# MESH OPTIMIZATION BASED ON THE CENTROIDAL VORONOI TESSELLATION

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Abstract. The subject of mesh generation and optimization is very important in many scientific applications. In this paper, we investigate the issue of mesh optimization via the construction of Centroidal Voronoi Tessellations. Given some initial Delaunay meshes with only average quality, it is shown that the CVT based mesh optimization generates a robust, high quality mesh which does not rely critically on the choice of the initial mesh. In comparison, other smoothing techniques, such as the classical Laplacian smoothing, tend to be more sensitive to the initial distributions of vertices. Thus, the CVT based optimization may be advocated as a prefered choice for mesh optimization and smoothing.

**Key Words.** Voronoi tessellations, Delaunay triangulation, optimal tessellations, mesh optimization, mesh smoothing, Centroidal Voronoi tessellation

### 1. Introduction

The automatic unstructured triangular/tetrahedral mesh generation for complex geometries is essential to the efficient solution of complex problems in various applications such as CFD, CEM and oil reservoir simulations. The advancing front techniques, Octree methods and Voronoi Delaunay-based methods are three well-studied techniques in unstructured mesh generation[1, 2, 3, 4, 5]. Regardless of the method chosen, the resulting unstructured mesh often requires further improvement and optimization. For example, much attention has been paid to the almost regular triangular/tetrahedral meshing used in conjunction with the Yee's scheme in computational electro-magnetics and the MAC method in CFD[37, 38, 39]. Such simulation requirement poses challenges on mesh improvement and optimization, especially in complicated domains.

Traditionally, the procedures for unstructured mesh optimization generally fall into the following basic categories [12, 29, 30, 31, 32, 33, 34, 35]: geometric optimization, meaning mesh smoothing or vertices relocation without changing the node connectivity, through strategies such as the Laplacian smoothing and its variants; topological optimization, consisting of local reconnections such as edges/faces flipping, while keeping node positions unchanged; and vertex insertion or deletion, referring to operations such as the sink insertion [42]. These techniques are often combined and performed in an iterative manner, and they form the core of the classical optimization methods. More recently, there have also been some studies on the

<sup>2000</sup> Mathematics Subject Classification. 65D18, 65N50, 68U07, 65Y20.

Research is supported in part by NSF DMS-0409297 and CCF-0430349. Part of this work was completed while the authors were at the Academy of Mathematics and Systems Science, Chinese Academy of Sciences, through the support of the Chinese Academy of Sciences and the China State Major basic research fund G1999032800. Special thanks also to Prof.Jiachang Sun, the guest editor of this special issue, for organizing the SCPI04 international conference.

use of global optimization approaches, such as the use of Winslow transforms, harmonic mappings and algebraic or geometric mesh quality measures [29, 30, 31, 32].

In this paper, we focus on the application of Centroidal Voronoi tessellations (CVTs) to mesh optimizations. The concept of CVT has been used in diverse applications, such as data and image analysis, communication and sensor network, clustering, vector quantization, flow control, dimension reduction and resource allocation [6, 8, 9]. CVTs are defined as special Voronoi tessellations of a region such that the generating points of the tessellations are also the mass centroids of the corresponding Voronoi regions with respect to a given density function[6]. In the application to quality mesh generation, a CVT configuration provides an optimal points distribution (with respect to a given density), its dual centroidal Voronoi-Delaunay triangulation (CVDT) provides a high quality triangular (or tetrahedral) mesh[7, 12]. The optimality can be illustrated through the minimization of an associated error or cost functional, and it can also be validated by the celebrated Gersho's conjecture which predicts the asymptotic equi-partition of the local error. CVTs can often be constructed through the iterative Lloyd algorithm which moves the generators to the mesh centers and re-start the Voronoi-Delaunay construction. Thus, if Lloyd iteration is applied to an initial Delaunay triangular mesh to construct a CVDT or a constrained CVDT of a given domain, the final triangular mesh becomes a natural optimization of the initial mesh. CVT based mesh optimization has been successfully applied to 2D/3D isotropic cases [7, 12, 16], and it has also been generalized to anisotropic and surface mesh generation [10, 15]. A brief survey can be found in [18].

