Heterogeneous Material Modeling with Distance Fields

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Abstract

We propose a universal approach to the outstanding problem of computer modeling of continuously varying distributions of material properties satisfying prescribed material quantities and rates on a finite collection of geometric features. The central notion is a parameterization of the shape's interior by distances from the material features - either exactly or approximately; this parameterization supports specification, interpolation, and optimization of desired material distributions in a systematic and controlled fashion. We demonstrate how the approach can be implemented within the existing framework of solid modeling and its numerous advantages, including:

- precise and intuitive control using explicit, analytic, differential, and integral constraints specified on the original (not discretized) geometric model;
- applicability to material features of arbitrary dimension, shape, and topology; and
- guaranteed smoothness and analytic properties for superior performance, analysis and optimization.

Last, but not least, the proposed approach subsumes and generalizes a number of other proposals for heterogeneous material modeling for FGM, heterogeneous solid modeling, and solid free-form fabrication.

Keywords: Solid modeling, heterogeneous materials, functionally graded materials, distance fields, meshfree

1 The Material Modeling Problem

1.1 Motivation

The main objective of this research is to extend the success of Solid Modeling techniques to modeling and representation of solids with continuously varying heterogeneous and anisotropic material properties. Such components are becoming increasingly important due to emerging techniques in design and manufacturing of functionally graded materials and solid free-form fabrication techniques. Applications of heterogeneous and anisotropic materials range from aircraft structures to

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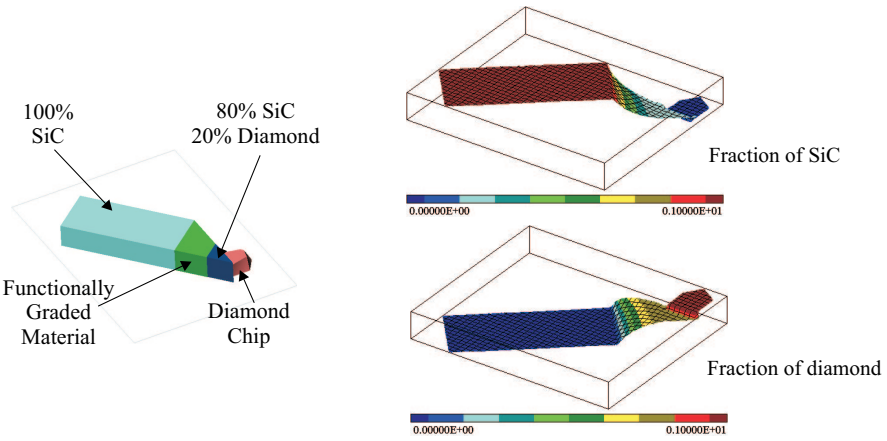
medical products [13, 6, 26]. In order to take full advantage of these existing technologies, the progress in material science, design and manufacturing methods must be matched by significant extension of existing methods for computer-aided representation, design, and manufacturing process plan technique. The task is non-trivial because the modern geometric and solid modeling technology has been developed under the assumptions of material homogeneity.

Informally, we can summarize the material modeling problem as follows: given a geometric representation of solid and/or collection of *material features* with known material properties, construct one or more *material functions*, subject to some given *constraints* (design, manufacturing, etc.) Each material function represents some material property that varies, usually continuously, from a point to point throughout the space, including the boundary and the interior of the solid.



(a) Diamond cutter tool consists of several distinct material regions

(b) Fractions of each material vary throughout the solid but always add to 1

Figure 1: A typical material modeling problem requires construction of material property functions that interpolate known material features subject to specified constraints and physical laws

Consider a simple but typical example that is depicted in Figure 1(a) and discussed in [6].Three material features are identifiable in the above example: the diamond chip and the two solid subsets of the shank (block region with 100% SiC, prismatic region with 80% SiC and 20% diamond,) where material properties are known. Two material functions need to be constructed (one for SiC and another one for diamond), subject to the following constraints: continuous interpolation of the material fractions on each of the features, fractions must add to 1, and the rate of material change is linear in the distance from each feature. In a more general case, material features can be of any dimension, shape or topology; the material distributions may be given as known continuous functions $f(x, y, z)$; the interpolation laws may include arbitrary weights and be subject to algebraic, differential, or integral constraints.

The recent surveys [19, 17] describe the technical challenges of this task and compare several known approaches from the perspective of applications, namely design, analysis, manufacturing process planning, and data exchange. To summarize:

- Material functions should match as exactly as possible their specified behaviors on material features. Material features can be of any dimension and shape.

