ARTICLES

Design of inhomogeneous materials with given structural properties

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We describe a technique applicable to optimize certain quantities associated with the two-phase structure described by a model of penetrable grains. The solution is given in a form of an intensity surface that controls locations of the grains. Particular examples include maximization of the expected phase 2 volume and design of functionally graded materials with a given density profile.

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I. INTRODUCTION

A popular stochastic model for two-phase random media is provided by Poisson ensembles of fully penetrable and uncorrelated spheres [1,2] (or more general grains). The density of spheres is usually assumed to be independent of the locations so that statistical properties of the microstructure is translationally invariant (homogeneous). Because spheres are used, this model corresponds to rotationally invariant (isotropic) random media. Significant work has been done to optimize the design of homogeneous materials, both in the context of bounds [3] and of design [4]. Quintanilla and Torquato [5] studied an inhomogeneous random medium in which uncorrelated spheres are still used but the density of spheres varies with the locations. They derived analytical expressions for the canonical n-point microstructure function and the lineal-path function.

In the present paper we continue to study such inhomogeneous random media. We do not attempt here to relate the mechanical and effective transport properties of the material to its microstructure, but rather assume such relations known. Provided the spatially inhomogeneous density can be controlled, our main aim is to design the material in order to optimize the corresponding quantities associated with its two-phase microstructure.

At the first approximation, the properties of such heterogeneous media depend on the volume fractions of the phases (see, e.g., [6]). As a simple example, one may want to locate spheres at random in order to minimize the volume fraction of phase 1 (the part exterior to the spheres), or equivalently, to maximize the volume fraction of phase 2 (the spheres). This becomes a computational geometry problem if the total number of spheres is fixed and predetermined. However, in many cases [1,2,7] the total number of spheres is random and follows a Poisson distribution. Thus, it is natural and reasonable to assume that the centers of these fully penetrable random spheres form a spatial Poisson point process. In such cases the optimal locations of centers may vary depending on the total number of spheres available. The objective function then becomes a function of a non-negative measure representing the spatial density (also called the intensity measure) of the Poisson point process of the sphere centers [8]. The optimization problem can then be reformulated as the search for an ''optimal'' (not necessarily unique) intensity measure of the Poisson point process. This optimization problem is usually constrained by fixing the total mass of the intensity measure (representing the resources available). However, other constraints may also be used, e.g., one may want to identify an optimal intensity measure with a given barycenter. There are numerous other functions that may be optimized, for example, the perimeter or surface area, or functions that characterize fluctuations of the volume fraction such as the entropy

$$-\int p(\mathbf{x})\log p(\mathbf{x})\,d\mathbf{x},$$

where $p(\mathbf{x})$ is the one-point phase probability function [1,5].

More complex constraints arise in the design of functionally graded (gradient) materials (FGM) [9]. An FGM consists of two (or more) phases, and its composition varies in some spatial direction for specific requirements. Grading the internal microstructure of a composite material enables ones to integrate the material and structural considerations into the

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design. The gradients are introduced intentionally and are quantitatively controlled in order to optimize specific properties for use in real environments. ''A major problem in the design of an FGM, aside from that of materials selection, lies in determining the optimum spatial dependence for the composition [10].'' The proposed optimization technique solves this problem for FGM materials modeled by Poisson ensembles of fully penetrable spheres.

The outline of this paper is as follows. Section II introduces a mathematical model used to describe heterogeneous materials. Sections III and IV present a general approach to find an optimal intensity measure and the corresponding steepest descent algorithm. Section V describes how to apply the algorithm in order to find an intensity measure maximizing the mean volume of phase 2 and presents various examples. Section VI shows how to determine the intensity measure to achieve a predetermined mean phase 1 volume. Section VII deals with a more general case of functionally graded materials.

II. MATHEMATICAL MODEL

The construction of an ensemble of fully penetrable and uncorrelated spheres involves two steps.

First, points determining locations of the centers are placed randomly and independently on a region D which is a subset of the d-dimensional Euclidean space. Because of the randomness and independence, it is quite natural to assume that no two points coincide and the numbers of points in disjoint subregions are independent. Such a collection of points can be modeled very well by a Poisson (point) process. A Poisson process is characterized by its intensity, which describes the mean number of points in subregions. Mathematically, a Poisson process Φ with intensity measure $\Lambda(\cdot)$ is a random collection of points in D such that the number of points of Φ in a bounded subregion $B\subseteq D$ follows a Poisson distribution with mean $\Lambda(B)$ and the number of points in disjoint subregions are mutually independent. For example, Quintanilla and Torquato [5] simulated planar random media with the following $\Lambda(\cdot)$:

$$\Lambda(B)=\int_B A\|\mathbf{x}\|^2 d\mathbf{x}, \quad \Lambda(B)=\int_B A\ln\left(\frac{K}{C-x_1}\right)d\mathbf{x},$$

$$\Lambda(B)=\int_B A\exp(-\|\mathbf{x}\|)d\mathbf{x}, \quad \Lambda(B)=\int_B A\exp(-x_2)d\mathbf{x},$$

where A, K, and C are constants, $\mathbf{x}=(x_1,x_2)$ and $\|\mathbf{x}\|$ is the Euclidean distance between $\mathbf{x}$ and the origin, see also Quintanilla [1]. Each of these examples expresses $\Lambda(\cdot)$ as an integral in the form

$$\Lambda(B)=\int_B \lambda(\mathbf{x})d\mathbf{x}, \tag{1}$$

where $\lambda(\cdot)$ is called the density function. If the density is a constant, the Poisson process Φ is said to be homogeneous. Whenever $\lambda(\cdot)$ is not a constant, Φ is called inhomogeneous. However, it is not always possible or necessary to express $\Lambda(B)$ in the form of Eq. (1). For instance, if Λ attaches non-negative masses to single points (i.e., possesses an atomic part), then the right-hand side of Eq. (1) should include a sum of measures of singletons located within B.

The second step of the construction of an ensemble is to associate each point with a sphere. The most obvious way is to place fully penetrable spheres of independent random radii centered at these points.

