Modeling and Designing Components with Locally Controlled Composition

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Abstract

SFF processes have demonstrated the ability to produce parts with locally controlled composition. In the limit, processes such as 3D Printing can create parts with composition control on the length scale of 100 microns. To exploit this potential, new methods to model, exchange, and process parts with local composition need to be developed. An approach to modeling a part's geometry, topology, and composition will be presented. This approach is based on subdividing the solid model into sub-regions and associating analytic composition blending functions with each region. These blending functions define the composition throughout the model as mixtures of the primary materials available to the SFF machine. Various design tools will also be presented, for example, specification of composition as a function of the distance from the surface of a part. Finally, the role of design rules specifying maximum concentrations and concentration gradients will be discussed.

Introduction

This research into modeling and designing components with locally controlled composition is part of a larger project funded by the National Science Foundation titled "The Distributed Design and Fabrication of Metal Parts and Tools by 3D Printing." The overall goal of this project is to identify the barriers preventing designers from accessing the unique and useful capabilities of SFF processes such as 3DP and provide solutions. One of the identified barriers is the inability for designers and manufacturers to work with models of graded compositions. To address this issue, we are researching methods to represent, design, exchange, and process these models with the intention of promoting the use and research of Local Composition Control through 3DP by a wider audience.

Background: Local Composition Control (LCC) through 3D-Printing (3DP)

Solid Freeform Fabrication (SFF) refers to a class of manufacturing processes that build objects in an additive fashion directly from a computer model. Although most build from a single material and in layers, a few SFF processes possess the capability to fabricate objects from multiple materials in a near point-wise fashion. The combination of these two features allows for the possibility of Local Composition Control (LCC) through which graded compositions can be manufactured from the base materials available to the SFF machine[1,2]. One such SFF process capable of LCC is 3D Printing[1].

Conventional 3DP manufactures a part by selectively binding powder together according to a computer model. The build cycle begins by spreading a layer of powder over the print bed. A print head then traverses the bed, selectively depositing binder over the regions corresponding to the interior of a slice of the

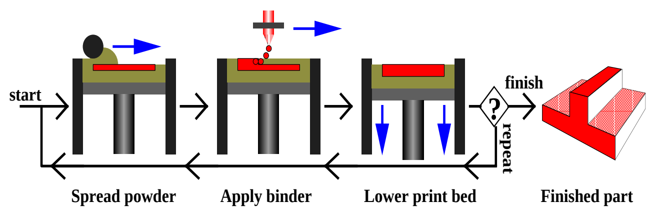

Figure 1. Conventional 3DPrinting process.

computer model. After the binder dries, the print bed is lowered and another layer of powder is spread. The process of spreading powder, depositing binder, and lowering the print bed is repeated, as shown in Figure 1, until the entire volume of the object is printed. At the end of the process, the bound powder becomes the manufactured object, effectively rendering the computer model as a physical object. Currently, metal and ceramic parts are being manufactured through 3DP, but the potential exists to build with any material supplied in powder form.

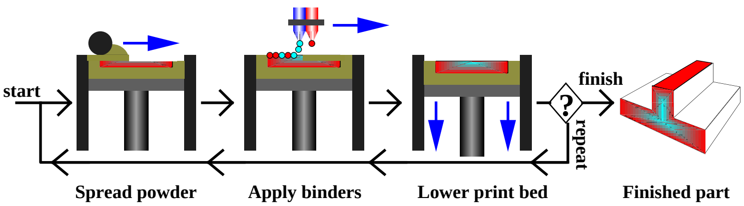

Figure 2. LCC through 3D Printing of multiple binders.

Similar to how an ink-jet printer prints color documents, 3DP can achieve LCC with multiple materials. This is accomplished by using a print-head with several jets, each depositing binders and /or slurries of unique material. By varying the pattern in which the jets deposit material on the powder-bed, the material composition can be controlled on the scale of the binder droplets (≅100µm). Regions of uniform and graded compositions can be created in a manner analogous to how continuous tone images are rendered on a hard-copy device from primary colors. With this capability, graded compositions can be designed along with the geometry of the part, tailoring the part's physical properties for a specific purpose or function. Such compositions have become known as Functionally Graded Materials (FGMs).