- Material functions should possess analytic and smoothness properties that are consistent with physical considerations, adopted analysis techniques, and/or manufacturing methods.
- Intuitive and efficient controls must allow users to specify explicit, differential, integral or analytic constraints on material functions and to modify them using a small number of meaningful parameters. Many of such constraints are application specific; for example, when the solid is composed from several materials, individual material functions represent a fraction of volume occupied by a particular material and must add to 1 at any point in the solid.
- The representation of material properties must be compatible with current or proposed standards for geometric modeling representations as described in ISO 10033 standard [5, 15]. This is essential to support exchange data between design, analysis and manufacturing process plan domain.

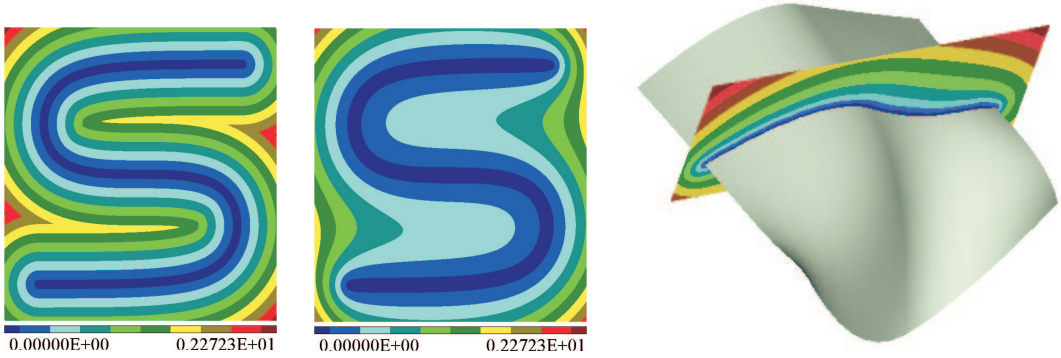
With the exception of the heuristic procedural method in [16], all proposed approaches to material modeling require some form of *spatial discretization* of the solid's interior. These include voxel-based [3, 25], finite-element based [18, 20], mesh-based [12, 8], and set-based [10, 9], or layer-based [24] schemes. Such discretizations amount to representation conversions that are expensive to compute and lead to many complications. First of all, all discretization methods introduce errors because they must approximate the geometry of solids and material features, as well as prescribed material properties. Secondly, the ability to satisfy the constraints and to assure smoothness properties places substantial restrictions on the types of allowed discretizations and approximations. Thirdly, modifying and controling material models becomes next to impossible, because every change may require recomputing both discretization and approximation of the material functions. Last, but not least, such representations are awkward for data exchange and standardization due to errors, approximations, and large size. Comparing these difficulties to the list of the requirements above, it seems clear that approaches to material modeling based on spatial discretizations are not likely to provide the required level of support. The heuristic approach in [16] offers no guarantees but corresponds to a special restricted case of material modeling in our framework [2].

1.2 Distance is the key

Much of the existing literature on material modeling points in the direction of one natural parameter: the distance from a material feature. For design purposes, it is convenient and intuitive to specify how material composition changes as a function of the distance from the material feature (recall the example in Figure 1). Capabilities of manufacturing processes for functionally-graded materials are also commonly described by their ability to modify material as functions of distance (determined either analytically or experimentally) [13, 7]. The most common types of material functions constructed by methods based on spatial discretization appear to be either the Euclidean distance function, weighted distance functions or simple functions of a distance function [4, 25, 24, 12, 8].

However, two possible difficulties may arise in relying on distance fields: computational cost and loss of differentiability at equidistant points. Computing the distance from a point to geometric primitives (typically a curve or surface) usually requires a numerical iterative procedure [14], which may result in a high computation cost. In the context of material modeling, the lack of smoothness in a material function constructed as a function of distance will result in stress concentrations or other undesirable singularities. We propose to eliminate both of these limitations of

the exact distance fields by replacing them with various smooth approximations, while preserving most of the attractive properties of the distance fields. In particular, we can replace the exact distance fields with their approximations constructed by the theory of $R-$functions [21] (See Figure 2).



