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Optimal design of functionally graded materials using a procedural model and particle swarm optimization

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ABSTRACT

A new method for the optimal design of Functionally Graded Materials (FGM) is proposed in this paper. Instead of using the widely used explicit functional models, a feature tree based procedural model is proposed to represent generic material heterogeneities. A procedural model of this sort allows more than one explicit function to be incorporated to describe versatile material gradations and the material composition at a given location is no longer computed by simple evaluation of an analytic function, but obtained by execution of customizable procedures. This enables generic and diverse types of material variations to be represented, and most importantly, by a reasonably small number of design variables. The descriptive flexibility in the material heterogeneity formulation as well as the low dimensionality of the design vectors help facilitate the optimal design of functionally graded materials. Using the nature-inspired Particle Swarm Optimization (PSO) method, functionally graded materials with generic distributions can be efficiently optimized. We demonstrate, for the first time, that a PSO based optimizer outperforms classical mathematical programming based methods, such as active set and trust region algorithms, in the optimal design of functionally graded materials. The underlying reason for this performance boost is also elucidated with the help of benchmarked examples.

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1. Introduction

Designing objects with Functionally Graded Material (FGM) distributions has been the subject of substantial research interest in recent years. This popularity is largely due to the many excellent and unique properties that FGM objects possess: for instance, the combined advantages of different materials, improved material compatibilities and good adaptability to versatile working conditions [1].

In the past few decades, considerable attention has been devoted to FGM representations (Computer-Aided Design), design validation (Computer-Aided Engineering), fabrication (Computer-Aided Manufacturing) and material heterogeneity optimization. These efforts were primarily targeted at answering the following questions [2]:

- (1) How best to *represent* a FGM object's geometries and material distributions?
- (2) Does the designed FGM object fulfil the user's functional requirements? How to *validate* its functional property or performance?

- (3) Is it physically realizable? How to make it?
- (4) Subject to the given constraints and external stimuli, how to identify the *optimal* design among different *representable*, *validated* and *manufacturable* models?

In the literature, problems (1)–(3) have been extensively investigated, and many well-established approaches to tackle the CAD [3–14], CAE [5,7,15–18] and CAM [19–26] problems have been found. In contrast, fewer investigations have been conducted into the optimal design of functionally graded materials.

Many existing FGM models were originally proposed for the purpose of computer *visualization*, *rapid prototyping* or design *evaluation* [4,14,27–29], and a large number of parameters or design variables are required to model heterogeneous FGM distributions [30]. Such representations can seldom be migrated unchanged to optimal design problems because the high dimensionality of the representations may impose significant computational overheads, making them prohibitively expensive or impractical for use in design optimization. For instance, it is feasible to represent the material heterogeneity with a 1024×1024 pixel bitmap where the intensity of a pixel denotes the volume fraction of materials. However, it is likely to be problematic to attempt design optimization with over one million design variables, as the computational cost entailed is hardly affordable even for modern computers. Other straightforward (e.g. explicit function based)

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models are better suited for FGM optimizations: when the material variations are represented with *explicit*, *analytic* functions [5,15, 16,31], the optimization search space can be confined within reasonably limited domains (e.g. pre-set functional formalism), and optimal solutions can be obtained much more efficiently and economically. However, only in rare cases can a material distribution be represented in such *explicit* and *analytic* forms. This becomes especially difficult when the objects under design have complex material distributions, where a *single analytic* function fails to characterize the material heterogeneity throughout the entire domain [1,32].

This paper is motivated by a desire to tackle the aforementioned challenges and to investigate effective approaches to tackle FGM design optimization problems. We propose the use of a procedural model to represent generic heterogeneous objects and employ Particle Swarm Optimization (PSO) as the mathematical optimizer. In contrast to most explicit functional models, the proposed procedural model allows more than one explicit function to be used to describe complex material variations. With such a model, the material composition at a given location is not calculated by simple evaluation of an analytic function, but obtained by execution of series of customizable procedures. The model therefore enables generic and diverse types of material variations to be represented, and most importantly, by a reasonably small number of design variables. The PSO method is inspired by the natural process that intimates the social sharing of information among conspeciates [33]. PSO has proved to be especially suited to finding the global optimum for problems of multimodality and nondifferentiability [34]. By leveraging the benefits of the procedural model and PSO optimizer, we show that optimal FGM design can be flexibly and efficiently conducted.

