

Optimal power diagrams via function approximation

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ABSTRACT

In this paper, we present a novel method for generating cell complexes with anisotropy conforming to the Hessian of an arbitrary given function. This is done by variationally optimizing the discontinuous piecewise linear approximation of the given functions over power diagrams. The resulting cell complexes corresponding to the approximations are referred to as Optimal Power Diagram (OPD). A hybrid optimization technique, coupling a modified Monte Carlo method with a local search strategy, is tailored for effectively solving the specific optimization task. In contrast to the Optimal Voronoi Tessellation (OVT) method (Budnitskiy et al., 2016), our OPD method does not restrict the target functions to be convex, providing more diverse classes of tessellations of the domain. Furthermore, our OPD method generally yields smaller approximation errors than the OVT method, which uses underlaid approximants. We conduct several experiments to demonstrate the efficacy of our optimization algorithm in finding good local minima and generating high-quality anisotropic polytopal meshes.

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1. Introduction

Meshes are important representations used in a wide range of applications, including geometric modeling, computer graphics, mechanical engineering and simulations. The complex geometric objects are represented as an assembly of discrete elements, e.g., triangles, quadrilaterals and polygons in 2D as well as their counterparts in higher dimensions. Numerous algorithms have been developed to produce high-quality isotropic meshes, and some of them are commercially available. While the problem of isotropic meshing has been well studied, the research on converting complex objects into an anisotropic mesh is relatively behind.

Anisotropic meshes are often advantageous in terms of computational cost and solution accuracy in finite element simulations for resolving physical problems with solutions changing more rapidly in one direction than others. In shape/functional approximation, anisotropic meshes also provide better interpolations/approximations of geometries/functions having strong directionality with fewer elements. However, many recent attempts have been exclusively focused on extending isotropic meshing to anisotropic simplicial meshing and quadrilateral/hexahedral meshing, due to their popularity. In this paper, we propose a novel Optimal Power Diagram (OPD) method for generating anisotropic

meshes formed by convex polygons/polyhedrons. The specific contributions of this paper are as follows:

1. We extend the Optimal Voronoi Tessellation (OVT) energy function that was previously used for generating anisotropic polygonal/polyhedral meshes. From the point view of functional approximation, the OVT energy function describes the error between a convex function and its underlaid polytope in the L_1 norm. We relax the constraints for both the approximant and the target function of the OVT energy function. More precisely, the target function is not necessarily convex, which is approximated by linear functions individually defined over sub-regions in the L^2 norm.
2. We use power diagrams to represent the tessellations of a given domain, so that the energy minimization problem can be tackled efficiently. Minimizing the generalized energy boils down to finding the optimal partition of the domain, which is difficult in general cases. As a matter of fact, it is NP-hard to decide if a bivariate function can be approximated by a piecewise linear function with a pre-specified number of facets and within an approximation error threshold, as has been shown in [1]. To make the problem solvable, we restrict the partitions to power diagrams, which have many important applications in various fields. Actually, this is not even a restriction for cell complex generation of volumes, as an arbitrarily simple cell complex in 3D can be represented by a power diagram [2].

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3. A hybrid optimization algorithm is presented to efficiently solve the specific minimization problem in this paper. It is very challenging to minimize the modified energy function, due to its highly non-linear and non-convex nature. Our hybrid optimization method, combining a local search with a global optimization technique, reduces the chance of getting stuck at poor local minima and converges fast to a deep enough local minimum. Moreover, a comprehensive initialization method is proposed to tremendously improve the results.

The remainder of this paper is organized as follows. We review the related works in Section 2 and introduce some preliminary concepts and notations in Section 3. In Section 4, we extend the OVT energy function and derive closed-form expressions for its derivatives. In Section 5, we provide the overview and technical details of our hybrid optimization method for the minimization of the proposed energy function. Finally, after giving some experimental results and comparisons with the OVT method in Section 6, we conclude this paper with discussions and limitations in Section 7.

2. Related work

In this section, we give a brief review of references that are most related to this work, with a focus on methods for anisotropic mesh generation.

Anisotropic simplicial meshing. Anisotropic simplicial meshes are triangulations of a given domain whose elements stretch along the desired directions. The anisotropy at each point of the domain is usually given as a symmetric matrix. The eigenvectors and eigenvalues of the matrix describe the desired stretching directions and magnitudes of mesh elements. Delaunay refinement is a widely used technique for generating high-quality isotropic simplicial meshes [3]. By taking anisotropy into account, various extensions to Delaunay refinement have been proposed to generate anisotropic Delaunay meshes [4–7]. Anisotropic mesh quality can be measured in different ways and optimized by combining the operations of vertex redistribution and retriangulation [8,9]. By embedding the anisotropic space into a higher dimensional isotropic one, anisotropic meshes can be obtained via constructing isotropic meshes in the embedded space [10–12].

Anisotropic Voronoi. The concept of Centroidal Voronoi Tessellation (CVT) has been successfully applied to high-quality isotropic mesh generation [13]. CVTs can be generalized to anisotropic Voronoi tessellations, by using different distance definitions [14–17]. Generally, the bisectors between sites are no longer straight under the generalized distance measures, making the precise construction of anisotropic Voronoi cells computationally cumbersome. Approximation methods are thus adopted to compute anisotropic Voronoi diagrams, by clustering discrete elements of a given mesh [18,17,19] or constructing restricted Voronoi diagrams instead [15,20]. In our method, power diagrams are used as the representation of convex tessellations of the domain, which allow more flexibility than Voronoi diagrams in optimization [21] and can be efficiently computed by off-the-shelf computational geometry libraries.

Function approximation based methods. Anisotropic meshes can be obtained by minimizing the approximation error between a target function f and its piecewise linear approximation. The optimal simplices with a minimal approximation error have been shown to be stretched along the two principal directions of f , with an aspect ratio equal to $\sqrt{|k_{\max}/k_{\min}|}$, where k_{\max} and k_{\min} are the principal curvatures [22,23]. Chen et al. [24,25] proposed the concept of optimal Delaunay triangulation which minimizes the linear interpolation error for a given convex function. Fu et al. [26]

generalized optimal Delaunay triangulation to anisotropic metrics by constructing convex functions that locally match a given anisotropic metric. The anisotropy of the resulting mesh elements conforms to the Hessian of an input target function. A CVT can also be defined from a variational point of view, which minimizes the error between a paraboloid $f(\mathbf{x}) = |\mathbf{x}|^2$ and its underlaid piecewise linear approximation. Budninskiy et al. [27] gave an anisotropic extension of CVTs, called Optimal Voronoi Tessellations (OVTs), which optimizes the piecewise linear approximation of convex functions over anisotropic cell complexes. Several other methods for generating function-dependent Voronoi diagrams have been studied in [28,29]. In this paper, we present an extension of OVTs based on the approximation of functions that are not necessarily convex.

Global optimization. Due to the highly non-linear and non-convex nature of the CVT energy, the commonly used local search methods such as the Lloyds iteration and quasi-Newton methods tend to get stuck at shallow local minima. Several global techniques were developed to search a deep enough local minimizer and even a global minimizer. For example, a Monte Carlo-minimization (MCM) based framework [30] was adopted to compute Euclidean CVT in [31], in which the Monte Carlo method was used to pass from one local minimum to the next local minimum obtained by the L-BFGS method, and ultimately to the global minimum. Similar methods were also used for generating constrained centroidal Delaunay meshes [32] on surfaces and computing the optimal Delaunay triangulation in 3D space [33]. A differential evolution based method was developed to compute the globally optimal geodesic CVT energy on triangle meshes [34]. In this paper, we tailor the MCM method to our specific problem and provide a comprehensive initialization technique to speed up the convergence.

