Modeling Functionally Graded Porous Structures with Stochastic Voronoi Diagram and B-Spline Representations

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***Abstract*—Functionally Graded Materials (FGMs) have been extensively studied in the past few decades. With increasingly powerful computers and highly precise measuring technologies, initial macro-scale volume fractions based FGM characterization has been extended to microstructural models, enabling more delicate and accurate description of FGMs in computer-aided design and analysis. This paper presents a new design approach to modeling porous structures with graded porosities and pore distributions. A novel digital model based on stochastic Voronoi diagram and B-Spline representation is proposed. Using such a model, generic porous structures with graded and irregularly shaped pores can be easily designed. The proposed approach is therefore useful for downstream model validations, simulations as well as microstructural optimizations.**

***Keywords*—shape; functionally graded; porous structure; Voronoi diagram; B-Spline; irregular shapes; probability density function**

I. INTRODUCTION

The advantages of using Functionally Graded Materials (FGMs) have been increasingly recognized in recent years. Compared with homogeneous solids, FGM objects have played indispensible roles in many applications where multi-fold, sometimes contradictive functional requirements are expected [1, 2]. In the past few decades, tremendous research efforts have been devoted to this cutting edge technology, and rich applications in mechanical, biomedical and other fields have been reported. For details of the various investigations on these subjects, the readers are referred to some recent reviews, e.g. [2-5], to cite a few.

Among existing efforts on functionally graded materials, an overwhelming majority is based on the compositional heterogeneity model, where the material distributions characterized at macroscopic scale are primary concerns. Under such a premise, a variety of FGM models were proposed based on specific material variation functions or patterns, for instance exponential function [6] based *unidirectional* FGM models, heterogeneous feature tree [7] based *bidirectional* models and spline tensor product [8] based *tri-variate* models.

With increasingly powerful computers and highly precise instruments such as magnetic resonance imaging (MRI), scanning electron microscope (SEM), Energy Dispersive Spectroscopy (EDS) etc., initial macro-scale volume fractions based FGM characterization has been extended to *microstructural* models in recent studies [9-12]. Using microstructural representations, more delicate and accurate description of FGMs can be used in computer-aided design and analysis. For instance, traditional effective property (e.g. Elastic modulus and Poisson ratio etc.) estimation of FGMs is mostly based on rule-of-mixture or empirical formulae [10, 13-17], and the reliability and accuracy of these estimates are usually ad hoc or case specific. Moreover, the volume fraction oriented FGM models can reflect macroscopic characteristics only, and many microscopic phenomena (e.g. local stress concentrations and crack initiation [10]) are likely neglected due to the averaging effects [10].

In view of the apparent merits of microstructural characterization of functionally graded objects, an appropriate representation for graded porous structure is highly expected. Most of existing micro-porous models are directly reconstructed from measurement data, however it is non-trivial, even if possible, to *edit* such micro structures to design *new* artifacts with *graded*, *irregular* pore shapes and distributions.

This paper is motivated to present a novel digital model based on stochastic Voronoi diagram and B-Spline representations, which allows users to easily design functionally graded porous structures at microscopic level. Most importantly, the proposed CAD models are *editable*, and generically similar but topologically and geometrically different porous structures can be efficiently generated at interactive time.

Before presenting the detailed CAD representation in Section 3, Section 2 briefly reviews related work in microscopic representation of porous structures, and the motivations and emphasis of this research is highlighted. Based on the proposed model in Section 3, Section 4 presents the methods for tailoring the grade porosity and pore distributions and finally this paper is concluded in Section 5.

II. RELATED WORK

Graded porous structures have manifested many appealing properties in bio-implants design (e.g. skeletal and femur replacement [18, 19]). The majority of existing investigations is of experimental nature, and the focus is on using different fabrication approaches to generate controlled porosity gradients. The fabricated graded porous structures are then tested and compared in terms of the physical performances such as biocompatibility, bone ingrowth or mechanical strengths. For these type of studies, as the digital models are unavailable, numerical simulation and microstructural optimization are therefore unable to be conducted.

To get the digital microstructural model for a micro-porous structure, Cannillo et al. [20] cut a specimen and the cross-section was observed by SEM and an image-based finite element analysis was then applied. Li et al. [21] used optical microscopy to characterize the microstructure of the FGMs while Teng et al [22] employed Back-scattered Electron Image (BEI) of polished FGM samples. These approaches rely on different micrographs, and in order to get the internal microstructures, cutting or dissection of the samples is usually unavoidable.

