&= \int_\Omega (\tilde{\mathbb{K}}^{\frac{1}{2}} \cdot \nabla(\tilde{\theta} - \theta^0)) \cdot \tilde{\mathbb{K}}^{\frac{1}{2}} \cdot \tilde{\mathbb{K}}^{-1} \cdot ((\mathbb{K}^0 - \tilde{\mathbb{K}}) \cdot \nabla\theta^0)\; d\Omega \\
&\leq \underbrace{\left(\int_\Omega \nabla(\tilde{\theta} - \theta^0) \cdot \tilde{\mathbb{K}} \cdot \nabla(\tilde{\theta} - \theta^0)\; d\Omega\right)^{\frac{1}{2}}}_{||\tilde{\theta} - \theta^0||_{K(\Omega)}} \\
&\quad \times \left(\int_\Omega ((\mathbb{K}^0 - \tilde{\mathbb{K}}) \cdot \nabla\theta^0) \cdot \tilde{\mathbb{K}}^{-1} \cdot ((\mathbb{K}^0 - \tilde{\mathbb{K}}) \cdot \nabla\theta^0)\, d\Omega\right)^{\frac{1}{2}}.
\end{aligned} \tag{9}
$$

Therefore, the upper bound is

$$
||\tilde{\theta} - \theta^0||^2_{K(\Omega)} \leq \int_\Omega ((\mathbb{K}^0 - \tilde{\mathbb{K}}) \cdot \nabla\theta^0) \cdot \tilde{\mathbb{K}}^{-1} \cdot ((\mathbb{K}^0 - \tilde{\mathbb{K}}) \cdot \nabla\theta^0)\, d\Omega \stackrel{\text{def}}{=} \Lambda(\theta^0). \tag{10}
$$

To derive this result, we used the Cauchy–Schwarz inequality and the fact that a symmetric positive-definite matrix has a unique square root, $\tilde{\mathbb{K}} = \tilde{\mathbb{K}}^{\frac{1}{2}} \cdot \tilde{\mathbb{K}}^{\frac{1}{2}}$. Note that the Λ bound depends only on $\mathbb{K}^0$, $\tilde{\mathbb{K}}$, and θ^0. Early variants of this class of bound for more structured elastic media can be found in Zohdi [15] and Zohdi et al. [16].

5. A numerical example: A special case

Let us consider a special case, where we decompose $\tilde{\mathbb{K}}$ into

$$
\tilde{\mathbb{K}} = \mathbb{K}^0 + \Delta\mathbb{K}^0(\boldsymbol{x}) = \mathbb{K}^0 \cdot (\mathbf{1} + \boldsymbol{B}(\boldsymbol{x})), \tag{11}
$$

where $\Delta\mathbb{K}^0(\boldsymbol{x}) = \mathbb{K}^0 \cdot \boldsymbol{B}(\boldsymbol{x})$ represents the degree of heterogeneity of the material. By construction, $\tilde{\mathbb{K}} = \mathbb{K}^0 \cdot (\mathbf{1} + \boldsymbol{B}(\boldsymbol{x}))$ is symmetric and positive definite. Inserting this expression into equation (10) yields

