International Journal of Fracture **114:** L15–L20, 2002.

ON THE TAILORING OF MICROSTRUCTURES FOR PRESCRIBED EFFECTIVE PROPERTIES

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Abstract. The focus of this communication is the development of genetic algorithms to handle material design problems where particulate microstructures are sought which deliver prescribed effective responses. In the problem formulation, constraints are incorporated on the distortion of the otherwise smooth internal fields corresponding to a pure (inhomogeneity-free) matrix material, due to the presence of particles. The key conceptual feature is that the microstructural variables are represented by a "genetic string", and a "survival of the fittest" algorithm is applied to a population of such strings in order to determine an optimal set of microstructural material design parameters.

1. Introduction. Materials with tailored microstructures consisting of randomly distributed particles suspended in a binding matrix are now widely employed in structural designs. We refer the reader to Torquato [21] for recent surveys. The microscale mechanical properties of such materials are characterized by a spatially variable elasticity tensor $\mathbb{E}$, while the effective macroscopic response is characterized by $\langle \boldsymbol{\sigma} \rangle_\Omega = \mathbb{E}^* : \langle \boldsymbol{\epsilon} \rangle_\Omega$, where $\langle \cdot \rangle_\Omega \stackrel{\text{def}}{=} \frac{1}{|\Omega|} \int_\Omega \cdot \, d\Omega$, and where $\boldsymbol{\sigma}$ and $\boldsymbol{\epsilon}$ are the stress and strain tensor fields within a statistically representative volume element (RVE) of volume $|\Omega|$. Direct numerical simulation to determine $\mathbb{E}^*$ is computationally enormous, due to the fact that the microstructure must be resolved by the discretization mesh. Therefore, it is advantageous to use analytical effective property approximations during the initial stages of the design and development of new tailored solids. Such approximate methods require minimal computational effort, thus allowing one to perform rapid analyses for large numbers of multiphase solid combinations controlling parameters such as the constituent volume fractions and phase contrasts. Afterwards, when the number of feasible microstructural design combinations have been sufficiently narrowed down, one can perform further indepth studies, applying computationally intensive numerical simulations, or more involved laboratory tests, to a reduced set of design alternatives. As an example, consider the widely used Hashin and Shtrikman bounds [9], [10], for isotropic materials with isotropic effective responses

$$\boxed{\begin{array}{l} \kappa^{*,-} \stackrel{\text{def}}{=} \kappa_1 + \dfrac{v_2}{\frac{1}{\kappa_2-\kappa_1} + \frac{3(1-v_2)}{3\kappa_1+4\mu_1}} \leq \kappa^* \leq \kappa_2 + \dfrac{1-v_2}{\frac{1}{\kappa_1-\kappa_2} + \frac{3v_2}{3\kappa_2+4\mu_2}} \stackrel{\text{def}}{=} \kappa^{*,+}, \\ \mu^{*,-} \stackrel{\text{def}}{=} \mu_1 + \dfrac{v_2}{\frac{1}{\mu_2-\mu_1} + \frac{6(1-v_2)(\kappa_1+2\mu_1)}{5\mu_1(3\kappa_1+4\mu_1)}} \leq \mu^* \leq \mu_2 + \dfrac{(1-v_2)}{\frac{1}{\mu_1-\mu_2} + \frac{6v_2(\kappa_2+2\mu_2)}{5\mu_2(3\kappa_2+4\mu_2)}} \stackrel{\text{def}}{=} \mu^{*,+}, \end{array}} \tag{1}$$

where κ_2 and κ_1 are the bulk moduli and μ_2 and μ_1 are the shear moduli of the respective phases ($\kappa_2 \geq \kappa_1$ and $\mu_2 \geq \mu_1$), and where v_2 is the second phase volume fraction. Such bounds are the tightest possible on isotropic effective responses, with isotropic two phase microstructures, where only the volume fractions and phase contrasts of the constituents are known. *During effective material design development, when selecting particulate micro-additives for a base matrix, information about the changes in the otherwise (relatively) smooth internal fields, corresponding to the matrix material alone, is valuable to characterize a new tailored material's performance.* One way to characterize the smoothness of the microscopic field behavior is via concentration tensors, which provide a measure of the deviation away from the mean fields throughout the material. By direct manipulation we obtain