The capability of producing FGM could be utilized by a wide variety of industries. Some applications being studied at MIT include:

1. Wear resistance and increased strength of a mechanical part through the controlled variation of its FGM composition[3].
2. Design of electrical components by controlling the electrical properties on a local scale.
3. Variation of medicine placement within an FGM pill to optimally deliver drugs to a patient through the "controlled release" of the drug over time[4].

Information Flow of FGM Solid Models

Despite the advanced capabilities of SFF machines, access to this new technology is limited by how information is represented, exchanged, and processed. Designers need new CAD tools to capture their ideas for FGM parts and manufacturers need algorithms capable of converting these models into machine instructions for their fabrication. To address these shortcomings and make LCC processes like 3D Printing available to the design community, this project is developing new methods for the design, representation, exchange, and processing of FGM models.

In current SFF practice, a model is communicated between the designer and manufacturer in terms of a tessellation of the model's boundary, usually in the form of a .STL file[5]. Only communicating information about the bounding surfaces, material information about the model is not conveyed, presenting a barrier to designers who wish to use LCC to create parts graded compositions.

Similar to how computer users regularly use desktop printers to produce hardcopy of their documents, 3DP can potentially permit a clean separation between the design of a part and its manufacture. For this to happen, a method for completely representing a part must be established, allowing its neutral exchange between designers and manufacturers. For traditional CAD models, this can be accomplished through the use of the IGES or STEP formats. For models consisting of FGM, however, the representation must go one step further and allow the representation of graded material compositions. This representation, along with tools for the design, inspection, and processing of FGM models, will increase access to SFF manufacturing with LCC by allowing more efficient flow of information between designers, manufacturers, and researchers.

Representation of FGM Models

In order to represent an object within the computer, a data structure representing all of the relevant information for its fabrication must be established. In traditional CAD systems, solid modeling methods maintain information about an object's geometry (shape) and topology (adjacency relationship between the geometric elements of its surface)[6]. Some CAD systems also provide the capability to associate material information with regions, facilitating the representation of composite structures. With the possibility of fabrication with LCC, a solid modeling method for 3DP must go one step further and represent smoothly varying compositions. Similar to how sculpted geometry can be represented as analytic functions (such as NURBS surfaces) methods to analytically describe how an FGM composition varies within a part need to be established. To provide this capability, an FGM solid modeling method must decompose the interior of the object into simpler sub-regions, each of which references information about the composition variation over its domain. To accomplish this goal, an FGM solid modeling method based on a representation known as the cell-tuple data structure[7] is under development. This structure naturally lends itself to the representation of models in terms of sub-regions over which the FGM information can be incorporated, similar to how the geometric information is maintained.

In the traditional cell-tuple structure, a model is decomposed into a set of cells with each cell representing a topological feature in the model, such as a vertex, edge, face or region. The topology of the model (or how the cells are connected together) is maintained by a graph of cells. The shape, position, and orientation of the model are determined by geometric information associated with each cell. Figure 3 illustrates this concept for a simple model of a tetrahedron with cells representing the different topological elements. For larger models, the interior may be decomposed into a single region, as in the .STL file, or subdivided into many smaller regions, similar to a finite element mesh.

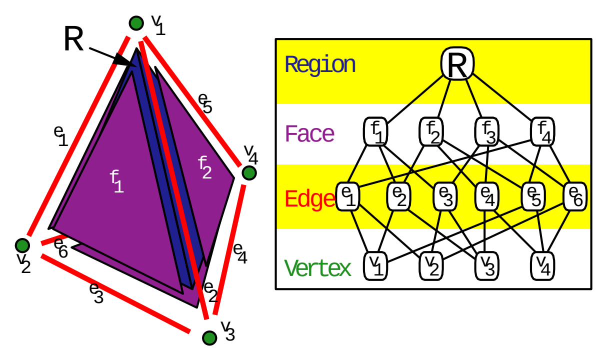

Figure 3. Model of a tetrahedron and its graph of cells.

To represent a FGM model within the cell-tuple structure, composition information, as well as geometric information, is associated with each cell. This information begins with the concept of a material system consisting of the primary materials available to an SFF machine capable of LCC: $\vec{S} = \{m^1, \ldots, m^N\}$. The composition of the model M is represented as a vector valued function $\vec{C}$ defined over the model's interior: $\vec{C} = \vec{C}(\vec{x})$ for $\vec{x} \subseteq M$. Each component of

$\vec{C}$ represents the volume fraction of the corresponding material in the material system $\vec{S}$ present at point $\vec{x}$ within the model.