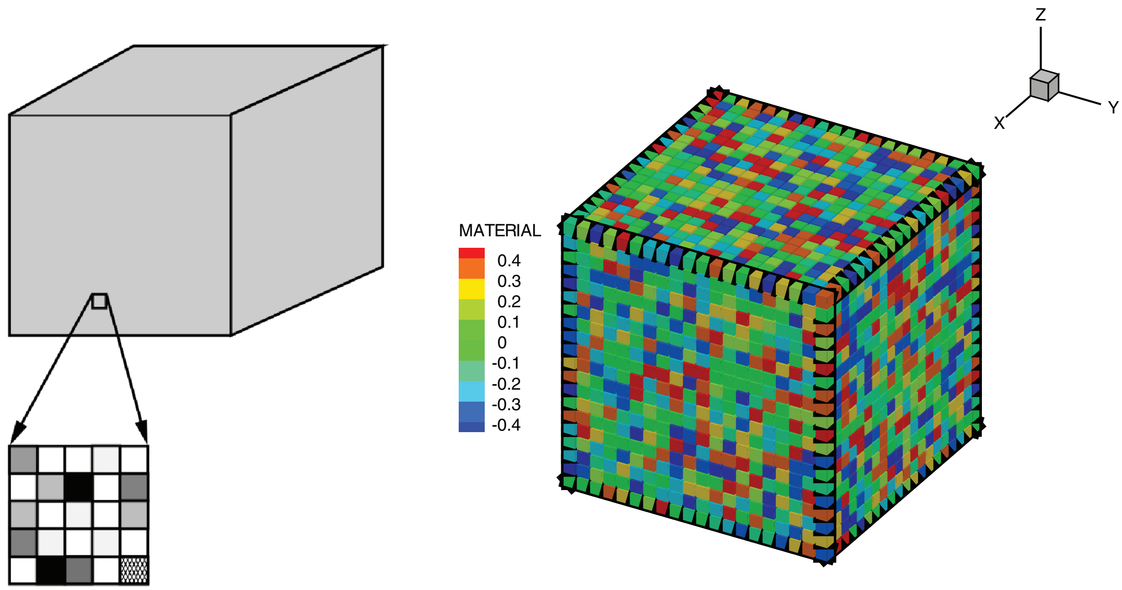

Figure 1. Left: A schematic three-dimensional cubical domain composed of a $200 \times 200 \times 200$ array of eight million heterogeneous sub-blocks which are perfectly bonded together. The variation from sub-block to sub-block was dictated by $\beta(\boldsymbol{x})$, which was chosen to be between $-1 < -\gamma \leq \beta(\boldsymbol{x}) \leq \gamma < 1$. Right: A $20 \times 20 \times 20$ portion (one-thousandth of the volume) of the domain for $\gamma = 0.4$. The color coding illustrates a normalized deviation from a mean conductivity value.

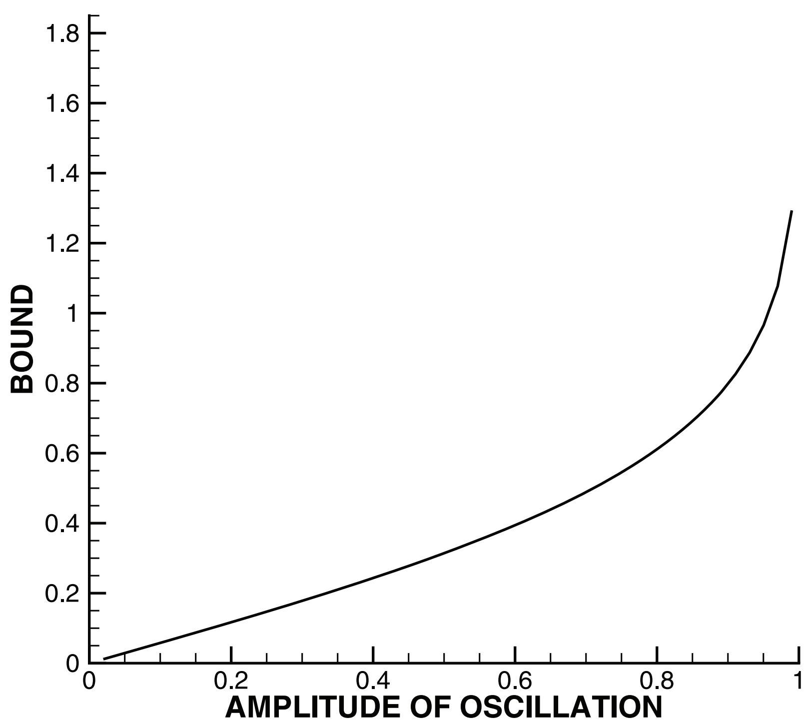

Figure 2. The behavior of the normalized, nondimensional bound $\hat{\Lambda}(\theta^0)$ for increasing amplitude limits (γ), for the three-dimensional cubical domain.

$$||\tilde{\theta} - \theta^0||^2_{K(\Omega)} \leq \int_\Omega (\mathbb{K}^0 \cdot (\boldsymbol{B}(\boldsymbol{x}) \cdot \nabla\theta^0)) \cdot \left(\mathbb{K}^0 \cdot (\mathbf{1} + \boldsymbol{B}(\boldsymbol{x}))\right)^{-1} \cdot (\mathbb{K}^0 \cdot (\boldsymbol{B}(\boldsymbol{x}) \cdot \nabla\theta^0))\, d\Omega. \tag{12}$$

As a further restricted special case, let us assume a type of (isotropic) heterogeneity (operating on the diagonal of the conductivity, $\mathbb{K}^0$) of the form

$$\mathbf{1} + \boldsymbol{B}(\boldsymbol{x}) = (1 + \beta(\boldsymbol{x}))\mathbf{1}, \tag{13}$$

where $-1 < \beta(\boldsymbol{x}) < 1$. Equation (12) then collapses to

$$||\tilde{\theta} - \theta^0||^2_{K(\Omega)} \leq \int_\Omega \nabla\theta^0 \cdot \mathbb{K}^0 \cdot \nabla\theta^0 \left(\frac{\beta(\boldsymbol{x})^2}{1 + \beta(\boldsymbol{x})} \right) d\Omega. \tag{14}$$

