Computer-Aided Design of Porous Artifacts

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Abstract

Heterogeneous structures represent an important new frontier for 21st century engineering. Human tissues, composites, “smart” and multi-material objects are all physically manifest in the world as three-dimensional (3D) objects with varying surface, internal and volumetric properties and geometries. For instance, a tissue engineered structure, such as bone scaffold for guided tissue regeneration, can be described as a heterogeneous structure consisting of 3D extra-cellular matrices (made from biodegradable material) and seeded donor cells and/or growth factors.

The design and fabrication of such heterogeneous structures requires new techniques for solid models to represent 3D heterogeneous objects with complex material properties. This paper presents a representation of model density and porosity based on stochastic geometry. While density has been previously studied in the solid modeling literature, porosity is a relatively new problem. Modeling porosity of bio-materials is critical for developing replacement bone tissues. The paper uses this representation to develop an approach to modeling of porous, heterogeneous materials and provides experimental data to validate the approach. The authors believe that their approach introduces ideas from the stochastic geometry literature to a new set of engineering problems. It is hoped that this paper stimulates researchers to find new opportunities that extend these ideas to be more broadly applicable for other computational geometry, graphics and computer-aided design problems.

Key words:
Computer-Aided Design, Representation, Heterogeneous Models, Solid Modeling, Porous models, Bio-Medical Applications

PACS: pacs code, pacs code, pacs code
1 Introduction

This paper presents a mathematical framework to computer-aided representation of and modeling with heterogeneous solids. The major research contribution of this paper is the study of how porosity can be effectively represented and modeled in a manner compatible with the established mathematics and techniques of solid modeling and Computer-aided Design. While density has been studied much in past literature [33,20,45,32,17,29,22,34,1,23], porosity is a relatively new problem for computer-aided design and of great importance in bio-medical and tissue engineering domains. The representation we present effectively unifies model density and porosity using stochastic geometry techniques adapted from the geophysics community [33,20,45,32,17].

Heterogeneous solid modeling is an emerging area with wide-spread applications in computer-aided design, manufacturing, bio-medicine, pharmacology and geology and physics. Existing research on heterogeneous modeling has focused primarily on the needs of the manufacturing processes solid free-form fabrication, usually with the goal of improving the fidelity of the manufacturing process to produce usable parts, rather than mere prototypes. Other researchers have studied how to model material gradients and multi-material objects. This paper introduces the porosity problem, specifically in the context of computer-aided design of replacement bio-tissues, such as human bone, whose porosity is illustrated in Figure 1. It is our ultimate goal to augment existing CAD representations and modeling techniques with porosity information and show how advanced modeling systems can be used to develop smart and multi-material models for use in the design and fabrication of tissue engineering structures and scaffolds. The improved capacity to model and generate porous designs implies far-reaching implications for bio-medical engineering.

Current methods for representing porosity represent only the density of the object, the volume fraction, or represent the internal porosity structure exactly. The first approach, while concise, is unable to take into consideration connectivity, pore size, or pore structure. The latter approach quickly results in huge files. We observe that every bone is different and, for most design, modeling and analysis applications, the exact internal geometric and topological structure of a bone is not needed. Ideally, one would like a means of storing the important properties of porous objects in a concise and efficient manner. Conversion to and from this representation as well as the application of operators would be accurate and efficient.

Section 2 presents background work that others have done on heterogeneous solid modeling. Section 3 builds up a theoretical base for representing and modeling porous solids. Section 5 discusses our implementation and empirical results. Section 7 concludes the paper and highlights important points.

2 Background

The potential to design and fabricate multi-material objects is very promising. The ability to design and fabricate such objects relies on representations to model these structures and algorithms and
fabrication techniques necessary to process them into reality. This challenging problem has been met with significant advancements based on the work of several groups of people, each approaching similar problems of heterogeneous modeling in unique ways. We present a brief overview, organized loosely by university or research group.

Research at MIT has progressed with the 3D Printing process by the efforts of N. M. Patrikalakis, T. R. Jackson, H. Liu, E. M. Sachs, and others. Here, research has focused on representations, designing, information flow, and the preparation of models for the 3D Printing process. Representations covered there include the voxel representation [23,8,22], where the solid is divided into rectangular prisms, and each prism has its own internal properties. This is their last stage in the transfer process before 3D printing. They experimented with the tetrahedral mesh approach [23,31,8,30,22], where the model is split into a tetrahedral mesh with material information stored at the vertices. This material is spread throughout the tetrahedra through the use of blending functions.

The MIT group has also touched on two popular boundary representations. They used the B-rep [23,8,22] (with NURBS) for use in designing the boundary of their models. Then, they converted these into the triangulated form (STL) [24,22]. From here, the models were broken down into a tetrahedral mesh [23,31,8,30,22] or cell-tuple structure [23,24,43,22] for processing. MIT also worked with the radial edge structure [23,22].

To supplement their 3D Printing facilities, they have developed a series of processing and post-processing algorithms. These include a bucketing scheme to speed up the distance-to-surface computations, ray and plane casting algorithms, and point classification algorithms. They further adapted the half-toning algorithms familiar to ink jet printing for use in post-processing. These algorithms are discussed in [31,31,8,30,44,7,22].

MIT also investigated using procedural storage [9] and assembly tree schemes [9]. Their investigations included detailed memory analyses of their structures [23,8].

Research elsewhere is pioneering forward with other representations and other fabrication techniques. University of Michigan has based its research on layered manufacturing [36,35]. Their research is due to V. Kumar, D. Dutta, M. J. Pratt, L. Patil, and others. They are studying the usage of r-sets [28,35,27], ISO 10303 (STEP) [36,35], and a representation based on fiber bundles [27]. They also have a representation based on atlases and attribute models [27].

Research at the University of Austin, by the efforts of S. Park, R. H. Crawford, and J. J. Beaman, have focused on selective laser sintering [25]. They have been working with a representation based on gradients [34] and a procedural representation [34], where information is stored in functions that can be evaluated when necessary.

The University of Maryland, by the efforts of M. Kumar and S. Gupta, has worked on using molding to create multi-material by splitting a piecewise homogeneous model into homogeneous sections for molding [11]. The University of Rochester has worked on a part description language [43].

