Optimum Node Positioning in Adaptive Grid Refinement and the Delaunay-Voronoi Algorithm

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Abstract:

This paper presents a method for optimum placement of nodes in grid generation for process simulation together with an algorithm for updating the grid after each addition of a new node to ensure that the Delaunay property is satisfied. Placement of nodes is decided on by considering the optimum error in evaluating the integral $\int_V C(x)dx$. The best error estimate is obtained when the node coincides with the centroid (the center of mass) of its own Voronoi region and moreover when the Voronoi region is symmetric. After addition of a node the grid is updated to maintain the Delaunay property using the Delaunay-Voronoi algorithm.

Introduction

In process simulation, we are concerned with solving the diffusion equation

$$\frac{\partial C}{\partial t} = \nabla.(D\nabla C),\ t \geq 0,\ x \in \Omega \subset \mathbf{R}^d,\ d = 2,3$$

where D is the diffusion coefficient. In solving the problem numerically, we are concerned with the error in computing the integral $\int_V C(x)dx$ where V is the region of influence of the node $\overline{x}$ (the Voronoi region (see [4]) of the node $\overline{x}$.) Previously, we have considered the problem of node removal in a grid where mesh is too fine for the problem, (see [1], [2], and [3].) The removal algorithm identified nodes to be removed by their low discretizaton error. We now turn our attention to addition of nodes. When a grid is adapted, new nodes are added in areas where, due to larger variation in $C(x)$, it is deemed that greater resolution is needed. To decide on the optimum placement of these new nodes, we consider which position will give the best error in evaluating $\int_V C(x)dx$.

The best error for this calculation is $O(h^3k, hk^3)$ when $C(x)$ is approximated by its Taylor series evaluated at the node $\overline{x}$, the generator of the Voronoi region V, and moreover, when the node is the centroid (center of mass) of its own Voronoi region. Such a Voronoi tesselation is called a centroidal Voronoi tesselation. (see [5]). After addition of a new node, the grid quality must be maintained. A desirable property of the grid is that it has the Delaunay property. The grid is updated, after addition of each new node, to ensure that it has the Delaunay property. The algorithm to achieve this is called the Delaunay-Voronoi algorithm.

The actual position of a new node is at the centroid of surrounding nodes to ensure that the node is at the centroid of its own Voronoi region. This position is decided on by considering the smallest order error in evaluating the integral $\int_V C(x)dx$ using a Taylor series as stated above. Hence the error in evaluating $\int_V C(x)dx$ is used as an error indicator in deciding on the positioning of nodes.

In adding nodes during grid adaption, a check is used whereby a new node is added if and only if the geometric grid quality is improved. If the geometric grid quality is not improved, then the new node is not added.

Error Indicator for Evaluation of $\int_V C(x)dx$

The best error for this calculation of $\int_V C(x)dx$.is $O(h^3k, hk^3)$, when $C(x)$ is approximated by its Taylor series evaluated at the node $\overline{x}$, the generator of the Voronoi region, V, and moreover, when the node is the centroid (center of mass) of its own Voronoi region.

In fact, in two spatial dimensions, we have that

$$\begin{aligned}\int_V C(x)dx \simeq \int_V \Bigg\{ & C(\overline{x},\overline{y}) + \overline{h}\frac{\partial C(\overline{x},\overline{y})}{\partial x} + \overline{k}\frac{\partial C(\overline{x},\overline{y})}{\partial y} + \\ & \frac{\overline{hk}}{2}\frac{\partial^2 C(\overline{x},\overline{y})}{\partial x \partial y} + \frac{\overline{h}^2}{2}\frac{\partial^2 C(\overline{x},\overline{y})}{\partial x^2} + \\ & \frac{\overline{k}^2}{2}\frac{\partial^2 C(\overline{x},\overline{y})}{\partial y^2} + O(\overline{h}^3, \overline{k}^3, \overline{h}^2\overline{k}, \overline{hk}^2)\Bigg\} d\overline{h}d\overline{k}\end{aligned}$$