$$\begin{aligned} \langle \boldsymbol{\sigma} \rangle_\Omega &= v_1 \langle \boldsymbol{\sigma} \rangle_{\Omega_1} + v_2 \langle \boldsymbol{\sigma} \rangle_{\Omega_2} \\ &= v_1 \mathbb{E}_1 : \langle \boldsymbol{\epsilon} \rangle_{\Omega_1} + v_2 \mathbb{E}_2 : \langle \boldsymbol{\epsilon} \rangle_{\Omega_2} \\ &= \mathbb{E}_1 : (\langle \boldsymbol{\epsilon} \rangle_\Omega - v_2 \langle \boldsymbol{\epsilon} \rangle_{\Omega_2}) + v_2 \mathbb{E}_2 : \langle \boldsymbol{\epsilon} \rangle_{\Omega_2} \\ &= \underbrace{((\mathbb{E}_1 + v_2(\mathbb{E}_2 - \mathbb{E}_1)) : \boldsymbol{C})}_{\mathbb{E}^*} : \langle \boldsymbol{\epsilon} \rangle_\Omega \end{aligned} \tag{2}$$

where

$$\underbrace{\left(\frac{1}{v_2}(\mathbb{E}_2 - \mathbb{E}_1)^{-1} : (\mathbb{E}^* - \mathbb{E}_1)\right)}_{\stackrel{\text{def}}{=} \boldsymbol{C}} : \langle \boldsymbol{\epsilon} \rangle_\Omega = \langle \boldsymbol{\epsilon} \rangle_{\Omega_2}. \tag{3}$$

We may write, for the variation in the stress $\boldsymbol{C} : \mathbb{E}^{*-1} : \langle \boldsymbol{\sigma} \rangle_\Omega = \mathbb{E}_2^{-1} : \langle \boldsymbol{\sigma} \rangle_{\Omega_2}$, which reduces to $\mathbb{E}_2 : \boldsymbol{C} : \mathbb{E}^{*-1} : \langle \boldsymbol{\sigma} \rangle_\Omega \stackrel{\text{def}}{=} \overline{\boldsymbol{C}} : \langle \boldsymbol{\sigma} \rangle_\Omega = \langle \boldsymbol{\sigma} \rangle_{\Omega_2}$. $\overline{\boldsymbol{C}}$ is known as the stress concentration tensor. Once either $\overline{\boldsymbol{C}}$ or $\mathbb{E}^*$ are known, the other can be determined. In the case of isotropy we may write

$$\overline{C}_\kappa \stackrel{\text{def}}{=} \frac{1}{v_2} \frac{\kappa_2}{\kappa^*} \frac{\kappa^* - \kappa_1}{\kappa_2 - \kappa_1} \qquad \text{and} \qquad \overline{C}_\mu \stackrel{\text{def}}{=} \frac{1}{v_2} \frac{\mu_2}{\mu^*} \frac{\mu^* - \mu_1}{\mu_2 - \mu_1}. \tag{4}$$

Clearly, the microstress fields are minimally distorted when $\overline{C}_\kappa = \overline{C}_\mu = 1$.

2. Computational material design. In a material design setting, we are primarily concerned with the construction of an inverse problem, where combinations of particulate and matrix materials are sought to minimize objective functions such as $\Pi = \left(\frac{\|\mathbb{E}^* - \mathbb{E}^{*,D}\|}{\|\mathbb{E}^{*,D}\|} \right)^2$, where $\mathbb{E}^{*,D}$ is a prespecified desired effective response, and where $\mathbb{E}^*$ is the effective response produced by a trial microstructure. A microstructural design can be defined through an N-tuple design vector, denoted $\boldsymbol{\Lambda} \stackrel{\text{def}}{=} (\Lambda_1, \Lambda_2, ..., \Lambda_N)$, consisting of the mechanical properties and volume fraction of the particulates. For both manufacturing and physical reasons, generally, each design variable will have a constrained design search space. For example, the volume fraction must nonnegative and no greater than unity. Specifically, our objective is to computationally design the macroscale effective bulk and shear moduli κ^* and μ^*, using convex combinations of the Hashin-Shtrikman bounds as approximations for