A. Pasko and V. Adzhiev have developed a representation designed for modeling in higher di-
mensions and for holding multiple attributes. In this representation, primitives consist of functions
defined either by equation or in some other way [1].

Lastly, efforts of W. Sun and X. Hu have developed a Boolean Reasoning method for combining
and analyzing models using constructive solid geometry (CSG) [41].

3 A Brief Stochastic Geometry Primer

Stochastic geometry is the study of random processes whose outcomes are geometrical objects
or spatial patterns. This section gives a basic introduction to stochastic geometry and is intended
for those readers not intimately familiar with the mathematics of stochastic structures. Readers
knowledgeable about this material may safely skip this section.

Geometric objects should be assumed to lie in \( \mathbb{R}^2 \) or \( \mathbb{R}^3 \), although this treatment in general holds
for \( \mathbb{R}^k \) or some more general set. One important definition is needed for the Boolean model. Let
\( A \oplus B = \{ x + y | x \in A, y \in B \} \) (Minkowski addition). One might think of this as taking a copy of \( A \)
and pasting it at each point in \( B \). The operation is commutative and associative.

3.1 The Stochastic Point Process

3.1.1 General

**Definition.** A point process is the family of all sequences of points satisfying two special con-
ditions: (1) The sequence is locally finite. Each bounded subset must contain a finite number of
points. (2) The sequence is simple. That is, it contains no duplicates. These sequences can in gen-
eral be considered as a random set, when order is not important.

**Measure of a Point Process.** A point process \( \Phi \) has associated with it a measure, which is
denoted as \( \#_\Phi(B) \). This measure maps each random sequence \( \rho \) of this point process into the
number of points in the sequence \( \rho \) that lie in some bounded set \( B \).

**Distribution of a Point Process.** This measure generates a distribution \( P \). The distribution \( P(Y) \)
is \( P(\rho \in Q), Q \subset \Phi \).

**Stationarity and Isotropy.** A stationary point process is one whose properties are invariant
under translation. Let \( \Phi_x \) denote the point process formed by translating \( \Phi \) by some vector \( x \).
\( P(\#_\Phi(B) = Y) = P(\#_{\Phi_x}(B) = Y) \). (This says that the probability of any particular sequence \( \rho \in \Phi \)
applied to \( B \) having measure \( Y \) does not change if \( \Phi \) is translated.)
An isotropic point process is one whose properties are invariant under rotation. \( P(\#_{\Phi}(B) = Y) = P(\#_{r\Phi}(B) = Y) \), where \( r \) is some rotation. A motion invariant point process is one that is both stationary and isotropic.

**Intensity measure.** The intensity measure is the expected value of \( \#_{\Phi}(B) \). That is, \( \Lambda(B) = E(\#_{\Phi}(B)) \). This is just the expected number of elements in \( B \) also in \( \rho \). If the point process is stationary, \( \Lambda(B) = \lambda V(B) \), where \( \lambda \) is the intensity of the point process and \( V(B) \) is the volume (in the appropriate dimension).

**Contact Distributions.** The contact distribution function \( H_B(r) \) is defined as the probability that \( rB \) does not intersect \( \Phi \), where \( r \) is a nonnegative scalar and \( B \) is a set. Expressed in the notation introduced above, we have \( H_B(r) = 1 - P(\#_{\Phi}(rB) = 0) \). If we let \( B \) be the unit sphere, we are left with the spherical contact distribution.

### 3.1.2 Marked Point process

A marked point process is a point process where each point has some value associated with it (these values are called marks). If the marks are removed, one is left with a point process. Marks may be mathematical (eg, size) or non-mathematical (eg, color). Though marked point processes can be treated as point processes, it may be useful to distinguish the two, since some operations (such as rotations and translations) may be best not applied to the marks.

### 3.1.3 Moment Measures

The general \( n \)-th order moment measure of a point process \( \Phi \) is defined as \( \mu^{(n)}(B_1 \times \cdots \times B_n) = E(\#_{\Phi}(B_1) \cdot \cdots \cdot \#_{\Phi}(B_n)) \). If \( B_i = B \) then we are left with the \( n \)-th moment, \( \mu^{(n)}(B^n) = E(\#_{\Phi}(B^n)) \). This leads to \( \text{cov}(A, B) = E(\#_{\Phi}(A)\#_{\Phi}(B)) - E(\#_{\Phi}(A))E(\#_{\Phi}(B)) \) and \( \text{var}(B) = \text{cov}(B, B) = E(\#_{\Phi}(B)^2) - E(\#_{\Phi}(B))^2 \).

If the underlying point process is stationary, the moment measures \( \mu^{(n)}(B_1 \times \cdots \times B_n) \) are unaffected when all sets \( B_i \) are translated by the same vector \( x \).

Another moment, called the factorial moment, is like the above moments, except that expectation is performed only on combinations containing distinct elements. Factorial moments are related to moments by an inclusion-exclusion principle. Factorial moments are a bit easier to calculate than moments.

### 3.1.4 Uniform Point Process

This point process consists of a single point \( \xi \), uniformly distributed on a compact subset \( W \) of the whole space. \( P(\xi \in A) = V(A)/V(W) \), where \( A \subset W \) and \( V \) represents the volume, in the
appropriate dimension. \( P(\xi \in A) = 0 \), if \( A \cap W = \emptyset \).

### 3.1.5 Binomial Point Process

When \( n \) independent points \( \xi_1, \ldots, \xi_n \) are uniformly distributed over the same set \( W \), the result is a binomial point process of \( n \) points. \( P(\xi_1 \in A_1, \ldots, \xi_n \in A_n) = V(A_1) \cdot \ldots \cdot V(A_n) / V(W)^n \). The points of this set are unordered and can be considered as a set when order is not important.

Recall that \( \#\Phi(A) \) is the number of points of the point process that are in \( A \). \( \#\Phi(\emptyset) = 0 \) and \( \#\Phi(W) = n \). If two sets are disjoint, then the measure of their union is the sum of their measures.

If \( A \subset W \), then \( \#\Phi(A) \) follows a binomial distribution with parameters \( n = n \) and \( p = V(A) / V(W) \). The intensity (points per unit volume) is \( \lambda = np / V(A) \). The measure is not independent, even for disjoint subsets. For example, if \( \#\Phi(A) = m \), then \( \#\Phi(W - A) = n - m \).