Rather than relying on SEM or other types of measuring instruments to capture the microstructure of porous objects, many fractal based representations have also been proposed. Among others, many well-known deterministic fractals have been used, for instance the Koch snowflake, Sierpinski carpet and Menger sponge fractals etc. [23-25]. Unfortunately these representations seem to be less applicable to modelling microstructures of *graded* pores.

Manually, the microstructure of graded pores and pore distributions can be modeled using mature CAD software packages, for instance the one shown in Fig.1. However such models are mostly limited in representing regularly shaped pores. To model irregular porous objects as commonly seen in SEM images, current CAD modelling approaches are usually inadequate.

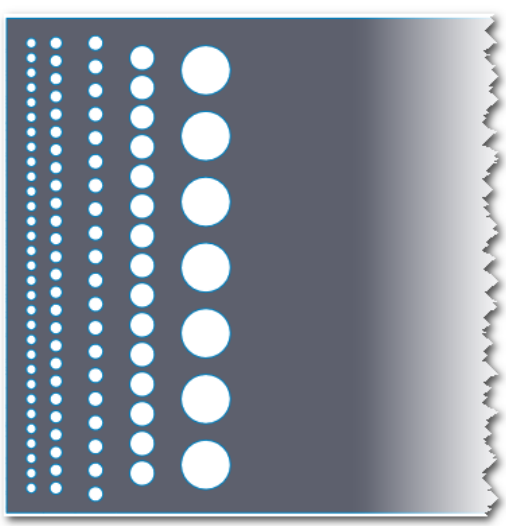


Fig. 1 Uniformly distributed circular shaped pores with graded pore sizes.

The purpose of this paper is to bridge such a gap and propose a new representation to model porous structures with graded pore distributions. In contrast with existing approaches, the proposed digital model can properly maintain the expected pore shape *irregularity* as well as the *graded* pore sizes and distributions. This model is extended from Kou and Tan's hybrid Voronoi-Spline representation [26] which is further discussed below.

III. Stochastic Voronoi Diagram and hybrid Voronoi-Spline (HVS) representation

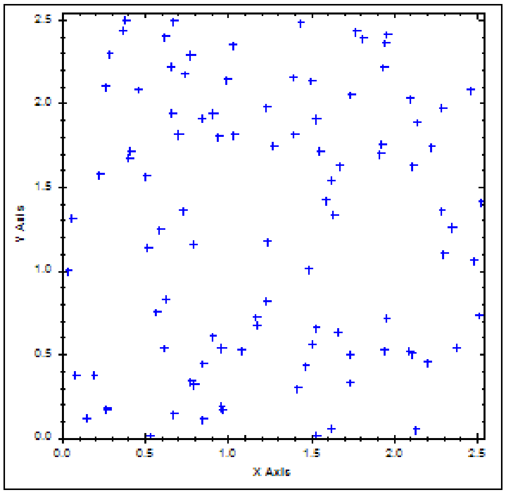
The use of Voronoi diagram and B-Spline representation to model irregular porous structure was reported in [26]. This simple and effective representation was inspired by Schaefer and Keefer's *random colloid-aggregation* model [27] that explains the formation *mechanism* of random porous materials. To make this paper self-contained, the underlying principle of Kou-Tan model is briefly presented here and more details can be found in [26].

Schaefer and Keefer [27] contended that the random porous structure formed in polymerization process is a result of random aggregate of silica particles. Kou and Tan imitated the physical process of polymerization using the following procedures:

- To simulate Schaefer and Keefer's "jungle gym" structure, Voronoi tessellation is first generated to discretize the design domain into a series of compartments, as shown in Fig. 2. The Voronoi generator points are generated with a *uniform* distribution (i.e. a constant Probability Density Function (PDF)) defined on the entire geometric domain).
- Some randomly selected compartments are then merged together to imitate the "random colloid aggregations". To accomplish this, each Voronoi cell is randomly associated with an attribute, as represented with different colors in Fig. 3 (a); adjacent Voronoi cells with the same attributes are merged together, as shown in Fig. 3 (b). In addition to the convex Voronoi polygons, this random Voronoi cell merge generates new concave polygons, and the irregularity of the porous structure can be enhanced.
- The vertices of these irregular convex and concave polygons are modeled as control points of closed B-Spline curves, as shown in Fig. 4 and Fig. 5. The fitted B-Spline curves are employed to represent the boundaries of the irregular-shaped pores. Note that before fitting the B-Spline curves, the merged polygons are scaled down with a scale factor t, $0 < t \leqslant 1$, and the purpose of such processing is to avoid over-small interstices between adjacent pores. As shown in Fig. 4, the smaller this scale factor is, the larger the interstices are.