3. Background

In this section, we introduce preliminary concepts and notation that will be used throughout the entire paper.

Power diagram. Let $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^n$ be a set of n distinct sites in a compact domain $\Omega \subset \mathbb{R}^d$ and $W = \{w_i\}_{i=1}^n$ be a set of real numbers. Each site \mathbf{x}_i is associated with a real number w_i , called the weight of \mathbf{x}_i . Then the power cell Ω_i of \mathbf{x}_i is

$$\Omega_i = \{\mathbf{x} \in \Omega \mid \|\mathbf{x} - \mathbf{x}_i\|^2 - w_i \leq \|\mathbf{x} - \mathbf{x}_j\|^2 - w_j, \forall i \neq j\},$$

where $\|\cdot\|$ denotes the Euclidean norm. The power diagram of the weighted point set $(\mathbf{X}, W) = \{(\mathbf{x}_1, w_1), \dots, (\mathbf{x}_n, w_n)\}$ is the cell complex formed by the collection of power cells $\{\Omega_i\}_{i=1}^n$. The power diagram is a generalization of the Voronoi diagram, which coincides with the Voronoi diagram of the sites \mathbf{X} when all the weights are the same [35].

Optimal Voronoi tessellations. Let $f : \Omega \rightarrow \mathbb{R}$ be a convex function in the compact domain $\Omega \subset \mathbb{R}^d$, and $\mathbf{X} = \{\mathbf{x}_i\}_{i=1}^n$ be a set of n distinct sites in Ω . For each site \mathbf{x}_i , we denote $T_i(\mathbf{x})$ the tangent hyperplane of $f(\mathbf{x})$ at \mathbf{x}_i . Then optimal Voronoi tessellations [27] are minimizers of

$$\mathcal{E}_{\text{OVT}}(\mathbf{X}, \mathcal{V}) = \|f - f_T\|_{L^1} = \sum_{i=1}^n \int_{V_i} (f(\mathbf{x}) - T_i(\mathbf{x})) d\mathbf{x}, \quad (1)$$

where f_T is a piecewise linear approximation of the target function f , formed by the set of tangent hyperplanes $\{T_i(\mathbf{x})\}_{i=1}^n$, and $\mathcal{V} = \{V_i\}_{i=1}^n$ is a tessellation of the domain. Since the function f is convex, tangent hyperplanes $T_i(\mathbf{x})$ are always below it, that is, $f(\mathbf{x}) \geq T_i(\mathbf{x})$ for all i . It has been shown in [27] that for a given set of sites \mathbf{X} , the optimal tessellation \mathcal{V} is the projection of the upper envelop of $\{T_i(\mathbf{x})\}_{i=1}^n$, which can be efficiently obtained by constructing a

power diagram of a set of shifted and weighted sites $\{(\mathbf{p}_i, w_i)\}_{i=1}^n$. We have

$$\mathbf{p}_i = \frac{1}{2}\nabla f(\mathbf{x}_i), \quad w_i = \frac{1}{4}|\nabla f(\mathbf{x}_i)|^2 + f(\mathbf{x}_i) - \nabla f(\mathbf{x}_i) \cdot \mathbf{x}_i.$$

The OVT energy function in Eq. (1) can be minimized by a Lloyd-based approach which alternately optimizes the locations of sites and updates the tessellation of the domain. Note that for the case of $f(\mathbf{x}) = |\mathbf{x}|^2$, \mathcal{V} is simply the Voronoi tessellation of X , and the OVT energy function coincides with the centroidal Voronoi tessellation energy function [13].

4. Optimal power diagrams

According to [22,23], the optimal aspect ratio of linear elements is dictated by the local Hessian of a target function f , regardless whether f is convex or not. In this section, we describe how to modify the OVT function in Eq. (1) to compute anisotropic cell complexes which are cast as the optimal piecewise linear approximations of given target functions that are not necessarily convex.

4.1. Formulation

Suppose $f : \Omega \rightarrow \mathbb{R}$ is a real-valued function and is continuous in the compact domain $\Omega \subset \mathbb{R}^d$. Given a tessellation \mathcal{V} of the domain Ω , we can construct the best L^2 fitting hyperplane of $f(\mathbf{x})$ for each cell V_i , denoted by $P_i(\mathbf{x})$. Then we approximate f with a discontinuous piecewise linear function $f_P(\mathbf{x}) = \sum_{i=1}^n P_i(\mathbf{x}) \mathbf{1}_{V_i}(\mathbf{x})$, where $\mathbf{1}_{V_i}$ is the indicator function of a cell V_i . We formulate our energy function as follows:

$$\mathcal{E}(\mathcal{V}, \mathcal{P}) = \|f - f_P\|_{L^2}^2 = \sum_{i=1}^n \int_{V_i} (f(\mathbf{x}) - P_i(\mathbf{x}))^2 d\mathbf{x},$$

where $\mathcal{P} = \{P_i(\mathbf{x})\}_{i=1}^n$ is a set of linear functions. As the function f is not convex and the fitting hyperplanes cannot guarantee to be always below or above the function f , we measure the approximation error between f and f_P using the L^2 norm instead of the L^1 norm in the OVT function.

The determination of the best tessellation \mathcal{V} and the corresponding best-fit hyperplanes is generally NP-hard [1]. To simplify the computation, we restrict the tessellation to a power diagram, which is uniquely determined by the site positions X and the weights W . Note that, the L^2 -norm best-fit hyperplane on each cell is determined once the tessellation is given. We denote by $P_i^*(\mathbf{x})$ the best linear fit on a cell V_i . Hence, the above energy function essentially depends on the site positions and weights as follows:

$$\mathcal{E}_{OPD}(X, W) = \|f - f_P\|_{L^2}^2 = \sum_{i=1}^n \int_{V_i} (f(\mathbf{x}) - P_i^*(\mathbf{x}))^2 d\mathbf{x}. \quad (2)$$

Thus we refer to minimizers of the above energy function as Optimal Power Diagrams (OPD).

4.2. Derivatives of energy function

We now derive the gradient of our energy function for later use. First, we consider the derivative of energy function with respect to site position \mathbf{x}_i . Applying the general Leibniz rule [36] to Eq. (2), we have

$$\begin{aligned} \frac{\partial \mathcal{E}_{OPD}(X, W)}{\partial \mathbf{x}_i} &= \sum_{j \in J_i \cup \{i\}} \int_{V_j} \frac{\partial}{\partial \mathbf{x}_i} |f(\mathbf{x}) - P_j^*(\mathbf{x})|^2 d\mathbf{x} \\ &+ \sum_{j \in J_i} \int_{V_{ij}} (|f(\mathbf{x}) - P_i^*(\mathbf{x})|^2 - |f(\mathbf{x}) - P_j^*(\mathbf{x})|^2) \frac{\partial \mathbf{x}}{\partial \mathbf{x}_i} \mathbf{n} ds, \end{aligned}$$

where J_i is the indexes of sites with cells adjacent to V_i , $V_{ij} = \partial V_i \cap \partial V_j$ is the common boundary of V_i and V_j , and \mathbf{n} is the outward unit normal vector on the boundary of V_i . According to the envelope theorem, the first term in the above equation vanishes. Now, let us consider the evaluation of $\partial \mathbf{x} / \partial \mathbf{x}_i$ in the second term. Note that,

$$(\mathbf{x} - \frac{\mathbf{x}_i + \mathbf{x}_j}{2}) \cdot (\mathbf{x}_j - \mathbf{x}_i) = w_i - w_j, \quad \text{for } \mathbf{x} \in V_{ij}.$$