### 3.1.6 Poisson Process

Consider the binomial process. If \( n \to \infty \), \( p \to 0 \) and \( W \) enlarges to fill the whole space, such that \( np \) is constant (for any \( A \)), the result is a Poisson point process. \( \#\Phi(A) \) is now of Poisson distribution with mean \( \lambda V(A) \). \( \lambda \) is the intensity.

### 3.2 The Boolean Model

**Definitions.** The Boolean model consists of a Poisson point process (the points of which are called germs). Associated with each point is a closed set called the primary grain. The underlying point process has intensity \( \lambda \), as it did when discussed earlier. The primary grains need not be the same. The \( i \)th germ (point) is \( x_i \), and the \( i \)th primary grain is \( \Xi_i \).

A simple example of a Boolean model is a point process with a disc centered at each point. Here, the primary grains are the discs, centered at the origin. The germs are the underlying point process composed of points at the centers of the disks.

The Boolean model is subject to a regularity constraint: \( E(V(\Xi_0 \oplus K)) < \infty \), where \( K \) is any compact set and \( \Xi_0 \) is a random compact set with the same distribution as \( \Xi_i \), but independent of it. This ensures that only finitely many of these grains will overlap any given compact set.

\( \Xi = \bigcup_{i=1}^\infty (\Xi_i \oplus x_i) \) is the notation for the entire Boolean model. This is just the union of all primary grains, shifted to the corresponding points of the point process. \( \Xi \) is itself closed, but it need not be connected.

**Stationarity and Isotropy.** If the underlying point process is stationary (its properties are invariant under translation) then the Boolean model will also be stationary. If the grains are isotropic,
then the Boolean model will also be isotropic. The condition, however, is not required. If the Boolean model is both stationary and isotropic, it is invariant under rigid transformation.

**Capacity Functional.** The capacity functional or hitting distribution is defined as $T_ξ(K = P(ξ ∩ K ≠ Φ))$. The distribution of a Boolean model is uniquely determined by its capacity functional. Application of the Poisson assumption and the assumption of stationarity yields the formula $T_ξ(K) = 1 - e^{-λE(V(ξ₀ ⊕ K))}$.

**Basic Characteristics.** The volume fraction $p$ is the mean fraction of occupied volume per unit volume. $p = E(V(ξ ∩ B))$, $V(B) = 1$. If the germs are stationary, this simplifies to $p = P(o ∈ ξ)$, where $o$ is the origin. When $K = \{o\}$ above, the formula simplifies to $p = T_ξ(\{o\}) = 1 - e^{-λE(V(ξ₀))}$, under the assumption of stationarity.

**Contact Distribution Functions.** A contact distribution (or hitting distribution) function for a stationary random closed set $ξ$ is defined in terms of a convex test set $B$ by the equation $H_B(r) = 1 - \frac{P(ξ ∩ rB = Φ)}{1 - p}$. The spherical contact distribution is obtained by letting $B = b(o, 1)$, the unit ball. It is also called the law of first contact. If convex grains are assumed, this simplifies down to $H_s(r) = 1 - e^{-4πλrE(R^2) + 3rE(R) + r^2}$. This distribution will be discussed later and is relevant to the work in this paper.

### 3.3 Background Materials from Geophysics

The basis for this primer has been the two excellent books on the subject[2,39], with the first more introductory and the second more detailed. The porosity representation we develop adapts work of geophysicists, specifically the work of R. Hilfer, C. Manwart, and S. Torquato. They consider the solid as a set of voxels [33,20,45,32,17,3,26], and they use stochastic functions to try to reconstruct the original model’s porous structure as best as possible using simulated annealing [33,45,17], a pressure correction algorithm [20], and Monte Carlo methods [32]. In this work, stochastic functions give them a distribution corresponding to internal porosity of the sandstones they were attempting to model. They also did significant work on analyzing these synthetic (and real) sandstone models [33,20,32,45,17,3,5,4,21,37]. They concerned themselves heavily with analysis (two-phase flow, [16,19]; erosion-dilation, [42,15]; connectivity, [3]; percolation, [4,21,14,13,15]; dielectric response, [13,18,37,15]; corrosion, [26]; and various other analyses, [3,15]).

The principle issue with their methodology is that it is intended for reconstruction of shapes and it is not intended for design or CAD-like modeling. Its main purpose is to create virtual models with specific internal geometry that matches the specific internal geometry of a sandstone sample. Hence, they learn (via the simulated annealing and other techniques) the specific distribution function associated with a specific piece of rock. In our work, we have extended aspects of their
representation to work with CAD models in a CSG modeling environment to produce a modifiable representation for any manner of porous object.

4 Our Technical Formulation

We wish to both represent and design with heterogeneous objects with porosity. Our approach to the representation and modeling is as follows:

Representation We develop a stochastic representation of both model density and porosity. A challenge with modeling materials such as human bone is that the specific internal geometry of identical bones can vary considerably from human being to human being. During the development process, bone growth proceeds organically and not according to rigid manufacturing parameters. Rather than modeling the specific internal geometry of a bone (which would be impossible, given that every bone is unique), we model the internal shape parameters as a stochastic process. Similar stochastic processes have been used to model other natural phenomenon, cellular automata and systems emergent behavior and structure. Drawing on work in geophysics, we present and evaluate three stochastic representations for model porosity and show how these can be used to create an implicit shape representation for the internal porosity of an object.

Modeling From a practical standpoint, a representation is only useful if it can be used to support design and manufacturing of heterogeneous objects. For the purposes of this paper we assume the underlying representation of the boundary of the model is based on constructive solid geometry (CSG). In CSG, a model is designed and represented starting with primitives, which are manipulated by combinations of (sometimes regularized) unions, intersections, and differences. Once all of these operations have been performed, the external geometry and topology of the artifact results. Traditionally, CSG has generally assumed that the contents of the models are compact and of a single material, whereas the contents of the outside is completely void. Some modelers do, however, permit the attachment of attributes to materials [10,40,6,38].