(a) (b) (c)

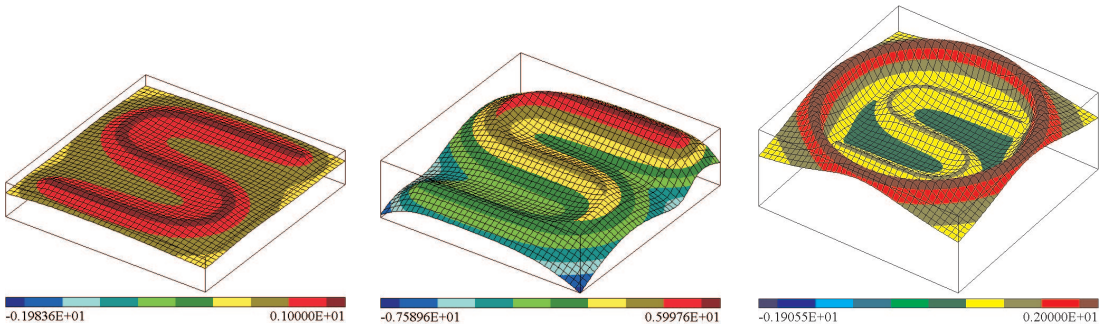
Figure 2: (a) The exact distance field of an S-shaped 4th-order B-spline curve; (b) An approximate distance field for the same curve normalized to the first order; (c) A section of an approximate distance field for a 4th-order B-spline surface normalized to the second order.

In the following section we describe with examples how material functions can be constructed and controlled with the distance fields of a single and multiple material features in our modeling scheme. We often used two-dimensional examples for the explanation because they are much easier to understand and visualize. However, all constructions and techniques apply to three-dimensional material modeling problems without any changes. Composition of several materials and other vector-valued material properties are modeled as vector-valued material functions in Section 3. A more detailed discussion of our approach, including theoretical details and many additional examples, can be found in [2].

2 Single and Multiple Material Features

The simplest problem of material modeling involves a single material feature. The material function P is constructed and controlled by specifying the value and derivatives at the feature. Using the distance function of the material feature, value and derivatives of P, specified at the material feature, is extended to the whole domain. Such material function construction method relies on the generalized Taylor series expansion by powers of a distance field of the feature and we showed that any material function can be constructed with our approach [21, 2]. Material functions in Figure 3(a) and (b) are examples of the construction with a single feature. For both of the distributions values of material functions attenuate with the exponential function of distance from the 'S' curve (4-th order B-splne curve). In Figure 3(a) a constant value of 1 is specified at the feature but for (b) the function varies linearly from one end of the 'S' curve to the other end and the gradient value of -4 is specified to all points of the curve.

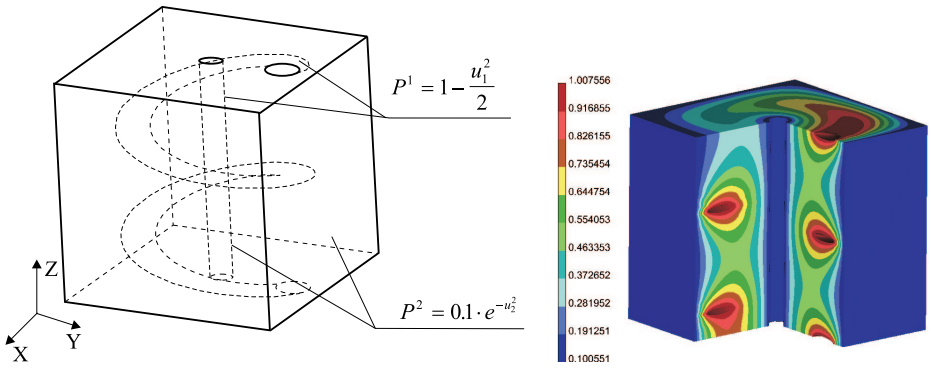
A more typical situation with heterogeneous material modeling involves several material features with known material characteristics. This task reduces to construction of a single material function $P^{\square}$ that interpolates given n material feature functions P^i, $i = 1, \ldots, n$. The interpolation



(a) (b) (c)

Figure 3: (a) Material function $e^{(-1.5u)}$ is prescribed in terms of distance u to the S-shaped feature. (b) Non-constant material function on a feature with derivative control: material function $ye^{(-1.5u)}$ and gradient -4 is specified on the feature. (c)Inverse distance interpolation of two material functions with derivative control: $P^1 = 1 - 1.5u$ (gradient specified at the curve is -1.5) is associated with the S-curve and $P^2 = 2$ is associated with the circular ring.

technique, which is employed to construct the single material function, is known as *inverse distance weighting* or as Shephard's method when used for scattered data interpolation [23, 11, 22]. The underlying notion of the interpolation method is that the influence of a feature decreases in proportion to the distance from the feature. Such interpolation technique does not require spatial discretization of the domain and applies to material features of arbitrary shape, topology and dimension. It also preserves exactly the values and derivatives specified on each material feature. The material distribution function in Figure 3(c) was constructed with two material features: the 'S'-shaped curve and an annulus region. The function specified at the 'S' curve was $(1 - 1.5u)$, where u is the distance function of the 'S' curve. The constant material function 2 was specified at the annulus feature.