There are many possible approaches to defining the composition function $\vec{C}(\vec{x})$. For parts similar to traditional composite structures, constant values can be associated with each sub-region within the model. For graded compositions, however, analytic functions must be defined, capable of representing smooth variations in the volume fractions of the materials over the domain of each sub-region.

With the cell-tuple structure's capability to represent models as subdivided manifolds, models can be arbitrarily subdivided into topologically simpler domains over which composition functions can be defined. In our approach, we are simplifying the problem by beginning with models subdivided into tetrahedral meshes, permitting the use of standard meshing algorithms to convert solid models to our cell-tuple representation. Over each tetrahedral domain, the composition is formulated in terms of a set of *control compositions* $\vec{c}_{\vec{i}}$ (see Figure 4) and basis functions $B^n_{\vec{i}}(\vec{u})$, where $\vec{i} = (i, j, k, l)$ is the index of the control composition, $B^n_{\vec{i}}$ is the Bernstein polynomial of degree n corresponding to index $\vec{i}$, and $\vec{u} = (u, v, w, t)$ is the barycentric coordinate within the tetrahedron[8]:

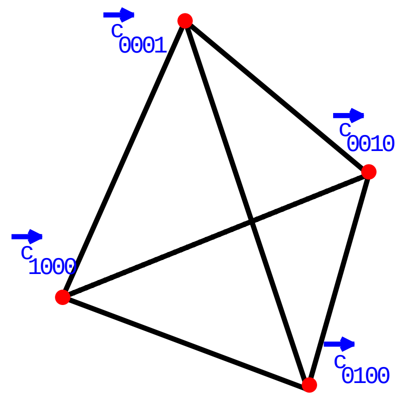

Figure 4. Wireframe view of a linear FGM tetrahedron with control compositions.

$$\vec{C} = \vec{C}(\vec{u}) = \sum_{|\vec{i}|=n} \vec{c}_{\vec{i}} B^n_{\vec{i}}(\vec{u}), \quad B^n_{\vec{i}}(\vec{u}) = \frac{n!}{i!\,j!\,k!\,l!} u^i v^j w^k t^l, \text{ and } |\vec{i}| = i + j + k + l \ .$$

Conceptually, the composition at a point can be considered as a blend of the control compositions with their influence determined by the value of their basis functions, analogous to the representation of NURBS surfaces with a mesh of control points. By defining compositions in terms of the Bernstein polynomials, the degree of composition variation is arbitrary, permitting the representation of regions of piece-wise uniform composition as well as higher order graded composition, as shown in Figures 5 and 6.

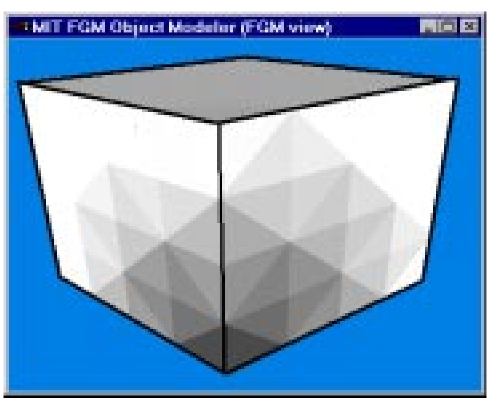

Figure 5. Cube consisting of 320 piece-wise constant FGM tetrahedra.

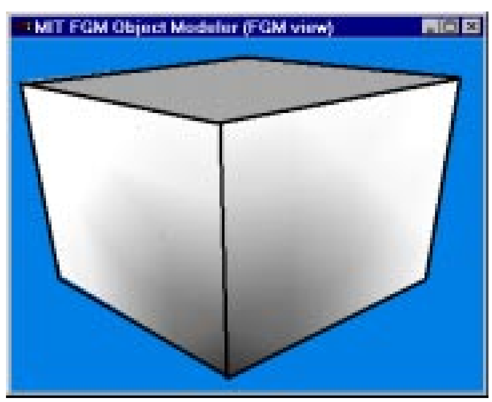

Figure 6. Cube consisting of 320 piece-wise linear FGM tetrahedra.