Furthermore, let us consider a scenario where the solution to the uniform material problem (θ^0) is a linear thermal field (with a constant temperature gradient, $\nabla\theta^0$). Because $\mathbb{K}^0$ is constant, equation (12) becomes

$$\frac{||\tilde{\theta} - \theta^0||^2_{K(\Omega)}}{||\theta^0||^2_{K^0(\Omega)}} \leq \frac{1}{|\Omega|} \int_\Omega \left(\frac{\beta(\boldsymbol{x})^2}{1 + \beta(\boldsymbol{x})} \right) d\Omega, \tag{15}$$

where $||\theta^0||^2_{K^0(\Omega)} = \nabla\theta^0 \cdot \mathbb{K}^0 \cdot \nabla\theta^0 |\Omega|$, $|\Omega|$ being the volume associated with the domain Ω. Finally, taking the square root of both sides yields the desired normalized, nondimensional bound:

$$\frac{||\tilde{\theta} - \theta^0||_{K(\Omega)}}{||\theta^0||_{K^0(\Omega)}} \leq \sqrt{\frac{1}{|\Omega|} \int_\Omega \left(\frac{\beta(\boldsymbol{x})^2}{1 + \beta(\boldsymbol{x})} \right) d\Omega} \stackrel{\text{def}}{=} \hat{\Lambda}(\theta^0). \tag{16}$$

As a numerical example, a cubical domain was selected, with a heterogeneous microstructure comprised of a $200 \times 200 \times 200$ array of heterogeneous, uncorrelated, sub-blocks (eight million in total), which are perfectly bonded together (Figure 1). For each sub-block, a random value of β (dictating a material mismatch) was chosen to be between $-1 < -\gamma \leq \beta \leq \gamma < 1$, where γ is an amplitude limit for $\beta(\boldsymbol{x})$. The normalized, nondimensional $\hat{\Lambda}(\theta^0)$ bound values for increasing amplitude limits (the horizontal axis, γ) are shown in Figure 2. For this example, $\hat{\Lambda}(\theta^0)$ exhibits virtually linear behavior for small values of $-\gamma \leq \beta(\boldsymbol{x}) \leq \gamma$, with superlinear growth at higher values of γ. Of course, this trend is dependent on the type of microstructure involved and the external loading. Generally, however, one can expect the difference in the fields to grow with increasing heterogeneity.

6. Summary

As indicated at the outset, new materials with heterogeneous, potentially unstructured microstructures are now widely used in high-tech applications. The result of this analysis was that the difference in thermal fields generated by heterogeneous media and uniform media can be quantified in a straightforward manner, with knowledge of only a (relatively) easy-to-compute thermal field associated with a uniform material, and the heterogeneous material properties. The extremely difficult-to-compute thermal field associated with the heterogeneous material does not need to be determined. The developed upper bound provides analysts with a quantitative, easy-to-compute way to characterize the effects of material heterogeneity which, in many cases, dictates the start of material failure at the macroscale. Finally, we remark that the analysis can be repeated in a virtually identical manner to bound displacement fields in elastic media possessing heterogeneous microstructures.

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Conflict of interest

None declared.

References

[1] Maxwell, JC. On the dynamical theory of gases. *Philos Trans Soc London* 1867; 157: 49.

[2] Maxwell, JC. *A treatise on electricity and magnetism.* 3rd edn. Oxford: Clarendon Press, 1873.

[3] Rayleigh, JW. On the influence of obstacles arranged in rectangular order upon properties of a medium. *Phil Mag* 1892; 32: 481–491.
[4] Torquato, S. *Random heterogeneous materials: Microstructure and macroscopic properties*. New York: Springer-Verlag, 2002.
[5] Jikov, VV, Kozlov, SM, and Olenik, OA. *Homogenization of differential operators and integral functionals.* Berlin: Springer-Verlag, 1994.
[6] Hashin, Z. Analysis of composite materials: A survey. *ASME J Appl Mech* 1983; 50: 481–505.
[7] Mura, T. *Micromechanics of defects in solids*. 2nd edn. Dordrecht: Kluwer Academic Publishers, 1993.
[8] Nemat-Nasser, S, and Hori, M. *Micromechanics: Overall properties of heterogeneous solids.* 2nd edn. Amsterdam: Elsevier, 1999.
[9] Huet, C. Universal conditions for assimilation of a heterogeneous material to an effective medium. *Mech Res Commun* 1982; 9(3): 165–170.
[10] Huet, C. On the definition and experimental determination of effective constitutive equations for heterogeneous materials. *Mech Res Commun* 1984 11(3): 195–200.
[11] Ghosh, S. *Micromechanical analysis and multi-scale modeling using the Voronoi cell finite element method.* Boca Raton, FL: CRC Press/Taylor & Francis, 2011.
[12] Ghosh, S, and Dimiduk, D. *Computational methods for microstructure-property relations.* New York: Springer, 2011.
[13] Zohdi, TI, and Wriggers, P. *Introduction to computational micromechanics.* Berlin: Springer-Verlag, 2008.
[14] Zohdi, TI. *Electromagnetic properties of multiphase dielectrics: A primer on modeling, theory and computation.* Berlin: Springer-Verlag, 2012.
[15] Zohdi, TI. Statistical ensemble error bounds for homogenized microheterogeneous solids. *Z Angew Math Phys* 2005; 56(3): 497–515.
[16] Zohdi, TI, Oden, JT, and Rodin, GJ. Hierarchical modeling of heterogeneous bodies. *Comput Meth Appl Mech Eng* 1996; 138: 273–298.