Title:
Material-Unit Network for Multi-Material-Property and Multiscale Components

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Introduction:
Currently, additive manufacturing technologies have already been widely used to fabricate parts with complex geometries. Porous structures with multiscale complexities can be fabricated by AM process without support structures [6]. To take advantage of design freedom provided by AM, several design methods for additive manufacturing [4] has been developed. However, it should be noted that most existing design methods only focus on structure’s geometry. Thus, most parts designed by existing DfAM methods are made of single materials [5].

To further improve the performance of designed products, concurrent optimization methods [2,3] which can update the distribution of material microstructures and structure’s macro geometry have been developed. Comparing to design optimization method focused on a single design scale, concurrent optimization methods can achieve better performance especially for design cases for multifunctional purposes. Even though, those concurrent optimization methods are promising in terms of their performance, none of the results of these optimization methods have been successfully fabricated by existing AM technologies. It is difficult to model the optimized results in existing commercial CAD software. The modeling techniques used in existing commercial CAD software only capable to deal with geometry with single material defined on a single design scale. To solve this problem, an innovative modeling framework is proposed in this paper to enable the modeling of structures with multiscale complexities.

Main Idea:
Multi-Material-Property Components

Fig. 1 represents the bone’s multi-scale configuration from the five scales of nanoscale, sub-microscale, microscale, mesoscale and microscale [1]. It can be seen that the whole bone has different constituent elements at different scales, and each element corresponds to different geometry, material and property information.

With the further development of AM technology, it can be inferred that this kind of configuration shown in Fig. 1 will be the main component of future products, and also the common object of future product manufacturing.

In this paper, an independent shape or structure with the following features in space is called a Multi-material-property Component:
① Limited size;
The shape and structure are composed of a set of geometric elements such as points, curves, surfaces and/or solids;

Within each geometric element (including a point), one or more materials are distributed in a certain way.

It can be seen from the above definition that the multi-material-property component studied in this paper not only retains the "limited size" of the traditional component structure, but also adds low-dimensional geometric elements such as points, curves and surfaces to the macro-structure composition, which is further speculated and expanded based on AM. On the microscopic aspect, the introduction of multi-material-property distribution has created conditions for further improving the performance of product components that that are traditionally distributed only with a single variety of materials.
Material-Unit Network

The results of all the multi-material-property operations of the above-mentioned component models are a group of material units which are adjacent to each other. We use graph to define and represent the operation result, which is called the material-unit network. Since the material unit and their adjacency relationships have certain specific properties and types, it is necessary to expand the concept of "graph" in mathematics before defining and establishing the material-unit network, and the extended graph is called "Extended Network".

The extended network is used to define and represent a component $C$, namely:

$$ C = (U, R) $$

where vertex set $U$ is the set of all component element and material unit (hereinafter collectively referred to as material unit) $u_i (i = 1, 2, ..., m)$, namely:

$$ U = \{u_1, u_2, ..., u_m\} $$

Edge set $R$ is the set of all relationships $r_j (j = 1, 2, ..., n)$ between $u_i (i = 1, 2, ..., m)$, namely:

$$ R = \{r_1, r_2, ..., r_n\} $$

The structure defined in Eqn. (2.1) is called the Material-Unit Network of a component. The intuitive definition of relationship $r$ is shown in Fig. 4, where 0 and 1 on the connecting line respectively define the correlation between material unit and relationships, and we agree that if there is no special annotation, 1 indicates correlation.

Fig. 4: Relationship of material unit: (a) Directed edge, and (b) Undirected edge.

1) Relationships Between Material Units

Let $r$ be any one of relationships of $R$, i.e., $r \in R$, then $r$ can be represented as

$$ r = u_i (g_j) | u_i \in U, i = 1, 2, ..., n_u > $$

which means that there is a relationship between the boundary element $g_j$ in $u_i (i = 1, 2, ..., n_u)$, $n_u = d(r)$.

