Heterogeneous Material Modeling with Distance Fields

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Abstract

We propose a universal approach to the problem of computer modeling of shapes with continuously varying material properties satisfying prescribed material conditions on a finite collection of material features and global constraints. The central notion is a parameterization of space by distances from the material features – either exactly or approximately. Functions of such distances provide a systematic and intuitive means for modeling of desired material distributions as they arise in design, manufacturing, analysis and optimization of components with varying material properties.

The proposed framework subsumes and generalizes a number of earlier proposals for heterogeneous material modeling. It is theoretically complete in the sense that it allows representation of *all* material property functions. We demonstrate that 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 native geometry; guaranteed smoothness and analytic properties without meshing; and applicability to material features of arbitrary dimension, shape, and topology.

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

1 The Material Modeling Problem

1.1 Motivation

Solid modeling of mechanical parts is now a mature technology that is the key to integration of design, analysis, manufacturing and other engineering activities [46]. While a number of difficult representational and integration problems are yet to be solved completely (for example, important technical problems remain in modeling of parametric families, interoperability, and integration of design and analysis), the general state of solid modeling is sufficient to support most of the activities in the product development cycle of traditional mechanical parts fabricated from homogeneous material.

The situation is drastically different for the emerging technologies focused on parts with *continually* varying material properties. Such parts are becoming increasingly important due to emerging techniques in design of functionally graded materials and solid free-form fabrication techniques that allow local material composition control. Powerful analysis and shape optimization methods (e.g., homogenization [2]) are available now for generating topologies for parts with variable material properties. Numerous applications of parts with *heterogeneously* and *anisotropically* varying materials are well documented [26, 14, 54] and include weight reduction, improved structural and other mechanical properties, promise of embedded sensors, and substantially improved motion and deformation control. Applications of heterogeneous materials range from aircraft structures to medical products. For example, implants (prosthesic hip, dental) are usually designed to have superior wear resistance, superior bonding with bones, maximize strength, and to exhibit biocompatibility. Being able to vary material properties locally and globally is the key to achieving all of these goals within a single solid component [26]. A number of promising free-form and layered fabrication techniques (such as photopolymer solidification, material deposition, powder solidification, lamination, and other layered

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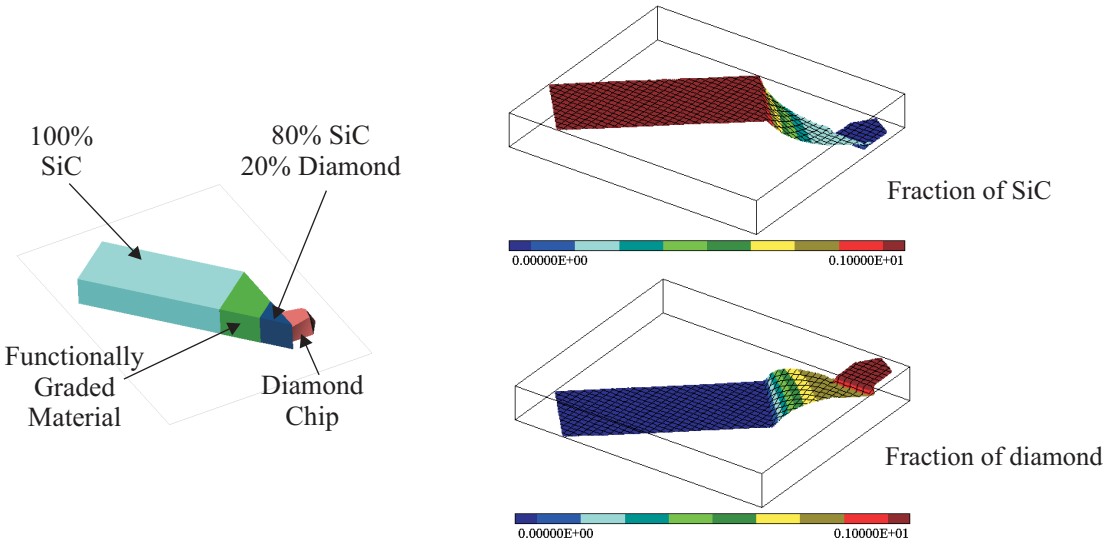
manufacturing methods [32]) hold the promise of making the manufacture of such parts and assemblies economically viable.

In order to take full advantage of these exciting technologies, the progress in material science, design, and manufacturing methods must be matched by significant extensions of existing methods for computer-aided representation, design, analysis, and manufacturing process planning. The task is non-trivial because the modern geometric and solid modeling technology has been developed under assumptions of material homogeneity [34]. Extensions of the classical solid modeling techniques are relatively straightforward for discretely varying material properties. They amount to choosing a particular method for representing a collection of geometric regions that may be heterogeneous in dimension, share boundaries, or contain each other. Several such schemes have been proposed [22, 21, 19].

Many researchers observed that material modeling is a type of physical field modeling, and as such, can be formulated as a problem in continuum mechanics. Some mathematical formulations are reviewed in [21], with a conclusion that a proper mathematical model for modeling material properties is a fiber bundle [57, 43] where the geometric model plays the role of the base space. Unfortunately, the correctness, or even profoundness of these observations, do not appear to offer concrete computational solutions.



(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. Plots in (b) correspond to the midsection of the cutter shown in (a).

Consider a simple but typical example that is depicted in Figure 1(a) and discussed in [14]. The solid object is partitioned into a diamond cutter (chip) and a shank that is manufactured from functionally graded composition of SiC and diamond. To control the composition, the shank is subdivided into three parts: block region with 100% SiC, prismatic region with 80% SiC and 20% diamond, and the transition region between them where the composition is a gradual blend of the two materials. Ideally, the blend should be smooth and may satisfy additional constraints prescribed by the designer or constrained by the manufacturing process. Figure 1(b) shows an interpolation between the respective fractions of the two materials that vary linearly with the distance between the two regions and add up to 1 at every point of the solid. It is clear that this problem may be formulated in terms of fiber bundles as suggested in [21], but such a formulation does not explicitly specify what exactly is given, how the variable material properties may be computed, represented, and controlled throughout the interior of the solid, or even when such problems are well posed and admit solutions.

The main contribution of this paper is in formulating the material modeling problem in a rigorous and computationally effective manner that appears to encompass most practical problems in material modeling. Our framework is based on the recognition that material modeling is a special type of boundary value problem whose solution is naturally parameterized by the distance fields of the material features. The theoretical and computational approach is inspired by our earlier work on meshfree engineering analysis [48, 47, 41, 40] using Rvachev's Function Method (RFM) of analysis [39, 38]. In particular, the approach is theoretically complete in that it allows representation of *all* material property functions. We demonstrate that 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 native geometry; guaranteed smoothness and analytic properties without meshing; and applicability to material features of arbitrary dimension, shape, and topology.

1.2 The Challenge

Informally, we can summarize the material modeling problem as follows: given a geometric representation of solid and/or a 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 point to point throughout the space, including the boundary and the interior of the solid. Three material features are identifiable in the above example: the diamond chip and the two solid subsets of the shank 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 pointsets of any dimension, shape, or topology; they may or may not be subsets of a solid object, but provide convenient means for defining material distribution throughout the solid [52]. The material distributions may be given as known continuous functions $f(x, y, z)$ that are subject to algebraic, differential, integral and/or interpolation constraints. The material features should be either disjoint or agree in the specified material properties. By definition, a material function will have a material discontinuity at points that are shared by boundaries of dissimilar material features, corresponding to the case of discrete heterogeneity. This formulation is general enough to include most material modeling problems. For example, most material composition operations, as described in [22, 50, 52] and others, reduce to geometric construction of a number of regions with given material properties (features) and regions where the material modeling problem must be solved.

To paraphrase, the problem is to fit a number of material functions to material features – in such a way that the material functions are properly constrained and smoothly parameterize the interior of the solid in terms of the material features in the solid's representation. The recent surveys [32, 30] 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 of 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 [12, 28]. This is essential to support exchange data between design, analysis and manufacturing process plan domain.

The main difficulty with the abstract formulations of the boundary value problems, and material modeling in particular, is that they do not suggest any representations for geometry and/or field. For example, the fiber bundle model assumes that the geometric domain and each material feature is represented by atlases of charts with C^∞

coordinate maps [21], but such representations are notoriously difficult to construct for most non-trivial solids and are rare in solid modeling. With the exception of the heuristic procedural method in [29], all proposed approaches to material modeling require some form of *spatial discretization* of the solid's interior. These include voxel-based [6, 52], finite-element based [31, 33], mesh-based [25, 19], set-based [22, 21, 52], and layer-based [51] 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 controlling 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 recently proposed implicit procedural scheme in [29] is an exception because it does not require any spatial discretization. Instead it proposes to represent material functions by known functions that describe material properties of elements in the boundary representation. While the approach appears to be heuristic and offers no guarantees, we will explain below how it corresponds to a special restricted case of material modeling in our framework.

1.3 Distance is the key

We have argued that material functions should be constructed, represented, and controlled in terms of intuitive parameters, presumably associated with the solid and/or its material features, and not in terms of *a posteriori* imposed spatial discretizations. But how are we to relate such parameters to global spatially-varying material functions without using some form of mesh? 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) [26, 17]. The importance of distance modeling has already been recognized by other researchers. 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 [8, 52, 51, 25, 19]. Inverse distance weighting can be used for interpolating boundary (or material) conditions prescribed on geometric features without meshing; the method was first described in [41] and used in a limited form in [50].