- Finally a Boolean subtraction of the pores from the external geometry is applied, and the irregular porous structure is obtained, as shown in Fig. 5 (b).

(a)



(b)

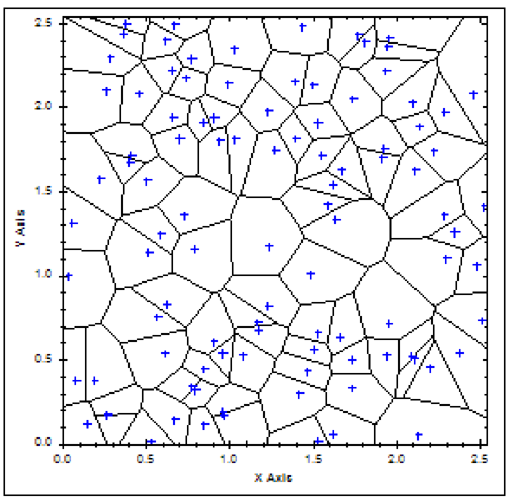
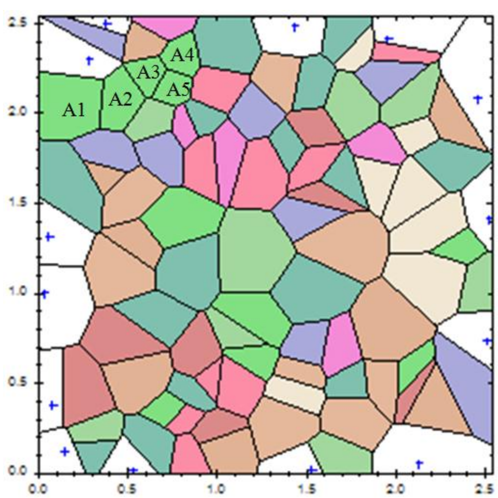


Fig. 2 Uniformly distributed random Voronoi sites and the generated Vornoi diagram (a) Voronoi sites; (b) Voronoi diagram

(a)



(b)

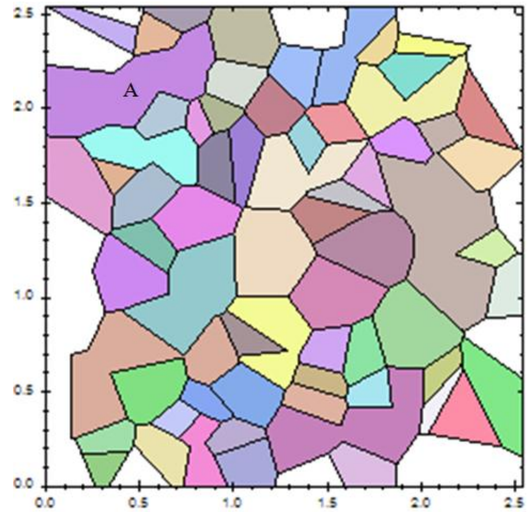
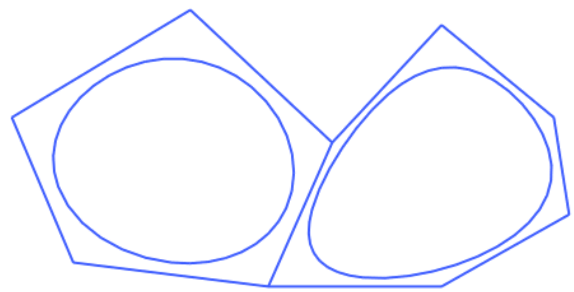
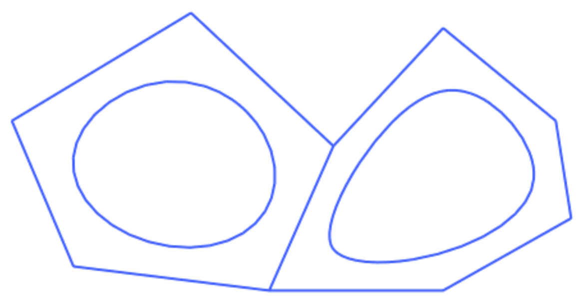


Fig. 3 Random attribute association and attribute based cell merging. (a) Attribute association; (b) Cell merging.