Differentiating both sides of the equation with respect to \mathbf{x}_i , we obtain

$$\frac{\partial \mathbf{x}}{\partial \mathbf{x}_i} (\mathbf{x}_j - \mathbf{x}_i) = \mathbf{x} - \mathbf{x}_i.$$

Thus, we have $\partial \mathbf{x} / \partial \mathbf{x}_i \mathbf{n} = (\mathbf{x} - \mathbf{x}_i) / |\mathbf{x}_j - \mathbf{x}_i|$. Then the derivative of $\mathcal{E}_{OPD}(X, W)$ with respect to \mathbf{x}_i can be simplified to

$$\begin{aligned} \frac{\partial \mathcal{E}_{OPD}(X, W)}{\partial \mathbf{x}_i} &= \\ \sum_{j \in J_i} \int_{V_{ij}} (|f(\mathbf{x}) - P_i^*(\mathbf{x})|^2 - |f(\mathbf{x}) - P_j^*(\mathbf{x})|^2) \frac{\mathbf{x} - \mathbf{x}_i}{|\mathbf{x}_j - \mathbf{x}_i|} ds. \end{aligned} \quad (3)$$

The derivative of $\mathcal{E}_{OPD}(X, W)$ with respect to w_i can be found in the same fashion:

$$\begin{aligned} \frac{\partial \mathcal{E}_{OPD}(X, W)}{\partial w_i} &= \\ \sum_{j \in J_i} \int_{V_{ij}} (|f(\mathbf{x}) - P_i^*(\mathbf{x})|^2 - |f(\mathbf{x}) - P_j^*(\mathbf{x})|^2) \frac{1}{2|\mathbf{x}_j - \mathbf{x}_i|} ds. \end{aligned} \quad (4)$$

5. Optimization algorithm

Minimizing the OPD energy function in Eq. (2) is difficult, due to its highly non-linear and non-convex essence. As shown in Fig. 2, the energy function presents many shallow local minima when we hold all variables except one site position or weight constant. Hence, directly applying a traditional local search method suffers from a common problem, i.e., trapping in local solutions. Whereas, conventional global optimization methods are usually very time-consuming. In this section, a hybrid local and global optimization method is adopted to efficiently solve our OPD energy function. Before getting into the details of our algorithm, we first provide some observations on the optimization of the OPD energy function, which relives the influence of variables to be optimized on the objective function and gives rise to an efficient optimization method based on block coordinate update.

Note that, the OPD energy function in Eq. (2) contains two types of variables (site positions and weights). One of the most straightforward methods for its optimization is using a gradient-based local search with a random initialization and without discriminating these two types of variables. As shown in Fig. 3(a), starting from a set of 1000 sites randomly sampled from the given domain and equal weights, a gradient-based local search method (the L-BFGS method in this paper) gets trapped in a shallow local minimum when we optimize all variables simultaneously, yielding a low-quality tessellation; see Fig. 3(b). Meanwhile, we find that optimizing site positions before optimizing all variables usually produces much better results, as shown in Fig. 3(c). Starting from the same random initialization in Fig. 3(a) and fixing the weights in the optimization, the L-BFGS method converges to a deeper local minimum, leading to a tessellation with much higher quality than the result in Fig. 3(b). The intermediate result in Fig. 3(c) can be further improved by applying local search again, with all variables involved in the optimization; see Fig. 3(d). More long and thin cells are introduced which better convey the expected anisotropy. The plot of approximation error versus optimization iteration number also illustrates that this block-coordinate-descent-like method

converges to a deeper local minimum. In other words, site positions are the most influential variables in the optimization process, while weights exert a smaller influence on the minimization of the objective function. Another benefit of optimizing site positions before weight optimization is that it reduces the chance of introducing large differences on weights. A power diagram coupled with weights varying over a wide range usually has sites locating outside the corresponding cells, as shown in Fig. 3(b), leading to a low-quality dual regular triangulation.

5.1. Overview of OPD optimization algorithm

Global minimization of a nonconvex objective function with many local minima is generally difficult, many efforts have been made to speed up the computation. Among them, the Monte Carlo-minimization (MCM) method [30], which combines the power of an efficient local search method to find local minima and that of the Monte Carlo method in global combinatorial optimization, is simple yet efficient to overcome the multiple-minima problem. Roughly speaking, the MCM method considers all local minimizers obtained by interleaving perturbation and local searching. A new local minimum is accepted if either it is better than the current local minimum, or it satisfies a pre-specified probability condition. Based on the above observations in Fig. 3, we modify the standard MCM method to efficiently minimize the OPD energy function. As shown in Fig. 4, taking a desired site number n and a target function $f(\mathbf{x})$ as input, our algorithm consists of three stages: initialization, position optimization and position-weight optimization. During position optimization and position-weight optimization, the following three steps are carried out to find the minimizer of the OPD energy function:

Step 1. Perturb the site positions or/and weights by using specific perturbation strategies. Denote the perturbed sites and weights by X' and W' , respectively.

Step 2. Optimize the site positions X' or/and weights W' simultaneously using the L-BFGS method, upon which the approximation error $\mathcal{E}_{OPD}(X', W')$ can be computed.

Step 3. If $\mathcal{E}_{OPD}(X', W') < \mathcal{E}_{OPD}(X, W)$, we accept new site positions and weights, i.e., $X \leftarrow X'$ and $W \leftarrow W'$. Otherwise, if $\mathcal{E}_{OPD}(X', W') > \mathcal{E}_{OPD}(X, W)$ in successive three times of perturbation and optimization, stop.

Note that, site positions are more important in the optimization of the OPD energy function, as we have observed previously. We can have an expectation that optimizing site positions thoroughly before optimizing all variables together will significantly speed up the convergence. Hence, our optimization algorithm is applied twice: the first time we only optimize site positions (position optimization) and the second time we optimize all variables to achieve a deeper local minimum (position-weight optimization). Details of the algorithm will be given in the rest of this section.

5.2. Initialization

Providing a good initial guess is critical for optimization to find a deep local minimum. Here, we generate an initial guess that is close to an optimal solution, which will considerably speed up the iteration progress.

Our initialization algorithm holds all the weights constant and takes a target $f(\mathbf{x})$, the desired site number n and a batch number m as input. We start with a small number of sites, and then add more sites adaptively in each subsequent iteration, guided by approximation errors, so that the approximation quality is improved progressively. The initialization phase consists of the following steps:

Step 1. The first batch of n/m sites, randomly sampled for the given domain Ω , are optimized using the L-BFGS method. Then, the approximation error on each cell of the tessellation can be computed.

Step 2. The n/m cells with the largest approximation errors are selected, with one new site inserted into each of them. In particular, we compute the principal axes of each selected cell using principal component analysis (PCA), and a new site is added next to the current site along the direction of the short axis. This new site placement operation is called *site insertion* in the following sections.

Step 3. To escape from the current local minimum and find another possibly better local minimum, each site \mathbf{x}_i is perturbed by a small amount in an arbitrary direction:

$$\mathbf{x}'_i = \mathbf{x}_i + \lambda l_i \mathbf{v}$$

where l_i is the length of the short axis of the corresponding cell V_i , λ is a factor used to adjust the magnitude of the perturbation, and \mathbf{v} is a random vector within a unit 2D disk or 3D sphere. Hereinafter, this perturbation operation is referred to as *local perturbation*. Then, all the site positions are optimized by the L-BFGS method.

Step 4. If all batches of sites are added, stop; otherwise, update the approximation error on each cell and go back to Step 2.