Let us examine more carefully which properties of the (Euclidean) distance make it so useful for material modeling. For any closed set S, we will say that function $u : E^3 \rightarrow R$ is the *distance function* if it associates with any point p in space a non-negative real number equal to the Euclidean distance from p to S. In other words, for each pointset S, the distance function defines a scalar *distance field.* Figure 2(a) shows the isolines of the Euclidean distance field for the S-shaped curve in the plane. Properties of distance functions and fields have been studied extensively in the literature; in particular, we observe that:

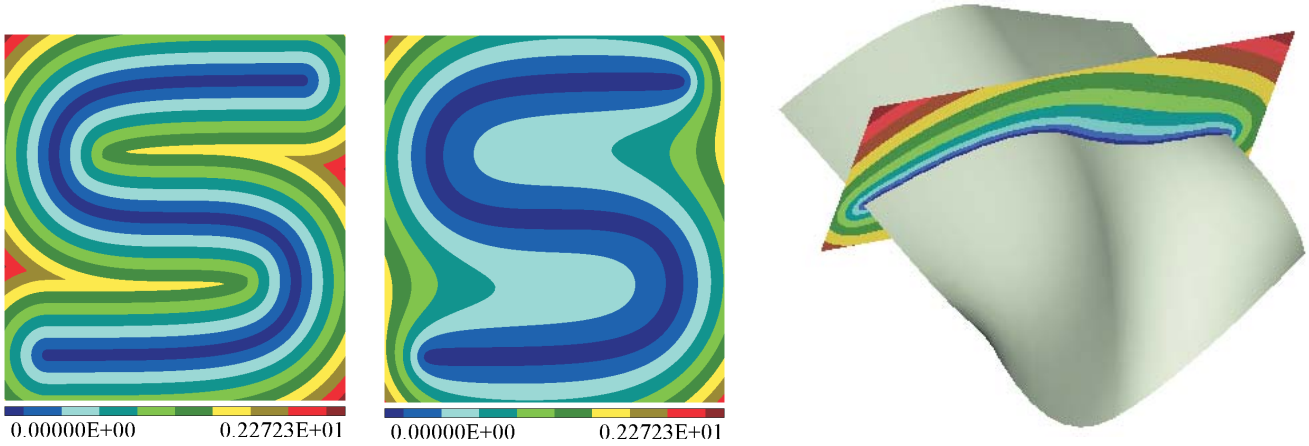
1. A point p belongs to the set S if and only if $u(p) = 0$, which means that the distance field defines S implicitly. The description applies uniformly to all closed sets irrespective of their geometric, analytic, and topological properties, because these properties are all encoded within the distance function.

2. For every value a of distance function u, $u^{-1}(a)$ is a non-empty subset of E^3. In other words, the distance provides a natural parameterization of the whole space by a single parameter – the distance to the set S.

3. The distance function u is not differentiable at the points on the boundary of S and at those points that are equidistant from two or more points of S.[1] These points are clearly visible in Figure 2(a). At all other points p, u is differentiable with $|\nabla u(p)| = 1$ and with all higher derivatives at p vanishing in the direction of the gradient.

The first property provides a simple yet powerful representation scheme for all closed subsets of Euclidean space. The second gives a simple method for extending properties of the set to the whole space. The third property assures that

[1] These special points provide a useful lower-dimensional characterization of set S in terms of its medial axis and Voronoi diagram.



(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.

this extension takes place in a gradual and predictable fashion. These properties of distance fields made them popular in many other applications: from computer graphics[9, 5] and geometric modeling[15], to robot motion planing [1, 24], biomedical applications [16], vision [53] and imaging [11]. These properties also explain why distance appears so natural and intuitive method for describing the material properties, but the power and the limitation of the approach are not obvious. We shall see later that, in fact, the distance-based approach to material modeling is also complete in the sense that it allows modeling of any and all material functions.

Two possible difficulties may arise in relying on distance fields: computational cost and loss of differentiability at equidistant points. When a set S is represented using n geometric primitives, it is reasonable to expect that the distance from a point p to S should be computable in $O(n)$, or even $O(\log n)$ if S is represented using some hierarchical structure. But unfortunately, computing the distance from p to a single geometric primitive (typically a curve or surface) usually requires a numerical iterative procedure [27]. At the same time, loss of differential properties may undermine some computational techniques and may not be acceptable in many engineering applications. 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.

Both of these limitations of the exact distance fields may be overcome 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 m-th order approximations in the following sense, originally described by Rvachev [38]. Suppose point p is a point on the boundary of set S, and ν is a unit vector pointing away from S towards some points that are closer to p than to any other point in S. In other words, ν coincides with unit normal on smooth points of the boundary, but the notion of the normal direction is also well defined at sharp corners. A suitable m-th order approximation of u is a function ω that is obtained by requiring that only *some* of the higher order derivatives vanish, that is for all points p on the boundary of S:

$$\frac{\partial \omega}{\partial \nu} = 1; \frac{\partial^k \omega}{\partial \nu^k} = 0; k = 2, 3, \ldots, m \tag{1}$$

Such a function ω is called *normalized*[2] to the m-th order. Normalized functions behave like a distance function near its zero set (corresponding to the boundary of set S) and tend to smoothly approximate the distance function away from S. However, normalization is a local property and cannot guarantee that the function behaves as the distance function away from the boundary points. Figure 2(b) shows an approximate distance field for the same S-curve normalized to

[2]This terminology is consistent with the term *normal* function that is often used synonymously with the distance function.

the first order. A higher order of normalization implies better approximation of the exact distance field, particularly near the boundary of S.

Normalized approximate distance fields exists for virtually all geometric objects of interest in engineering[45] and may be constructed by a variety of methods. In particular, the theory of R-functions [44, 38] offers a systematic and algorithmic method for constructing such functions automatically for curves, surfaces, and solids. This method was used to construct the field in Figure 2(b), as well as the approximate distance field for the 4th-order B-spline surface normalized to the second order shown in Figure 2(c). The implicit procedural method in [29] represents material properties by approximate distance fields constructed with Ricci functions [35] that smoothly approximate particular R-functions: $\min$ and $\max$. Many other choices of R-functions are available. Additional details on R-functions and implemented techniques can be found in [47, 4].

It should be apparent that normalized distance fields inherit most of the attractive characteristics of the exact distance field; they are also smooth on all points away from the boundary, but the accuracy of approximation and hence the uniformity of parameterization deteriorates as we move away from the point set of interest. In the remainder of the paper, the term 'distance field' will refer to any normalized distance field – either exact or approximate. We will also assume that a distance field may be constructed for any material feature. Such fields normalized to second order for the material features of the diamond tool are shown in Figure 3.

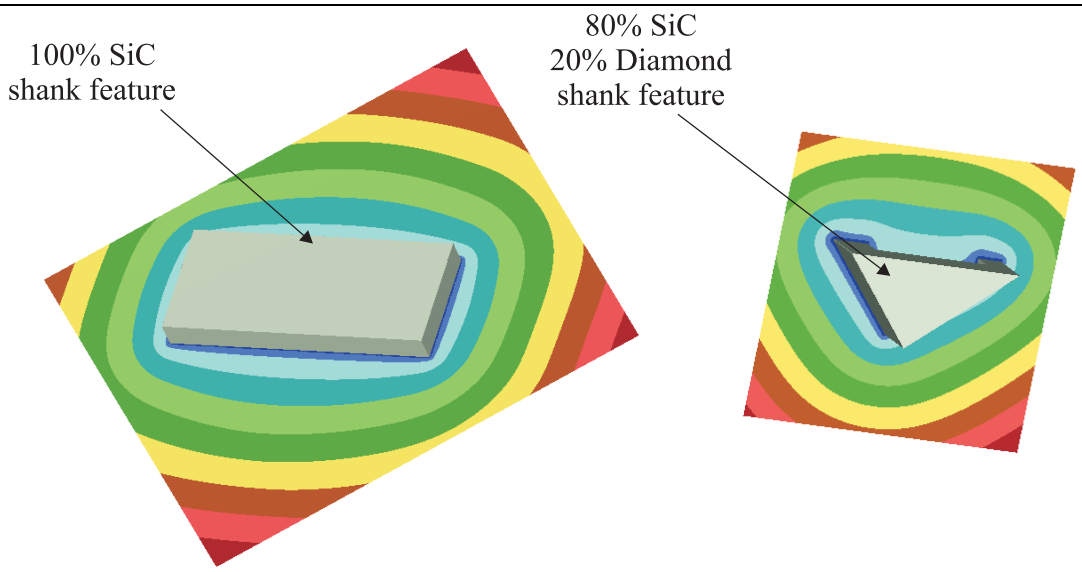


Figure 3: Approximate distance fields for two material features of the diamond cutter tool of Figure 1, are normalized to the second order, and the distance fields are shown on the midsection.