(a) Scale factor: t_a



(b) Scale factor: t_b

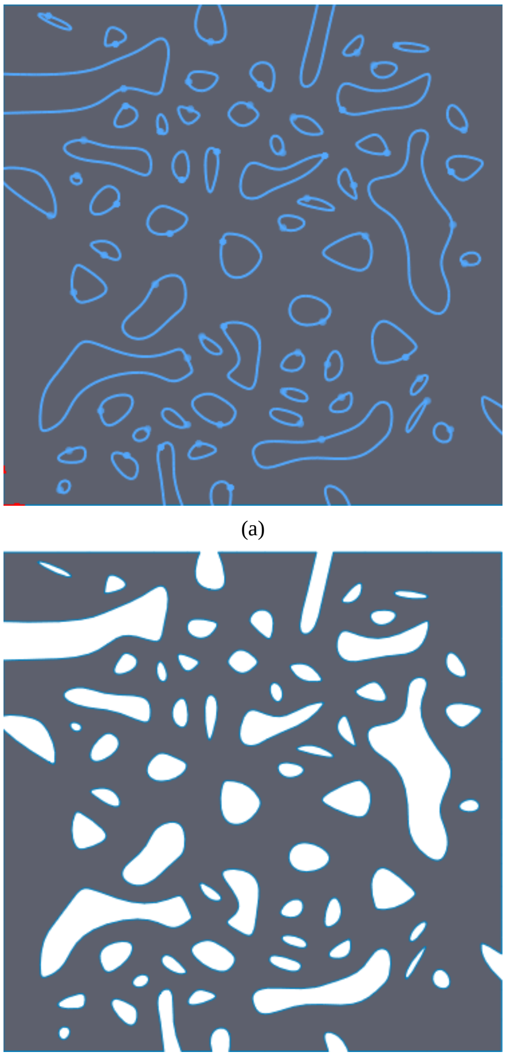
Fig. 4 Using scaled B-Spline curve to control the pore interstices. The scale factor $t_a > t_b$.

As is seen from Fig. 2 to Fig. 5, the pore size, shape, topology and distribution are closely related to the following parameters:

- The distribution of the Voronoi generator (Fig. 2);
- The associated attributes to each Voronoi cell (Fig. 3);
- The scale factor used (Fig. 4).

In [26], Kou and Tan used *uniformly* distributed Voronoi generators and a *constant* scale factor for all the fitted B-

Spline curves. We show in this paper that this flexible representation can be extended to model graded porous structure by using *non-uniformly* distributed Voronoi generators and *non-constant* scale factors.



(a)

(b)

Fig. 5 B-Spline curve based pore boundary and Boolean subtraction of spline curves from the external geometry

IV. TAILORING GRADED PORE SIZES AND PORE DISTRIBUTIONS

A. Modeling graded pore sizes with location dependent scale factors

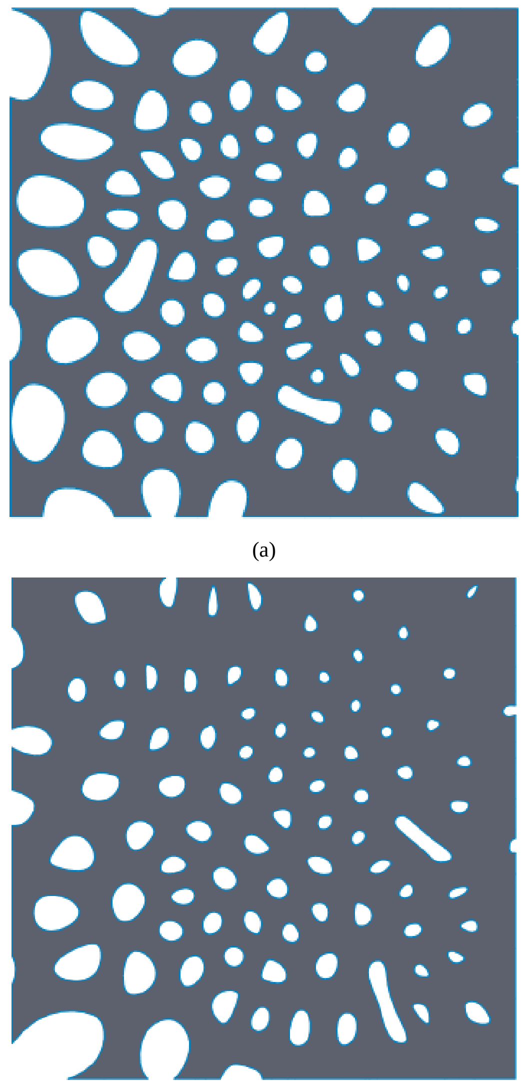
Instead of using a constant scale factor to scale all the B-Spline curves, in this paper, each B-Spline curve is separately associated with an independent scale factor. By gradually changing the scale factor, porous structures with graded pore sizes can be obtained. The results shown in Fig. 6 demonstrate the usage of this approach. Fig. 6 (a) and (b) show the result after applying horizontally and diagonally decreasing scale factors on spline curves fitted from uniformly distributed Voronoi generators.