Analytical analyses of such a model are possible if the distribution of the radii and the intensity measure of the Poisson process are known [1,2,7,5]. Actually, using spheres as building blocks does not simplify the analyses much. In other words, generalizing the model by replacing spheres by more general sets does not complicate the situation severely. Let us consider a sequence of independent and identically distributed random compact sets [11] $\Xi_1,\Xi_2,\ldots$ (called grains) which are not necessarily isotropic. A random set Ξ_0 having the same distribution as all Ξ_i, $i\geqslant 1$, is called the typical grain. The ensemble of the fully penetrable and uncorrelated grains

$$\Xi=\bigcup_{x_i\in\Phi}(x_i+\Xi_i),$$

is called a Boolean model [12,11], where here and thereafter $x+a\Xi=\{x+ay: y\in\Xi\}$. If the underlying Poisson process Φ is homogeneous, then we also say that Ξ is homogeneous. The total mass of Λ, $\Lambda(D)$, determines the mean total number of grains.

Consider a Boolean model inside a region D. The mean d-dimensional phase 2 volume V (that corresponds to length if $d=1$ or to area if $d=2$) can be calculated as

$$\langle V(\Xi\cap D)\rangle=\int_D p(\mathbf{x})d\mathbf{x}, \tag{2}$$

where $p(\mathbf{x})=\mathbf{P}(\mathbf{x}\in\Xi)$ is the one-point phase probability function for phase 2, see [1] and [5]. It is easy to see [12, p. 21] that

$$p(\mathbf{x})=1-\exp\left\{-\int_D \mathbf{P}(\mathbf{x}-\mathbf{y}\in\Xi_0)\Lambda(d\mathbf{y})\right\}. \tag{3}$$

Note that $\int_D \mathbf{P}(\mathbf{x}-\mathbf{y}\in\Xi_0)\Lambda(d\mathbf{y})$ equals $\langle\Lambda(x-\Xi_0)\rangle$. If Eq. (1) holds, then $\Lambda(d\mathbf{y})=\lambda(\mathbf{y})d\mathbf{y}$. If $\Xi_0=B_\xi(0)$ is a ball centered at the origin 0 of random radius ξ with $\mathbf{P}(\xi>t)=\overline{F}(t)$, then $\mathbf{P}(\mathbf{x}-\mathbf{y}\in\Xi_0)=\overline{F}(\|\mathbf{x}-\mathbf{y}\|)$. Furthermore, if the radius of the ball is deterministic and equal to r, then

$$p(\mathbf{x})=1-\exp\{-\Lambda[D\cap B_r(\mathbf{x})]\}. \tag{4}$$

III. OPTIMIZATION SETUP

In the following we keep the distribution of the typical grain fixed and aim to find a Λ that provides realizations of Ξ with required properties. The quantities of interest then become functions of the intensity measure Λ. Consider a general problem of minimizing a function $f(\Lambda)$ over all measures Λ satisfying some constraints:

$$f(\Lambda)\mapsto\min \quad \text{for } \Lambda\in\mathbb{M} \text{ and } H(\Lambda)=\mathbf{C}. \tag{5}$$

Here $\mathbb{M}$ denotes the family of all non-negative measures, and

$$H(\Lambda)=\left(\int_D h_1(\mathbf{x})\Lambda(d\mathbf{x}),\ldots,\int_D h_k(\mathbf{x})\Lambda(d\mathbf{x})\right) \tag{6}$$

maps $\mathbb{M}$ into the k-dimensional Euclidean space, so that $H(\Lambda)=\mathbf{C}=(C_1,\ldots,C_k)$ singles out those measures Λ for which $\int_D h_i(\mathbf{x})\Lambda(d\mathbf{x})=C_i$, $1\leqslant i\leqslant k$. We will also assume that $h_1,\ldots,h_k$ are linearly independent on D. Note that a maximization problem can be easily turned into a minimization problem by changing the sign of the objective function f.

An important example of a single constraint appears when $k=1, h_1(\mathbf{x})=1$ for all x. Thus

$$H(\Lambda)=\Lambda(D)=C, \tag{7}$$

specifying that the total mass of Λ is a constant C. The corresponding optimization problem is called the fixed total mass problem. Further examples of constraints (which can be applied simultaneously) are

$$h_2(\mathbf{x})=\mathbf{x},\quad h_3(\mathbf{x})=\|\mathbf{x}-\mathbf{x}_0\|^2,$$

where $h_2(\cdot)$ pinpoints the center of gravity of Λ and $h_3(\cdot)$ imposes a restriction on the inertia of Λ with respect to rotations around a given $\mathbf{x}_0$.

Assume that $f(\Lambda)$ is Fréchet differentiable (see, e.g., [13]) with a gradient $d_f(\mathbf{x},\Lambda)$, meaning that

$$f(\Lambda+\Upsilon)\approx f(\Lambda)+\int_D d_f(\mathbf{x},\Lambda)\Upsilon(d\mathbf{x})$$

up to terms of smaller orders than the total variation norm of a general signed measure Υ. Recall that the total variation norm of Υ is defined to be the sum of the total masses of the positive and negative parts of Υ.

Molchanov and Zuyev [8] showed that if Λ solves Eq. (5), then there exist some constants $u_1,\ldots,u_k$ such that

$$\begin{cases} d_f(\mathbf{x},\Lambda)=\sum u_i h_i(\mathbf{x}) & \Lambda \text{ almost everywhere,} \\ d_f(\mathbf{x},\Lambda)\geqslant\sum u_i h_i(\mathbf{x}) & \text{for all } \mathbf{x}. \end{cases} \tag{8}$$

In particular, for the fixed total mass problem Eq. (8) implies

$$\begin{cases} d_f(\mathbf{x},\Lambda)=u & \Lambda \text{ almost everywhere,} \\ d_f(\mathbf{x},\Lambda)\geqslant u & \text{for all } \mathbf{x}, \end{cases} \tag{9}$$

so that $d_f(\mathbf{x},\Lambda)$ is a constant u on the support of Λ and is at least u for all other $\mathbf{x}\in D$. First order optimality necessary conditions for more general constraints can also be found in [8] and [14].