Some earlier results reported on the CVT based mesh optimization show encouraging signs that it may be further developed into a robust procedure for improving the mesh quality. In this paper, we carry out more numerical studies on the effectiveness of its applications to the isotropic 2D and 3D mesh optimization and also make comparisons with other existing algorithms. For two dimensional examples, the Lloyd iterations with respect to the constant density yield meshes that are almost regular triangular meshes. The comparisons between the classical optimization techniques that combine mesh smoothing with edges/faces swapping and the CVT based optimization technique indicate that the classical optimization is much more sensitive to the initial mesh configuration or vertex distribution, while the CVT based optimization provide meshes that are largely independent of such initial conditions. Similarly, for the three dimensional application examples, we can also see that the CVT based optimization results in meshes that are of higher quality and are more structured than those obtained by the classical optimization.

The remaining part of the paper is organized as follows. The basic procedures of the mesh optimization based on the centroidal Voronoi tessellation are recalled in Section 2. The effects of the mesh improvement based on the CVT and comparisons with those of classical optimizations are discussed in Section3 and Section4, for 2D and 3D isotropic meshing respectively. A final conclusion is made in Section5.

#### 2. Mesh Optimization Based on Centroidal Voronoi Tessellation

Recently, the centroidal Voronoi tessellation (CVT) and its wide range of applications have been studied in [6, 7, 8, 9, 10, 11, 12]. Often, CVT provides optimal points placement with respect to a given density function. When the density function is chosen properly with respect to a giving sizing field, its dual structure, the so-called centroidal Voronoi Delaunay triangulation (CVDT), results in a highquality Delaunay mesh[7, 12]. We have applied this technique to mesh generation and optimization in isotropic 2D and 3D unstructured meshing[7, 12], and also generalized it to anisotropic and surface quality mesh generation[10, 15]. In the following, we recall some of the main concepts and properties of the CVT from [6], and present the algorithm for constructing CVDT for the optimization of any given Delaunay mesh.

**2.1.** Basic Concepts and Properties. Given a density function  $\rho$  defined on a region V, the mass centroid  $\mathbf{z}^*$  of V is defined by

$$\mathbf{z}^* = rac{\int_v \mathbf{y} 
ho(\mathbf{y}) d\mathbf{y}}{\int_v 
ho(\mathbf{y}) d\mathbf{y}}$$

We then have [6]:

**Definition 2.1.** Given the set of points  $\{\mathbf{z}_i\}_{i=1}^k$  in the domain  $\Omega$  and a positive density function  $\rho$  defined on  $\Omega$ , a Voronoi tessellation is a centroidal Voronoi tessellation (CVT) if  $\mathbf{z}_i = \mathbf{z}_i^*$ , i = 1, ..., k, i.e., the generators of the Voronoi regions  $V_i, \mathbf{z}_i$ , are themselves the mass centroids of those regions. The dual Delaunay triangulation is referred to as the Centroidal Voronoi-Delaunay triangulation (CVDT).

For any tessellation  $\{V_i\}_{i=1}^k$  of the domain  $\Omega$  and a set of points  $\{z_i\}_{i=1}^k$  (independent of  $\{V_i\}_{i=1}^k$ ) in  $\Omega$ , we can define the following *cost* (or *error* or *energy*) functional:

$$F(\{V_i\}_{i=1}^k, \{z_i\}_{i=1}^k) = \sum_{i=1}^k \int_{V_i} \rho(x) ||x - z_i||^2 dx \; .$$

The standard CVT's along with their generators are critical points of this cost functional. Using the concept of cost functional, we also have the definition of Constrained CVT (CCVT) and its duality constrained CCVT (CCVDT); see [6, 7, 12] for the details. Also, in [15], the definition of CVT has been generalized to anisotropic cases with a Riemannian metric and an one-sided distance.

Generally speaking, the practical construction of CVT and CVDT can be classified into two categories: the probabilistic and the deterministic methods [6, 20, 21, 23, 27, 28]. Here, we apply a deterministic algorithm based on the popular Lloyd's method [6, 19, 28] which is an obvious iteration between constructing Voronoi tessellations and centroids. And it enjoys the property that the functional F is monotonically decreasing throughout the iteration. A detailed description of the algorithm will be presented later. For studies on the probabilistic methods as well as their parallelization, we refer to [11].