1.4 Outline

The rest of the paper is organized as follows. In section 2, we explain how the distance fields may be used to solve the material modeling problem in the presence of a single material feature. Using generalized Taylor series expansion by powers of a distance field, we show that any material function may be constructed to satisfy a variety of prescribed constraints. Section 3 extends the results of section 2 for the case of multiple material features by application of transfinite weighted interpolation. The interpolation technique remains meshfree because the weights are constructed using functions of distance fields. Composition of several materials and other vector-valued material properties are modeled as vector-valued material functions in Section 4. Possible extensions and open research issues are discussed in the concluding section 5.

Throughout the paper, we will use two-dimensional examples because they are much easier to understand and visualize. Unless explicitly stated, all constructions and techniques apply to the three-dimensional material modeling problem without any changes — as illustrated by several three-dimensional examples.

2 Single Material Feature

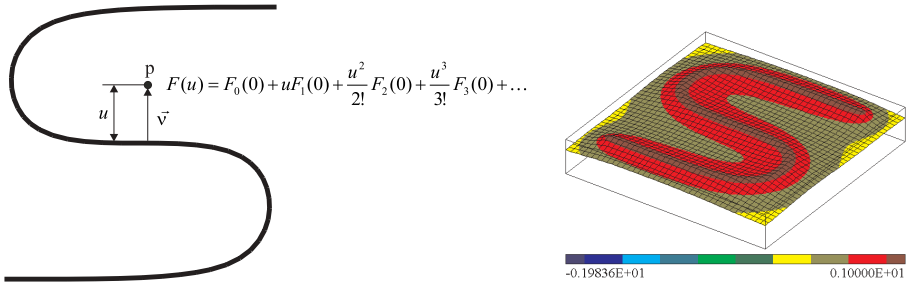
The simplest problem of material modeling involves a single material feature – a closed subset S with known material properties. We place no other restrictions on geometry, topology, or dimension of S; it may be a subset of a known solid, a part of the solid yet to be designed or an auxiliary geometry used as a reference datum for defining material distribution throughout the solid. It may be the only material feature or one of many material features that will be discussed in section 3. Following the discussion in the last section, we assume that S comes with a known normalized distance field u and material properties of S in a form of some material function $F_0(p),\ p \in S$. Below we show that any influence of such a feature may be extended and controlled throughout the space using distance to the feature as a parameter.

2.1 The Distance Canonical Form

In order to understand how the material properties may be controlled in terms of distance, let us suppose that we already constructed a desired material function $F(u, x, y, z)$ for the feature S. In general F may depend on any number of parameters in addition to spatial coordinates. Consider behavior of F as a function of distance u, while keeping all other variables fixed. By definition, for all points p of the boundary of material feature ∂S, $F(u(p)) = F(0)$ must be equal to the material conditions prescribed on S. As point p moves some distance away from the boundary of the feature S, we can express the value of $F(p)$ in terms of values and derivatives of $F(0)$ using the Taylor series expansion:

$$F(u) = F_0(0) + uF_1(0) + \sum_{k=2}^{m} \frac{1}{k!} F_k(0) u^k + u^{m+1}\Phi \tag{2}$$

This representation of a general field function was pioneered by Rvachev [38] and is illustrated in Figure 4. It is a straightforward generalization of the classical Taylor series, where the term $|x - x_0|$, measuring the distance to point x_0, is replaced by u, measuring the distance to a set of points S [37]. Thus, expression (2) is a representation of any function $F(u)$ as a polynomial in u of order m plus the remainder term $u^{m+1}\Phi$. The coefficients F_k in the classical Taylor series are kth order derivatives of function F with $F_0 = F(x_0)$. In Figure 4 we measure the change in the normal direction ν, and if the distance field u is normalized to mth order, then the corresponding Taylor coefficient F_k is kth partial derivative of F in the direction ν normal to the boundary of the material feature, with $F_0(0) = F(0)$. All coefficients $F_k(0)$ are evaluated on the boundary of S where $u = 0$, and $F_0(0)$ must coincide with the prescribed material distribution $f(p)$ on the boundary of the feature.



(a) (b)

Figure 4: (a) A material function F may be represented in the neighborhood of the material feature, in this case S-curve, by a Taylor's series expansion in the powers of a distance field u. (b) Material function $e^{-1.5u}$ is prescribed in terms of distance u to the S-shaped feature.

Based on the above generalized Taylor series expansion (2), an analogue of the classical Weierstrass theorem implies that any continuous material function on a solid may be approximated by a distance polynomial in u as closely as desired[40]. It is equally important that the distance polynomial expansion is unique and gives a systematic method for specification, construction, comparison, and modification of various material functions. Accordingly, we will refer to the generalized Taylor series form (2) as the *distance canonical form* for a material function. Practical use of this

form for material modeling amounts to selecting and controlling the coefficients of individual terms of the canonical form in order to satisfy design, analysis, or manufacturing constraints.

2.2 Explicitly defined material functions

Many material functions have been described in literature explicitly as functions of distance, based on experimental data or analytical studies [26, 3]. Any such material function of distance may be put in the canonical form by straightforward repeated differentiation with respect to the distance variable. For example, suppose the material function is known to be $F(u) = e^{(-1.5)u}$ (exponential material functions have been used to control the shear modulus in order to improve strength and bonding properties [3]). The first four terms of the corresponding distance canonical form are obtained by straightforward application of (2) as

$$F(u) = e^{(-1.5)u} = 1 - 1.5u + \frac{(-1.5)^2}{2!}u^2 + \frac{(-1.5)^3}{3!}u^3 + u^4\Phi,$$

where the last term is the unknown $O(u^4)$ remainder term. Each of the four terms is a function of $u^k, k = 0, 1, 2, 3$ and are shown in Figure 5. As $k \to \infty$, the series approaches the original function. But only a small number of terms may be needed in practical situations. For example, approximations of material functions $e^{(-1.5)u}$ using the first two terms and the first four terms respectively are shown in Figure 6. The same expansion and approximation procedure may be applied to any sufficiently smooth material function.

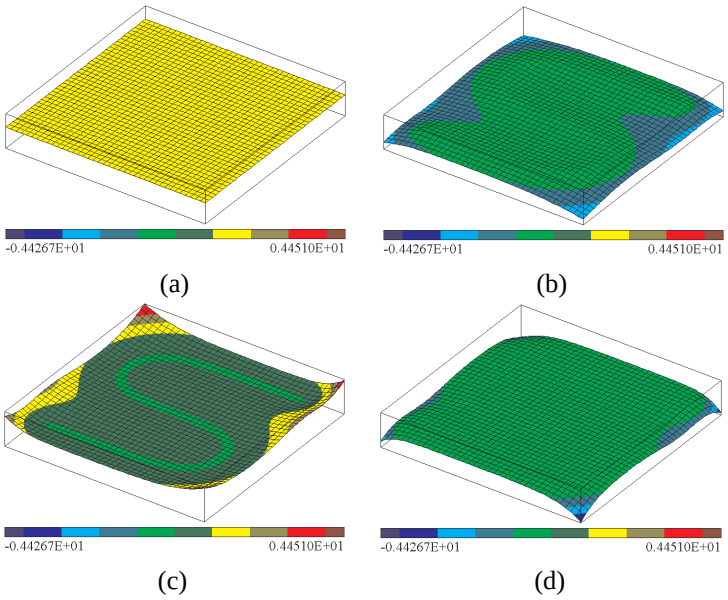
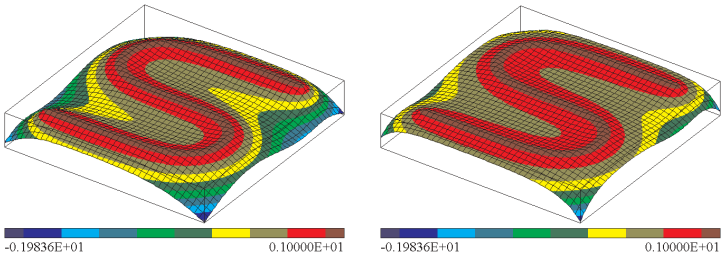


Figure 5: Terms in the distance canonical form of $F(u) = e^{(-1.5)u}$. (a) First term 1. (b) Second term $(-1.5)u$. (c) Third term $\frac{(-1.5)^2}{2!}u^2$. (d) Fourth term $\frac{(-1.5)^3}{3!}u^3$

Recall that the coefficients of the power terms in the distance canonical form correspond to the derivatives of $F(u)$ in the direction ν normal to the boundary of the feature S. For example, in the canonical form of the exponential function F above, the value of F on the boundary is $F_0 = 1$, the first derivative in the normal direction is $F_1 = -1.5$, the second derivative $F_2 = (-1.5)^2$ and so on. This immediately suggests a general method for specifying and controlling an arbitrary material function in terms of its behavior on the boundary of the material feature, namely by the values of the material function and its derivatives up to desired order in the direction of the outward normal to the boundary. When these values are constants, syntactic substitution into the distance canonical form yields the desired material function.



(a) (b)

Figure 6: Approximation of the material function $e^{(-1.5)u}$ shown in Figure 4(a) by the sum of generalized Taylor series terms shown in Figure 5: (a) First two terms $1 + (-1.5)u$. (b) First four terms $1 + (-1.5)u + \frac{(-1.5)^2}{2!}u^2 + \frac{(-1.5)^3}{3!}u^3$.