We show how to adapt CSG to model artifacts of varying density and porosity using our stochastic representations. This involves identifying a mathematically consistent manner for the stochastic representations of internal model properties to be unionited, intersected and subtracted. Given two models, A and B, we show the internal shape parameters for the resulting model C for each of the major Boolean operations. Hence, the resultant CSG models are not internally compact—model density may vary. Furthermore, these void places in the model are to be themselves represented by porosity. This gives the flexibility to decide not only how much void is inside a model but the general properties and arrangement of those void parts.

Validation Lastly, we provide some empirical data to demonstrate and validate the approach. Specifically, we use a well-known cellular automata-based technique to generate synthetic data
with varying density and porosity properties and evaluate how well the representation and modeling paradigm conforms to experimental data. Additionally, we provide an example of how the modeling technique can be used to represent a synthetic bone structure.

4.1 Model Representation

Models must have both external, boundary representation as well as internal representation. This section develops the boundary and internal representation of single model; the Section 4.2 will show how to design heterogeneous models with varying density and porosity using constructive solid geometry (CSG) operations and solids whose representations are those from this section. In this work, the structure of the CSG-tree will capture the internal properties of the final object based on stochastic Boolean operators applied to object primitives.

4.1.1 Boundary Representation

We are primarily concerned with the internal structures of objects. For simplicity, the boundary of the CSG primitives can use a number of suitable boundary representation structures (NURBS patches, implicit surfaces, etc). We note that this paper does not introduce new algorithms for manipulating bounding surfaces but will give a mathematical framework for representation of the internal properties. Our representation is compatible with any B-rep-based modeling paradigm.

4.1.2 Internal Representation

For the internal shape, a model has statistical parameters that represent the nominal porosity and density.

4.1.2.1 Representing Model Density. The density, \( \rho \), is represented as a value in the range \( 0 \leq \rho \leq 1 \). The density specifies what fraction of a certain volume is solid material. Alternatively, the density \( \rho \) is a probabilistic description of the likelihood of finding solid material at a given point inside the boundary of the model.

Note: this formulation can be used to derive several other useful representations of density. For example, one could consider an object as multi-material, where an extra material called void represents the porous regions. The volume fraction consisting of materials other than void is then the density of the object. In this case, it is sufficient to store the density itself. For the purposes of this paper, the density is assumed to be constant or a given and be altered by each Boolean operation.

4.1.2.2 Representing Model Porosity. The internal representation of this density information is quite different from the internal representation of the porosity information. Whereas density is a general property of a model’s interior, porosity refers largely to the specific geometry of the inside.
For example, a model with high density might have a single large pore or many infinitesimally small pores. Conversely, a model with low density might have a porous structure much like that of the human bones shown in Figure 1, where the pore sizes are relatively consistent and result in a highly connected internal structure. Hence, given a fixed model density, the specific internal porous geometry could vary greatly depending on the statistical distributions that describe the locations and sizes of the pores.

We will consider the interior geometry of a model as a point set \( S \). To quantify the porosity of the model, we use a function \( f() \), where \( f : S \in \mathbb{R}^3 \rightarrow \mathbb{R} \). This function \( f() \) takes a point in the interior of a solid \( x \in \mathbb{R}^3 \) and returns the value of an attribute \( v \in \mathbb{R} \) at that point. Multiple functions \( f() \) may be used, with their resulting attributes collected into a vector of dimension \( b \). More simply, \( f() \) takes a point in the 3-dimensional model and returns some value describing the internal properties of the model at that point. We define the probability distribution \( p(v) \) such that \( f() \) will result in a value \( v \in v \) with probability \( p(v) \), for each function \( f() \). Note that \( f(x) \) is the same function at points for a given model and that this function will vary internally when doing CSG-based design as described in Section 4.2. For a given model, we start with \( p(0) = \delta(0)\rho \), where \( \delta \) is the Dirac function and \( \rho \) is the density. The value 0 means that \( f() \) is zero when not in a pore, since \( f() \) is only meaningful for the pores (when considering materials, this is reversed). Defining \( p(0) \) in this way causes \( p \) to be a full probability distribution although for a given model there will be limits on the size a pore can be (i.e., one cannot have a pore of infinite radius). This implies that:

\[
\int_0^\infty p(v) \, dv = 1
\]

Consider \( V \) to be the volume of \( S \). Choosing an arbitrary function \( g(r) \) results in:
\[
V \int_0^\infty g(v)p(v) \, dv = \int_S g(f(x)) \, dx
\]

under the constraint that \( f(x) \) obey \( p(v) \). If \( g(v) = v \) then another useful identity is obtained:

\[
V \langle p(v) \rangle = V \int_0^\infty vp(v) \, dv = \int_S f(x) \, dx
\]

Multiple stochastic functions \( f() \) may be used. The \( b \) functions map a solid model \( S \) into the \( b \) distributions \( P = f(S) \).

Given two models, \( A \) and \( B \), with the same external boundary representation, we can consider an error function, \( E() \), that determines the difference between two sets of distributions that stochastically describe their internal geometries. Because \( P \) is stored in the model, and both \( f() \) and \( E() \) are stored globally in the representation, \( F : \mathbb{R}^b \to \mathbb{R} \) is defined by \( F(x) = E(f(x), P) \). \( f() \) assigns to each object a number signifying how close its distributions are to those of \( S \). \( f() \) has a large number of global and local minima (i.e., solids that have the same or similar distributions as \( S \)). One of those global minima is \( S \). A good choice of \( f() \) will tend to cause minima of \( f() \) to have properties similar to those of \( S \). In this way, a result similar to \( S \) can be reconstructed. In most cases, the exact location and size of pores is not needed; only the properties are important. It is these stochastic properties of the shape, and not the specific geometric configuration of pores, that this representation seeks to capture.

The next question to address is the choice for the stochastic function \( f() \). Good choices of \( f() \) will support the Boolean operations in a logical, efficient, and effective manner. Furthermore, the function \( f() \) should adequately describe the porosity of the function that models reconstructed from it will be sufficiently similar to the original in properties. We evaluated three functions based on those used by[33].

- The first choice of \( f : x \in \mathbb{R}^3 \to v = \in \mathbb{R} \) is based on the distance from points in pore space to the material matrix. Formally, consider the input of the function, a single point in pore space. Find the nearest point in/on material to this point, as shown in 2D in Figure 2(a). The distance from the input point to this material is \( v \). This is equivalent to finding the largest sphere centered at the given point that fits entirely inside pore space. \( v = 0 \) elsewhere.