The scale factors for the results in Fig. 6 (a) and (b) follow the variations described by Eq. (1) and Eq. (2) respectively, where t is the scale factor, x_{max} and y_{max} are the maximum coordinates of the design domain, x and y are the spatial coordinates of the centroid of the Voronoi polygon.

$$t(x) = 0.8 - 0.5\, {x}/{x_{\max}} \tag{1}$$

$$t(x,y) = 0.8 - 0.5\, {\sqrt{x^2 + y^2}}/{\sqrt{x_{\max}^2 + y_{\max}^2}} \tag{2}$$

The results in Fig. 6 clearly show the effect of using heterogeneous scale factors in pore size control. Note that pore shape irregularity is not lost in the graded porous structure modeling, this is different from the results shown in Fig.1.



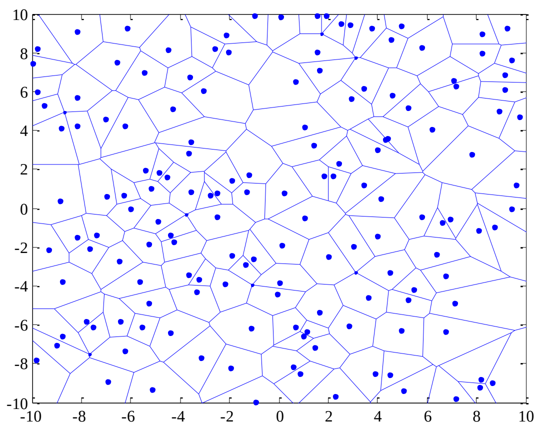
(a)

(b)

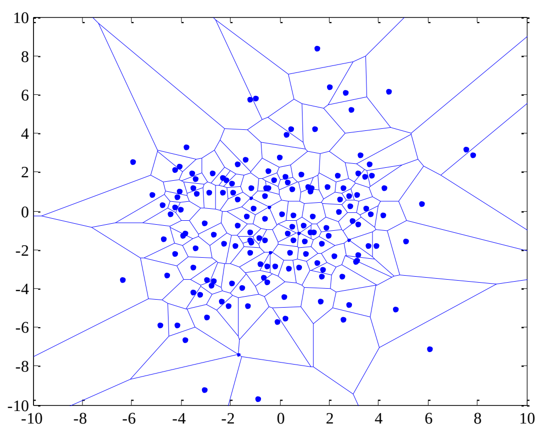
Fig. 6 Using horizontally and diagonally decreasing scale factors to control the graded pore sizes. (a) Voronoi sites with horizontally graded pore sizes; (b) Voronoi sites with diagonally graded pore sizes from lower left to top right.

B. Modeling graded porous structures using Probability Density Functions

Apart from using location dependent scale factors, a more straightforward method is to use Voronoi generators with a graded distributions. In this paper, we propose to use a Probability Density Function (PDF) to describe the relative likelihood for a Voronoi generator to occur at a given location in the design space.



(a)



(b)

Fig. 7 Comparison of using uniform and Gaussian distribution of 150 random points as Voronoi generators. (a) Voronoi sites with uniform distributions. (b) Voronoi sites with Normal distributions, with $\mu = (0, 0)$ and $\sigma = (10/3, 10/3)$.