In some applications, it may be desirable to vary both the material function and its normal derivatives throughout the material feature. Suppose $F_0 = F_0(p)$ is a given material distribution on the feature S and its normal derivatives are prescribed on the boundary of S as $F_k = F_k(p)$. One might be tempted to construct the material function as

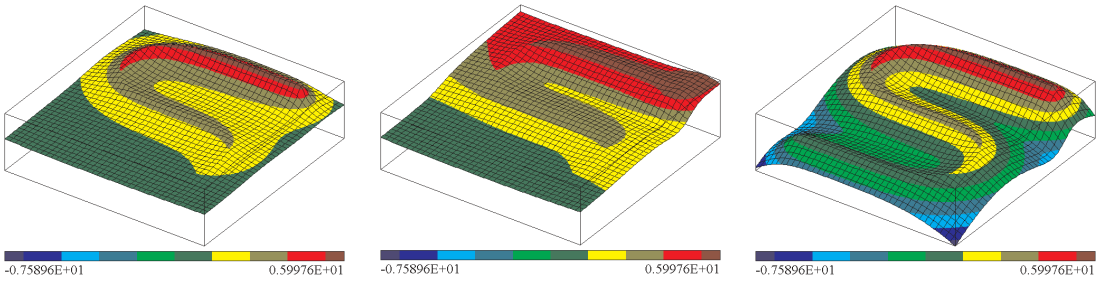
$$F(u) = F_0(p) + F_1(p)u + \frac{1}{2}F_2(p)u^2 + \frac{1}{6}F_3(p)u^3 + \ldots + u^{m+1}\Phi, \tag{3}$$

but this could be incorrect. For example, the first derivative of $F(u)$ at $u = 0$ yields $\frac{\partial F_0(p)}{\partial \nu} + F_1(p)$, which is equal to F_1 only if $\frac{\partial F_0}{\partial \nu} = 0$. Similarly, for $F_1(p)$ to qualify as the second coefficient in the canonical form, its derivatives in the normal direction must vanish or they will affect the values of the higher order terms in the canonical form. In other words, for the expression (3) to qualify as the distance canonical form (2), the coefficient of each term has to behave as a constant in the direction ν normal to the boundary. Formally, these conditions are identified in [38] as:

$$\frac{\partial^l F_k(p)}{\partial \nu^l}|_{u=0} = 0, \qquad (l = 1, 2, \ldots, m-k) \tag{4}$$

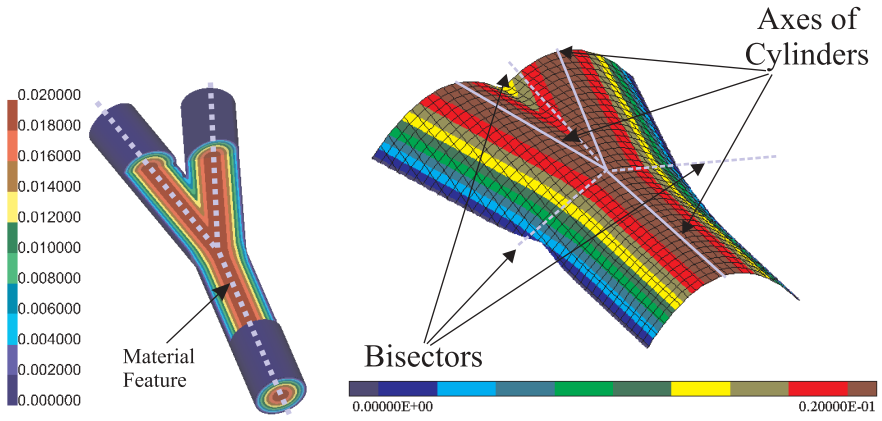
This requirement may appear to severely limit which functions may be prescribed by users or applications on the boundary of material features to serve as coefficients in the distance canonical form. Fortunately, every function $F_k(p)$ may be "conditioned" to satisfy the requirement (4) using a simple coordinate transformation $F_k^*(q) \equiv F_k(p - u\nabla u)$ proposed by Rvachev [38, 41]. If u is a normalized distance field, then in the neighborhood of the boundary, the conditioned function $F_k^*(q)$ returns the value of F_k at the closest point (p) on the boundary of the material feature. This implies that F_k and F_k^* have the same values on the boundary of the feature and that F_k^* behaves as constant in the neighborhood of the boundary in the normal direction ν. Additional details and examples, including a method to incorporate other types of directional derivatives, can be found in [41].

In Figure 7(a), function $F_0 = ye^{-1.5u}$ describes material variation on the material feature. The y direction coincides with the vertical direction of the letter S and corresponds to the direction of increasing values of F starting from 0 at the bottom of S. This function is not conditioned, because its first derivative is non-zero. Before we can prescribe derivative information, the function F_0 is conditioned through the coordinate transformation into another function F_0^* shown in Figure 7(b). The fact that the two functions agree on the points of the S-curve becomes clear in Figure 7(c) showing the material function $F = F_0^* - 4u$ after the gradient value of -4 is prescribed on all points of the curve. A three-dimensional example in Figure 8 shows a parabolic distribution of the graded refractive index (GRIN) within the Y-shaped solid. Many applications of GRIN are found in optical fibers for communication and precision lens for microoptics [26, 20]. In Figure 8, the material feature is the Y-shaped one-dimensional skeleton constructed as the union of the three axes of the cylinders. The refractive index is prescribed to vary as $(0.02 - 50u^2)$. This function is already conditioned because its derivatives vanish on $u = 0$ and no higher order derivatives are prescribed. It therefore qualifies as the first term of the distance canonical term. Figure 8(a) shows the resulting distribution with the distance field u normalized to the 12th order. Figure 8(b) shows a magnified planar section of the distribution, which is almost as uniform as with the exact distance field, but is also smooth everywhere including the points that are equidistant from the axes of the material feature.



(a) (b) (c)

Figure 7: Non-constant material function on a feature with derivative control: (a) material function $F_0 = ye^{-1.5u}$ is prescribed on the S-shaped feature; (b) conditioned function F_0^* agrees with F^0 on the feature but behaves as a constant function in the direction normal to the S-curve; (c) first derivative in the canonical form of the material function, $F_1 = -4$, is specified on all points of the curve in addition to its value F_0.



(a) (b)

Figure 8: Refractive index distribution of a radial GRIN Y-branching waveguide for optical communications. (a) Distribution $(0.02-50u^2)$ is specified explicitly for the Y-shaped one-dimensional skeleton. (b) Magnified distribution plotted as a surface over a 2D section: analytic everywhere away from the feature, including the points on bisectors where the exact distance field would not be differentiable.

2.3 Implicitly constrained material functions

Explicit control of material properties may not be adequate for a number reasons. Material distributions may not be specified in the closed form because they usually must follow complex physical laws and constraints for which closed form solutions are not available. The distance canonical form, and the associated explicit power series, provide only an approximation to a material distribution with at least three distinct sources of errors. By definition, as a Taylor series expansion, the distance canonical form represents the function locally, in our case near the boundary of the material feature. Secondly, explicit representation only approximates the material function when the remainder term is omitted. Finally, the accuracy of the distance canonical form depends on the accuracy of the distance field. Since we usually use only normalized (approximate) distance fields in order to assure differential properties, the accuracy of approximation may degrade substantially away from the feature.

Because the distance canonical form (2) applies to any and all functions, the remainder term may always be chosen to make the above inaccuracies arbitrarily small or to eliminate them altogether. The errors are measured against one or more constraints on the material function specified either by the user or an application. Such constraints could be local or global, and may include algebraic, differential, or integral conditions that implicitly define the material function. For most such constraints, the remainder term cannot be determined exactly; therefore we choose to represent the unknown function Φ in the remainder term $u^{m+1}\Phi$ by a linear combination

$$\Phi = \sum_{i=1}^{n} C_i \chi_i \tag{5}$$

of known basis functions χ_i from some sufficiently complete space, such as polynomials, B-splines, trigonometric polynomials, etc. Both errors and the basis functions χ_i are functions of spatial variables, and all modeling problems reduce to determination of the unknown coefficients C_i that satisfy the prescribed constraints on the material function either exactly or approximately.

Suppose we would like to constrain a material function $F(u)$ to behave as some continuous function $f(p)$ on points p away from the material feature. $F(u)$ already satisfies the material behavior on the feature; hence, the problem becomes one of minimizing the difference between $F(u)$ and $f(p)$ globally. The difference can be measured many different ways. For example, using the standard technique of least squares. In this case, we seek to minimize the integral

$$\int_\Omega (F(u) - f(p))^2 d\Omega = \int_\Omega \left(F_0(u) + uF_1(u) + \ldots + u^{m+1} \sum_{i=1}^{n} C_i \chi_i(p) - f(p) \right)^2 d\Omega \tag{6}$$

For a specific example, suppose a material function is defined explicitly as $F(u) = 1 - u^2$ on the S-shaped curve (see Figure 9(a)). As distance u increases, $F(u)$ quickly drops to 0 and then turns negative, which may not be desirable for some material properties. In order to keep the material function positive, we impose a global constraint that $F(u)$ must approximate the behavior of $f(p) = 1 - \frac{u}{1+u}$ globally. This function for the S-curve is shown in Figure 9(b). To compute the least square fit of $F(u)$ to $f(p)$, we choose functions $\{\chi_i\}$ to be a set of bi-cubic B-splines on a uniform Cartesian 81×81 grid. As is shown in Figure 9(c), the resulting function combines the benefits of the parabolic distribution near the S-curve feature and maintains positive values everywhere in space.