IV. STEEPEST DESCENT ALGORITHM

Algorithms of the steepest descent type and their various modifications are widely known in the optimization literature [15]. The most basic method of the gradient descent suggests moving from Λ_n (the approximate solution on step n) to $\Lambda_{n+1}=\Lambda_n+\Upsilon_n$, where Υ_n minimizes

$$\int d_f(\mathbf{x},\Lambda_n)\Upsilon(d\mathbf{x}) \tag{10}$$

over all signed measures Υ with the total variation $\varepsilon=\varepsilon_n$, the latter being the size of step n. At every step it is vital to ensure that the $\Lambda_n+\Upsilon_n$ is a non-negative measure that satisfies the imposed constraints.

Consider minimization problem (5) with only constraint (7) on the fixed total mass. In order to keep $\Lambda_n(D)$ fixed, the increment Υ_n at every step must deliver a total mass zero. The integral given by Eq. (10) is minimized over such Υ if $\Upsilon=\Upsilon_n$ has an atom of positive mass $\varepsilon/2$ attached to any point where $d_f(\mathbf{x},\Lambda_n)$ is minimal and an atom of negative mass $-\varepsilon/2$ to any point where $d_f(\mathbf{x},\Lambda_n)$ is maximal. However, adding a negative atom may render $\Lambda_{n+1}=\Lambda_n+\Upsilon_n$ nonpositive.

The optimal steepest descent direction in the fixed total mass problem on a discretized space D with only constraint Eq. (7) can be found as follows [16]. Find the points of global minimum of $d_f(\mathbf{x},\Lambda_n)$ and distribute somehow the total mass $\varepsilon/2$ over these points (one or several). Then determine t_ε (respectively s_ε) which is the smallest (respectively the largest) value such that the total Λ_n mass of points at which the gradient $d_f(\mathbf{x},\Lambda_n)$ is at least t_ε (respectively s_ε) are less than or equal to $\varepsilon/2$ (respectively greater than $\varepsilon/2$); let the total Λ_n mass of points where the gradient is at least t_ε be $m\leqslant\varepsilon/2$. Finally, assign zero mass to all these points and reduce the total mass of the points at which the gradient is between t_ε and s_ε by an amount $\varepsilon/2-m$. The obtained measure is Λ_{n+1}. If the value of the objective function f at Λ_{n+1} is less than at Λ_n then Λ_{n+1} is taken as the next approximate solution. Otherwise, the step size ε is adjusted and another step with the new step size is attempted. Many involved and efficient ways of choosing the step size can be implemented, for example, the Armijo method described in [15, Sec. 1.3.2].

The described algorithm surely leads to the global minimum when applied to convex objective functions. In the general case it may get stuck in a local minimum, a common feature for gradient algorithms applied in the context of global optimization [15]. The necessary condition for the optimum given by Eq. (9) is used as a stopping rule for this algorithm: the function $g(\mathbf{x})=d_f(\mathbf{x},\Lambda)$ is a constant and takes its minimal value on the support of an optimal Λ. Although, strictly speaking, the support of Λ on the discrete space D is the set $S=\{\mathbf{x}\in D:\Lambda(\mathbf{x})>0\}$, in practice one may wish to ignore the atoms of the mass less than a predetermined small threshold.

For the optimization problem Eq. (5) with many linear constraints given by Eq. (6), it is computationally more efficient to use an approximation to the exact steepest direction. For instance, we choose the negative component of the increment Υ proportional to Λ in every step and vary its positive part Υ^+, i.e., $\Lambda_{n+1}=\Lambda_n+\Upsilon^+-\gamma\Lambda_n$ for some $0<\gamma<1$. The value of γ characterizes the size of the step, although generally it is not equal to the total variation of Υ. It can be shown [17] that the positive part Υ^+ of the steepest increment measure consists of at most k atoms, where k is the number of constraints. These k atoms of masses $p_1,\ldots,p_k$ located at points $\mathbf{x}_1,\ldots,\mathbf{x}_k$ are chosen to minimize

$$\int d_f(\mathbf{x},\Lambda)\Upsilon^+(d\mathbf{x})=\sum d_f(\mathbf{x}_i,\Lambda)p_i \tag{11}$$

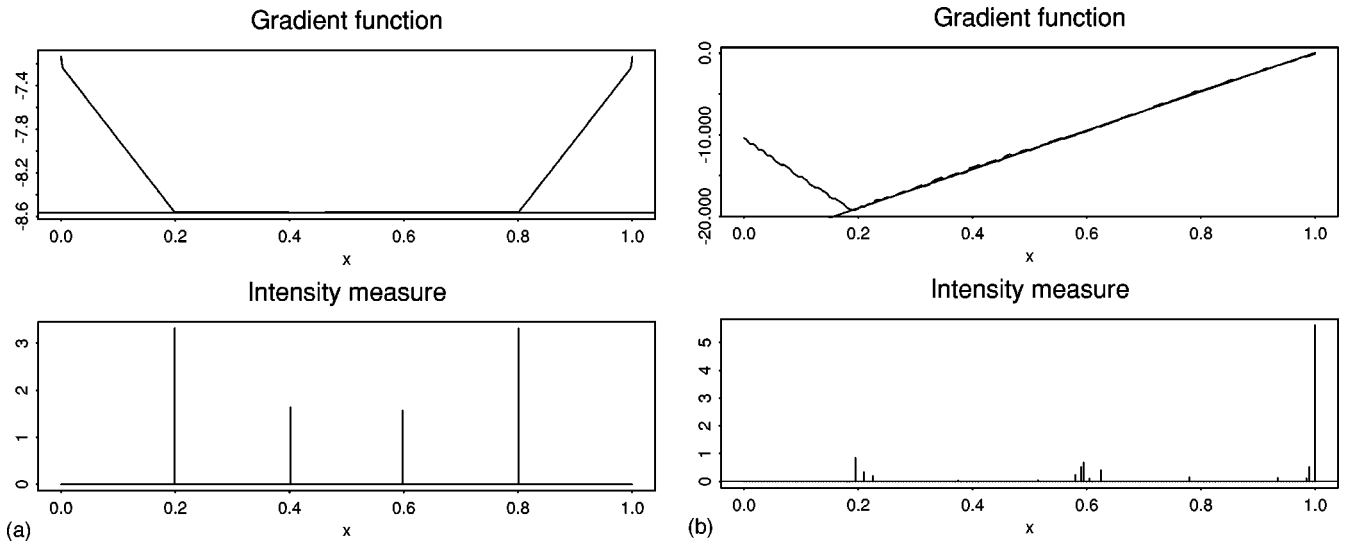

FIG. 1. Measures maximizing the mean phase 2 area and the corresponding gradient functions with grains are balls of radius $r=0.2$. (a) The only constraint on the total mass being 10; (b) under an additional constraint on the center of gravity located at 0.8.