2) Associated Unit

We call $u_i (i = 1, 2, ..., n_u)$ in Eqn. (2.4) the associated material unit, or Associated Unit for short, and $g_j$ is called the associated boundary element, or Associated Element for short. The set of all the associated material units of $r$ is called the associated unit set, denoted by $U(r)$, which is:
The set of all the associated elements is denoted as $B(r)$, which is:

$$B(r) = \{ g_i | u_i(g_i), u_i \in U, i = 1,2,...,n_u \}$$  \hspace{1cm} (2.6)

If both $b$ and $g$ are boundary elements of material unit $u$, and $b$ is the composition of $g$ or equals $g$, we unify the representations as $b \in g$.

(3) Overlapping Relationship

Let $r_1 = < u_1'(g'_1) | i = 1,2,...,n_1 >$ and $r_2 = < u_2'(g'_2) | i = 1,2,...,n_2 >$ be two relationships, if the following conditions are both met:

a. $d(r_1) = d(r_2)$, i.e., $n_1 = n_2$ ;

b. For any boundary element $g_2$ of $B(r_2)$, $\exists g_1 : g_1 \in B(r_1) \land g_2 \in g_1$, i.e., $g_2$ is also a boundary element of $B(r_1)$ or the composition of one of the boundary elements. Then $r_2$ is called the Overlapping Relationship of $r_1$.

Axiom: There is no overlapping relationship in a material-unit network.

(4) Cluster of Relationships between Material Units

In a material-unit network, set $u_1$ and $u_2$ be two material units, then all the relations between them are recorded as $R(u_1, u_2)$, namely:

$$R(u_1, u_2) = \{ r | u_1 \in U(r) \land u_2 \in U(r) \}$$  \hspace{1cm} (2.7)

That is to say, $R(u_1, u_2)$ is a set of all relations $r$ between associated unit $u_1$ and $u_2$, $R(u_1, u_2)$ is called the cluster of relationships between material units.

Example

Fig. 5: Example: (a) Microfibril component, (b) Relationships of material unit, and (c) Material-unit network.

A microfibril in nanoscale from Fig. 1 is used to illustrate material-unit network shown in Fig. 5, $u_i$ represents skin of microfibril and consists of Side $S_{1_1}$. $u_2, u_3$ is tropocollagen that makes up core of microfibril, which consist of Side $S_{2_1}$, Plane $S_{2_2}, S_{2_3}$ and Side $S_{3_1}$, Plane $S_{3_2}, S_{3_3}$ respectively. The relationships among $u_i, u_j$ and $u_k$ in the material-unit network are:

1. $r_1 = < u_1(s_{1_1}), u_2(s_{2_1}) >$,
2. $r_2 = < u_2(s_{2_1}), u_3(s_{3_1}) >$,
3. $r_3 = < u_1(s_{1_1}), u_2(s_{2_1}) >$,
4. $r_4 = < u_1(s_{1_1}), u_2(s_{2_1}) >$,
5. $r_5 = < u_2(s_{2_1}), u_3(s_{3_2}) >$,
6. $r_6 = < u_2(s_{2_1}), u_3(s_{3_2}) >$

Obviously, $r_3, r_4$ and $r_5, r_6$ are Overlapping relationships of $r_1$ and $r_2$ in turn.

Around the above mentioned material-unit network, the common object design pattern is used to define each object class, including refining and defining data members such as geometry, material, property, and related data processing functions of each object class, and on that basis, we establish...
the relationship between object classes, as shown in Fig. 6. "vertex" refers to the vertex of "graph", which is the abstraction of "material unit" and "component". This pattern is based on the "composite" object pattern.

**Conclusion:**
Based on developed material-unit network, a set of operations will be defined to enable the generation and modification of multiscale objects. These operations mainly include Boolean operation such as difference, union, intersection. Comparing to existing boolean operations algorithm, the developed operations and their related algorithms involve the calculation on both materials and geometries. Thus, more research needs to be done to investigate how to apply these operation algorithms on both materials and geometries.

**References:**