Hence

$$\begin{aligned}\int_V C(x)dx \simeq\ & 4C(\overline{x},\overline{y})hk + \frac{1}{2}\overline{h}^2\Big|_{\overline{h}=-h}^{\overline{h}=h}\overline{k}\Big|_{\overline{k}=-k}^{\overline{k}=k}\frac{\partial C(\overline{x},\overline{y})}{\partial x} + \\ & \frac{1}{2}\overline{h}\Big|_{\overline{h}=-h}^{\overline{h}=h}\overline{k}^2\Big|_{\overline{k}=-k}^{\overline{k}=k}\frac{\partial C(\overline{x},\overline{y})}{\partial y} + \\ & \frac{1}{8}\overline{h}^2\Big|_{\overline{h}=-h}^{\overline{h}=h}\overline{k}^2\Big|_{\overline{k}=-k}^{\overline{k}=k}\frac{\partial^2 C(\overline{x},\overline{y})}{\partial x \partial y} + \\ & \frac{1}{6}\overline{h}^3\Big|_{\overline{h}=-h}^{\overline{h}=h}\overline{k}\Big|_{\overline{k}=-k}^{\overline{k}=k}\frac{\partial^2 C(\overline{x},\overline{y})}{\partial x^2} + \\ & \frac{1}{6}\overline{h}\Big|_{\overline{h}=-h}^{\overline{h}=h}\overline{k}^3\Big|_{\overline{k}=-k}^{\overline{k}=k}\frac{\partial^2 C(\overline{x},\overline{y})}{\partial y^2} + \\ & O(h^4k, hk^4, h^3k^2, h^2k^3)\end{aligned}$$

and so

$$\begin{aligned}\int_V C(x)dx \simeq\ & 4C(\overline{x},\overline{y})hk + \frac{2}{3}h^3k\frac{\partial^2 C(\overline{x},\overline{y})}{\partial x^2} + \\ & \frac{2}{3}hk^3\frac{\partial^2 C(\overline{x},\overline{y})}{\partial y^2} + O(h^4k, hk^4, h^3k^2, h^2k^3)\end{aligned}$$

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where $\int_V C(x)dx \simeq 4C(\overline{x})hk$, and so the error is seen to be

$$\frac{2}{3}h^3k\frac{\partial^2 C(\overline{x},\overline{y})}{\partial x^2}+\frac{2}{3}hk^3\frac{\partial^2 C(\overline{x},\overline{y})}{\partial y^2}+O(h^4k, hk^4, h^3k^2, h^2k^3)$$

Notice that the condition of symmetry of the Voronoi region is what causes cancellation of the terms involving h^2k, hk^2, and h^2k^2.

Centroidal Voronoi Tesselations

A centroidal Voronoi tesselation is a Voronoi tesselation where the generators of the Voronoi cells and the centroids of those cells coincide (see [5]).

To generate a centroidal Voronoi tesselation, (see Figure 1 for a Voronoi tesselation versus a centroidal Voronoi tesselation) we add new nodes at the centroid of surrounding nodes. In fact, given points p_i, $i = 1, 2, ..., N$ and $\overline{p} = \frac{1}{N}\sum_{i=1}^{N} p_i$, the centroid of these points, $\overline{p}$, will be the centroid of its own Voronoi region. i.e. if we generate a grid where points are added at the centroids of surrounding points, then we will generate a centroidal Voronoi tesselation.

Delaunay-Voronoi Algorithm

To maintain good grid quality after addition of a new node, we need to update the grid so that it is Delaunay at each stage. In 2-dimensions, the Delaunay triangulation is the dual of the Voronoi tesselation,(see Figure 2). A property of the Delaunay triangulation is that the circumcircle (circumsphere in 3-dimensions) of the nodes contained in a face of the triangulation does not contain any of the other nodes. This property can then be used to update the grid at each stage to ensure that it has the Delaunay property. We test each face to see if the circumcircle(sphere) of the face contains the newly added node, (see Figure 3). The faces associated with the circumcircles (spheres) which contain the newly added node are glued together in a "Big Face". The newly added node is moved to the centroid of the "Big Face". We iterate the algorithm, testing the remaining faces to see if the centroid of the new "Big Face" lies in the circumcircle of any other faces. When the centroid of "Big Face" is not contained in the circumcircle of any other faces, "Big Face" is regridded using its centroid. This algorithm ensures that the grid is Delaunay after each addition of a node, and also ensures that the new grid generates centroidal Voronoi regions. This strategy means that it is also easy to interpolate the concentration to conserve the dose. The algorithm is known as the Delaunay-Voronoi algorithm, (see [6]).

Computing the Delaunay triangulation for N nodes has computational complexity $O(N \log N)$. This computational complexity is greatly reduced by updating the grid after each addition of a node. In fact, the number of faces whose circumcircles contain the newly added node is constant and so the computational complexity of maintaining a Delaunay grid after addition of nodes is linear in the number of newly added nodes.