and to maintain the imposed constraints (6). To satisfy the constraints $H(\Lambda+\Upsilon^+-\gamma\Lambda)=\mathbf{C}=(C_1,\ldots,C_k)$, we impose

$$H(\Upsilon^+)=\sum_{j=1}^{k} p_j h(\mathbf{x}_j)=\gamma\mathbf{C}. \tag{12}$$

For every k-tuple $(\mathbf{x}_1,\ldots,\mathbf{x}_k)$, Eq. (12) can be used to find $p_1,\ldots,p_k$ and then compute the right-hand side of Eq. (11). The k-tuple $(\mathbf{x}_1,\ldots,\mathbf{x}_k)$ and the corresponding weights $p_1,\ldots,p_k$ that minimize Eq. (11) subject to the nonnegativity constraint on $p_1,\ldots,p_k$ are then used to determine Υ^+.

Similarly, Eq. (8) provides a stopping rule for the algorithm. For example, under the two constraints on the total mass and the center of gravity, Eq. (8) requires that

$$\begin{cases} d_f(\mathbf{x},\Lambda)=u_1+u_2\mathbf{x} & \Lambda \text{ almost everywhere,} \\ d_f(\mathbf{x},\Lambda)\geqslant u_1+u_2\mathbf{x} & \text{for all } \mathbf{x}, \end{cases} \tag{13}$$

for some real numbers u_1 and u_2.

The described optimization routines can be obtained from the authors' web pages. They are realized in Splus/*R* statistical computing languages and organized as an *R*-bundle mesop.

V. MAXIMIZATION OF THE MEAN PHASE 2 VOLUME

Consider maximization of the mean phase 2 volume. It follows from Eqs. (2) and (3) that this problem is equivalent to minimization of the following objective function:

$$f(\Lambda)=\int_D \exp\left\{-\int_D \mathbf{P}(\mathbf{x}-\mathbf{y}\in\Xi_0)\Lambda(d\mathbf{y})\right\}d\mathbf{x}. \tag{14}$$

The exponential function is convex and so is f as a function of Λ, meaning that $f(t\Lambda_1+(1-t)\Lambda_2)\leqslant tf(\Lambda_1)+(1-t)f(\Lambda_2)$ for every $t\in[0,1]$ and every two measures Λ_1 and Λ_2. The convexity of f confirms that the steepest descent algorithm started with any initial measure indeed converges to a solution of Problem (5) for the objective function given by Eq. (14). Although the optimization problem is convex, it may have several solutions that provide the same values of the objective function. The gradient $d_f(\mathbf{y},\Lambda)$ can be easily calculated as the main term in the expansion

$$t^{-1}[f(\Lambda+t\Upsilon)-f(\Lambda)]\approx\int_D d_f(\mathbf{y},\Lambda)\Upsilon(d\mathbf{y}) \quad \text{for } t\downarrow 0.$$

Substituting f from Eq. (14) yields

$$d_f(\mathbf{y},\Lambda)=-\int_D \mathbf{P}(\mathbf{x}-\mathbf{y}\in\Xi_0)\times\exp\left\{-\int_D \mathbf{P}(\mathbf{x}-\mathbf{z}\in\Xi_0)(d\mathbf{z})\right\}d\mathbf{x}. \tag{15}$$

In particular, if Ξ_0 is a deterministic ball of radius r, then by Eq. (4) one has

$$f(\Lambda)=\int_D \exp\{-\Lambda[B_r(\mathbf{x})]\}d\mathbf{x},$$

$$d_f(\mathbf{y},\Lambda)=-\int_{D\cap B_r(y)} \exp\{-\Lambda[B_r(\mathbf{x})]\}d\mathbf{x}.$$

The formulas for the objective function and the gradient are then used in the steepest descent algorithm described in Sec. IV.

Below we provide several examples for $D=[0,1]$ (the unit segment) and $D=[0,1]^2$ (the unit square) and the typical grain being either deterministic or random ball. Note that numerical implementation of algorithms inevitably requires discretizing D by imposing a sufficiently fine mesh. In all cases starting measures for descent algorithms were uniform distributions over the mesh vertices.