The problem of constructing material distribution given its values and derivatives on some point sets may be viewed as a problem of surface fitting, where surface is really a material distribution. Thus, the differential and integral constraints used in computer-aided geometric design of surfaces [18, 42, 41] may be handled in a similar manner using variational or other numerical methods. For instance, suppose we want to choose the remainder term so that $F(u)$ satisfies the differential constraint $\nabla F(u) = f(p)$. This means that we need to determine the coefficients C_i of the basis functions that minimize the functional $\int_\Omega (\nabla F(u) - f(p))^2 d\Omega$. Figure 9(d) shows the result computed using the least squares method for $f(p) = -2$ on the same 81×81 grid of bi-cubic B-spines. Note that the scale in Figure 9(d) is different from Figures (a) and (b) and clearly shows that $F(u)$ turns negative away from the material feature.

The above examples are also indicative of the computational machinery that is required for enforcing the constraints: differentiating the functions under the integral signs with respect to the unknown coefficients C_i, integrating them over the domain (usually represented by a solid model), and using the integrals to assemble a system of algebraic (often linear) equations in C_i. Solving for C_i and substituting $\sum_{i=1}^{n} C_i \chi_i$ for Φ in the distance canonical form (2)

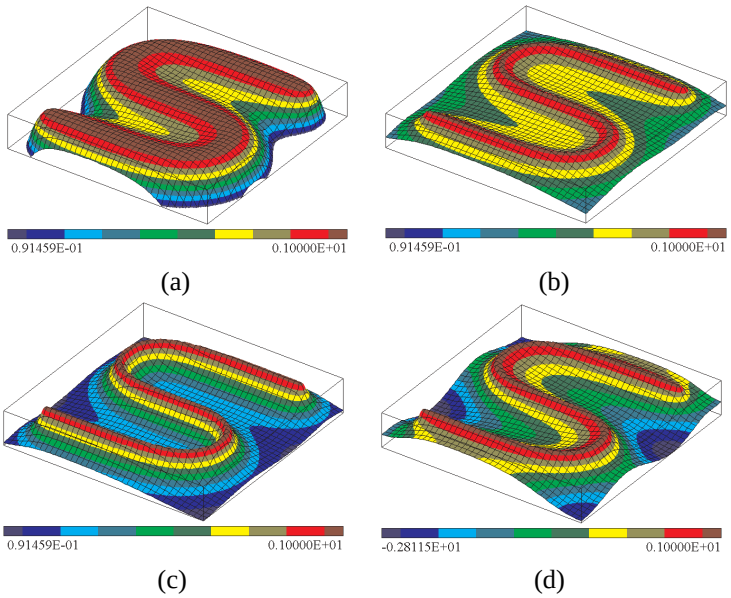


Figure 9: Constraints on material function can be enforced by approximating the residual; in this case using bi-cubic B-splines on a uniform Cartesian 81×81 grid. (a) Explicitly constructed material function $F(u) = 1 - u^2$; (b) Algebraic constraint function $f(p) = (1 - \frac{u}{1+u})$; as $u \to \infty$, $f(u(p)) \to 0$. (c) Least square fit of the material function in (a) to the constraint function in (b). (d) A function $F(u)$ that minimizes the functional $\int_\Omega (\nabla F + 2)^2 d\Omega$ with $F_0(u) = 1 - u^2$.

gives the desired material function. In contrast to the mesh-based methods, our approach does not require spatially conforming discretization. By construction, the canonical distance form (2) satisfies all prescribed material conditions on the material feature exactly. Integration and visualization over the solid may or may not require spatial discretization, depending on the basis functions and sampling method, but never a *conforming* discretization. In the context of material modeling, this independence of material representation from any particular mesh or spatial discretization, allows seamless integration of geometric and material modeling with effortless changes and intuitive control. One potential disadvantage of the distance-based method is that the constructed functions depend on the distance field of the material feature and hence are not known *a priori*; this means that differentiation of such functions must be performed at run time at some computational cost. Additional details on these and other computational utilities can be found in [55].

3 Multiple Material Features

A more typical situation with heterogeneous materials involves several material features $S_i,\ i = 1, \ldots, n$ with known but distinct material characteristics. For example, recall that the diamond cutter tool discussed in section 1.1 relies on two material features with distance fields shown in Figure 3. Another simple two-dimensional example is shown in Figure 10. Given material value P_0^i and derivative information $\{P_k^i\}$ on the ith feature S_i, we can construct individual material functions P^i using the distance canonical form and techniques of the last section. In this section, we show that these individual material functions may be combined into a single material function $P^\square(P^1, P^2, \ldots, P^n)$ in a meshfree manner while preserving the exactness, completeness, and intuitiveness of the distance-based representation scheme.

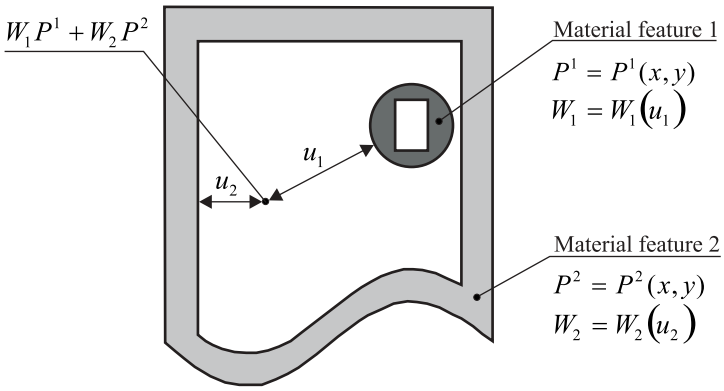


Figure 10: Example of material interpolation problem: construct a material function that combines material functions of individual features.

3.1 Transfinite interpolation

As stated above, the problem is not well defined, because there are many different ways to "combine" individual material functions. At the very least, the combined material function must preserve the values and derivatives specified on each material feature. In other words, $P^{\square}$ must *interpolate* the values and derivatives of P^i on every feature S_i. When S_i themselves are sets of points (curves, surfaces, solids), the interpolation is called *transfinite*. The most common form of interpolation relies on a convex combination of P^i

$$P^{\square}(p) = \sum_{i=1}^{n} P^i(p) W_i(p),\ i = 1, \ldots, n, \tag{7}$$

with each weight function W_i controlling the influence of the material function associated with feature S_i. The desirable properties of the weights W_i are well known [18, 41]:

- The requirement that $P^{\square}(p) = P^i(p)$ for points on the ith material feature implies $W_i(p) = \delta_{ij}$. In other words, each $W_i(p)$ should be identically 1 on points $p \in S_i$ and should be identically 0 for points $p \in S_j,\ j \neq i$ (points on the other material features.)
- Completeness of the interpolation method in terms of its ability to reproduce constants and polynomials require that the weight functions $W_i(p)$ form a partition of unity in the sense $\sum_{i=1}^{n} W_i(p) = 1, 0 \leq W_i(p) \leq 1$.
- The weight functions W_i should be as smooth as needed to assure the smoothness of properties of the combined function $P^{\square}$.
- The weights should have intuitive meaning in order to control the influence of individual material features relative to each other.

In principle, various interpolation techniques, for example those that have been studied extensively in computer-aided geometric design[18], could be used to solve the material interpolation problem. But the ideal interpolation method should not require spatial discretization of the domain and should handle material features of arbitrary shape, topology, and dimension. Below we propose such a method for transfinite interpolation as an extension of the technique described in [41]. The key ingredient is once again the normalized distance field because it abstracts the geometric and topological details of the material features while providing a convenient parameter (distance) for intuitive and meshfree interpolation.

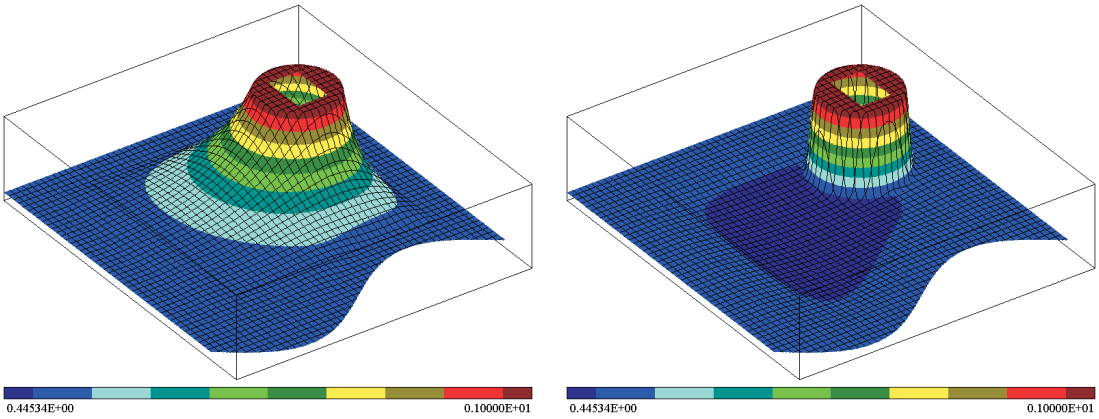
3.2 Inverse Distance Weighting

Perhaps the most popular method for designing weight function $W_i(p)$ is based on the distance from p to the source feature S_i that is responsible for the material function P^i. For example, in Figure 10, if the distance $u_1(p)$ from

material feature S_1 is greater than the distance $u_2(p)$ from material feature S_2, then it may be desirable to expect that $W_1(p) > W_2(p)$ because S_1 should also have a larger influence than S_2 at point p. In other words, the weight $W_i(p)$ should be inversely proportional to some power of distance $u_i^k(p)$. Normalizing by the sum of all weights so that each weight function varies between 0 and 1, yields

$$W_i(p) = \frac{u_i^{-k}(p)}{\sum_{j=1}^{n} u_j^{-k}(p)} = \frac{\prod_{j=1;j\neq i}^{n} u_j^k(p)}{\sum_{j=1}^{n} \prod_{j=1;j\neq i}^{n} u_j^k(p)} \tag{8}$$

It is straightforward to check that the weights $W_i(p),\ i = 1,\ldots,n$ satisfy all of the postulated properties; the last expression on the right provides an equivalent but numerically more stable form. The resulting method of interpolation is known as the inverse distance weighting, or as Shepard's method when used for scattered data interpolation [49, 23]. Figure 11(a) shows inverse distance interpolation for the problem in Figure 10 with first-order normalized distance fields and $k = 1$.