2.2. Application to Quality Mesh Generation. The construction of CVDT (or CCVDT) through the Lloyd iteration can be viewed from a different angle as a smoothing process of an initial mesh. The CVDT concept provides a good theoretical explanation to the smoothing process: by successively moving generators to the mass centers (of the Voronoi regions), the cost functional is reduced. Here, *smoothing* means both node-movement and node reconnection. If the density function can be chosen according to the sizing function, the cost functional may be related to the distortion of the mesh shape and quality with respect to the mesh sizing. Thus, the process of iteratively constructing CVDTs, like the the Lloyd's algorithm, contributes the reduction of the global distortion of element shape and sizing. The final CVDT would have the minimal distortion, and hence shares good elements quality with respect to the sizing distribution[7, 12].

A practically useful property of the CVT and CVDT is the equi-distribution of cost[6, 7, 12]. It is not difficult to show that in the one dimensional case,

$$\int_{V_i} \rho(x) (x - x_i)^2 dx \approx c \qquad \forall$$

for some constant c when the number of generators goes to infinity. This means, asymptotically speaking, the cost is equally distributed in the Voronoi intervals[6]. For the multidimensional CVT, the Gersho conjecture [26] predicted that asymptotically, as the number of generators becomes large, all Voronoi regions are approximately congruent to the same basic cell that only depends on the dimension. The basic cell was shown to be the regular hexagon in two dimensions[24], and the dual cell is the regular triangle, thus explaining why the CVDTs in 2D tend to provide high quality meshes. The conjecture remains open for three and higher dimensions [25, 26] while further numerical substantiation has been provided in [25] to the fact that the basic cell in 3D is the conjectured BCC lattice polyhedra [16]. The conclusion of the conjecture would lead to the cost equi-distribution principle. Moreover, for large scale problems involving millions of grid points, the conjecture also would imply that the unstructured Delaunay mesh may in fact be locally well-structured. Even though the conjecture is still open in three and higher dimensions, it is nevertheless practically prudent to apply the equi-distribution of the cost functional based on the conjecture. With the cost functionals being related implicitly to the distortion of the elements quality [7, 12], the equi-distribution principle can then be understood as the equi-distribution of the distortion of the elements quality. In other words, asymptotically, almost regular triangulation/tetrahedralization can be generated. This idea has been applied to quality isotropic 2D and 3D mesh generation and optimization [7, 12] where various meshing examples have provided support to the claim of good element quality. More recently, similar techniques were also successfully generalized to the anisotropic case and quality surface grid generation in [10, 15, 17].

We now briefly recall how to construct the CVDT using the Lloyd method as an natural optimization for the constrained Delaunay meshing of a given domain. Given a bounded domain and a prescribed element sizing, suppose a constrained boundary Delaunay triangulation/tetrahedralization of the domain with respect to the sizing has been generated and stored[12, 13, 14, 16], we then perform the optimization procedure, or say the Lloyd iteration, as follow:

# Algorithm 2.1. (The Lloyd iteration) Given a set of vertices.

1) Construct the Voronoi region for each of the interior points that are allowed to change their positions, and construct the mass center of the Voronoi region with a properly defined density function  $\rho(p)$  derived from the sizing field H(p). Here,  $\rho(p) = C/H(p)^{2+d}$ , where d is the dimensions, C is a scaling constant (may be simplified to identity).

2) Insert the computed mass centers into the constrained boundary Delaunay triangulation/tetrahedralization through a constrained Delaunay insertion procedure[5, 12, 35].

3) Compute the difference  $D = \sum_{i=1}^{k} ||P_i - P_{imc}||^2$ ,  $\{P_i\}$  is the set of interior points allowed to change,  $\{P_{imc}\}$  is the the set of corresponding computed mass center. 4) If D is less than a given tolerance, terminate; otherwise, return to step 1.

Later in the paper, the Lloyd iteration given above is applied to optimize various constrained isotropic Delaunay mesh examples in 2D and 3D respectively. The mesh improvement effects are probed with respect to different initial points distribution and the final element qualities of the converged CVDTs. Comparisons with the classical mesh optimization techniques are also made. We note that generalizations of the Lloyd method as well as its parallel implementations have been provided in our earlier works[11].

To further demonstrate the effect of the CVT based mesh optimization, the Laplacian smoothing and its variant (edge length weighted Laplacian smoothing) together with local Delaunay edges swappings are performed to the same initial meshes until convergence. The final results are compared which further highlight the more effectiveness of the CVT-based optimization.