Example 1. (One dimensional case.) Consider the fixed

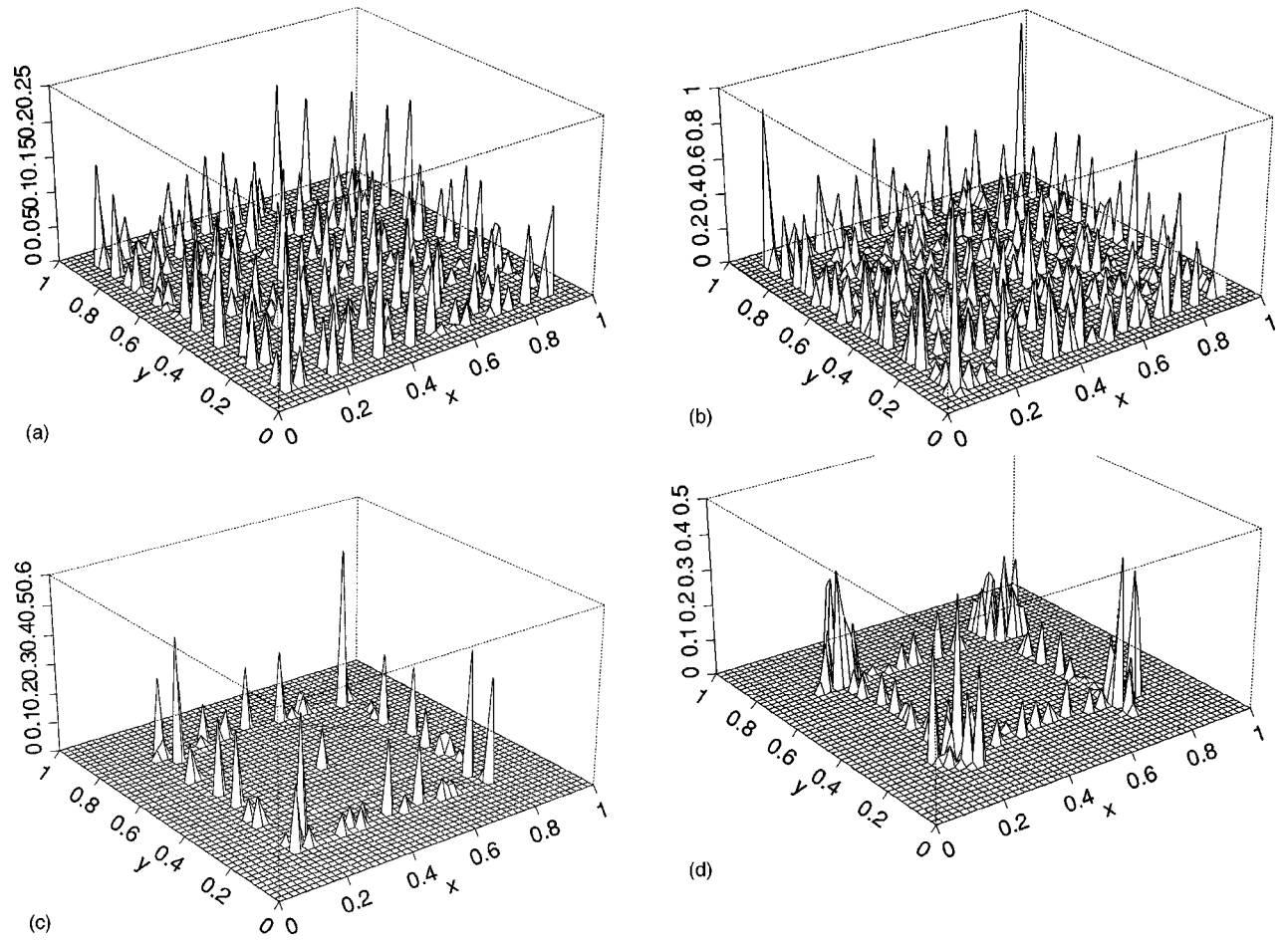

FIG. 2. Measures maximizing the mean phase 2 area in two dimensions with the fixed total mass C. The typical grain is a ball of radius r. (a) $C=10$, $r=0.1$; (b) $C=50$, $r=0.1$; (c) $C=10$, r is exponentially distributed with mean 0.1; (d) $C=10$, $r=0.3$.

total mass problem in one dimension $D=[0,1]$ with mesh size 0.005. Figure 1(a) shows the plots of masses of the obtained optimal Λ for the grains being fixed ball with radius 0.2. The corresponding plot of the gradient $d_f(\mathbf{x},\Lambda)$ confirm that the necessary optimality condition is satisfied, i.e., the gradient is minimal and constant on the support of Λ. Compare this to the theoretical solution available for this model—optimal Λ has four atoms: $\Lambda(0.2)=\Lambda(0.8)=10/3$ and $\Lambda(0.4)=\Lambda(0.6)=10/6$. In order to avoid comutational problems with rounding off when the radius of the ball is a multiple of the mesh size, the algorithm was actually run for the ball of radius 0.199999. Figure 1(b) shows the solution of the same problem as above with an additional constraint on Λ that its center of gravity is located at 0.8. Note that the gradient is linear on the support of Λ as it should be for an optimal Λ by Eq. (13).

Example 2. (Two dimensional case.) Let $D=[0,1]^2$ be discretized by using a square grid with mesh size 0.02. Figure 2 shows several results for the fixed total mass problem. Generally, the optimal measures have a well-identifiable ''comb'' pattern, which is typical in deterministic dense packing, but the probabilistic setup manifests in different masses attached to various nodes of the grid. An increase in radius or its randomness results in a sparser ''comb.''

It is possible to generalize the setup to minimize the mean of an integral of a function $\theta(\cdot)$ over phase 1, so that the objective function is given by

$$f(\Lambda)=\int_D \theta(\mathbf{x})\exp\left\{-\int_D \mathbf{P}(\mathbf{x}-\mathbf{y}\in\Xi_0)\Lambda(d\mathbf{z})\right\}d\mathbf{x},$$

and Eq. (15) holds with $d\mathbf{x}$ replaced by $\theta(\mathbf{x})d\mathbf{x}$. A constant $\theta(\mathbf{x})$ corresponds to the original problem of minimizing the mean phase 1 volume.

Another function of interest may be the entropy of phase 1 in a two-phase medium given by

$$g_1(\Lambda)=-\int_D [1-p(\mathbf{x})]\log[1-p(\mathbf{x})]d\mathbf{x},$$

with $p(\mathbf{x})=p(\mathbf{x},\Lambda)$ given by Eq. (3). This entropy function is not convex in Λ, so that additional computation has to be performed to finding an optimal Λ. The methods are known from the literature on global optimization and may include starting the descent from various initial measures or allowing the algorithm to go sometimes in the direction of increase of the objective function with the hope to visit the attraction domains of different minima.