  The reverse of this function requires that the input is a material point, and the same measure is performed but with material space. This becomes \( v \). In this case, \( v = 0 \) if the input point is in void.

  We use these two choices and collect the results in a vector. The reason for applying the same measurement to both material and pore is that it permits effortless inversion of the model. This will aid in subtraction when doing Boolean operations. When applying these functions we wrap around to avoid boundary problems. This is what you would expect if the cubes we are using were tiled.
Fig. 2. Three choices for the stochastic function, \( f() \), to represent internal model porosity.

This function is quit similar to the spherical contact distribution, but there are some subtle differences. Eg, it cares about the point under consideration, unlike the contact distribution which does not care.

- The second choice of \( f() \) is based on the largest cube that can be centered at the given point as shown in Figure 2(b). This representation is otherwise the same as the first scheme. There is a reverse of this one, too. We do not use these functions.

- For the third choice of \( f() \), consider the longest segment that can be embedded in pore space and pass through the point. This involves checking the embedding in every direction and taking the length of the shortest such segment as the measure, as shown in Figure 2(c). The same is done for the material as with the first case. We do not use these functions, either.

An Example: The UC Berkeley Bone. The full cycle starts with a material sample. For this, we chose to work with a bone model from UC Berkeley’s tissue engineering group. This bone is a VRML file with 280,474 points and 564,320 faces that describes the structure of a porous bone and is shown in Figure 3(a).

The second stage of the data path is voxelization. To convert from a triangular mesh to a set of voxels, we fit the mesh to a lattice and run lines down the center of each string of cells in the lattice in one direction. We then intersect these lines with the mesh. We then classify the centers of the cells as in or out by counting the number of intersections between the cell’s center and the outside of the model. We take a cell to be part of the model when its center is. We store this as a simple list of voxel coordinates. Our lattice is 100 by 100 by 100. The resulting model contains 325,026 voxels, giving the model a density of 0.325. The voxelized Berkeley bone is shown in Figure 3(b).

The third stage is calculating the distributions. This step is described in greater detail elsewhere in this paper. We will not describe this stage here. The distributions are shown in Figure 3(c).

The fourth stage would normally be the modeling phase, where inversions, unions, and intersections an be performed with multiple primitives to yield a new distribution. For the purposes of this example, we only wish to reconstruct the distribution we started with.
Fig. 3. The stages of the full data cycle for the Berkeley bone.

The fifth stage is reconstruction. We start the reconstruction process with a grid of voxels. Our grid is $32 \times 32 \times 32$. We then randomly set voxels as being material, until the desired density is met. We then apply simulated annealing to improve the distribution’s fit with the original. Updates to the grid are done by selecting a voxel and walking randomly around the model until another voxel of the same type (material or pore) is found. We back up and choose that voxel. We then swap these two voxels, update the distribution, and choose to accept or reject the modification according to its affect on the fit of the model and the cooling schedule. We permit the annealing process to continue until the solid is completely frozen. The result is a model with similar density and distribution as the original model. The simulated model is shown in Figure 3(d).

The sixth stage is to convert the model back into a triangular mesh. We converted our voxel representation back into STL for the fabrication process.

The seventh and final stage is fabrication. Pictures of the fabricated models are shown in Figure 3(e) and Figure 3(f).

**Example Artifact: A Femur Cross-Section.** Figure 4(a) shows an approximation of a femur as a cylinder with rings with increasing porosity as the center of the cylinder is approached. The porosity is 10% at the perimeter and 90% porous in the center. Varying the porosity in this way
may be used to model not only the density but also the porosity of the bone.

4.2 Modeling and Design with Heterogeneous Solids

A heterogeneous 3D model, $M$, is represented as a CSG tree with the porosity and boundary information for each model stored in the leaves and regularized Boolean operations stored in the nodes. Modeling with CSG requires a set of objects (solids, halfspaces, etc.) which will be used as building blocks for the artifact. In the context of this paper, we assumed the boundaries of the primitive are suitable for traditional CSG operations and that the density and porosity of the regions bounded by these patches are represented as in Section 4.1. Hence, we need mathematics describing the results of CSG-like operations for the internal model properties under these operations.

To perform design with CSG, we require the ability to manipulate objects through the Boolean operations of regularized union ($\cup^*$), intersection ($\cap^*$), and subtraction ($-^*$). Standard regularized Boolean operations were not developed to model with the stochastic representations of density and porosity. In this section we develop Boolean operations that preserve the stochastic properties of the internal geometry.

4.2.1 Density-Preserving Operations

The density must undergo the operations of union ($\cup$), intersection ($\cap$), and subtraction ($-$). Regularization of the resulting solid may be necessary.

The probability of finding material at a certain point in region $A$ is $\rho(A)$, and the probability of finding material in region $B$ is $\rho(B)$.

- Consider the intersection of these two solids $A$ and $B$. Four cases can occur at any point. Both regions can have material. This case occurs with probability $\rho(A)\rho(B)$. In this case, the resulting region $C = A \cap B$, will possess material at the same location. In all other cases, one or both of the regions $A$ and $B$ will be void. In these cases, the regions do not intersect, so that the region $A \cap B$
is also void at that point. Because material occurs at a given point with probability, the density is $\rho(A \cap B) = \rho(A)\rho(B)$.

- Next consider the union $C = A \cup B$ with $A$ and $B$ as before. The probability that a point is not material is $\overline{\rho(B)} = 1 - \rho(B)$ Thus, the chances of $B$ being void are $1 - \rho(B)$. $\rho(A \cup B) = (\text{prob. of } A) + (\text{prob. of } B) - (\text{prob. of } A \text{ and } B) = \rho(A) + \rho(B) - \rho(A)\rho(B)$.
- Finally, consider the difference $A - B$. This is the probability of $A$ having material and $B$ not having material. Thus, $\rho(A - B) = \rho(A)(1 - \rho(B)) = \rho(A) - \rho(A \cap B)$.

We note that these Boolean operations are not quite the same as the ones most are used to from computer-aided design. Additionally these operators, while developed for CAD, do have analogues in geophysics [2,17].