To be more precise, the Laplacian smoothing here takes the following simplest form: a new position  $P_{new}$  for an interior vertex  $P_i$  is computed by the formula:  $P_{new} = \frac{1}{N_i} \sum_{j=1}^{N_i} P_j$ , with  $P_j$  being the adjacent vertices, and  $N_i$  the number of adjacent vertices to  $P_i$ . It is heuristically simple and often has reasonable convergence rate. It also smoothes local sizing and improves the quality of the worst element. However, for a general initial mesh, its convergence does not guarantee the global quality improvement and the element validity (i.e. sometimes, inverted elements are generated). This is in part due to the fact that it is not related to a rigorously proved reduction of some global measure. Its improvement to three dimensional tetrahedral mesh is even more limited, and thus its application should be more cautiously used[29, 30, 34, 35]. With such limitations, several variants have been developed to retain the efficiency of Laplacian smoothing while improving its robustness[4, 29, 30, 34]. Here, we apply the edge-length weighted version for which the position of  $P_{new}$  is related to the global sizing field and the optimality of element quality.

We now briefly recall the general procedure which is based on the edge unit length computation (for details, see [35, 36]). Let P be an interior free vertex, and  $K_i$  be the set of elements sharing P. Let  $P_i$  be the vertices of  $K_i$  other than P. Each point  $P_i$  is associated with an optimal point  $P_i^*$  such that  $\overline{P_iP_i^*} = \overline{P_iP}/l(P_iP)$ , for which  $l(P_iP_i^*) = 1$  holds. The computation of the edge length  $l(P_iP)$  can be found in [36]. Then,  $P_{new}$  is defined as the centroid of  $(P_i^*)$ .

In the above Laplacian smoothing or it variant, it is not sufficient to only consider the improvement made through vertices movement, for the new triangulation after the Laplacian smoothing may no longer be Delaunay. Hence, it is necessary to add local topological operations such as edges swappings into the improvement of the mesh so as to keep the Delaunay property of the triangulation. Usually, they are coupled in an iterative manner. Here, the Laplacian smoothing and the edgelength weighted version are both coupled with the local edges swapping and these combined optimizations are called the Delaunay-Laplacian (DL) optimization and the Weighted Delaunay-Laplacian (WDL) optimization.

### 3. Optimization effects for 2D test examples

We note that, for a triangle A, its quality can be often defined by  $Q = 4\sqrt{3}|A|/\sum L_i^2$ where |A| is the area of the element and  $L_i$  is the length of the *i*-th edge. In order to study the effects of CVT-based optimization for a given 2D mesh, two test examples are investigated here. One is a quadrilateral domain with uniform sizing and the other is a washer shaper with nonuniform sizing. The points of the two initial meshes are all generated using the advancing-front technique[1, 2]. Then, perturbations are performed to the initial points so as to produce triangular meshes with bad qualities. Such perturbations may be produced with a combination of random movements and movements to form clusters. To improve the meshes, Lloyd iterations are performed, leading to converged CVDTs which are almost regular with respect to the specified sizing and element quality.



FIGURE 1. A quadrilateral domain and a perfect mesh (top) and the meshes after perturbations (bottom).

The first example is a quadrilateral domain which can be meshed with all equilateral triangles. The domain and a perfect regular mesh is shown in Fig3. Such as initial regular mesh is generated in advancing-front method and then the interior points are repositioned by random perturbations or by perturbations to cluster all points to the center of the domain. The two meshes after the relocation of vertices are also shown in Fig3. Obviously the elements are of low qualities after the perturbations. To improve these meshes, DL, WDL, and CVT based optimizations are performed respectively. The final converged meshes are different from each other, which indicate different optimization effects. The meshes after the DL optimization are shown in Fig3 and the element qualities of the meshes are presented in Table 1 (RandPert and ClusPert refer to the randomly perturbed and the clustered initial distributions respectively). Both meshes and the mesh quality data demonstrate that the DL optimization is very sensitive to the initial vertex distribution and is it is not effective especially for the mesh with vertices that are highly clustered. This is due to the fact that the optimization is done with no respect to any global sizing measure. Thus, most of the initial vertices still remain in the center, see the right of Fig3. The meshes generated by the WDL optimization are significantly better with much more improvement. The mesh sizing is in more conformity with the given uniform sizing, and element quality is also better. The meshes and the element quality data are given in Fig3 and Table 2. It can be seen that the final converged or optimized mesh is still somewhat different from the regular initial mesh, thus showing the sensitivity of WLS to the initial vertex distribution. But the Lloyd iterations (or the CVT based optimization) for these two different initial meshes converge to the same mesh: the original regular mesh shown in Fig3 (so that we do not actually need to provide any quality data), a demonstration that the CVT based optimization is very effective and it performs better than the other two classical ones due to their less sensitivity on the initial vertex distribution.