Note that, as an initialization for a new round of local search in Step 3, the positions of newly added sites in Step 2 is of critical importance. Similar to previous observations, a random placement of newly added site at each selected cell would also lead to unsatisfying results. Examples are shown in Fig. 5. By randomly placing a new site at each selected cell, our initialization algorithm results in shallow local minimizers, especially when the input target function shows strong anisotropic property, see Fig. 5(a). Whereas, adding new sites at short axes gives a better anisotropic approximation to the input function, and leads to a much deeper local minimizer, see Fig. 5(b). This site insertion method does no harm for the isotropic case, see Fig. 5(d), which generates similar results to the random insertion method in Fig. 5(c).

It is also worth pointing out that it is hard to determine the right number of batches such that the approximation can reach the best quality. Generally speaking, having fewer sites inserted in each step needs more iteration steps, leading to slower approximation and smaller approximation error. While having more newly-inserted sites in each approximation step needs fewer iteration steps, but may result in larger approximation error. The worst case is adding all sites at once, as shown in Fig. 3(c), which results in a much shallower local minimum than the result obtained by adding new sites in batches in Fig. 5(b). Empirically, we insert n sites by 20 batches, which reaches a good balance between computation time and approximation quality.

5.3. Perturbation

The results of our comprehensive initialization can be further improved by the aforementioned MCM global optimization which involves perturbation and local searching.

Position perturbation. The proposed perturbation strategy sequentially applies two types of perturbations: *global perturbation* and *local perturbation*. In global perturbation, 1% of the sites whose cells have the smallest approximation errors are removed. In compensation, each of 1% of the cells with the largest approximation errors is split by adding a new site, using the site insertion operation in Step 2 of Section 5.2. In local perturbation, each site is perturbed as Step 3 of Section 5.2. Note that, the factor λ plays an important role in adjusting the perturbation magnitude. Too

small λ may lead to a failure of escaping from the current local minimizer. Whereas, too large λ would amount to re-starting the optimization from a random initialization. Empirically, λ is set to be 0.2 in all our experiments. As can be observed in Fig. 6(b), our global optimization method helps find a deeper local minimum, benefiting from the perturbations. It is also worth pointing out that, it is the cooperative effect between global and local perturbations that allows our algorithm to reach deep local minima. As shown in Fig. 6, the local minimum obtained by solely using local perturbation is shallower than the local minimum obtained by using both global and local perturbations in position optimization.

Weight perturbation. In the position-weight optimization, weights provide additional degrees of freedoms and allow a better approximation to the given function. After adding perturbation to sites, a local perturbation is also added to each weight. In particular, each weight w_i is randomly perturbed by a magnitude less than βl_i , where l_i is defined in Step 3 of Section 5.2 and β is an adjustable factor empirically chosen as $\beta = 0.1$. Results in Fig. 7 indicate that the approximation result obtained from position optimization is further improved in the following position-weight optimization, as more degrees of freedom are exploited to control the local anisotropy.

5.4. Terminating condition

In our modified MCM method, a deep local minimum is found in a more aggressive way, i.e., a worse local minimum is always rejected, instead of accepting it according to a probability in the original MCM method. Our algorithm terminates when it fails to decrease the energy after successive three times of perturbation or reaches a pre-defined maximum iteration number. Benefiting from the delicate initialization, our method usually achieves satisfying results within 20 iterations of position optimization and 5 iterations of position-weight optimization. Thus, in all our experiments (except the experiment shown in Fig. 3), the maximum iteration numbers of position optimization and position-weight optimization are set to 20 and 5, respectively.

6. Results

In this section, we present several experimental results to demonstrate the effectiveness of our OPD method and compare it with the OVT method. Voronoi cells restricted to a given domain are computed using an efficient clipping method proposed in [37]. All the experiments were performed on a machine with a 3.3 GHz Intel Xeon processor and 12 GB RAM.

Non-convex function approximation. We first conduct our algorithm on several non-convex functions in the 2D case to demonstrate the capability of our algorithm in generating anisotropic tessellations. Anisotropy described by the Hessian of the given non-convex functions may change greatly from region to region. The experimental results shown in Figs. 1(c), 8, 9 and 12 indicate that the generated tessellations well capture the expected anisotropic variations.

Density control. By adding a non-negative scalar function to modulate the L^2 norm in the OPD energy function (2), our method is capable of generating anisotropic mesh with density adapting to the scalar function. In particular, we compute the minimizer of the modified energy function

$$\mathcal{E}_{OPD}(X, W) = \sum_{i=1}^n \int_{V_i} \rho(x)(f(\mathbf{x}) - P_i^*(\mathbf{x}))^2 d\mathbf{x}, \quad (5)$$

whose derivative can be derived in the same manner as Eq. (2). Fig. 9 shows that the generated meshes adapt to both the predicted anisotropy and density.

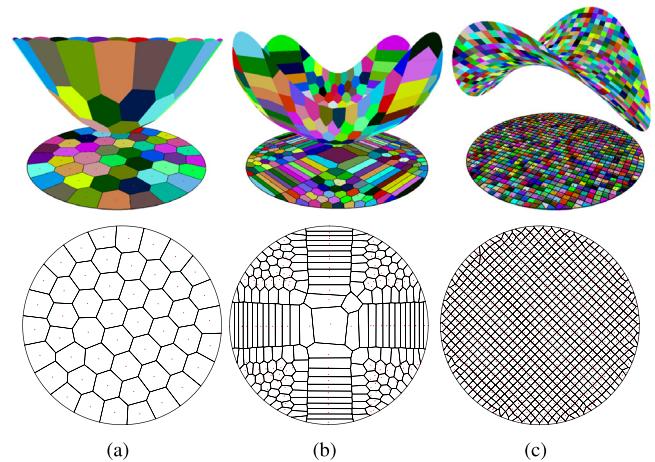


Fig. 1. Optimal power diagrams based on discontinuous piecewise linear approximations of different target functions: (a) $f(x, y) = x^2 + y^2$; (b) $f(x, y) = x^4 + y^4$; and (c) $f(x, y) = xy$.

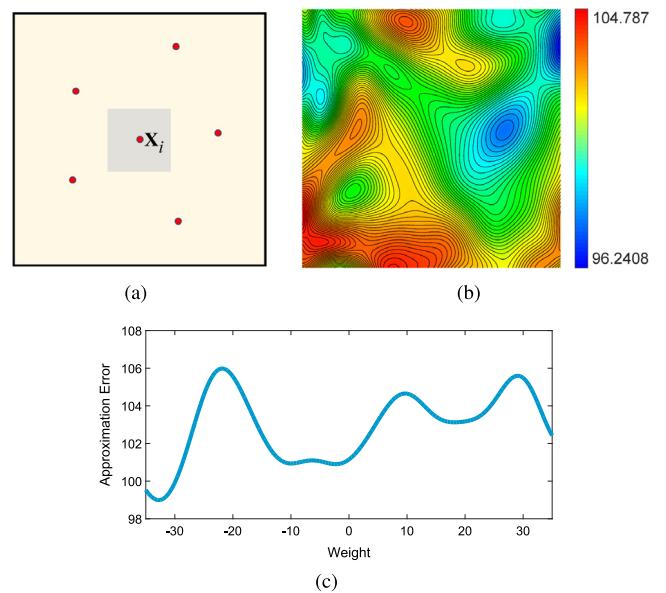


Fig. 2. Energy landscape near \mathbf{x}_i , with an input function $f(x, y) = \sin(\pi(x + 0.5))\cos(\pi y)$. (a) All sites and weights are held constant except the position or weight of site \mathbf{x}_i ; (b) variations of the energy function with respect to site \mathbf{x}_i ; and (c) plot of approximation error with respect to weight w_i varying from -35 to 35 .