**Examples of the Density Operators.** Consider a 50% dense cylinder $A$ and a 40% dense block as shown in Figure 5(a). $A \cap B = C$. The density of the cylinder at which the geometry intersects is $\rho(A)\rho(B) = (.50)(.40) = .20$. The portions not contained within the geometry of both have zero density, since $\rho(A) = 0$ or $\rho(B) = 0$ here. The resulting solid is a 20% dense object at the intersection of the geometries of $A$ and $B$.

For the union, consider a 50% dense cylinder $A$ and a 30% dense block $B$ as shown in Figure 5(b). $A \cup B = C$. At the intersection of their geometry, the density of $C$ is $\rho(A) + \rho(B) - \rho(A)\rho(B) = .50 + .30 - (.50)(.30) = .65$. The portion of $C$ contained in the block $B$ but outside the cylinder $A$ has density $\rho(B) - \rho(A)\rho(B) = 0 + \rho(B) - (0)(\rho(B)) = \rho(B)$. The portion of $C$ contained inside the cylinder $A$ but not inside the block $B$ has density $\rho(A) + \rho(B) - \rho(A)\rho(B) = \rho(A) + 0 - (\rho(A))(0) = \rho(A)$. The portion of $C$ at the intersection of $A$ and $C$ has density .65; the rest of $C$ has the same density as the corresponding portions in $A$ and $B$.

Consider a subtraction between a 50% dense cylinder $A$ and a 40% dense block as shown in Figure 5(c). $A - B = C$. At the intersection of $A$ and $B$, the density is $\rho(A)(1 - \rho(B)) = (.50)(1 - .40) = .30$. At points outside of $A$, the density is $\rho(A)(1 - \rho(B)) = (0)(1 - \rho(B)) = 0$. At portions outside of $B$, the density is $\rho(A)(1 - \rho(B)) = \rho(A)(1 - 0) = \rho(A)$. Thus, $C$ is just $A$, but with the intersection reduced in density to 30%.

4.2.2 Porosity-Preserving Operations

This section begins by considering $p_A$ as $p_{A0}$ and so on for brevity. The general case is treated later. Performing Boolean operations on the porosity requires that one be able to obtain a new distribution $p_C$ from the original distributions $p_A$ and $p_B$. The stochastic function $f()$ is global and is the same
for all objects. In general, the distribution that is obtained by Boolean operations applied to the input distributions will not be unique. The geometry of the original objects themselves determine the exact properties of the resulting solid. It is, however, possible to calculate a likely distribution that one might expect to obtain. The means of calculating such a distribution is dependent on the function $f()$ used to create the distribution. Calculating this new distribution is a very difficult task.

In developing these operators, we will employ the function $f_i()$, which finds the sphere of largest radius centered at the desired point in pore space which has an empty intersection with the model. Development of operators based on the other stochastic function would proceed in a similar manner.

**Intersection.** If two objects, $A$ and $B$, were to intersect, the result, $C$, would have less material and more pore space. The size of the smallest sphere is at least as large as either of the original objects. This suggest the following calculation of the new distribution:

$$
p_C(x) = p_A(x) \int_0^x p_B(t) dt + p_B(x) \int_0^x p_A(t) dt
$$

This formula can be derived mathematically using methods of Stochastic geometry. First, it is necessary to build up a formula for $\int_0^r p(t) dt$. Consider $M_A$ to be the material portion of $A$. $b(o,r)$ is the ball of radius $r$ centered at the origin. $M_A \oplus b(o,r)$ includes everything in the material portions of $A$, as well as everything no more than $r$ away from the material portions. $V(M_A \oplus b(o,r))$ is the volume of $A$ that is material or at most $r$ from material. $V(M_A \oplus b(o,r))/V(U)$ is then the volume fraction for this region, where $U$ is the universe of interest. But this is precisely what $\int_0^r p(t) dt$ represents. Remember that the pores are being considered here.

$$
\int_0^r p_A(t) dt = \frac{V(M_A \oplus b(o,r))}{V(U)}
$$

Similar formulas hold for $p_B$ and $p_{A \cap B}$:

$$
\int_0^r p_B(t) dt = \frac{V(M_B \oplus b(o,r))}{V(U)}
$$

Now for the intersection version, we can simplify this down, but only as far as an inequality. We assume strict equality for purposes of calculations. Note that independence between $A$ and $B$ is required for the fourth step to hold.
\[
\int_0^r p_{A \cap B}(t) \, dt = \frac{V(M_{A \cap B} \oplus b(o, r))}{V(\mathbb{U})} \\
= \frac{V((M_A \cap M_B) \oplus b(o, r))}{V(\mathbb{U})} \\
\geq \frac{V((M_A \oplus b(o, r)) \cap (M_B \oplus b(o, r)))}{V(\mathbb{U})} \\
= \frac{V(M_A \oplus b(o, r)) \cdot V(M_B \oplus b(o, r))}{V(\mathbb{U})} \\
= \int_0^r p_A(t) \, dt \int_0^r p_B(t) \, dt
\]

The formula originally presented is obtained by differentiating this equation.

**Union.** If two objects, \(A\) and \(B\), were to be united, the result, \(C\), would have more material and less pore space. The size of the smallest sphere is at most as large as either of the original objects. This suggests the following calculation of the new distribution:

\[
p_C(x) = p_A(x) \int_x^\infty p_B(t) \, dt + p_B(x) \int_x^\infty p_A(t) \, dt
\]

The union formula is obtained in a similar manner as the intersection one. In this case, however, strict equality is obtained.

\[
\int_0^r p_{A \cup B}(t) \, dt = \frac{V(M_{A \cup B} \oplus b(o, r))}{V(\mathbb{U})} \\
= \frac{V((M_A \cup M_B) \oplus b(o, r))}{V(\mathbb{U})} \\
= \frac{V((M_A \oplus b(o, r)) \cup (M_B \oplus b(o, r)))}{V(\mathbb{U})} \\
= \frac{V(((M_A \oplus b(o, r))' \cap (M_B \oplus b(o, r))')')}{V(\mathbb{U})} \\
= 1 - \frac{V((M_A \oplus b(o, r))' \cap (M_B \oplus b(o, r))')}{V(\mathbb{U})} \\
= 1 - \frac{V((M_A \oplus b(o, r))') \cdot V((M_B \oplus b(o, r))')}{V(\mathbb{U})}
\]
\[ 1 - \left( 1 - \frac{V(M_A \oplus b(o, r))}{V(\Omega)} \right) \left( 1 - \frac{V(M_B \oplus b(o, r))}{V(\Omega)} \right) = 1 - \left( 1 - \int_0^r p_A(t) \, dt \right) \left( 1 - \int_0^r p_B(t) \, dt \right) \]

As before, the formula is obtained by differentiating this equation.