Although beginning with meshed tetrahedral models, the cell-tuple data structure is sufficiently general to represent a model as any valid subdivided manifold. This will permit FGM objects to be efficiently and accurately modeled from a suitable collection of FGM cells. Regions of uniform composition, for example, could be represented with a single region cell of constant composition, bounded by an arbitrary number of faces (similar to the traditional Boundary Representation and .STL representation). For graded regions, a collection of FGM cells starting with the tetrahedron can be defined, permitting different subdivision schemes of the object's interior. Hexahedral, wedge, and pyramid finite elements, for example, could eventually be defined with formulations for their geometry and graded composition in terms of tensor product B-splines or mixed tensor product B-splines and barycentric polynomials[9]. These formulations permit specification of continuous compositions at the interface of the cells using elementary properties of Bernstein polynomials and B-splines. However, specification of compositions with higher order derivative continuity is more complex and is not addressed in this paper.

The main components of our FGM solid modeling system are shown in Figure 7. Models created on a commercial CAD system are meshed into finite elements and then loaded into the data structure. As described above, model's topology is maintained by the cell-tuple structure as a graph of cells. Each cell in the model references information about its own geometry, a set of control compositions, and blending functions to define the variation in composition. The material system is composed of the primary materials available to the SFF machine. The SFF machine is assumed to have the capability to selectively place primitive of each material during the build process. Similar to how an ink-jet printer strategically places drops of the primary colors on a page to represent continuous tones, the model processor will generate the machine instructions to accurately fabricate the desired compositions. The processing of FGM models for fabrication will be based on halftoning algorithms similar to those used in image processing[10].

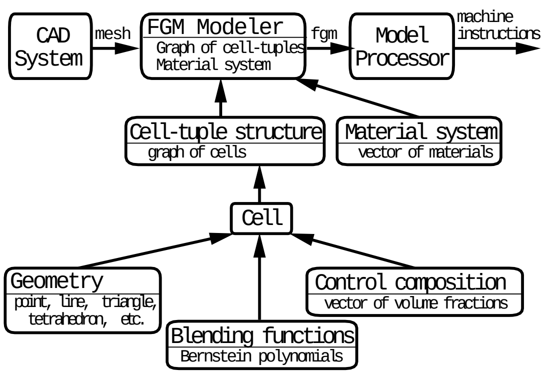

Figure 7. Components of FGM object modeler.

Methods for Designing FGM Models

With each *control composition* in our data structure representing a degree of freedom, the task of designing the FGM can be non-intuitive and confusing at the very least, if not impossible considering that a model may have millions of FGM sub-regions. To aid the designer, tools for simplifying and automating the design of FGM compositions are being developed. One approach being explored is the design of compositions in terms of distance functions.

The design of FGM compositions in terms of distance functions begins with the selection of a feature from which the composition will be designed. This may be a fixed reference in the coordinate system of the model, such as a point, line, or plane, or a feature of the model, such as its boundary or a particular face. Next, the designer specifies a variation for the FGM in terms of distance from the feature: $\vec{C}_{design} = \vec{C}(r)$, where r is the distance of a point from the reference feature. With a reference feature selected and a FGM variation designed, an algorithm automatically assigns values to the model's control compositions to define its FGM.

Design example 1: FGM design of a pulley.

Figure 8. Pulley model.

To illustrate the concept of designing FGM as a function of distance from a line, consider the FGM design of a pulley in Figure 8. The designer, using a 3DP machine capable of building stainless steel parts with local control over the concentration of carbide wishes to optimally design an FGM composition resistant to wear. First, the CAD model is meshed into tetrahedral domains and loaded into the composition design system. The designer then specifies the pulley's axis of rotation as the reference feature from which the composition will vary. The final step in the design process is the design of the composition variation of the pulley as a function of distance from the axis. In this case, the concentration of carbide is greatest near the hub and rim where wear is greatest, as shown in Figure 9. The control compositions are then automatically assigned to the model, creating the desired FGM pulley as shown in Figure 10. A view of a pulley spoke showing the FGM tetrahedra is given in Figure 11, illustrating how the composition is defined over tetrahedral sub-regions.