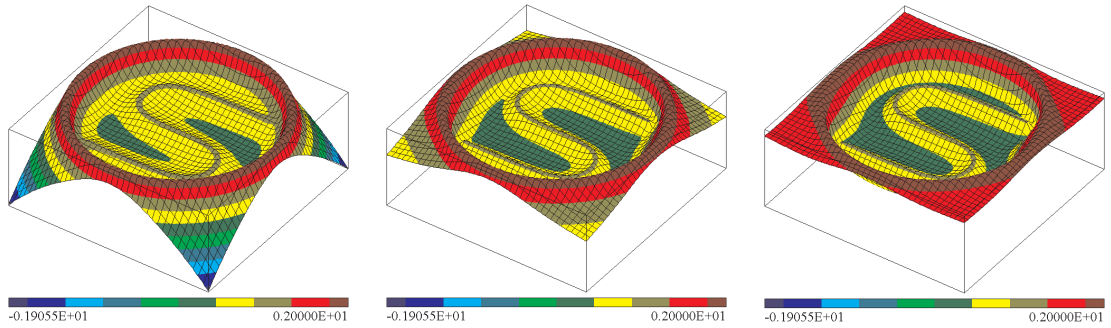


(a) (b)

Figure 11: Transfinite interpolation of the material functions in Figure 10: specified material properties $P^1 = 1$ and $P^2 = 0.5e^{-u_2^2}$ are interpolated using first-order normalized distance fields. (a) Inverse distance interpolation; (b) weighted inverse distance interpolation with influence functions with $\lambda_1 = e^{60u_1}$ and $\lambda_2 = 1$.

It is well known that the exponent k of the term u_i^k controls the smoothness of the function on the points of the material feature S_i where $u_i(p) = 0$ [18]. In particular, the power k should exceed the highest power of the term P_k^i in the canonical distance form (2) for the material function P^i [41]. In general terms, $P^{\square}$ and P^i have the same values of derivatives in any direction up to the order $k-1$ at the i-th feature, and this property does not depend on how P^i was constructed. The inverse distance weight (8) can also accommodate different exponents (and smoothness) for each material feature by replacing terms u_i^k with $u_i^{k_i}$. An example is shown in Figure 12. Material functions associated with the two features are interpolated using inverse distance weight with different degree of smoothness: $k_2 = 1$ on the circular ring, but k_1 for S-curve feature varies. In Figure 12(a), $k_1 = 1$ means that the derivatives on the S-curve are not preserved by the interpolation. Figure 12(a) shows the interpolated function with $k_1 = 2$ which guarantees that the first derivatives on the S-curve are now interpolated exactly at all points. Finally, raising $k_1 = 3$ even further has the effect of flattening the material function on S-curve thereby diminishing the zone of its influence.

Inverse distance weighting is simple, intuitive, and in many ways natural. For example, when $k_1 = k_2 = 1$, the inverse distance weights W_i for two material features are respectively $W_1 = u_2/(u_1 + u_2)$ and $W_2 = u_1/(u_1 + u_2)$. When the features are isolated points and u_i are exact distances, W_1 and W_2 are the barycentric coordinates of the line segment through the points. For arbitrary material features, these weights implement the linear interpolation between the material functions on individual features, such as that shown in Figure 1. Additional details and examples of the transfinite interpolation using inverse distance weighting can be found in [41].



(a) (b) (c)

Figure 12: Inverse distance interpolation of two material functions with derivative control: $P^1 = 1-1.5u$ is associated with the S-curve and $P^2 = 2$ is associated with the circular ring. (a) $k = 1$ for the S-curve and no derivative control; (b) $k = 2$ means that the first derivatives on S-curve are interpolated exactly; (c) $k = 3$ further decreases the influence of the S-curve feature

3.3 Weighted and Constrained Interpolation

The weight W_i is the primary means for describing the contribution of the material function P^i associated with the material feature S_i. In essence, the *relative* influence of these weights describes the global material property law, and the inverse distance weighting is only one of many possible ways to construct the weight functions W_i. A more general method for constructing the weight functions associates an *influence* function $w_i(p)$ with each material feature. Then each weight function W_i of the material feature S_i is simply the normalized influence function

$$W_i(p) = \frac{w_i(p)}{\sum_{j=1}^{n} w_j(p)}. \tag{9}$$

Selecting the influence functions in the form $w_i = u_i^{-k}$ yields the inverse distance weights (8). Other choices of influence functions would result in other material property laws. For example, if all influence functions are set $w_i(p) = 1,\ i = 1, 2, \ldots, n$, then the weight functions become $W_i = 1/n$ and the linear combination (7) of material functions becomes a weighted average of the individual functions P^i. The latter example shows that not every choice of influence functions is appropriate, because the resulting weight functions $W_i(p)$ may not satisfy the requirements postulated above in section 3.1.

Since most global material property laws are likely to be expressed in terms of influences of individual material features, it is convenient that the influence functions w_i themselves should be functions of distance. For example, choosing influence functions $w_i(p)$ in the form of $(\lambda_i(u_i)u_i)^{-k}$, with $\lambda_i > 0$, generalizes the inverse distance interpolation into a *weighted* inverse distance method. The latter allows a more precise control of how the influence of a particular feature S_i diminishes with increase in distance u_i. Popular choices of the influence coefficients λ_i include exponential functions, polynomials with local support, cubic splines and trigonometric functions [23]; other choices are possible depending on the application. A straightforward computation confirms that the resulting weight functions W_i satisfy all postulated requirements. Specifically, $W_i(p) = \delta_{ij}$, $\{W_i(p)\}$ form the partition of unity, $W_i(p)$ is differentiable up to the order $k-1$ at the material feature S_i and interpolates derivatives of specified P_i up to the order $k-1$.

An example of transfinite interpolation with influence coefficients $\lambda_1 = e^{60u_1}$ and $\lambda_2 = 1$ respectively for the two material features in Figure 10 is shown in Figure 11(b). The influence zone of the material feature 1 is diminished substantially in comparison to its influence zone in Figure 11(a) where $\lambda_1 = \lambda_2 = 1$. A three-dimensional material modeling example is shown in Figure 13. 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. The weighted inverse distance interpolation using first-order normalized distance fields is shown in Figure 14.

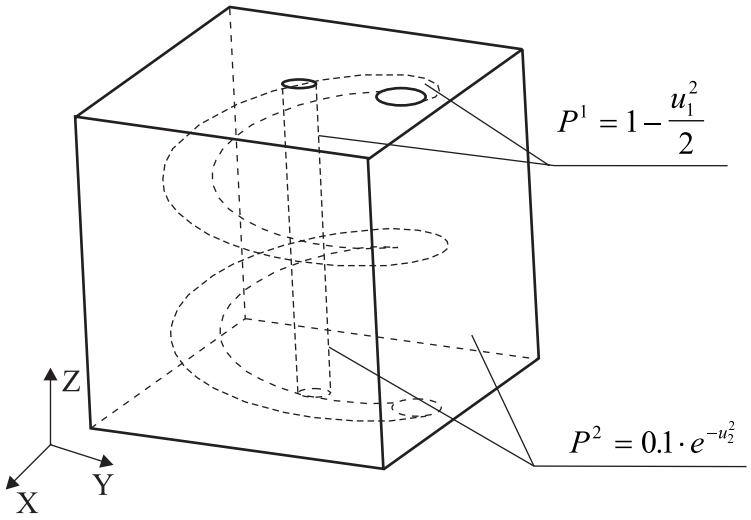
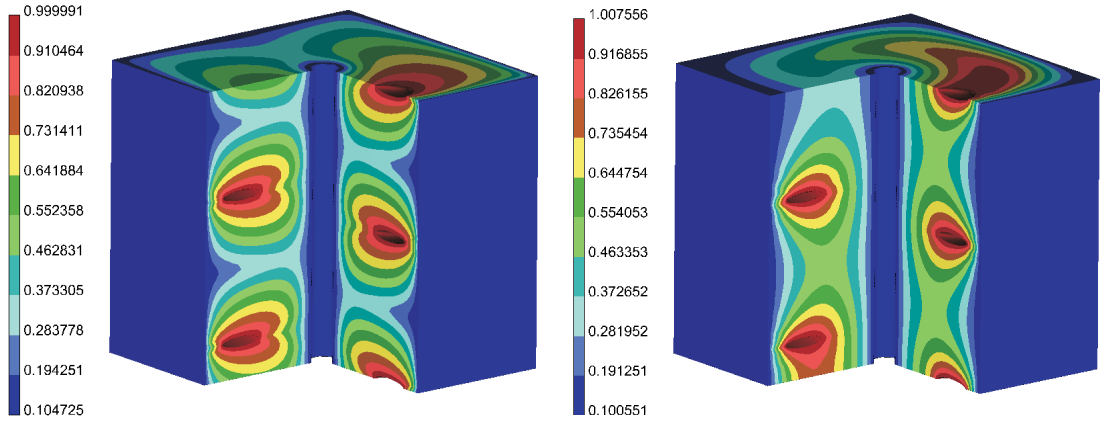


Figure 13: Three-dimensional material modeling problem requires constructing a material function for the solid from the material functions associated with the two features as shown.