Up until now, only the porosity distribution has been considered. Now treat both distributions at once using the above union and intersection equations. For intersection:

\[ p_C = p_A \cap p_B = \{p_{A0}, p_{A1}\} \cap \{p_{B0}, p_{B1}\} = \{p_{A0} \cap p_{B0}, p_{A1} \cup p_{B1}\} \]

and similarly for union:

\[ p_C = p_A \cup p_B = \{p_{A0}, p_{A1}\} \cup \{p_{B0}, p_{B1}\} = \{p_{A0} \cup p_{B0}, p_{A1} \cap p_{B1}\} \]

**Inversion and Subtraction.**  Inversion (\(\neg\)) of the model is accomplished by:

\[ p_B = \neg p_A = \neg \{p_{A0}, p_{A1}\} = \{\neg p_{A0}, \neg p_{A1}\} = \{p_{A1}, p_{A0}\} \]

and by using inversion, subtraction (\(\neg\)) is achieved by applying the intersection and the inversion:

\[ p_C = p_A - p_B = p_A \cap \neg p_B = \{p_{A0}, p_{A1}\} \cap \neg \{p_{B0}, p_{B1}\} = \{p_{A0} \cap p_{B1}, p_{A1} \cup p_{B0}\} \]

**Examples of the Porosity Operators.**  A 2D illustration of the behavior of the three Boolean operations is shown in Figure 6. The first two images represent the input models, \(A\) and \(B\). The white parts represent pores and the colored portions represent material.

The remaining three represent the union (\(\cup\)), intersection (\(\cap\)), and difference (\(\neg\)) between the input solids \(A\) and \(B\). The red portions are the actual output of the operations. The blue and yellow portions show, for purposes of demonstration and clarity only, where the original input models are situated relative to the output. These are not part of the output.
5 Empirical Results

5.1 Validation of Modeling Operators.

To test the proposed method for combining distributions, we first generated two $100 \times 100 \times 100$ voxelized cubes, $A$ and $B$. Then, a third cube $A \cup B$ was calculated explicitly by applying the union, subtraction and intersection voxel by voxel.

For the first set of tests, we calculated the voxelized cubes by starting with a completely solid $100 \times 100 \times 100$ cube. We then generated spheres with radii according to an exponential distribution, scaled and shifted to reasonable values (at least two voxels in radius). These spheres were removed from the cube until the density reached 0.7 of the total volume, as shown in Figure 7(a) and Figure 7(b).

For the second set of tests, a $100 \times 100 \times 100$ cube is filled to density 0.3 with voxels, randomly placed. Then, an algorithm mimicking termites [12] was performed on the cube. In this algorithm, a population of termites is placed in the cube. The termites move around. When they hit a piece of material, if they have a woodchip, they drop it. If they do not, they pick up the one they ran into. Otherwise, they just go straight. When they hit material, they turn. The direction of the turn is random. The algorithm terminates after a specified number of iterations. The algorithm tends to cluster the voxels into clumps, which get larger and fewer in number as time goes one. The number of voxels with woodchips does not change, so the density is constant. After these cubes are generated, they are stored, loaded into an analysis program, and inverted. (This swaps the pore and material portions, making the density 0.7.) A sample cross-section from such a cube is illustrated in Figure 7(c).

The distributions $p(A)$, $p(B)$, and $p(A \cup B)$ were calculated by searching outwards from each voxel until a voxel with the opposite type (pore or material) was found. Then, the distance was calculated and the appropriate counter was incremented. Separate counters were kept for each type. The result is a histogram for pores and a histogram for material.

The distributions $q$ were generated by applying the suggested formula for union. This requires a union of the material distribution and an intersection of the pore distribution. The union of a distribution was suggested as:
Fig. 7. Cubes used for Boolean operations.

\[ p_C(x) = p_A(x) \int_0^x p_B(t) \, dt + p_B(x) \int_0^x p_A(t) \, dt \]

which becomes:

\[ p_C(x) = p_A(x) \sum_{i=0}^x p_B(i) + p_B(x) \sum_{i=0}^x p_A(i) - p_A(x)p_B(x) \]

due to voxelization. Similarly the suggested intersection:

\[ p_C(x) = p_A(x) \int_x^\infty p_B(t) \, dt + p_B(x) \int_x^\infty p_A(t) \, dt \]

becomes:

\[ p_C(x) = p_A(x) \sum_{i=x}^{m'} p_B(t) + p_B(x) \sum_{i=x}^m p_A(t) - p_A(x)p_B(x) \]

where \( m \) is the size of largest nonzero element in \( p_A(t) \), and \( m' \) is the size of the largest nonzero element in \( p_B(t) \).

Figure 8 shows the result of a the union operation on two cubes formed by removal of random spheres from a cube. The green distribution represents the probability that a point in material space will have a pore a given distance away. This is the radius of the largest sphere that can be inserted at a point and fit entirely in the material of the solid. The red distribution represents the probability that a point in pore space will have material a given distance away. This is the radius of the largest sphere that can be inserted at a point and fit entirely within the pore of the solid.
Cube A is shown in Figure 8(a), and cube B is shown in Figure 8(b). The distribution calculated from the formulas, shown in Figure 8(d), should be similar to the distributions calculated from the Boolean operations applied to the voxels, shown in Figure 8(c).

The colors in Figure 9 have the same meaning as before. Cube A is shown in Figure 9(a), and cube B is shown in Figure 9(b). These cubes, unlike those in the last example, are formed by running the termite simulation on a cube of randomly placed voxels. Again, the figure calculated by performing the voxel-by-voxel union operation, shown in Figure 9(c), should be similar to the distribution calculated from the the formulas, shown in Figure 9(d).