The second example is for meshing a washer-shaped domain shown in Fig 4. The initial vertices are also generated by the advancing-front method. As in the above, the interior vertices are perturbed or clustered near the inner circle. The two distorted meshes are shown in Fig 4. These two meshes are then improved



FIGURE 2. Meshes after the DL optimization of example 1 with randomly perturbed and clustered initial meshes.

Example 1	RandPert	ClusPert
average quality	0.986	0.927
minimum quality	0.776	0.391
minimum angle	35.24	13.89
maximum angle	98.95	121.0

TABLE 1. Mesh quality data after the DL Optimization



FIGURE 3. Meshes after the WDL optimization of example 1 with randomly perturbed and clustered initial meshes.

Example 1	RandPert	ClusPert
average quality	0.991	0.940
minimum quality	0.871	0.600
minimum angle	41.67	30.0
maximum angle	88.73	120.0

TABLE 2. Mesh quality data after the WDL Optimization.

through DL, WDL and the CVT based optimization. Concerning the optimization effects, similar conclusions as in the previous example can be drawn. The meshes in Fig 5 and elements quality statistics contained in Table 3 further clarify that the simple DL optimization is not effective for sizing related mesh improvement; while Fig 6 and Table 4 demonstrate that the WDL optimization is much more effective, both in terms of the sizing consistency and the element quality. However, observing the different mesh configurations near the inner circle (see Fig 6), there are still noticeable differences in the two converged meshes after the WDL optimization. The meshes shown in Fig 7 after the CVT based optimizations and their mesh quality data given in Table 5 once again illustrate that the Lloyd iteration can lead to almost regular triangular meshes with the values of average quality up to 0.99. The converged results are insensitive to the given initial vertex distribution.



FIGURE 4. Perturbed initial meshes for example 2.



FIGURE 5. Meshes after the DL Optimization of example 2.

Example 2	RandPert	ClusPert
average quality	0.978	0.926
minimum quality	0.798	0.328
minimum angle	34.98	11.3
maximum angle	97.35	120.1

TABLE 3. Mesh quality data after the DL Optimization

Example 2	RandPert	ClusPert
average quality	0.973	0.958
minimum quality	0.751	0.447
minimum angle	34.1	20.3
maximum angle	103.6	134.9

TABLE 4. Mesh quality data after the WDL Optimization.

Example 2	RandPert	ClusPert
average quality	0.989	0.991
minimum quality	0.861	0.854
minimum angle	40.1	41.1
maximum angle	88.4	91.3

TABLE 5. Mesh quality data after CVT-based optimization



FIGURE 6. Meshes after the WDL Optimization of example 2.



FIGURE 7. Meshes after CVT based optimization of example 2.

# 4. Optimization effects in 3D applications

We now present two application examples in 3D to investigate the effect of the CVT based optimization in more practical situations. One example is a cube containing an interior sphere, a case often considered in simple external flow field simulations. The other is the femur reconstructed from CT scans or cross sectional contours and used for a biomedical simulation such as the fracture prediction and simulation[40, 41]. In the above simulation examples, the generated mesh quality is often closely related to the computational efficiency, especially when explicit marching schemes are used, and hence it is necessary to construct quality tetrahedral meshes in such applications [40, 41].

For both examples, initial tetrahedral meshes are constructed by the classical constrained Delaunay tetrahedralization method which includes surface mesh generation, initial unconstrained Delaunay 3D triangulation of boundary points, constrained boundary recovery, interior refinement and mesh optimization. Here, for simplicity, interior vertices are generated along interior edges by the method of [35]. For mesh optimization, two methods are applied. One is the classical *Combined Optimization* which includes optimization based on the Laplacian smoothing, edges/faces flipping and the iterations between them [2, 4, 29, 33, 34]. In each iteration, three to five Laplacian smoothings are performed and complex edges or faces flippings are conducted to improve the minimal dihedral angles. The other method is the CVT based optimization which has been shown to be a successful approach for generating various high quality 3D meshing examples in [12], and more recently, for probing the qualities of optimal CVTs and the Gersho conjecture in three dimensions in [16]. Also, CVT has been applied together with simple swappings to remove slivers[12, 16].