3D results. Our algorithm is naturally applicable for 3D mesh generation and provides the same control over anisotropy and density. Fig. 10 shows an example of anisotropic meshing on a simple spherical domain, and the cutaway views show that the cells precisely get aligned to the expected anisotropy. In Fig. 11, our method generates a sequence of meshes from isotropic mesh to anisotropic meshes (with aspect ratios being 1, 2 and 8, respectively) on a geometric model. The cutaway views show that the aspect ratio of cells are effectively controlled by the input function. In Fig. 12, a cube model is decomposed to cells with spatially-varying anisotropy and density. Once again, the predicted anisotropy and density are well captured, as can be observed in exterior and cutaway views.

Comparison with the OVT method. We evaluate our OPD method via a comparison with the OVT method [27]. Three measures of the cells V_i , including the Hessian variation, shape ratio

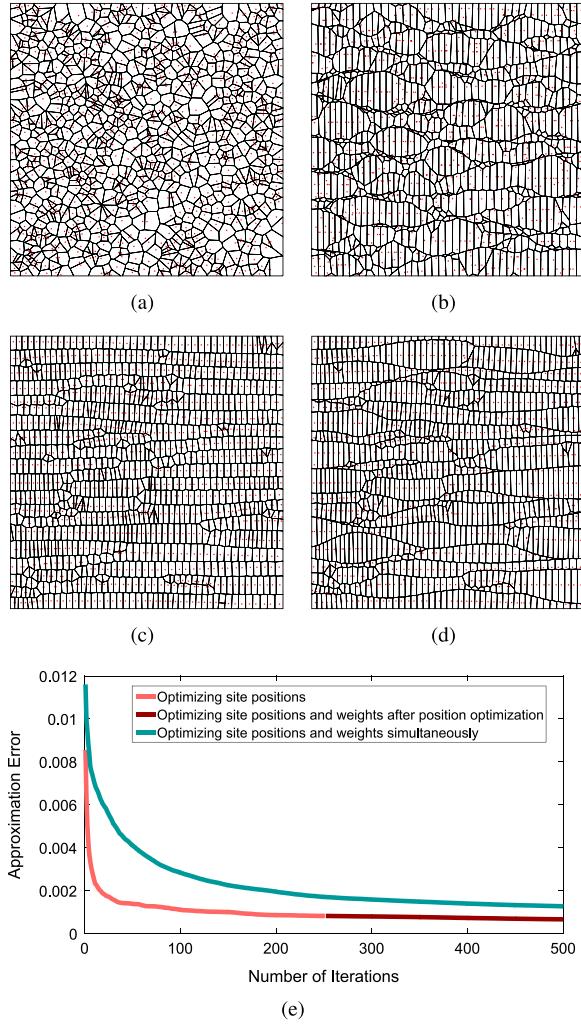


Fig. 3. Influence of variables on the objective function, where $f(x, y) = 100x^2 + y^2$, $-1 \leq x, y \leq 1$. (a) Random initialization of 1000 sites; (b) result obtained by directly optimizing all site positions and weights, with $\varepsilon_{OPD} = 1.273 \times 10^{-3}$; (c) result obtained by only optimizing site positions from the random initialization in (a), with $\varepsilon_{OPD} = 8.239 \times 10^{-4}$; (d) result obtained by optimizing all site positions and weights from the intermediate result in (c), with $\varepsilon_{OPD} = 6.607 \times 10^{-4}$; and (e) plot of approximation error versus iteration number, obtained by updating variables in different orders.

and modified area, are adopted here to evaluate the mesh quality as follows:

- Hessian variation: $\max_{\mathbf{x}, \mathbf{y} \in V_i} \|Hess[f](\mathbf{x}) - Hess[f](\mathbf{y})\|_F$, where $Hess[f](\mathbf{x})$ is the Hessian of function $f(\mathbf{x})$ and $\|\cdot\|_F$ is the Frobenius norm.
- Shape ratio: $\max_{\mathbf{x}, \mathbf{y} \in V_i} \left[\sqrt{(\mathbf{x} - \mathbf{y})^t \bar{H}_{V_i} (\mathbf{x} - \mathbf{y})} \right] \left[|V_i| \sqrt{\det \bar{H}_{V_i}} \right]^{-\frac{1}{d}}$, where \bar{H}_{V_i} is the averaged Hessian of f within a cell V_i .
- Modified area: $(\bar{\rho}_{V_i}^d \det \bar{H}_{V_i})^{\frac{1}{d+2}} |V_i|$, where $d = 2, 3$, and $\bar{\rho}_{V_i}$ is the average density within a cell V_i .

Generally speaking, the cells of a high-quality tessellation have similar Hessian variations, shape ratios and areas. Figs. 13–15 show a comparison of our OPD method with the OVT method on generating meshes conforming to anisotropic metrics induced by 2D/3D convex functions. From the tessellation results, we can observe that our OPD method produces meshes with visually more

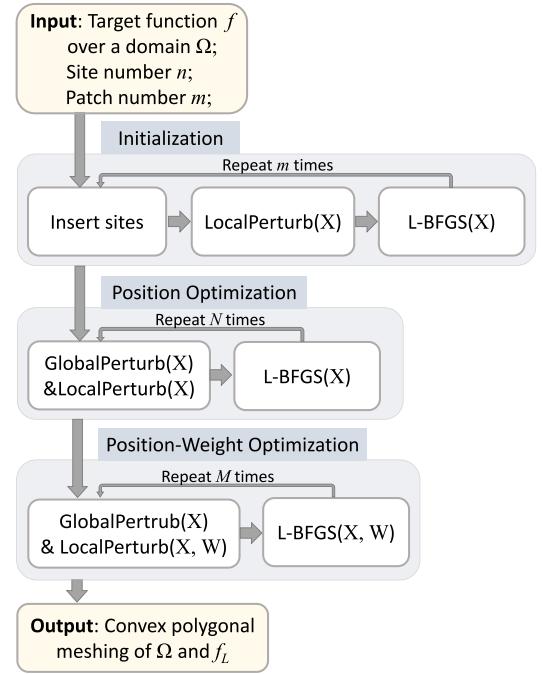


Fig. 4. Overview of our OPD optimization algorithm.

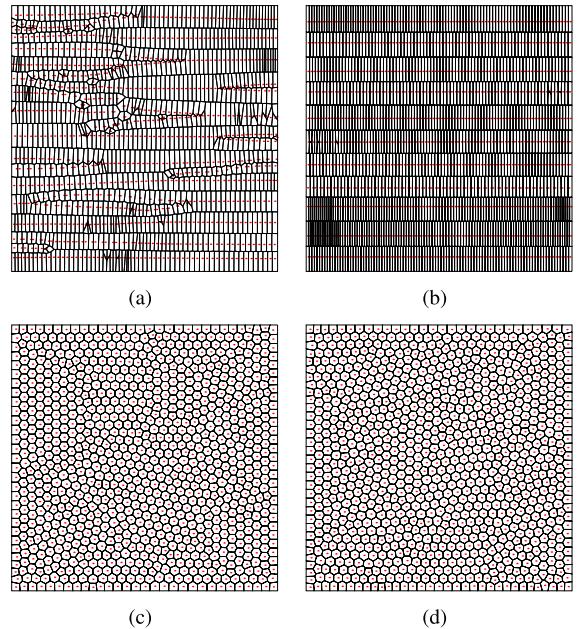


Fig. 5. Comparison of new site insertion methods with different initializations. (a) and (c) are results using a random insertion method for new sites; and (b) and (d) are results using the PCA based new site insertion method. Top row: $f(x, y) = 100x^2 + y^2$, $-1 \leq x, y \leq 1$, with $\varepsilon_{OPD} = 4.124 \times 10^{-4}$ (a) and $\varepsilon_{OPD} = 8.492 \times 10^{-5}$ (b). Bottom row: $f(x, y) = x^2 + y^2$, $-1 \leq x, y \leq 1$, with $\varepsilon_{OPD} = 6.044 \times 10^{-7}$ (c) and $\varepsilon_{OPD} = 6.095 \times 10^{-7}$ (d).

regular cells. Histograms display the distributions of the three aforementioned measures on each resulting mesh, which indicate that our OPD method achieves a better performance than the OVT method. Histograms of Hessian variations in Figs. 13 and 15 are not given as the Hessian is constant on each cell. The color-coded approximation errors in both L^1 and L^2 norms also reveal that our OPD method provides better approximation to the given functions.