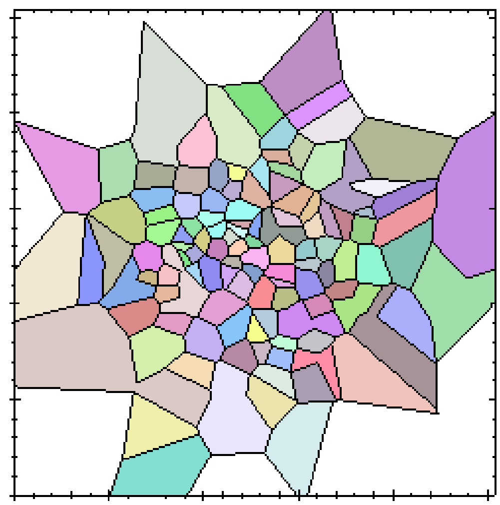
As an example, the use of two-dimensional Gaussian distributions (also known as normal distributions) to generate Voronoi points is compared against uniformly distributed generators, as illustrated in Fig. 7. In Fig. 7 (b), the *x* and *y* coordinates are independently generated following a two-parameter distribution, as formulated by Eq. (3):

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \qquad (3)$$

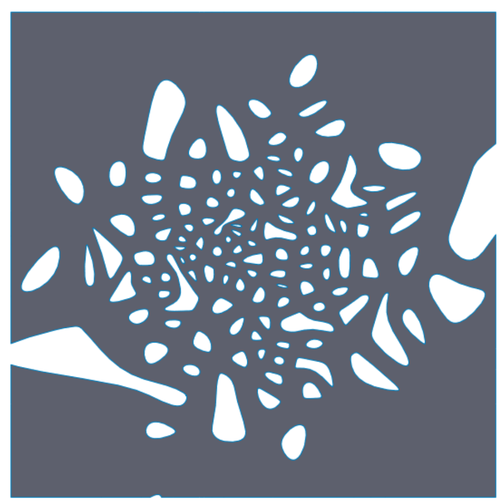
where parameters μ and σ are the mean and standard deviation. The non-uniform distributions shown in Fig. 7 (b) are generated from uniform distributions followed by a transformation procedure. The most straightforward but less efficient transformation is the inverse Cumulative Distribution Function (CDF) [28] based technique, while the rejection sampling [29] (also known as acceptance/rejection) method and finite mixtures method [30] are computationally more efficient.

Note that the probability of a point coordinate (either *x* or *y*) falling inside the range $[\mu - 3\sigma, \mu + 3\sigma]$ is 99.72%, given the range of Voronoi generators, the standard deviation can be implicitly determined. In Fig. 7 (b), the standard deviations for Gaussian distribution of *x* and *y* are determined by Eq. (4):

$$\sigma_x = \frac{X\max - X\min}{6}, \sigma_y = \frac{Y\max - Y\min}{6} \qquad (4)$$



(a)



(b)

Fig. 8 Using radially decreasing scale factors to control the graded pore sizes. (a) Voronoi diagrams generated from Gaussian distributions, 150 Voronoi generators. (b) Radially graded porous structures created using the proposed approach.

Fig. 8 shows the result of using Gaussian distributed Voronoi generators in modeling graded porous structures where the pore sizes grows along radial directions.

C. Implementations

A prototype CAD module, “iPorous Modeler”, is developed to implement the proposed modeling approach. The module is developed in C# language in 64 bit Windows 7 using SolidWorks API. Fig. 9 shows a snapshot of the implemented graphical user interface.

approaches are presented to tailor the graded pore structures. Using the graded scale factors, the graded values are deterministically calculated as formulated by Eq. (1) and (2), for instance. Using PDF based approaches presented in Section B, a constant scale factor is used, however the control polygons are modulated by specific probability density functions, and the pore size and pore distributions can still be regulated with expected gradients. In statistics, there have been lots of other predefined PDFs which are not elaborated in this paper. Many of such PDFs have direct physical meanings, for instance, the sum of two uncorrelated Gaussian distributions used in Fig. 7 (b) and Fig. 8 (b) is actually a *Rayleigh* distribution, commonly used to model the effects of radio signal propagations. The PDF based approach is therefore very attractive to be used in physics based modeling and simulations.