VI. BOOLEAN MODELS WITH A PREDETERMINED MEAN PHASE 1 VOLUME

It is easy to modify the approach in order to be able to find models with a predetermined value of the objective function. For example, consider the following equation:

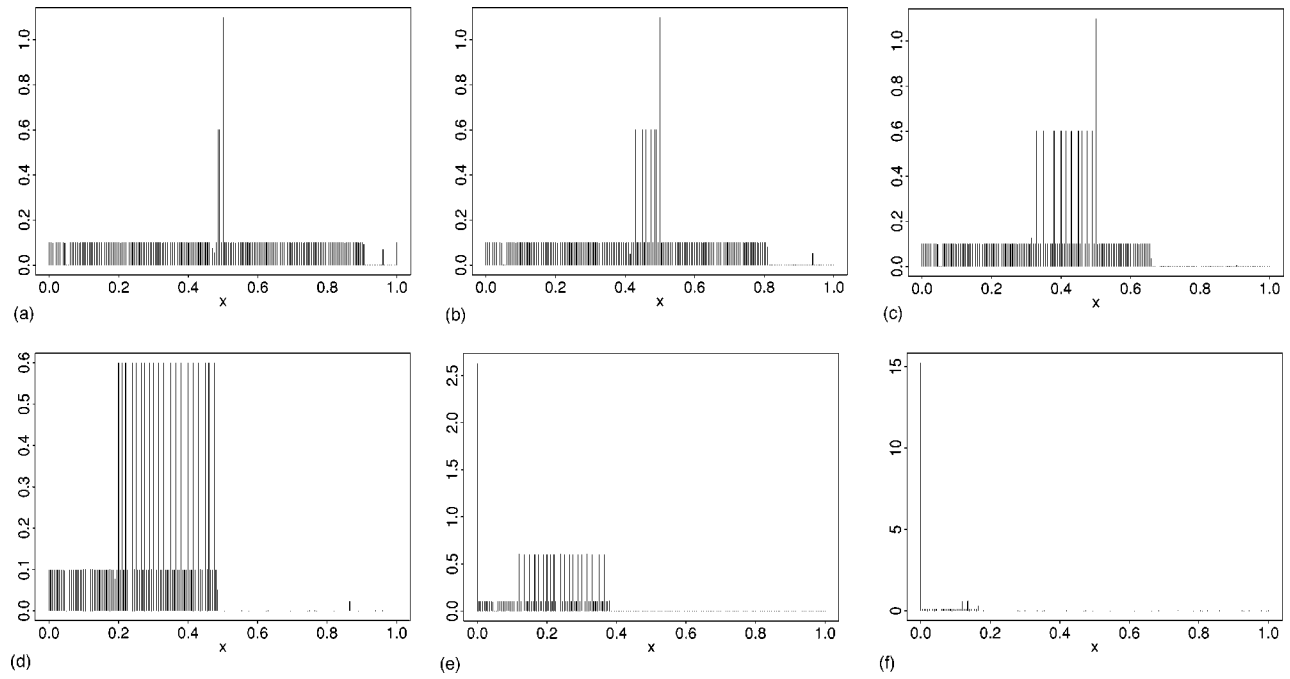

FIG. 3. Intensity measures providing the mean proportion of phase 1 area of (a) 5%; (b) 10%; (c) 20%; (d) 30%; (e) 40%; (f) 60%. The total mass is 20 and grains are balls with exponentially distributed radii of mean 0.1.

$$f(\Lambda)=a, \tag{16}$$

where $f(\Lambda)$ is given by Eq. (14). The solution of Eq. (16) is a measure that provides two-phase media with the mean phase 1 volume equal to a. Consider a new objective function

$$f_a(\Lambda)=[f(\Lambda)-a]^2.$$

The corresponding gradient is

$$d_{f_a}(\mathbf{x},\Lambda)=2[f(\Lambda)-a]d_f(\mathbf{x},\Lambda) \tag{17}$$

that is then used to perform the steepest descent.

Example 3. Consider a one-dimensional problem for grains being balls having exponentially distributed radii with mean 0.1. The total mass of Λ is fixed at 20. Figure 3 shows a solution of Eq. (16) for various values of a. The way the algorithm was programmed, the obtained solutions are somewhat trivial in that they have no phase 2 in a part of the material. More practically sensible solutions can be obtained either by starting algorithm from different initial measures or by adding new constraints, say on the maximal possible value of density $\lambda(\mathbf{x})$.

Clearly, Eq. (16) may have no solution if a is too small or too big, so that it lies out of the range of values that are possible for all intensity measures with a given total mass. In such cases the minimization problem leads to a $f(\Lambda)$ which is as close to a as possible. The smallest possible phase 2 volume is obtained if the whole intensity is concentrated at a corner of D and is $2^{-d}(1-e^{-C})\mu$, where C is the total mass