(a) (b)

Figure 14: Transfinite interpolation of the material features in Figure 13: (a) Inverse distance interpolation. (b) Interpolation of (a) further constrained to satisfy the Laplace equation.

In the above discussion of transfinite interpolation methods we made no assumptions on the form of material functions P^i associated with individual features. They can be represented as known functions of the distance field $P^i(u_i)$ or of spatial variables $P^i(x, y, z)$, by the canonical distance form with or without the remainder term, explicitly or implicitly. In all cases, the transfinite interpolation method provides *explicit* means for combining the material functions into a single global function $P^{\square}(p)$. This means that, in addition to possible inaccuracies in individual P^i, the transfinite interpolation itself has a limited precision for the reasons we already discussed in section 2.3. Once again, the constructed interpolating function $P^{\square}(P^1, P^2, \ldots, P^n)$ may be adjusted to satisfy a variety of additional constraints. Without loss of generality, let P^i be represented by the first m_i terms of the distance canonical form (2), and $P^{\square}$ is a transfinite interpolation (7) of $P^i,\ i = 1, \ldots, n$. It is shown in [40] that representation in the form

$$F = P^{\square} + \Phi \prod_{i=1}^{n} u_i^{m_i} \tag{10}$$

is complete in the sense of Weierstrass theorem, and therefore includes every admissible material function. The second term is essentially a product of the remainder terms for each individual material function P^i. The power m_i of u_i indicates that derivatives up to order $m_i - 1$ have been satisfied on the ith material feature. The unknown function Φ can be represented by a linear combination of basis function (5) with coefficients C_i chosen to satisfy the desired constraints. For example, Figure 14(b) shows the material function in Figure 14(a) constrained to approximate the Laplace's equation $\nabla^2 F = 0$. The shown material function was computed using the Ritz method via minimization of the functional

$$I = \iint_{\Omega} \left(\nabla \left(u\Phi\right)\right)^2 d\Omega + 2 \iint_{\Omega} \nabla \left(u\Phi\right) \nabla P^{\square} d\Omega$$

over the shown solid. In this case, the unknown function Φ was represented by a linear combination of tensor-product (tri-cubic) B-splines defined over a $31 \times 31 \times 31$ uniform (non-conforming) Cartesian grid. It should be clear that both interpolation and approximation of the constraint can be computed in a meshfree manner.

4 Vector Valued Material Properties

4.1 Constraints on scalar components

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 [21]. In all cases, the vector valued material function $\mathbf{F} : E^3 \rightarrow M$ where M is usually an application specific manifold. Locally every manifold can be viewed as a copy of R^n, and we can consider $\mathbf{F}(p)$ to consist of a finite number of scalar component material functions $(U(p), V(p), W(p), \ldots)$.

Each scalar component function can be treated independently using the techniques of sections 2 and 3, but the component functions are also constrained by the manifold M. For example, when $\mathbf{F}$ represents orientation of the material grain, $\mathbf{F}(p)$ must be a unit vector at every point $p \in E^3$. When $\mathbf{F}$ represents composition of several materials, each component function models a fraction of the total volume, and the sum of all components must be equal 1 at every point of space (recall the diamond cutter example in Figure 1). Many other and multiple constraints are possible depending on the properties of the manifold space M.

A general approach to modeling a vector material function with n components subject to k constraints is to construct $n-k$ components separately and then use the constraints to solve for the remaining k component functions. For example, if $\mathbf{F}(p) = (U(p), V(p), W(p))$ is a unit vector function, we can construct $U(p)$ and $V(p)$ to be sufficiently smooth functions with values in the range $(-1, 1)$ and define $W(p)^2$ to satisfy $1 - U(p)^2 - V(p)^2$. On the other hand, if $U(p)$ and $V(p)$ are volume fractions used in material composition, then we can define the third fraction as $W(p) \equiv 1 - U(p) - V(p)$ in order to enforce the constraint. There are two potential difficulties with this approach:

Existence: even when the solution to the constrained problem exists, it may be difficult to compute, and it may be invalidated if the component functions are constructed separately without additional constraints. Clearly, it makes no sense to impose the unit vector constraint if one of the component functions exceeds the value of 1.

Uniqueness: in general, there is no reason to expect that the above method of construction of $\mathbf{F}$ is unique. In the case of material composition modeling, if we construct $V(p)$ and $W(p)$ first, there is no reason to expect that $U(p) = 1 - V(p) - W(p)$ is the same component function that we would get if we were to model $U(p)$ directly first.

Material modeling techniques that do not guarantee existence and uniqueness of the solution are of questionable value, because they are not likely to reflect realistic physical conditions. It is also clear that these issues have to be resolved in the context of specific applications. When a vector function $\mathbf{F}(p)$ is a solution of a boundary value problem, its existence and uniqueness follow directly from the classical conditions on well-posed problems [10]. In this case, $\mathbf{F}(p)$ can be constructed by approximating the (vector-valued) remainder term in the distance canonical form using the meshfree techniques described in section 2.3 and 3.3. The same theoretical results also guarantee the completeness of the solution [39, 40]. In the following section, we establish sufficient conditions for existence and uniqueness of the material composition modeling using normalized distance fields.

4.2 Material Composition Modeling

In a general case, the material volume of a solid is composed from m different materials. The fraction of each material at every point p of the solid is represented by a scalar material component function $P^{\square,j}(p),\ j = 1, 2, \ldots, m$. In other words, the challenge is to construct a vector valued material function with the constraint that its scalar components must form a partition of unity:

$$\mathbf{P}(p) = (P^{\square,1}, P^{\square,2}, \ldots, P^{\square,m}) \text{ such that } \sum_{j=1}^{m} P^{\square,j} = 1 \tag{11}$$

Each jth material function $P^{\square,j}(p)$ must interpolate the material functions $P^{i,j},\ i = 1, 2, \ldots, n$ associated with n material features of the solid using some weight functions W_i. If each scalar component function $P^{\square,j}$ is constructed separately, then satisfying the partition of unity constraints appears non-trivial in general. We now show that when the weights W_i satisfy the conditions postulated in section 3.1, the interpolated scalar component functions preserve the partition of unity property if it is satisfied by the individual feature functions $P^{i,j}$.

Theorem 1 *Let $P^{i,j} \geq 0$ be jth material fraction function associated with the ith feature and let the material fraction function $P^{\square,j}$ be constructed as a convex combination of $\{P^{i,j}\}$ with the same weights W_i for every feature as*

$$P^{\square,j} = \sum_{i=1}^{n} P^{i,j} W_i, \quad j = 1, 2, \ldots, m$$

Then

$$\sum_{j=1}^{m} P^{\square,j} = 1 \qquad \text{iff} \qquad \sum_{j=1}^{m} P^{i,j} = 1$$

The proof follows from the straightforward application of the definitions of the weighted interpolation and the requirement that the weights themselves form a partition of unity. Let us sum all global m material fraction functions:

$$\sum_{j=1}^{m} P^{\square,j} = \sum_{j=1}^{m} \sum_{i=1}^{n} P^{i,j} W_i = \sum_{i=1}^{n} \left(\sum_{j=1}^{m} P^{i,j} \right) W_i = \sum_{i=1}^{n} W_i = 1$$

The practical consequence of this theorem is a broad applicability of the proposed approach to material composition modeling. For example, in the case of diamond cutter example of Figure 1, constant fractions of two materials, SiC and diamond, are prescribed on two features: 0.2 and 0.8 on the first feature and 1.0 and 0.0 on the second feature. Each of the constant fraction correspond to the first terms in the distance canonical forms for the respective material fraction functions, implying that

$$P^{1,1} = 0.2,\ P^{1,2} = 0.8,\ P^{2,1} = 1.0,\ P^{2,2} = 0.0$$

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). The above theorem guarantees that 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. In fact, we only need to construct one of the two functions, say $P^{\square,1}$. The theorem guarantees that material function $P^{\square,2} = 1 - P^{\square,1}$ is identical to the one that is constructed directly with inverse distance weighting.