For the example with a cube containing a sphere as shown in Fig 8, the cutting views of its two optimized meshes are shown in Fig 9, and the element quality data of the initial mesh, the mesh after combined optimization, and the mesh after the CVT based optimization with or without simple swappings, are given in Table 6. Here, element quality formulae follows that in [12, 16]. The bad elements or the *good elements* are defined as those whose quality number is less than 0.3 or larger than 0.5 respectively. From the cutting view, it can be seen that the CVT based optimization generates more structured mesh than the counterpart obtained via the combined optimization. From the mesh quality data in Table6, first, it indicates that the combined optimization is very effective in removing slivers or bad-quality tetrahedra (bad elements), thus making the technique very popular among commercial meshing softwares [4, 29, 35]. In comparison, nevertheless, the CVT based optimization can produce a mesh CVDT with an average element quality about 0.81, better than the value 0.71 in the mesh obtained by the classical combined optimization. Moreover, the CVDT has a larger number of tetrahedra whose quality are closer to that of the regular one. Also, it can be found that there is a small number of sliver-like elements (bad elements) in the CVDT and they are neighboring the boundary of the domain as similarly reported in [12, 16]. But just like in [12, 16], using simple edge or face swappings (SWAP), these very bad elements can be all deleted as demonstrated by the quality statistics of the mesh produced with CVDT + SWAP. The final mesh is superior to the mesh after the combined optimization both in terms of the minimum element quality (relating to slivers), the average element quality (the global quality), and the more structured configuration.

The surface mesh, the cutting view of tetrahedral mesh, and the quality statistics of the meshes of the second example, i.e., the femur are presented in Figures 10 and 11, and Table 7 respectively. Both the mesh structure and the element quality data show similarity to those of the first example and it further demonstrate that the CVT based optimization is more effective than the classical combined optimization. And in the dynamic analysis of the fracture prediction of the femur, it is found that the generated CVDT results in larger time steps than that from the classical optimization and this significantly saves simulation time [40, 41].

#### 5. Conclusions and future work

In our present study, numerical investigations are conducted in both 2D and 3D on the effect of CVT based optimizations. It can be seen that CVT based optimizations, or say, the convergence of Lloyd iterations, is much less sensitive to the initial vertex distribution than the classical and weighted Laplacian based optimization. The CVT based optimization is clearly more effective that the classical counterparts. Also, the converged mesh is more geometrically structured, largely due to

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	Init	CombOpt	CVDT	CVDT+SWAP
number of elements	26060	24364	23880	23779
0.7 < Q < 1.0	9882	14579	19814	21475
0.5 < Q < 0.7	12212	9183	3734	2090
0.3 < Q < 0.5	2990	601	201	214
0.0 < Q < 0.3	976	1	131	0.0
$Q_{min}$	0.0024	0.243	0.09	0.352
bad elements (%)	3.74	0.5	0.8	0.0
good elements( $\%$ )	84.7	97.5	98.6	99.1
average quality	0.641	0.719	0.803	0.810

TABLE 6. Elements quality statistics of optimized meshes of a cube containing a sphere

	Init	CombOpt	CVDT	CVDT+SWAP
number of elements	31511	29441	25808	25757
0.7 < Q < 1.0	12140	16941	20602	22347
0.5 < Q < 0.7	14346	11577	4589	3101
0.3 < Q < 0.5	3774	919	399	309
0.0 < Q < 0.3	1251	4	218	0
$Q_{min}$	0.007	0.267	0.084	0.311
bad elements (%)	3.97	0.01	0.8	0.0
good elements(%)	84.0	96.8	97.6	98.8
average quality	0.639	0.713	0.791	0.803

TABLE 7. Elements quality statistics of optimized meshes of a femur



FIGURE 8. The frame line (left) and the surface mesh (right) of a cube containing a sphere

the nice properties of the CVDT and due to the accompanied Gersho conjecture which states that asymptotically the converged CVDT is a regular triangular mesh in two space dimension and a BCC lattice based Delaunay mesh in the three dimensional space [24, 25, 26]. Such a conjecture has been proved in two dimension and more recently, its three dimensional version has been numerically substantiated via abundant numerical examples [16]. Hence, one may expect that the final converged CVDT mesh is more structured locally and is of higher quality than that constructed using the classical optimization method.



FIGURE 9. The cutting view of meshes after the Combined Optimization (left) and the CVT based Optimization (right)







FIGURE 11. The cutting view of meshes after the Combined Optimization(left) and the CVT based Optimization(right)

We note that in more recent years, there have also been many studies on the global optimization methods [29, 30, 31, 32]. We will leave a more careful comparison with such global methods to future works.