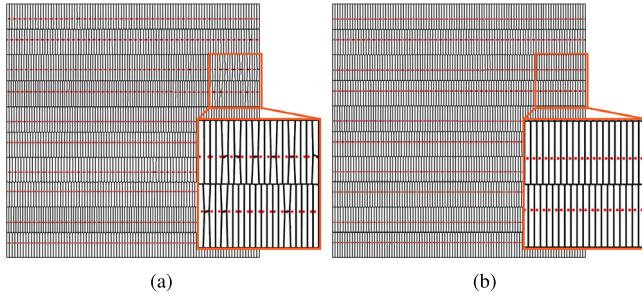


Fig. 6. Influence of global perturbation on site position optimization. (a) Result using only local perturbation, $\varepsilon_{OPD} = 7.396 \times 10^{-5}$; and (b) result using both global and local perturbations, $\varepsilon_{OPD} = 7.115 \times 10^{-5}$.

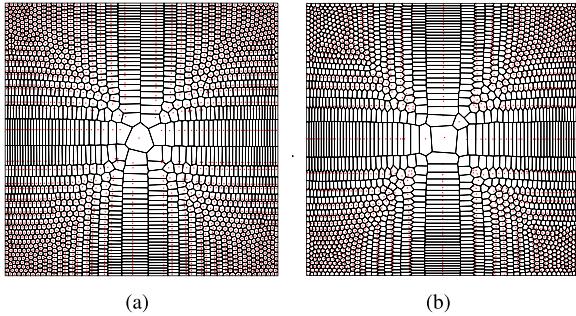


Fig. 7. $f(x, y) = x^4 + y^4 + (x - 3)^2 + (y - 3)^2, -10 \leq x, y \leq 10$ with 2,000 sites. (a) Result after position optimization; and (b) result of position-weight optimization, taking the tessellation in (a) as input.

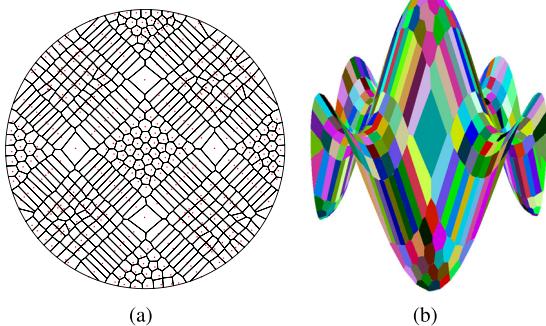


Fig. 8. Resulting tessellation (a) and piecewise linear fit (b) of a non-convex target function $f(x, y) = \sin(\pi(x + 0.5)) \cos(\pi y), x^2 + y^2 \leq 1$ with 500 sites.

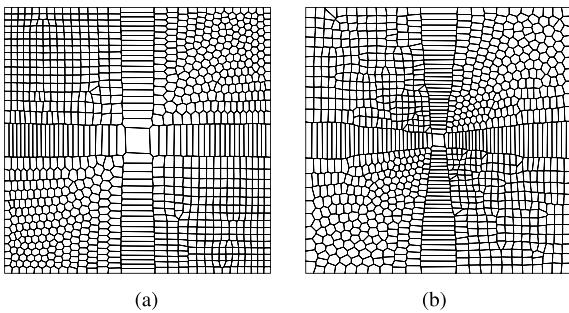


Fig. 9. Density control. Resulting tessellations for a non-convex target function $f(x, y) = x^3 + y^3, -1 \leq x, y \leq 1$ with a constant density in (a) and a nonuniform density function $\rho(x, y) = 1.0/((x^2 + y^2)^2 + 0.001)$ in (b).

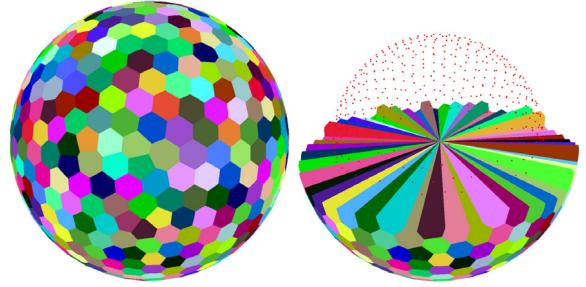


Fig. 10. Tessellation of sphere for a non-smooth target function $f(x, y, z) = \sqrt{x^2 + y^2 + z^2}$ with 800 sites.

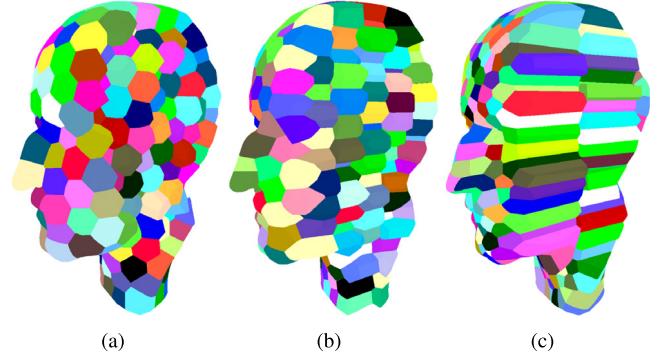


Fig. 11. 3D optimal power diagrams with increasing anisotropy. (a) Isotropic; (b) 2:1:1; and (c) 8:1:1.

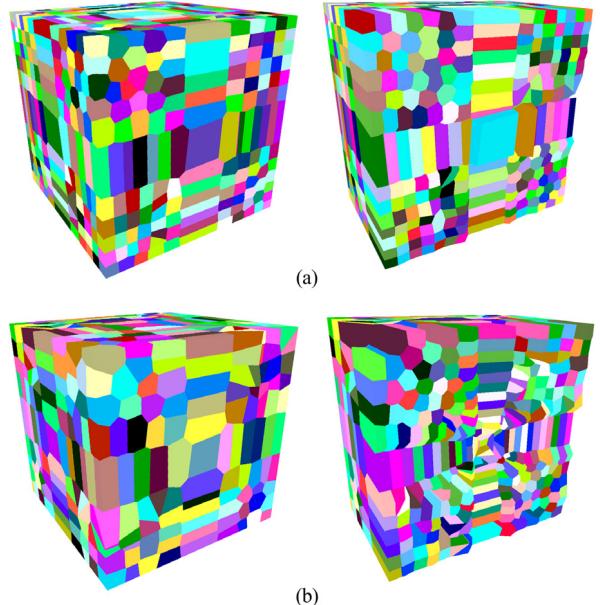


Fig. 12. Exterior and cutaway views of tessellations for a non-convex target function $f(x, y, z) = x^3 + y^3 + z^3, -1 \leq x, y, z \leq 1$ with a constant density in (a) and a nonuniform density function $\rho(x, y, z) = 1.0/((x^2 + y^2 + z^2)^2 + 0.001)$ in (b).