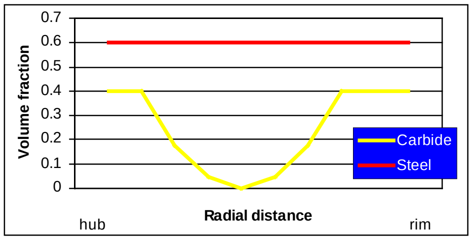

Figure 9. Variation of carbide concentration in pulley.

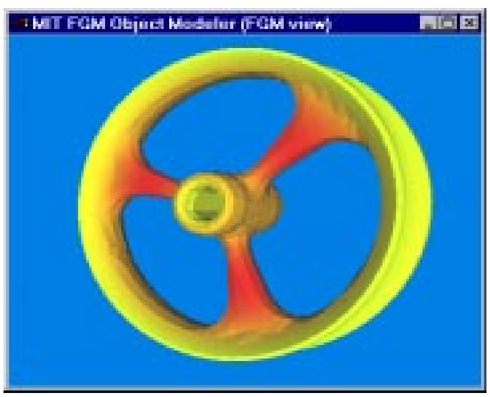

Figure 10. Composition variation over pulley with increased hardness at rim and

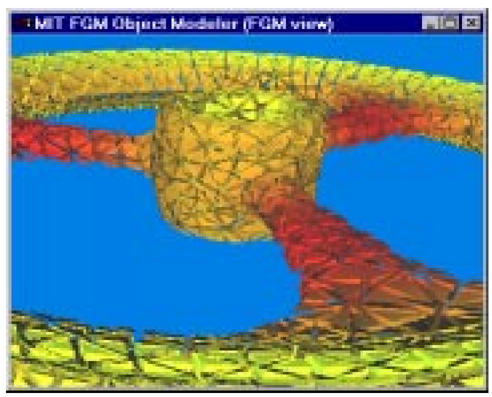

Figure 11. View of spoke decomposed into FGM tetrahedra.

Design example 2: FGM design of a drug delivery device for controlled release.

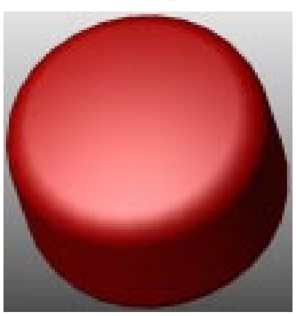

Figure 14. Model of pill.

With the ability to rapidly build objects through LCC, customized drug delivery devices can be created, optimally tailoring the release of drugs into the body. The design of the pill's FGM involves the controlled placement of medicine as a function of distance from its boundary. Knowing that the rate at which medicine is released into the body is governed by the rate at which the pill dissolves, the medicine concentration profile within the pill can be tailored for optimal release[4]. In this case, the powder bed is the pill matrix and the drug placement is controlled by the print-head. Figure 14 shows the initial model of a pill

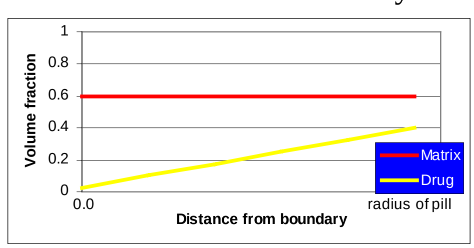

Figure 15. Design of drug concentration profile from the pill boundary.

before it is meshed into tetrahedra. The designer then specifies the concentration profile of the drug as a function of distance from the boundary, as given in Figure 15. The control compositions are then assigned, with each one's concentration determine by its distance to the nearest exterior boundary of the pill. Figure 16 shows a sliced view of the FGM pill with the variation in composition represented as colors on the internal surfaces of the tetrahedra. Figure 17 is the same pill but rendered with shrunken tetrahedra.

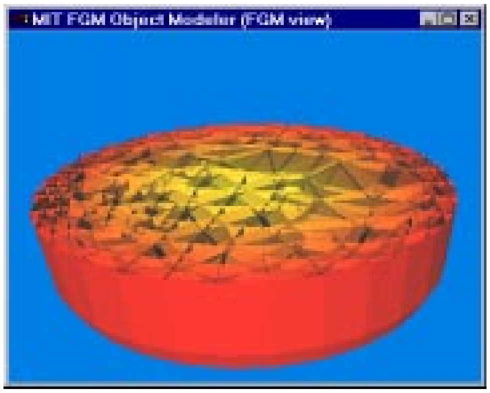

Figure 16. Clipped view of FGM pill.