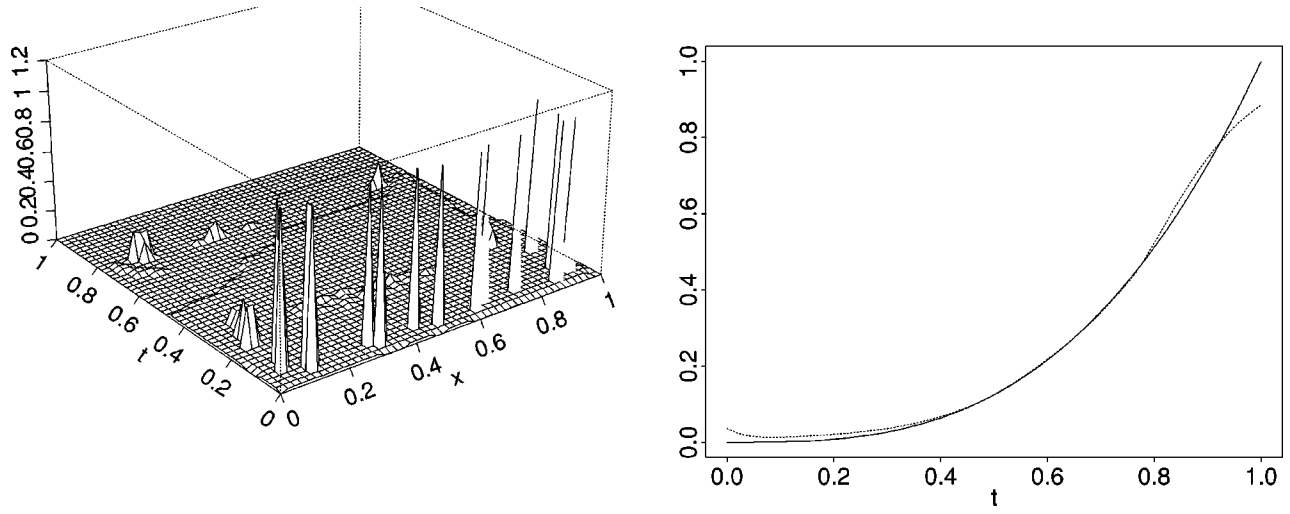

FIG. 4. Measure with a total mass of 50, providing a functionally graded material with a given target density profile $h(t)=t^3$ (solid line) and the corresponding density profile $q(t,\Lambda)$ (dotted line) according to the optimal measure obtained.

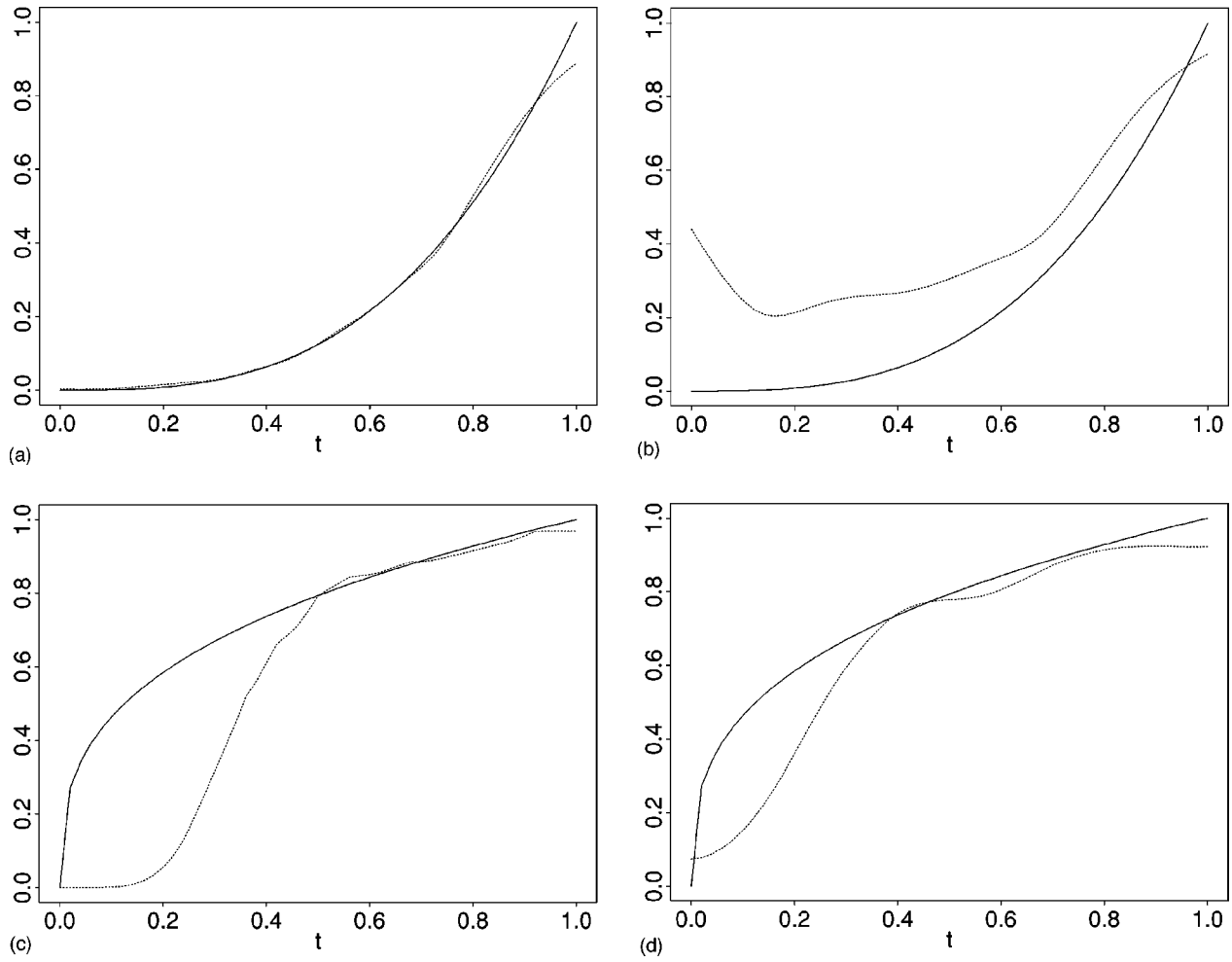

FIG. 5. Target density profiles h (solid lines) and the calculated density profiles $q(t,\Lambda)$ (dashed lines) for optimal measures with a total mass 50, assuming that the two-phase media on slices taken at each height t are homogeneous. (a) $d=1$, $h(t)=t^3$; (b) $d=2$, $h(t)=t^3$; (c) $d=1$, $h(t)=t^{1/3}$; (d) $d=2$, $h(t)=t^{1/3}$.

of Λ and μ the mean volume of grains. The smallest phase 1 volume can be obtained by minimizing $f(\Lambda)$ as described in Sec. V. Because f is a continuous function, all intermediate values a of mean phase 1 volume are realizable for suitable intensity measures, so that $f(\Lambda)=a$ has a solution for all such a.

However, the objective function f_a is not convex in Λ, and so an additional analysis is needed to confirm that the obtained solution indeed minimizes the objective function. A natural stopping criterion for the steepest descent algorithm in this case is to stop when $f_a(\Lambda)$ reaches its true minimum (being zero) within some degree of accuracy.