Naturally, let us point out that in order for the CVT based optimization to be successfully applied to large scale quality meshing, especially in the applications areas such as oil reservoir simulations, and wave scattering simulations for three dimensional CEM, the Lloyd iteration needs to accelerated in order to make the CVT based optimization scheme more competitive both quality wise and efficiency

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wise. The acceleration can be realized through the localization of the Delaunay triangulation or through the use of Multigrid type methods. Such initiatives are under current investigations [20, 21]. Connections between meshes and algebraic solvers and their *co-adaptations* are also useful issues to be examined further [22].

#### References

- R. Lohner and P. Parikh, Generation of three-dimensional grids by the advancing-front method. Int.J.Num.Method.Fluids 1988; 8: 1135-1149.
- [2] D. Marcum, and N. Weatherill, Unstructured Grid Generation using iterative point insertion and local reconnection. AIAA Journal 1995; 33: 1619-1625.
- [3] MS. Shephard and MK. Georges, Automatic three-dimensional mesh generation technique by the finite element octree technique. Int. J. Num. Method Engrg. 1991; 32: 709-749.
- [4] N. Weatherill and O. Hassan, Efficient three dimensional Delaunay triangulation with automatic point creation and imposed boundary constraints, Int. J. Num. Method Engrg. 1994; 37: 2005-2039.
- [5] H. Borouchaki and SH. Lo, Fast Delaunay triangulation in three dimensions. Computer Methods in Applied Mechanics and Engineering 1995; 128: 153-167.
- [6] Q. Du, V. Faber and M. Gunzburger; Centroidal Voronoi tessellations, Applications and algorithms, SIAM Review, (1999), 41: pp.637-676.
- [7] Q. Du and M. Gunzburger, Grid Generation and Optimization Based on Centroidal Voronoi Tessellations, Applied and Computational Mathematics, 133 (2002), pp.591-607.
- [8] Q. Du, M. Gunzburger, and L. Ju, Meshfree, probabilistic determination of point sets and support regions for meshless computing, Comput. Methods Appl. Mech. Engrg., 191 (2002), pp. 1349-1366.
- [9] Q. Du, M. Gunzburger, L. Ju and X. Wang, Centroidal Voronoi tessellation algorithms for image compression and segmentation, to appear in J. Math Imaging and Vision, 2006.
- [10] Q. Du, M. Gunzburger and L. Ju, Constrained Centroidal Voronoi Tessellations on General Surfaces, SIAM J. Sci. Comp, 24, pp.1499-1506, 2003.
- [11] Q. Du, M. Gunzburger, L. Ju, Probablistic methods for centroidal Voronoi tessellations and their parallel implementations, Journal of Parallel Computing, 28, pp.1477-1500, 2002.
- [12] Q. Du, and D. Wang, Tetrahedral mesh generation and optimization based on Centroidal Voronoi Tessellations. Int. J. Num. Method Engrg., 56, pp.1355-1373, 2002
- [13] Q. Du, and D. Wang, Boundary recovery for three dimensional conforming Delaunay triangulation. Computer Methods in Applied Mechanics and Engineering, 193, pp.2547-2563, 2004.
- [14] Q. Du, and D. Wang, Constrained boundary recovery for three dimensional Delaunay triangulation, Int. J. Num. Method Engrg., 2004, 61: 1471-1500.
- [15] Q. Du and D. Wang, Anisotropic Centroidal Voronoi Tessellations and their applications, SIAM SIAM J. Sci Comp., 26, pp.737-761, 2005.
- [16] Q. Du and D. Wang, On the Optimal Centroidal Voronoi Tessellation and the Gersho's conjecture in the three dimensional space, Computers and Mathematics with Applications, 49, pp.1355-1373, 2005.
- [17] Q. Du and D. Wang, Approximate Constrained Centroidal Voronoi Tessellation on Surfaces and the Application to Surface Mesh Optimization, preprint, 2005.
- [18] Q. Du, and Desheng Wang, New progress in robust and quality Delaunay mesh generation, to appear in J. Computational Applied Mathematics, 2006.
- [19] Q. Du, M. Emelianenko and L. Ju, Convergence Properties of the Lloyd Algorithm for Computing the Centroidal Voronoi Tessellations, to appear in SIAM J. Numer. Anal., 2006.
- [20] Q. Du and M. Emelianenko, Uniform convergence of a nonlinear optimization-based multilevel quantization Scheme, preprint, 2005.
- [21] Q. Du and M. Emelianenko, Acceleration schemes for computing centroidal Voronoi tessellations, to appear in special issue of Numerical Linear Algebra with Applications, 2006
- [22] Q. Du, Z. Huang and Desheng Wang, Mesh and Solver Co-adaptation in Finite Element Methods for Anisotropic Problems, Numerical Methods for Differential Equations, 21, pp.859-874, 2005.
- [23] T. Kanungo, D. Mount, N. Netanyahu, C. Piatko, R. Silverman and A. Wu, An efficient kmeans clustering algorithm: Analysis and implementation, IEEE Trans. Pattern Anal. Machl Intel. 24, (2002), pp.881–892.
- [24] D. Newman, The Hexagon theorem, IEEE Trans. Infor. theory, 28, 1982, pp.137-139.