the effective moduli, i.e. $\kappa^* \approx \theta\kappa^{*+} + (1-\theta)\kappa^{*-}$ and $\mu^* \approx \theta\mu^{*+} + (1-\theta)\mu^{*-}$ where $0 \leq \theta \leq 1$. The micro-macro objective function is

$$\Pi = w_1(\tfrac{\kappa^*}{\kappa^{*,D}} - 1)^2 + w_2(\tfrac{\mu^*}{\mu^{*,D}} - 1)^2 + \hat{w}_3(|\tfrac{\overline{C}_\kappa - 1}{\phi_\kappa}| - 1)^2 + \hat{w}_4(|\tfrac{\overline{C}_\mu - 1}{\phi_\mu}| - 1)^2, \tag{5}$$

where (I) if $|\overline{C}_\kappa - 1| \leq \phi_\kappa$, then $\hat{w}_3 = 0$, (II) if $|\overline{C}_\kappa - 1| > \phi_\kappa$, then $\hat{w}_3 = w_3$, (III) if $|\overline{C}_\mu - 1| \leq \phi_\mu$, then $\hat{w}_4 = 0$ and (IV) if $|\overline{C}_\mu - 1| > \phi_\mu$, then $\hat{w}_4 = w_4$. The design variables are $\mathbf{\Lambda} = \{\kappa_2, \mu_2, v_2\}$, and their constrained ranges are $\kappa_2^{(-)} \leq \kappa_2 \leq \kappa_2^{(+)}$, $\mu_2^{(-)} \leq \mu_2 \leq \mu_2^{(+)}$ and $v_2^{(-)} \leq v_2 \leq v_2^{(+)}$. There are two characteristics of such a formulation which make the application of standard gradient type minimization schemes, such as Newton's method, inapplicable: (I) the incorporation of limits on the microfield behavior, as well as design search space restrictions, renders the objective function not continuously differentiable in design space and (II) the objective function is nonconvex, i.e. the system Hessian is not positive definite (invertible) throughout design space.

3. Nonconvex/nonderivative search methods: genetic algorithms. The lack of *robustness* of classical gradient based deterministic optimization processes can be rectified by application of a family of methods usually termed "genetic" algorithms. Essentially, genetic algorithms are search methods based on the probabilistic principles of natural selection. There are a variety of such methods, which employ concepts of species evolution, such as reproduction, mutation and crossover. Such methods stem from the pioneering work of John Holland and his colleagues in the late 1960s and early 1970s at the University of Michigan (Holland [11]). For introductions to the basics of such methods, the interested reader is referred to Goldberg [7], Davis [3] and Onwubiko [19]. A recent overview of the state of the art of the field can be found in a collection of recent articles edited by Goldberg and Deb [8]. Here we concentrate on constructing a genetic-type algorithm for nonconvex inverse problems of micro-macro material design where the microstructural parameters form a "genetic string", and a "survival of the fittest" is then applied to a population of such strings. Algorithmically, the approach is:

STEP 1 : RANDOMLY SELECT N STARTING GENETIC STRINGS $\mathbf{\Lambda}^i$, $(i = 1, ..., N)$:
$\mathbf{\Lambda}^i \stackrel{\text{def}}{=} \{\Lambda_1^i, \Lambda_2^i, ...,\}$ *(FOR EXAMPLE* : $\mathbf{\Lambda}^i \stackrel{\text{def}}{=} \{\kappa_2^i, \mu_2^i, v_2^i\}$)
STEP 2 : COMPUTE FITNESS ($\Pi(\mathbf{\Lambda}^i)$) OF EACH GENETIC STRING : $(i = 1, ..., N)$
STEP 3 : RANK THE GENETIC STRINGS, $\mathbf{\Lambda}^i$ (i = 1, ..., N)
STEP 4 : MATE NEAREST PAIRS (PRODUCE OFFSPRING) (i = 1, ..., N)
$\boldsymbol{\lambda}^i \stackrel{\text{def}}{=} \Phi^i\mathbf{\Lambda}^i + (1-\Phi^i)\mathbf{\Lambda}^{i+1}$ $\quad$ $\boldsymbol{\lambda}^{i+1} \stackrel{\text{def}}{=} \Phi^{i+1}\mathbf{\Lambda}^{i+1} + (1-\Phi^{i+1})\mathbf{\Lambda}^{i+1}$
$0 \leq \Phi^i = \text{RAND} \leq 1$ $\quad$ *(DIFFERENT FOR EACH COMPONENT)*
STEP 5 : ENFORCE DESIGN CONSTRAINTS : $\kappa_2^- \leq \kappa_2^i \leq \kappa_2^+$, $\mu_2^- \leq \mu_2^i \leq \mu_2^+$, ...
STEP 6 : KILL OFF BOTTOM M < N STRINGS. OPTIONAL : KEEP TOP K PARENTS
STEP 7 : REPEAT WITH TOP GENE POOL PLUS M NEW ONES : $\mathbf{\Lambda}^i = \boldsymbol{\lambda}^i$, $(i = 1, ..., N)$
TERMINATION : CONTINUE UNTIL $||\Pi|| \leq$ TOL

(6)

We remark that, in this algorithm, the definition of "fitness" of a genetic string indicates the value of the objective function. In other words, the most fit genetic string is simply the one with the smallest objective function. STEPS 1-7 attempt to first collect genetic strings associated with multiple local minima and then to successively mate them to determine the most fit genetic string. It is remarked that if the function Φ is allowed to be greater than unity, one can consider the

resulting convex combination (offspring) as a "mutation". This was not employed in this work. It may seem somewhat superfluous to retain the top (K) parents in such an algorithm, however, if one considers that the objective functions are highly nonconvex, i.e. nonmonotone objective function behavior between parents in design space, there exists a strong possibility that the inferior offspring will replace superior parents. However, with top parent retention, the minimization of the cost function is guaranteed to be monotone. Typically, with the presented algorithm (Box 6), after a few generations, a dominant genetic string will appear.

4. Numerical examples. As an example, we considered a base matrix material (aluminum) of fixed material values, $\kappa_1 = 77.9$ GPa and $\mu = 24.9$ GPa. The desired values were $\kappa^{*,D} = 100$ GPa, $\mu^{*,D} = 50$ GPa, ϕ_κ=0.5 and ϕ_μ=0.5. The (constrained) design variable's ranges were $0.1\kappa_1 = \kappa_2^{(-)} \leq \kappa_2 \leq \kappa_2^{(+)} = 10\kappa_1$, $0.1\mu_1 = \mu_2^{(-)} \leq \mu_2 \leq \mu_2^{(+)} = 10\mu_1$ and $0 = v_2^{(-)} \leq v_2 \leq v_2^{(+)} = 0.66666$. The weights were set to $w_1 = w_2 = 1$ and $\hat{w}_3 = \hat{w}_4 = 1000$. We used $\theta = 0.5$ for the Hashin-Shtrikman bound combination. The number of genetic strings was set to 1000, for ten generations, keeping the offspring of the top 100 parents after each generation. Two cases were considered: (I) Additionally keeping top $K = 100$ parents after each generation, thus with 800 new genetic strings infused and (II) Not keeping top $K = 100$ parents after each generation, thus with 900 new genetic strings infused. Table 1 and Figure 1 depict the results. After ten generations, a dominant genetic appeared for each approach ((I) and (II)). The minimization of the cost function is guaranteed to be monotone, if the top parents are retained. As the results illustrate, not retaining the parents is suboptimal due to the possibility that inferior offspring will replace superior parents. Furthermore, parent retention is computationally less expensive, since these designs do not have to be reevaluated, although this was not a concern for the types of simulations presented in this work, since the total simulation time was on the order of a few seconds. However, it is a concern for large scale numerical simulations involving spatial discretization, which we briefly discuss next.