(a) (b)

Figure 4: Material modeling with differential constraint. (a) Three-dimensional material modeling problem requires constructing a material function for the solid from the material functions associated with the two features as shown. (b) Constructed material distribution constrained to satisfy Laplaces equation.

The formulation based on generalized Taylor series expansion of the representation scheme

also makes possible to control material function with differential, integral, analytic and explicit constraints [2]. For example, Figure 4(b) shows the specified material function in Figure 4(a) constrained to approximate the Laplaces equation $\nabla^2 P^{\square} = 0$. Material functions for two material features are specified: $P^1 = 1 - u_1^2/2$ for the material feature defined as the union of all vertical faces (circular hole and four vertical faces of the cube), and $P^2 = 0.1e^{-u_2^2}$ for the spiral canal surface through the interior of the solid.

3 Vector Valued Material Properties

The proposed approach to material modeling extends directly to a more general case where a material property is a vector valued function. Common examples of such properties include material anisotropic grain orientation represented by a vector field, material composition represented by a vector of volume fractions, and vector of varying shape inclusion parameters in microstructure models. These and other vector and tensor valued properties of materials are discussed and compared in [9]. Each scalar component function can be treated independently using the techniques of section 2, but the component functions are also constrained to satisfy additional conditions. For example, when composition of several materials is represented, each component function $P^{\square,j}(p),\ j = 1, 2, \ldots, m$ models a fraction of the total volume, and the sum of all components must be $\sum_{j=1}^{m} P^{\square,j} = 1$ at every point of space. In [2], we showed that this constraint on volumetric factions can be maintained automatically using generalized inverse distance interpolation of the material feature functions $P^{i,j}$ satisfying the partition of unity condition, where $P^{i,j}$ is the jth material fraction function associated with the ith feature.

For example, in the case of diamond cutter example of Figure 1, constant fractions of two materials, SiC and diamond, are prescribed on three features: $P^{1,1} = 1.0,\ P^{1,2} = 0.0,\ P^{2,1} = 0.8,\ P^{2,2} = 0.2\ P^{3,1} = 0.0,\ P^{2,2} = 1.0$. These constant fraction functions are interpolated into two material fraction functions: $P^{\square,1}$ for SiC and $P^{\square,2}$ for the diamond. Each function was constructed using transfinite interpolation with inverse distance weights as shown in Figure 1(b). By construction, the two material functions add to 1 at all points of the cutter, simply because each feature was prescribed fractions of materials that add up to 1.

4 Conclusions

In the context of material modeling, the distance fields provide a natural parameterization of the space and allow formulation and solution of the material modeling problem in a manner that covers most practical situations in modeling, design, and manufacturing. The theoretical completeness of the formulation guarantees that any and all material functions may be represented to a desired precision as functions of the distance fields associated with material features [2]. We conjecture that the practical methods described in this paper are sufficient for handling most applications involving heterogeneous materials.

This paper considered relatively simple constraints on material properties. Additional research is needed on material functions to represent general tensorial properties, possibly anisotropic, with or without symmetry, and perhaps with periodicity such as found in composite materials. We already observed that material modeling can be viewed as a particular kind of a boundary value problem. One could also argue that the material modeling is a more general problem, because physical fields (temperature, stress, electric charge, etc.) are essentially material functions that

are defined by boundary conditions and constrained by suitable differential equations. A natural extension of our work is combining material modeling and engineering analysis within the same meshfree computational framework. In fact, the same distance fields provide a natural representation for any number of distinct physical fields over the same geometric domain, suggesting a possible approach to handling multi-physics problems. On the other hand, geometric domain itself may be also defined implicitly by a threshold of the constructed material density function[1]. Sensitivity analysis with respect to either geometric parameters or material changes, as well as shape and material optimization, can be performed in a meshfree manner using the same computational utilities and avoiding the usual difficulties with (re)meshing [27].

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