7. Conclusion

We present a cell complex generation framework using OPD, achieving tessellations with well controlled local anisotropy and density. Our OPD method extends the existing OVT method by removing the convex restriction on the approximated function and replacing tangent planes with general planes as approximants.

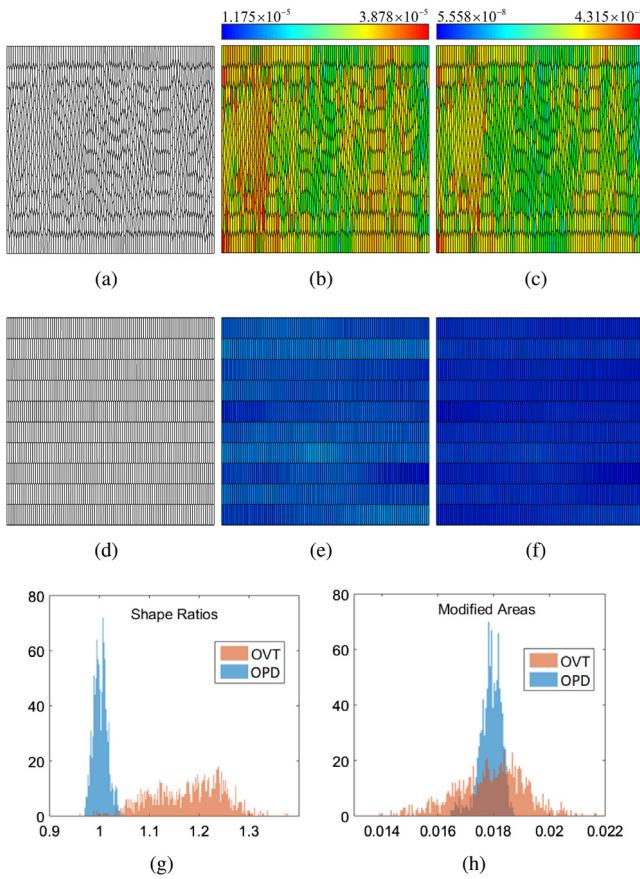


Fig. 13. Comparison of our OPD method with the OVT method on a convex function with a constant Hessian $f(x, y) = 100x^2 + y^2$, $-1 \leq x, y \leq 1$. (a–c) Results from the OVT method; (d–f) results from our OPD method; and (g–h) histograms of shape ratios and modified areas. (a, d) Resulting tessellations; (b, e) color-coded errors in the L^1 norm; and (c, f) color-coded errors in the L^2 norm. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

A combined local-global optimization technique, coupled with comprehensive initialization and perturbation schemes, is tailored for solving the specific optimization problem. Experimental results demonstrate that our method is capable of generating more diverse tessellations with expected density and anisotropy and providing a better approximation to the given function than the OVT method.

Limitation and future work. In practical applications, one may desire to generate meshes adapted to a given tensor field. However, an arbitrarily prescribed tensor field is not the Hessian of any function in general. Hence, the aforementioned anisotropic technique cannot be directly used for this situation. One promising solution is to find a function whose Hessian provides the best fit to the prescribed anisotropy using a fitting method. Compared with the optimization method of computing OVT, our hybrid optimization often suffers from the high computational cost, despite of successes in finding optimal local minima. The running time of our OPD method for each example is given in Table 1. As part of our future work, we will focus on speeding up the optimization.

Although in this paper we only focus our research endeavors on generating anisotropic cell complexes for function approximation, potential applications of cell complex generation are much broader. For example, shape functions defined over polygonal/polyhedral elements are often desirable in finite element analysis and isogeometry analysis. We plan to further refine our

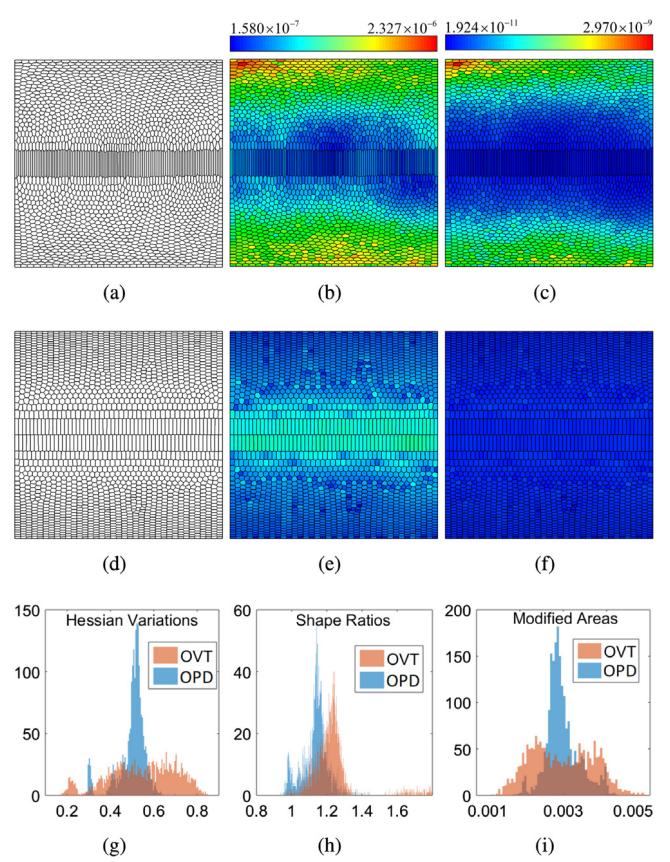


Fig. 14. Comparison of our OPD method with the OVT method on a convex function with varying Hessian $f(x, y) = x^2 + 10^{-5}y^2 + y^4$, $-1 \leq x, y \leq 1$ with 2000 sites. (a–c) Results from the OVT method; (d–f) results from our OPD method; and (g–h) histograms of Hessian variations, shape ratios and modified areas. (a, d) Resulting tessellations; (b, e) color-coded errors in the L^1 norm; and (c, f) color-coded errors in the L^2 norm. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

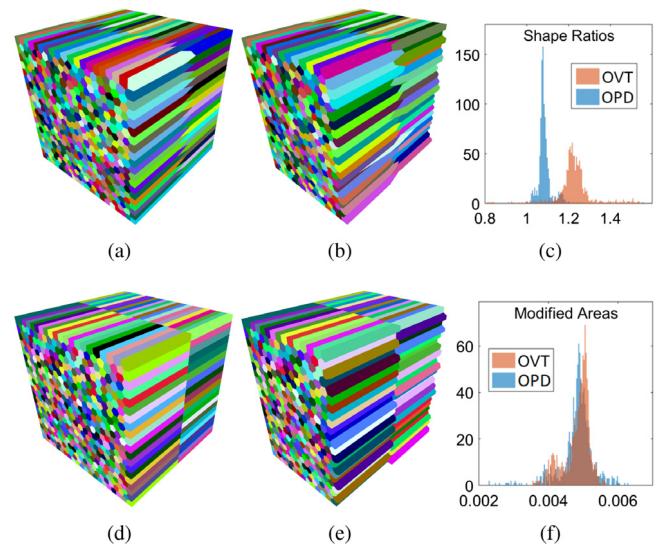


Fig. 15. Comparison of our OPD method with the OVT method in the 3D case $f(x, y, z) = x^2 + y^2 + 0.01z^2$, $-1 \leq x, y \leq 1$. (a, b) Result and cutaway view from the OVT method; (d, e) result and cutaway view from our OPD method; and (c, f) histograms of shape ratios and modified areas, respectively.

Table 1

Statistics of running time.