5. Final comments. The presented genetic minimization schemes can be used for optimization involving many more design parameters, such as topological variables. Reviews of methods of topology optimization for quasi-regularly structured (checkerboard-like) materials are given in Bendsoe [2], Kikuchi et. al [15] and recently in Sigmund [20]. Such techniques have been recently extended in Hyun and Torquato [14] and Torquato and Hyun [22]. Specifically for randomly dispersed particulate composites, deterministic optimization approaches can be found in Zohdi [25]. The presented genetic minimization schemes can also be used in conjunction with large-scale numerical methods, where the primary issue is the simulation of bodies containing large numbers of particulates or fibers. There exist a variety of methods to deal with large-scale computational micromechanical problems, for example multiscale methods, exemplified by Fish and Ghouli [4], Voronoi cell methods (Ghosh et al. [6]), transformation methods (Moulinec et al. [17]), hierarchical modeling methods (Huet [12], [13], Zohdi et al. [23],Oden and Vemaganti [18]), multipole methods (Fu et

al. [5]) and iterative micro-domain decomposition type strategies (Zohdi et al. [24]). Micro-domain decomposition methods are closely related to alternating Schwarz approaches (see Le Tallec [16] for reviews) and methods of equilibration (see Ainsworth and Oden [1] for reviews). Such iterative domain decomposition techniques can be incorporated into the genetic algorithm design methodology relatively easily, and are currently being implemented in a large-scale computational framework by the author.

RANK	$\frac{\kappa_2}{\kappa_1}$	$\frac{\mu_2}{\mu_1}$	v_2	Π
1	1.70504332	4.18105632	0.47901479	0.0000000669
2	1.79829428	4.73913286	0.43593674	0.0000002239
3	1.70429527	4.15100069	0.48157999	0.0000004331
4	1.73964619	4.40902794	0.46050216	0.0000005034
5	1.79563011	4.73965691	0.43711644	0.0000006076
1	1.74140577	4.41387024	0.45972867	0.0000003176
2	1.76652440	4.51961623	0.45075001	0.0000010890
3	1.76565742	4.49920830	0.45314006	0.0000013550
4	1.71215005	4.28228845	0.47080279	0.0000033655
5	1.71220297	4.30300751	0.46913710	0.0000057834

Table 1: Best microstructural designs after ten generations. TOP: Keeping parents and BOTTOM: Not keeping parents.

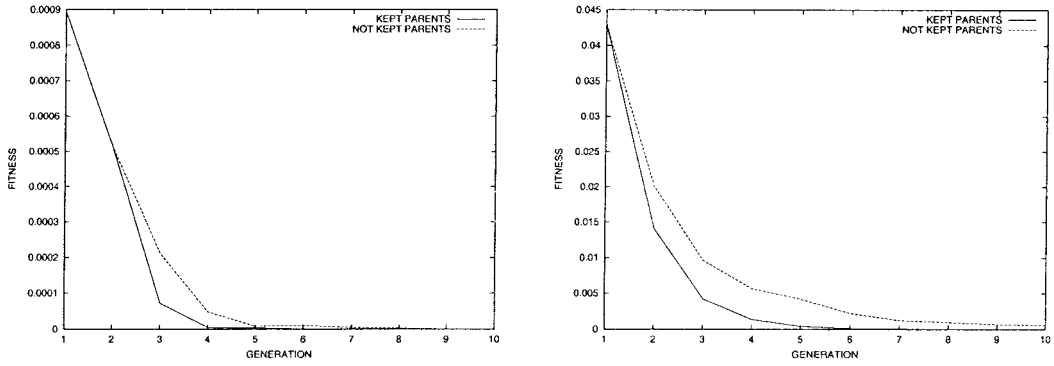

Figure 1: Generational values of (LEFT) the best design's objective function and (RIGHT) the average of the best 100 designs' objective functions.

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