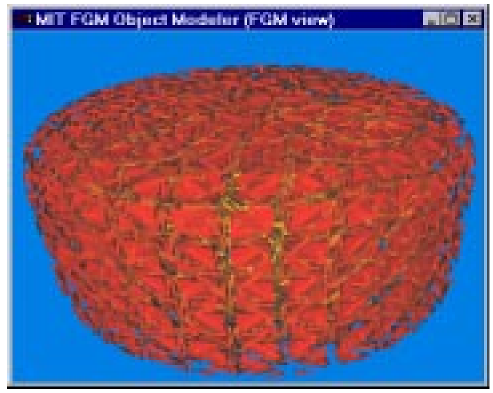

Figure 17. Decomposed view of pill.

Design Rules for FGM Models

The ability to represent complex FGMs does not guarantee the ability to manufacture the part. Due to the limited accuracy and resolution inherent in any process, some FGM models may not be fabricated to the designer's satisfaction. To avoid this situation, a set of "Design Rules" governing the design of FGMs need to be established. These Design Rules will be based upon the limitations in the manufacturing process (resolution, accuracy, layer thickness, etc.) and will inform the designer about the model's manufacturability. If the CAD model violates the Design Rules, the designer will be informed of the violation and will have the opportunity to redesign the object without the costly and disappointing process of manufacturing an unacceptable product. By providing tools to enforce Design Rule checking, some of the burden of ensuring part quality is reduced, allowing the designer to work with FGMs without being an expert in the manufacturing capabilities of the machine. Similar concepts involving minimum feature size were explored for macro-texturing for 3DP[11]. For FGM models, two Design Rules are being explored, governing the model's composition and its rate of change. Only the former is described here.

Design Rule limiting maximum and minimum composition.

Depending upon the material system used to fabricate the part, there is a limitation to the maximum and minimum volume fraction of each material that can be present and still guarantee successful fabrication. Hence, the first foreseen Design Rule would limit the maximum and minimum concentration of each material in an FGM model.

In 3DP, the material system is composed of the powder in the print-bed and several different binders and/or slurries (solutions without binding properties) jetted from the print-head. In order to form the print-bed a minimum amount of powder must be present, thereby imposing a lower limit on the amount of the powder in the FGM. Likewise, the maximum packing density will limit the maximum concentration of powder's material. During printing, the voids left in the print-bed are filled with material jetted from the print-head. Its porosity places a limit on the maximum total amount of jetted material it can hold. In addition, to form a solid part, a minimum about of binder is required to hold the powder particles together, placing a lower limit on the amount of binder throughout the interior of the model.

Enforcement of the Design Rules involves restricting the assignment of the FGM $\vec{C}(\vec{x})$ such that $DR^{\min,j} \le C^{j}(\vec{x}) \le DR^{\max,j}$, where j is the material index and C^{j} is the corresponding volume fraction of material. For a system of three materials (powder, binder, slurry), a sample set of Design Rules governing the permissible compositions is given in Table 1. These Design Rules are applied to the hypothetical FGM model in Figure 18. For this example, the composition grades from powder and slurry at the top and bottom faces to powder and binder at the mid-plane. Due to the requirement of a minimum amount of binder, the compositions at the top and bottom need to be redesigned in order to guarantee a solid part.

Material system	$DR^{\min,j}$	$DR^{\max,j}$
m^1 = Powder	0.7	0.8
m^2 = Binder	0.1	0.3
m^3 = Slurry	0.0	0.3

Table 1. Design rule limiting volume fractions of material.

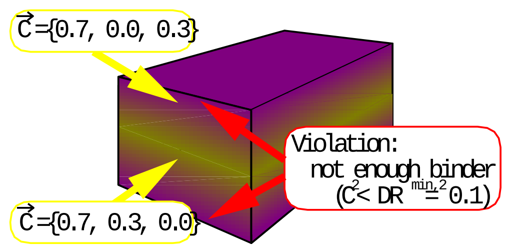

Figure 18. Extreme volume fraction of materials in FGM violate design rules.

Acknowledgements.

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