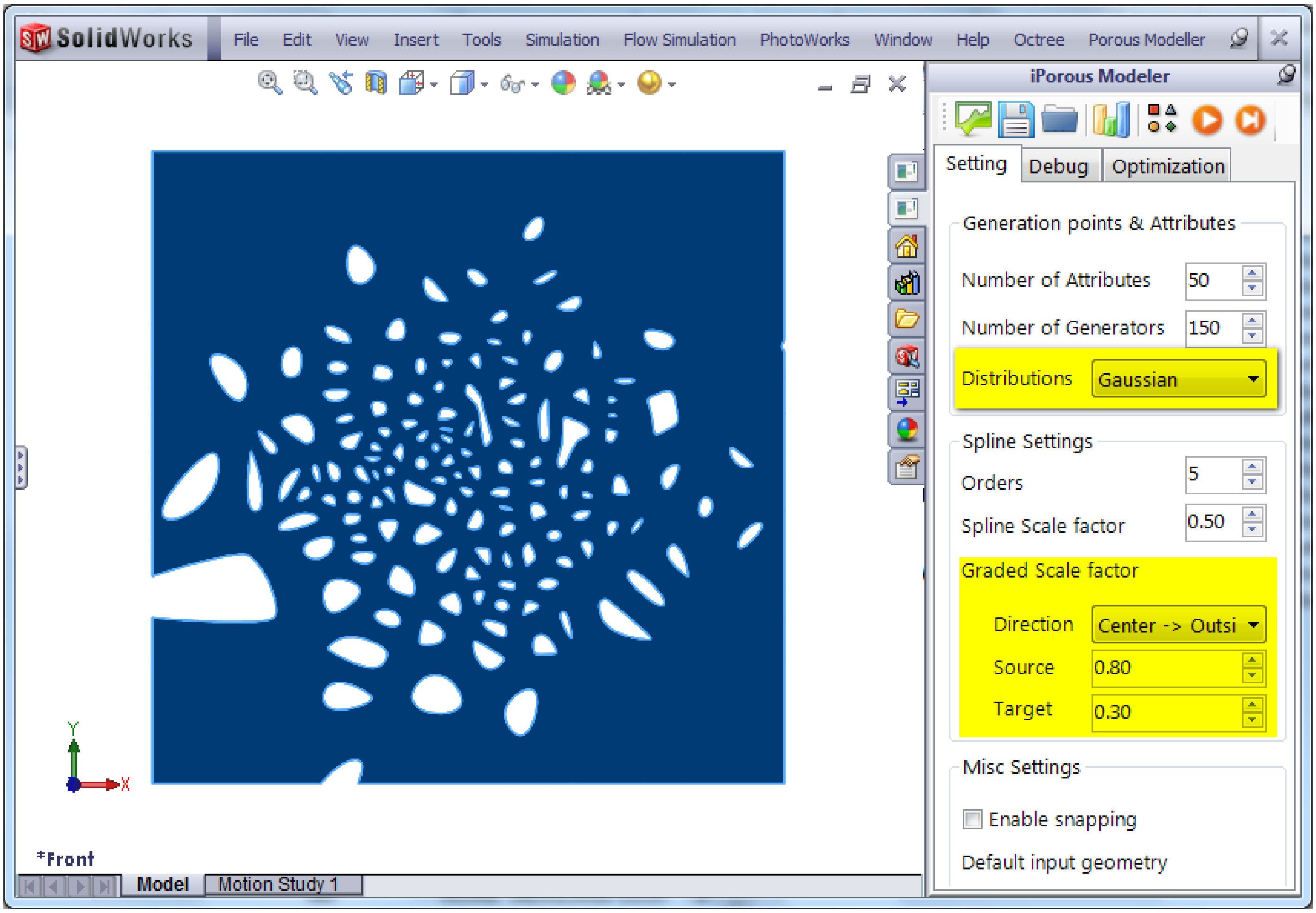


Fig. 9 Graphic user interface of the implemented CAD module.

In this CAD module, the users can either select the distribution of the Voronoi generators in the drop-down list or customize graded scale factors by inputting the values.

All the 2D porous structures in this paper are generated with this module. The average time used to construct a 2D model is no more than 0.5 seconds, and the average model file size is smaller than 300 KB.

V. Conclusions and Discussions

A new design approach to modeling porous structures with graded porosities and pore distributions is presented in this paper. A novel digital model based on stochastic Voronoi diagram and B-Spline representation is proposed. Two

Experiments show that using the proposed model, generic porous structures with graded pore shapes and distributions can be easily designed; meanwhile the expected irregular pore shapes can be properly maintained, making the designed porous structures more natural and realistic.

Acknowledgment

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