- [25] E.S. Barnes and N.J.A. Sloane, The optimal Lattice quantizer in three dimensions, SIAM J. Algebraic Discrete Methods, 4, 30-41, 1983.
- [26] A. Gersho, Asymptotically optimal block quantization, IEEE Trans. Inform. Theory, 25, 1979, pp.373-380.
- [27] R. M. Gray and D. L. Neuhoff, Quantization, IEEE Trans. Inform. Theory, 44 (1998), 2325-2383.
- [28] S. Lloyd, Least square quantization in PCM, IEEE Trans. Infor. theory, 28, 1982, pp.129-137.
- [29] L. Freitag, P. Knupp, T. Munson, and S. Shontz. A Comparison of Optimization Software for Mesh Shape Quality Improvement Problems, p29-40, Proceedings of the 11th International Meshing Roundtable, Ithaca NY, 2002.
- [30] L. Freitag, P. Knupp, Tetrahedral mesh improvement via optimization of the element condition number, Int. J. Numer. Meth. Engr., 53:1377-1391, 2002.
- [31] P. Knupp, Matrix Norms and the Condition Number: A general framework to improvemesh quality via node-movement, 8th International Meshing RoundTable, Lake Tahoe, pp13-22, 1999.
- [32] L. Freitag and P. Knupp, Tetrahedral Element Shape Optimization via the Jacobian Determinant and Condition Number, 8th International Meshing RoundTable, Lake Tahoe, pp247-258, 1999.
- [33] L. Freitag and C. Olliver-Gooch, Tetrahedral mesh improvement using swapping and smoothing. Int. J. Num. Method. Engrg. 1997; 40: 3979-4002.
- [34] EA. Dari and GC. Buscaglia, Mesh Optimization: how to obtain good unstructured 3-D finite element meshes with not-so-good mesh generators. Structural Optimization 1994; 8: 181-188.
- [35] PL. George, Delaunay Triangulation and Meshing: Application to Finite Elements. Editions HERMES, Paris, 1998.
- [36] H. Borouchaki and P.Frey, Adaptive Triangular-Quadrilateral Mesh Generation. Int. J. Num. Meth. Engrg. 1998; 41: 915-934.
- [37] N. Madsen, Divergence preserving discrete surface integral methods for Maxwell's equations using nonorthogonal unstructured grids, J. Computational Physics, 1995;119: 35-45.
- [38] I. Sazonov, D. Wang, O. Hassan, K. Morgan and N. Weatherill, A stitching method for unstructured mesh generation for co-volume solution techniques, Computer Methods in Applied Mechanics and Engineering, 2005, in press.
- [39] A.G.Churbanov, A unified algorithm to predict compressible and imcompressible flows. In CD-Rom Proc. ECCOMAS Computational Fluid Dynamics Conf., Swansea, Wales, 2001.
- [40] T.D.Fawcett, Creating and validating heterogeneous tetrahedral finite element models of the femur from Computed Tomography (CT) images, Sept. 2004, Master thesis, Civil and Computational Engineering Centre, University of Wales Swansea.
- [41] C.A.Pridham(Beng) Hons, Tetrahedral finite element (FE) meshes to model femoral fractures generated from CT scans taken from the Visible Human Project.Sept. 2004, Master thesis, Civil and Computational Engineering Centre, University of Wales Swansea.
- [42] H. Edelsbrunner and D. Guoy, Sink Insertion for Mesh Improvement. International Journal of Foundations of Computer Science, 2002, 13: 223–242

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