The rest of this paper is structured as follows. Section 2 briefly reviews related work and current challenges, and the motivations of this work are identified. Section 3 focuses on the proposed methodology: the details of Heterogeneous Feature Tree (HFT) based procedural model and the PSO approach are presented. Implementation details, benchmarking examples and case studies are provided in Section 4. Concluding remarks and discussions are finally offered in Section 5.

2. Related work and motivations

Two of the most important issues in the optimal design of FGM objects are the *representation* of the FGM object and the *optimization method* used. The FGM representation determines how a functionally graded material distribution is encoded or abstracted into a parametric model, where the design variables are identified and the material heterogeneity is formulated with functions of these variables. The optimization method, either sensitivity based or sensitivity-free, influences the global optimality of solutions as well as the computational efficiency of the process.

2.1. FGM representation and design parameterization

In terms of the design parameterization scheme, existing approaches can be classified into two mainstream types. *Discrete models* partition the geometric domain of interest into a collection of lumps, and each lump is assumed to have a homogeneous or an interpolated material composition. Cho and Ha [35], Cho and Shin [16], Na and Kim [36] discretized the object under design into a number of homogeneous 1D *layers* in the optimal design of *unidirectional* FGM objects. The design variables of the optimization problem are the material compositions of each homogeneous lump, and the objective might be minimizing the peak thermal stress or the mass/weight of a component. For

Table 1Number of design variables in *discrete* model based FGM optimization.

FGM representations	Number of design variables	References
1D layers	10	Cho and Ha [35] Cho and Shin [16] Na and Kim [36]
2D rectangular elements 3D tetrahedral elements	72, 77 104	Cho and Ha [3] Hu et al. [26]

bidirectional FGM optimization problems, Cho and Ha [3] proposed a two-dimensional volume fraction optimization procedure for relaxing the effective thermal stress, and the 2D geometric domain is discretized into a collection of uniform rectangles. Hu et al. [26] further extended the discrete model in tri-variate FGM design in which a three-dimensional I-beam is discretized into tetrahedral elements. The material compositions defined at the tetrahedron vertices are regarded as design variables, and the material of any point inside a tetrahedron is defined with linear interpolation between the compositions of the nodes (i.e. the tetrahedron vertices).

Using discrete models, a large number of design variables are usually needed, which may significantly degrade computational efficiency. Table 1 lists the number of design variables used in typical discrete-model based FGM optimizations. It can be clearly seen that as the dimension of the object changes from 1D to 3D, the optimization search space is enlarged enormously. Note that the growth in the computational resource consumption (including CPU time and memory) is seldom linear but often involves steep nonlinear increases: this is understandable due to the intensive calculations required in finite difference based sensitivity analysis [37], as will be further elaborated in Section 2.2.

Instead of modeling FGM distributions with spatial discretization, functional models [1] avoid direct specification of material compositions at discrete sites, but rather use a function defined over a geometric domain to describe the material heterogeneity. In representing unidirectional functionally graded materials, Elishakoff et al. [5], Na and Kim [38], Ootao et al. [39] and Lin et al. [40] represented the material heterogeneity with power-law based distributions; while Eraslan and Akis [7] proposed exponential and parabolic functions. Huang et al. [15] described the FGM distribution with a parametric Bezier curve based representation. Biswas et al. [41] proposed using a generalized Taylor expansion to formulate material heterogeneities. Similar functional representations were also extended to model bidirectional and tri-variate FGM objects: Vel and Pelletier [42] formulated the FGM distributions with piecewise cubic Hermite polynomials and the materials defined on a 2D domain are interpolated from a collection of control points; Nemat-Alla [43] and Hedia et al. [44] employed multivariate polynomial functions to model 2D material heterogeneities; Schmitt et al. [45], Martin and Cohen [9] and Hua et al. [8] further extended such methods in the design of tri-variate FGMs, where FGM objects are modeled with B-spline/NURBS volumes using tensor product representations.

Using a functional model to represent FGM distributions, the design variables are in most cases the coefficients of analytical functions, for instance the power index for power-law based formulae or polynomial coefficients for Taylor expansions. This explicit and concise representation makes functional models well suited for material formulation in the optimal design of FGM: they are intuitive, easy to implement and computationally efficient, as only a few design variables are required to fully characterize the material distributions, see Table 2.

Despite the apparent advantages of functional models, it should be noted that explicit functional models also have certain

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