Figure	Site number	Initialization (s)	Position optimization (s)	Position-weight optimization (s)	Total time (s)
1(a)	50	0.1	1.6	2.4	4.1
1(b)	200	49	65	72	186
1(c)	800	32	18.8	17.6	68.4
7	2000	270	213	109	592
8	500	56	27.8	44.8	128.6
9	1000	57	59.7	43.3	160
10	800	780	246	1245	2271
11	500	860	414	283	1557
12(a)	2000	1731	3615	615	5961
12(b)	2000	1694	3521	354	5579
13	1000	63	67	23	153
14	2000	98	200	36	334
15	1000	598	1028	286	1912

algorithm by integrating more constraints on the geometry shape of cells and apply it to analysis and simulation tasks.

Acknowledgments

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References

- [1] Agarwal PK, Suri S. Surface approximation and geometric partitions. In: Proceedings of the fifth annual ACM-SIAM symposium on discrete algorithms, 1994, p. 24–33.
- [2] Aurenhammer F. A criterion for the affine equivalence of cell complexes in R^d and convex polyhedra in R^{d+1} . *Discrete Comput Geom* 1987;2(1):49–64.
- [3] Shewchuk JR. Delaunay refinement algorithms for triangular mesh generation. *Comput Geom* 2002;22(1–3):21–74.
- [4] Borouchaki H, George PL, Hecht F, Laug P, Saltel E. Delaunay mesh generation governed by metric specifications. Part I. Algorithms. *Finite Elem Anal Des* 1997;25(1–2):61–83.
- [5] Dobrzynski C, Frey P. Anisotropic Delaunay mesh adaptation for unsteady simulations. In: Proceedings of the 17th international meshing roundtable, 2008, p. 177–94.
- [6] Boissonnat J-D, Wormser C, Yvinec M. Anisotropic diagrams: Labelle Shewchuk approach revisited. *Theoret Comput Sci* 2008;408(2–3):163–73.
- [7] Boissonnat J-D, Wormser C, Yvinec M. Anisotropic Delaunay mesh generation. *SIAM J Comput* 2015;44(2):467–512.
- [8] Bossen FJ, Heckbert PS. A pliant method for anisotropic mesh generation. In: Proceedings of the 5th international meshing roundtable, 1996, p. 63–74.
- [9] Jiao X, Colombi A, Ni X, Hart J. Anisotropic mesh adaptation for evolving triangulated surfaces. *Eng Comput* 2010;26(4):363–76.
- [10] Zhong Z, Guo X, Wang W, Lévy B, Sun F, Liu Y, et al. Particle-based anisotropic surface meshing. *ACM Trans Graph* 2013;32(4):1–99.
- [11] Dassi F, Si H, Perotto S, Streckenbach T. Anisotropic finite element mesh adaptation via higher dimensional embedding. *Procedia Eng* 2015;124:265–77.
- [12] Dassi F, Perotto S, Si H, Streckenbach T. A priori anisotropic mesh adaptation driven by a higher dimensional embedding. *Comput Aided Des* 2017;85 (Supplement C):111–22, 24th International Meshing Roundtable Special Issue: Advances in Mesh Generation.
- [13] Du Q, Faber V, Gunzburger M. Centroidal Voronoi tessellations: applications and algorithms. *SIAM Rev* 1999;41:637–76.
- [14] Du Q, Wang D. Anisotropic centroidal Voronoi tessellations and their applications. *SIAM J Sci Comput* 2005;26(3):737–61.
- [15] Lévy B, Liu Y. L_p centroidal Voronoi tessellation and its applications. *ACM Trans Graph* 2010;29(4):1–11.
- [16] Sun F, Choi Y-K, Wang W, Yan D-M, Liu Y, Lévy B. Obtuse triangle suppression in anisotropic meshes. *Comput Aided Geom Design* 2011;28(9):537–48.
- [17] Richter R, Alexa M. Mahalanobis centroidal Voronoi tessellations. *Comput Graph* 2015;46(Supplement C):48–54, Shape Modeling International 2014.
- [18] Valette S, Chassery JM, Prost R. Generic remeshing of 3D triangular meshes with metric-dependent discrete Voronoi diagrams. *IEEE Trans Vis Comput Graphics* 2008;14(2):369–81.
- [19] Cai Y, Guo X, Liu Y, Wang W, Mao W, Zhong Z. Surface approximation via asymptotic optimal geometric partition. *IEEE Trans Vis Comput Graphics* 2017;23(12):2613–26.
- [20] Lévy B, Bonneel N. Variational anisotropic surface meshing with Voronoi parallel linear enumeration. In: Proceedings of the 21st international meshing roundtable, 2013, p. 349–66.
- [21] Xin S-Q, Lévy B, Chen Z, Chu L, Yu Y, Tu C, et al. Centroidal power diagrams with capacity constraints: computation, applications, and extension. *ACM Trans Graph* 2016;35(6):244.
- [22] Nadler E. Piecewise linear best L^2 approximation on triangulations. In: Approximation Theory V. 1986, p. 499–502.
- [23] Mirebeau J-M, Cohen A. Greedy bisection generates optimally adapted triangulations. *Math Comp* 2012;81(278):811–37.
- [24] Chen L, Xu J-C. Optimal Delaunay triangulations. *J Comput Math* 2004;299–308.
- [25] Chen L. Mesh smoothing schemes based on optimal Delaunay triangulations. In: Proceedings of 13th international meshing roundtable, 2004, p. 109–20.
- [26] Fu X-M, Liu Y, Snyder J, Guo B. Anisotropic simplicial meshing using local convex functions. *ACM Trans Graph* 2014;33(6):182.
- [27] Budninskiy M, Liu B, De Goes F, Tong Y, Alliez P, Desbrun M. Optimal Voronoi tessellations with Hessian-based anisotropy. *ACM Trans Graph* 2016;35(6):242:1–242:12.
- [28] Nivoliers V, Lévy B. Approximating functions on a mesh with restricted Voronoi diagrams. *Comput Graph Forum* 2013;32(5):83–92.
- [29] Chen Z, Xiao Y, Cao J. Approximation by piecewise polynomials on Voronoi tessellation. *Graph Models* 2014;76(5):522–31.
- [30] Li Z, Scheraga HA. Monte Carlo-minimization approach to the multiple-minima problem in protein folding. *Proc Natl Acad Sci USA* 1987;84(19):6611–5.
- [31] Lu L, Sun F, Pan H, Wang W. Global optimization of centroidal Voronoi tessellation with Monte Carlo approach. *IEEE Trans Vis Comput Graphics* 2012;18(11):1880–90.
- [32] Chen Z, Cao J, Wang W. Isotropic surface remeshing using constrained centroidal Delaunay mesh. *Comput Graph Forum* 2012;31(7):2077–85.
- [33] Chen Z, Wang W, Lévy B, Liu L, Sun F. Revisiting optimal Delaunay triangulation for 3D graded mesh generation. *SIAM J Sci Comput* 2014;36(3):A930–54.
- [34] Liu Y-J, Xu C-X, Yi R, Fan D, He Y. Manifold differential evolution (MDE): a global optimization method for geodesic centroidal Voronoi tessellations on meshes. *ACM Trans Graph* 2016;35(6):243:1–243:10.
- [35] Aurenhammer F. Power diagrams: properties, algorithms and applications. *SIAM J Comput* 1987;16(1):78–96.
- [36] Flanders H. Differentiation under the integral sign. *Amer Math Monthly* 1973;80(6):615–27.
- [37] Yan D-M, Wang W, Lévy B, Liu Y. Efficient computation of 3D clipped Voronoi diagram. In: International conference on geometric modeling and processing. Springer; 2010. p. 269–82.