Since the gradient given by the left-hand side of Eq. (17) vanishes only if $f(\Lambda)=a$ or $d_f(\mathbf{x},\Lambda)=0$ identically, f_a does not have any local minimum points but only stationary points of f, where $d_f(\mathbf{x},\Lambda)=0$, or where Λ solves Eq. (16). This confirms that if f is convex, the steepest descent algorithm indeed leads to the global minimum of f_a when it does not find a solution to Eq. (16). It should be noted that Eq. (16) may have a number of different solutions.

VII. OPTIMIZATION PROBLEMS FOR FUNCTIONALLY GRADED MATERIALS

A functionally graded material is a $(d+1)$-dimensional two-phase medium in $D\times[0,1]$, where the last coordinate (height) determines the grading of the material. The mean phase 1 d-volume of slices taken at height t is equal to

$$q(t,\Lambda)=\int_D \exp\{-\langle\Lambda[(\mathbf{x},t)-\Xi_0]\rangle\}d\mathbf{x},$$

which is called the density profile [18]. An intensity measure Λ on $D\times[0,1]$ that provides a functionally graded material with $q(t,\Lambda)$ mimicking a given function $h(t)$ is a measure Λ that minimizes the function

$$G_h(\Lambda)=\int_0^1 [q(t,\Lambda)-h(t)]^2 w(t)dt, \tag{18}$$

where $w(\cdot)$ is a given weight function used to emphasize particular ranges where a closer fit is required. The corresponding gradient is given by

$$d_{G_h}[(\mathbf{y},s),\Lambda]=-\left\langle \int_{\Xi_0+(\mathbf{y},s)} 2[q(t,\Lambda)-h(t)] \times e^{-\langle\Lambda[(\mathbf{x},t)-\Xi_0]\rangle} d\mathbf{x}w(t)dt \right\rangle,$$

cf. Eq. (15).

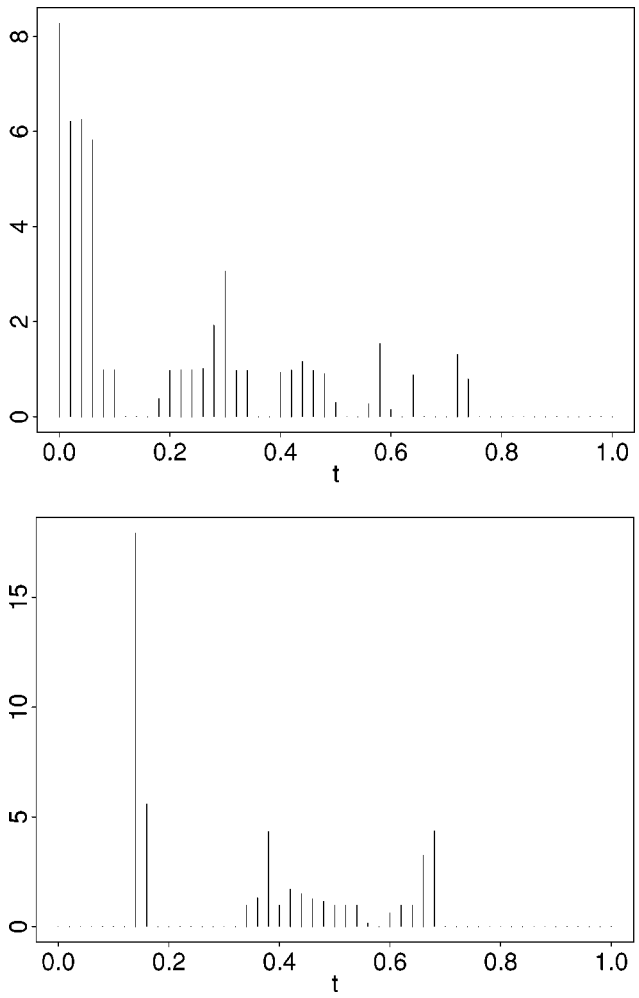

FIG. 6. The obtained optimal density functions $\lambda(s)$ corresponding to the cases shown in Figs. 5(a) and 5(b).

Example 4. Consider $D=[0,1]$ discretized with mesh size 0.05. Assume that grains are balls with exponentially distributed radii with mean 0.1. Figure 4 shows the perspective plot of a measure that minimizes Eq. (18) with $w(t)=1$ for a fixed total mass 50. The plot of h compared with the obtained functions q confirms that the fit is fairly good.

The computational time is reduced substantially in the case when the two-phase medium sliced at each height is required to be homogeneous, i.e., $\Lambda(d\mathbf{x}\,dt)$ has the form $d\mathbf{x}\,\lambda(t)dt$, where $\lambda(t)$ is the density function on $[0,1]$ (the range of heights t). In this case, an expression for $q(t,\Lambda)$ can be explicitly obtained as

$$q(t,\Lambda)=V(D)\exp\left\{-\int_0^1 \lambda(s)g(s-t)ds\right\}$$

for some function $g(s)$ depending on the grains. For example, if the typical grain is a ball with a (possibly random) radius ξ, then

$$g(s)=\kappa_d\langle\max(\xi^2-s^2,0)^{d/2}\rangle,$$

where κ_d is the volume of a d-dimensional unit ball (we assume that the values of ξ are smaller than the diameter of the maximal ball that fits in D).

Example 5. (Uniform spatial distributions) Figure 5 shows plots that compare the required density profile function h and the density profiles obtained from the optimal measures, assuming that the two-phase media on slices taken at each height are homogeneous. Figure 6 shows the corresponding density functions $\lambda(s)$.

Note that the function given by Eq. (18) is nonconvex. A convex problem can be posed in the context of functionally graded materials to minimize

$$H(\Lambda)=\int q(t,\Lambda)h(t)dt. \tag{19}$$

for a given function h.

VIII. CONCLUSIONS

We described a general framework for computation of the spatial densities of particles to obtain media with given geometrical microstructure that would enable design of materials with desirable effective properties. The latter calls for further studies to relate such macroscopic properties with microstructural information. The corresponding analysis includes optimization procedures based on the explicit expressions for the gradient and the necessary optimality conditions for functional depending on the density measures. Numerical algorithms are encoded in Splus/R statistical computing languages and are available from the authors' web pages.

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