Incorporated in the algorithm is a check, whereby a new node is added if and only if the geometric grid quality, Q, for the "Big Face" is improved by adition of the new node.

Geometric Grid Quality

The geometric grid quality of a collection of faces $\{F_1, ..., F_N\}$, where A_i is the area of the face F_i, and the face F_i has sides of lengths l_{i1}, l_{i2}, and l_{i3}, is defined by

$$Q = \sum_{i=1}^{N} \frac{A_i}{\sum_{j=1}^{3} l_{ij}^2},$$

It is expected that a centroidal Voronoi mesh will have excellent quality. For example, a perfect equilateral triangular mesh ($Q = 1$) is also centroidal. In test examples, (see Figures 4 and 5) geometric grid quality is seen to be improved when this algorithm is used, (see Figure 6 for percentage improvements in geometric grid quality concerning a particular input). Figures 4 and 5 show a spacer where the poly has ben finely gridded and adapted. The coarsely gridded oxide has also been adapted. Figure 4 uses the Delaunay Voronoi algorithm and Figure 5 does not.

Conclusions

We propose that grid should be adapted with addition of nodes at the centroid of suroundling nodes to generate Voronoi regions which are centroidal. Improvement in the error indicator function is ensured by this positioning of the new nodes and nodes are added if and only if the geometric quality is improved.

References:

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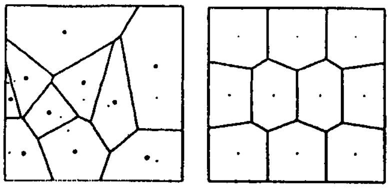

Figure 1: Voronoi versus centroidal Voronoi tesselations.

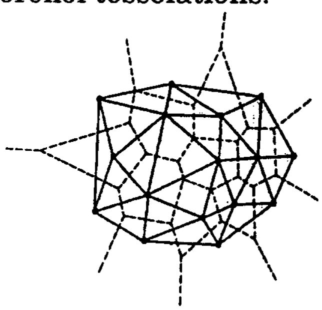

Figure 2: Delauney triangulation dual of the Voronoi diagram.

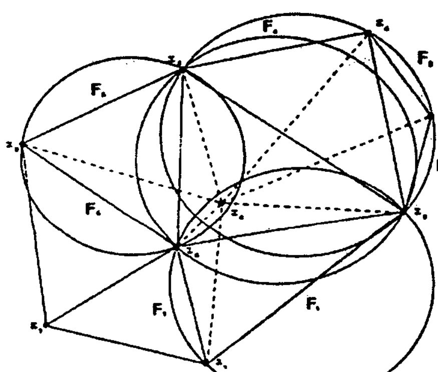

Figure 3: Delauney - Voronoi algorithm.

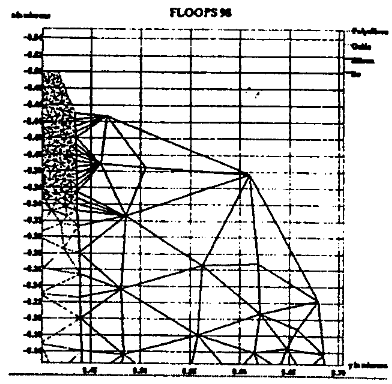

Figure 4: Grid with use of Delauney-Voronoi algorithm

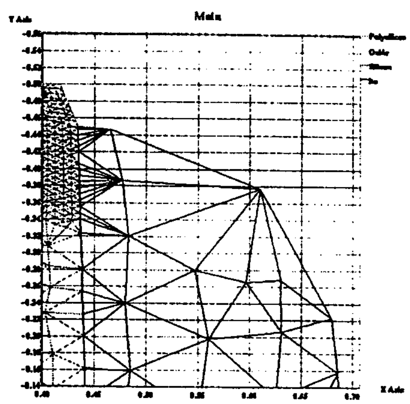

Figure 5: Grid without using Delauney-Voronoi algorithm.

Figure 6:
Improvement:
Max. int. angle:54%
Min. int. angle: 97%
Avg. element qual.:50%
Element qual> (worst): 77%
Element qual. (best): 15%
Joint qual.: 75%
Qual. <0.3: 16% becomes 0%
Qual. > 0.6: 28% becomes 86%