A more complex example is shown in Figure 15 where composition of three materials is defined over the two-dimensional shape with 2 material features in Figure 10. For each feature, three distinct material fraction functions are constructed using techniques of section 2, making sure that these functions form a partition of unity. Figure 15(a) shows the result of inverse distance interpolation between the two features, applied to each of the three materials. Figure 15(b) shows another interpolation, this time with different influence coefficients prescribed on each feature. In all cases, the results do not depend on the order in which the functions are constructed, and the partition of unity condition is guaranteed by the above theorem.

5 Conclusions

5.1 Advantages of modeling with distance fields

In retrospect, it seems surprising that distance fields have not played a more prominent role in computer aided design and analysis. With the exception of [13], distance fields do not seem to appear in most classifications of the representation schemes for solid models, even though they have been used in many fundamental geometric algorithms, such as blending [36] and medial axis transform [56, 7]. The two most likely reasons for this omission are the preoccupation of the solid modeling community with homogeneous solids and treatment of field problems as a separate discipline. In fact, distance fields may not be computationally convenient as a representation scheme because they do not offer local control or global guarantee of validity, as defined in [34]. But the distance field is also an *intrinsic property* of any unambiguously represented shape, and as such, does not really need to be represented separately. It is unique for any closed set, captures all its topological properties, and establishes the direct link between geometric and field modeling.

In the context of material modeling, we showed that 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. We conjecture that the practical methods described in this paper are sufficient for handling most applications involving heterogeneous materials. Other generalizations are straightforward. For example, we focused on Euclidean distance, but other distance measures, such as distance measured along a curve[50], surface, or using a different norm, may be more appropriate in some applications. The technical assumption that the material features are disjoint is not a limitation of the approach: whenever the features overlap their corresponding material functions must either agree or becomes discontinuous (for example when there is a discrete transition in material properties). Interpolating such discontinuities does not require special handling[41].

Parameterization of material functions by distances leads to a compact, canonical, and unique representation scheme for fields defined over geometric domains. To recap our findings, every field function over a set of material features may be represented by specifying:

- A normalization order for a normalized distance field (1) associated with each feature;
- Finite number of Taylor coefficients (constants or functions) in the distance canonical form (2) for each feature;
- An influence coefficient (constant or function) and distance exponent for every feature to be used in weights (9) for transfinite interpolation;
- Constraints on features or interpolated function;
- A finite number of linearly independent basis functions $\{\chi_i\}$ for representation (5) of function Φ in the remainder term.

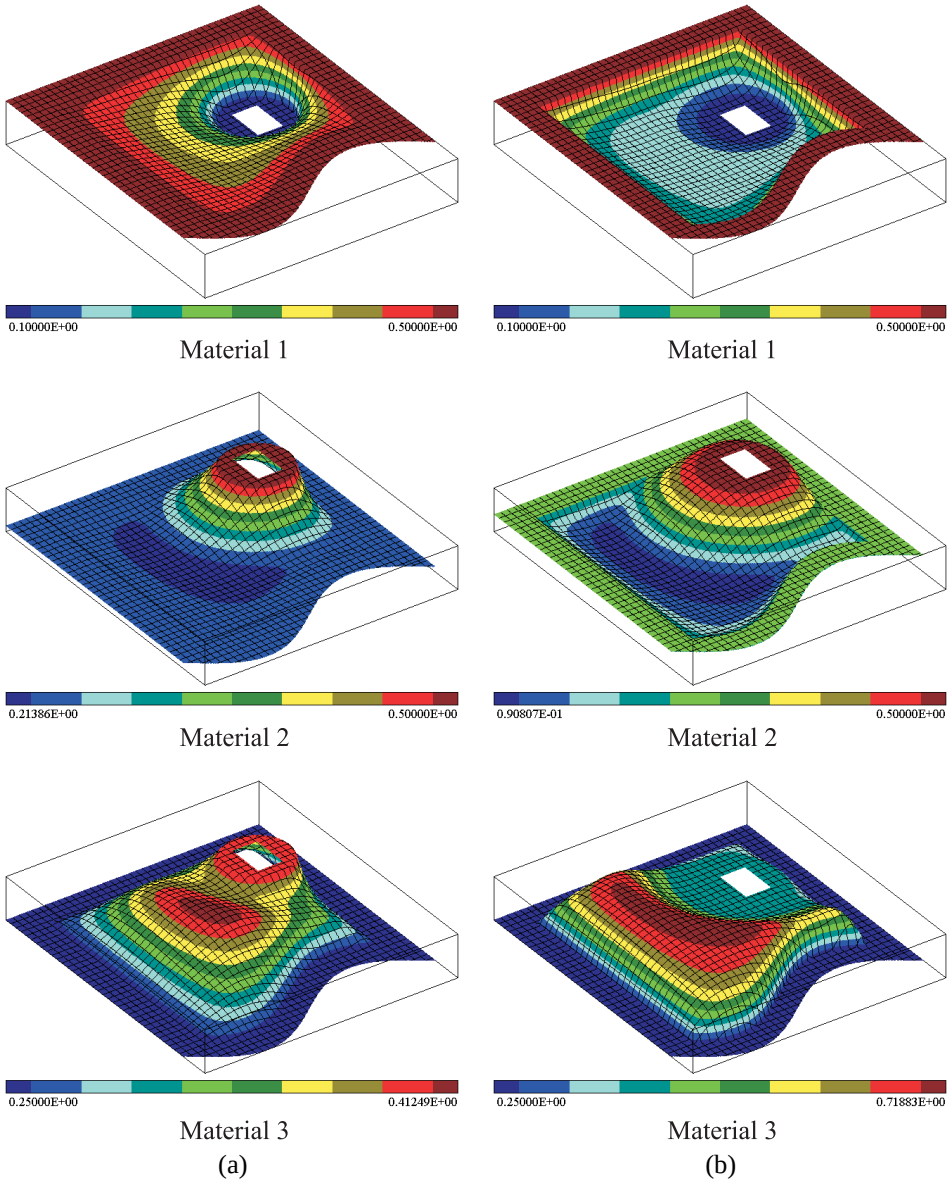


Figure 15: Composition of 3 materials over 2 material features in Figure 10. Material fraction functions associated with feature 1: $P^{1,1} = 0.5e^{-u_1^2}$; $P^{2,1} = 0.25$; $P^{3,1} = 1 - P^{1,1} - P^{2,1}$; Material fraction functions associated with feature 2: $P^{1,2} = 0.1(1 - 0.1u_2^2)$; $P^{2,2} = 0.5e^{-u_2^2}$; $P^{3,2} = 1 - P^{1,2} - P^{2,2}$. (a) Global material fraction functions constructed using inverse distance interpolation; (b) Global material fraction functions constructed using weighted inverse distance interpolation with distinct influence functions for each feature: $\lambda_1 = (0.1 + 10e^{-5u_1^2})$ and $\lambda_2 = (0.5 + e^{\frac{-u_2^2}{2}})$

This relatively compact representation specifies the desired material function *implicitly* as an element of a space of functions. Yet this representation can be considered unambiguous and unique in the sense that all functions satisfying this specification are practically indistinguishable. Indeed, in many cases, for example when the distance field is exact, or when the constraints correspond to a well-posed boundary value problem, the specified material function is unique. Thus, such a representation of material functions provides a basis for systematic design, analysis, comparison, and control of material functions, and is nearly ideal for use in data exchange standards [32, 30]. Like other 'unevaluated' representations, some queries on this representation may be relatively expensive, but this drawback fades away in comparison to the numerous advantages of the approach: flexible, intuitive, and independent control of material and/or geometric properties, freedom from spatial discretization and associated errors, and guaranteed completeness and analytical properties.

5.2 Extensions and promising directions

We have downplayed the issue of computing the (normalized) distance fields, not because it is not important, but because these computations may be performed by different means without affecting the fundamental formal properties of the proposed approach. The two most common approaches to representing distance fields are procedural (often using a numerical algorithm)[27] or by explicitly constructing the distance function. The procedural approach is problematic because it is likely to be expensive and may undermine the required analytic properties. The explicit exact distance fields can be constructed for simple domains (for example, linear polygons), but must be approximated for more general pointsets. Fortunately, the theory of R-functions provides a suite of systematic and automatic methods for constructing normalized fields of any order for semi-analytic sets [38, 44, 45, 47]. The task may be non-trivial for some parametric curves and surfaces, but is always possible as witnessed by examples in this paper; for details see [4].

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.) satisfy our definitions of material functions that are defined by boundary conditions and constrained by suitable differential equations. It should not come as a surprise that the approach to material modeling and all our results apply without modifications to any and all field problems arising in engineering analysis. In fact, much of the present work is an outgrowth of the earlier efforts on meshfree analysis and simulation [39, 40, 41, 48], and we have relied extensively on the computational utilities developed originally for that purpose [55]. The material functions are constructed directly from the native geometry, without meshing, and are guaranteed to be as smooth as desired. 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.

Bridging the gap between the geometric and field modeling via distance fields opens many new exciting possibilities in integrated shape-material modeling. Material features, and geometric models in general, are usually parameterized by engineering parameters. Through changes in geometry, these parameters indirectly control the distance fields, and therefore, all distance-based material and field constructions. On the other hand, the geometric domain itself may also be defined implicitly by a threshold of the constructed material density function[2]. 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.

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