The calculated porosity distributions tended to be similar to the distribution actual union. This is consistent with the equality in the derived formula. The calculated material distributions were similar to the actual distributions, but there was a noticeable and consistent deviation. The predicted distribution is greater than the actual for lower radii and less for the greater radii. This behavior can be explained by noting the inequality in the formula. The assumed equality is likely to become less accurate for larger radii. The calculated values for larger radii are understated. Because this causes the calculated values to be smaller, all values are adjusted to bring the area under the distribution to unity. This adjustment causes lower radii to go high (since the distribution is lifted without having fallen) and higher radii to go low (since they are not lifted as much as they fell).
5.2 Example: Simple Boolean Operation

Since we have the distributions describing the properties of a bone, we may use this as one of our primitives. We wish to create a bone scaffold suitable for supporting bone growth. Since we have this primitive, we may obtain the scaffold we desire by subtracting this distribution from a solid block. (Ie, a simple inversion.) The distribution obtained from this inversion is shown in Figure 10(a). This model was then reconstructed. The reconstructed model is shown in Figure 10(b). The fabricated model is shown in Figure 10(c).

5.3 Example: Modeling Porosity with a CSG Tree

Modeling with Boolean operations starts with primitives. In this example, we have chosen primitives with distributions shown in Figure 11(a). Primitives might be hardcoded in the system, obtained from existing porous primitives, or specified at design time.

The next step involves modeling with these primitives. In our case, we chose to model our result according to this equation: \( \text{Result} = ((A \cap B) \cap C')' \). The corresponding CSG tree is shown in Figure 11(a). The target in this example is a distribution that describes properties similar to the inverse of bone matrix.

In practice, one would attach these properties to geometry. In our case, we are only concerned with these properties. For this reason, geometry is not considered in this example.

The next step is to convert the model with attributes into a geometric model that can be fabricated. For this step, we apply the reconstruction techniques described earlier. The reconstructed geometry for our finished product is shown in Figure 11(b). The cube is \( 32 \times 32 \times 32 \).

The final step is to fabricate the finished product. A fabricated unit cell describing the properties of the product is shown in Figure 11(c). This end result is intended to be a growth bone matrix with properties similar to the inverse of bone matrix. In this way, bone matrix can fill the pores of the
reconstructed bone, and the reconstructed bone can degrade away over time.

5.4 Implementation.

Several programs were created during the course of this research. One program analyses these synthetic models, performs the explicit (voxel-by-voxel) Boolean operations, calculates their internal density and porosity distributions as well as the calculated distribution. Another program generates synthetic models using the sphere-based porosity function, by removal of spheres of varying sizes. Yet another program was written to perform simulated annealing and reconstruction. Each of these are ANSI C++ and compiled under G++ and run on Solaris. Some illustrations were made using C++, GLUT, and OpenGL. The distributions were plotted using GNUplot on Solaris.

The complexity of the code for generating synthetic 3D voxel-based models using removal of spheres is $\Theta(n^3)$, where the basic cube is $n \times n \times n$ voxel matrix. The memory requirement is also $\Theta(n^3)$, the volume of the cube. In our case, $n = 100$.

The complexity of the analysis code is $O(n^3 s^2)$, where $s$ is the average size of the spheres that could be fit at any point. Typically, $s$ will be quite small (in the case of the examples used in this paper, $s$ was rarely greater than 10.) The worst case for $s$ is just $\frac{n}{2}$. The resulting $O(n^5)$ time bound occurs when the cube is nearly empty or nearly solid. The memory requirement is again $\Theta(n^3)$, the volume of the cube.

The reconstruction code is written in ANSI C++, compiled and run under Solaris. The complexity
of this code is $O(n^3s^2 + In^3 + Is^6)$ in the worst case, where $I$ is the number of iterations performed. In practice, the last term is not too bad; $s$ tends to be small, and the constant is not too large. The memory requirement is $\Theta(n^3)$.

6 Discussion.

Through the use of stochastic functions in combination with density and the methods of CSG, we have laid a theoretical framework for representing and modeling porous, heterogeneous objects. We have extended the traditional Boolean operations of union, intersection, and subtraction into a domain where representing, manipulating, and modeling density is possible in a concise and logical manner.

We suggest the usage of stochastic functions as a means of representing porosity in addition to the density, making it possible to specify not only how much material and pore space exist but also describe the properties of the pores themselves (e.g., pore size or pore roughness). We also explored the theoretical basis for the Boolean manipulation of these stochastic functions without knowledge of the underlying geometry or the representation of individual pores. In doing so, we suggested a means of extending the Boolean operations to the domain of porous solids, where objects of varying geometry, density, and porosity may be used to aid in the design of more complex solids than was before possible.

The effectiveness and consistency of the Boolean density operations is theoretically and empirically sound. The proposed method of combining stochastic functions, though not perfect, is both theoretically sound and shows great promise.

Combining stochastic functions using a means independent of the geometry of the object has serious shortcomings. Because the geometry is not entirely described by the distributions, the combination of these distributions can be done only statistically. Considering the stochastic nature of the problem, the distributions calculated using the described formulas describes the actual distributions approximately. One might apply adjustments to the resulting distributions to correct error that systematically results in practice. This is especially useful where the inequality was replaced with equality for calculations.

7 Conclusions

The design and fabrication of heterogeneous structures requires new techniques for solid models to represent such 3D objects with complex internal shape and material properties. This paper introduced a novel representation of model density and porosity based on stochastic geometry and showed how to use this representation to create CSG-based models of heterogeneous objects. The authors believe that, while density has been previously studied in the modeling literature, representation and modeling with porosity is a new problem for solid modeling.
In a number of bio-material and composites applications, porosity is a critical design and fabrication parameter. Using our mathematical formulation, we performed a set of experiments that showed that the techniques can be implemented and that the results are well-behaved with respect to synthetic model data. We believe that results from these limited experiments indicate our technique could be the basis of a new set of data structures and algorithms for high-fidelity representations of heterogeneous objects. Our future work includes integration of these techniques into CAD, enabling interactive design, analysis and (eventually) manufacturing of customized heterogeneous materials.

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