THE MPAS MESH

Timothy Chui Feb. 28, 2019

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http://mpas-dev.github.io/atmosphere/tutorial.html

Overview of seminar series

- Introduction to MPAS
- The MPAS Mesh
- Introduction to Finite-Volume Methods
- MPAS Numerics and Dynamics



http://mpas-dev.github.io/atmosphere/tutorial.html

**MPAS Workshop

Table of Contents

- Definition of Spherical Centroidal Voronoi Tessellations (SCVT)
- Applications of (S)CVTs
- Mesh Generation for the Model for Prediction Across Scales (MPAS)
- Summary



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Spherical Centroidal Voronoi Tessellation





http://mpas-dev.github.io/atmosphere/tutorial.html

SCVTs and MPAS

http://mpas-dev.github.io/atmosphere/tutorial.html

- Want a multiresolution approach to global climate and weather modelling (don't want boundaries)
- Don't want any singularities (looking at you, lat-lon)
- Want ease of control in how you define what's "high resolution" (looking at you, stretched-grid)



Primary Goal

- Build a mesh that covers the whole globe... (global)
- ...that has flexible geometry... (multiresolution)
- ...and no boundaries or discontinuities (conformal)



www.shutterstock.com

Spherical Centroidal Voronoi Tessellation





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Tessellation



Study of Regular Division of the Plane with Reptiles (1939) – M.C. Escher Tiling of surface using geometric shapes without overlaps or gaps



http://www.designcoding.net/semi-regular-tesselation/

Voronoi Tessellation



- Tessellation of surface with tiles (regions) that are polygons each associated with a generating point
- All points in each region are closer to the region's generating point than to any other generating point



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- Tessellation of domain $\Omega \subseteq \mathbb{R}^N$ with *k* regions V_i that are each associated with a $\mathbf{z_i}$, $1 \le i \le k$
- All points *x* in V_i are closer to generating point *z_i* than to any other *z_j*, *j* ≠ *i*



• Points associated with a Voronoi region V_i make up a Voronoi set \widehat{V}_i

$$\widehat{V}_i = \{ \boldsymbol{x} \in \Omega \mid |\boldsymbol{x} - \boldsymbol{z_i}| < |\boldsymbol{x} - \boldsymbol{z_j}| \text{ for } j = 1, \dots, k, j \neq i \}$$

- Set of all Voronoi regions is the Voronoi tessellation ${\mathcal V}$ of Ω

$$\mathcal{V} = \{V_i\}_{i=1}^k$$

- This is associated with the set of generating points ${\boldsymbol Z}$ of ${\boldsymbol \Omega}$

$$\boldsymbol{Z} = \{\boldsymbol{z}_i\}_{i=1}^k$$

Voronoi Tessellation - Properties

- Geometric entity V_i is the same as the set-based entity \widehat{V}_i
- Voronoi regions do not overlap (intersections = empty set)

$$V_i \cap V_j = \emptyset$$
 for $i \neq j$

 Voronoi regions and their boundaries cover Ω completely, including its boundaries

$$\bigcup_{i=1}^{k} \overline{V_i} = \overline{\Omega}$$

(Ju et al. 2011)





 Edges between two cells bisects (and is orthogonal to) the line joining the two generators



 Connecting the generators of the cells forms the Delaunay triangulation of the mesh



 Circle centered at the vertex shared by the three cells should touch the three generators; <u>no generators inside</u> <u>the circle</u> (circumscription property/Delaunay condition)



- Left: bad (green rectangle within blue circle; purple rectangle within red circle)
- Right: good (meets Delaunay condition)

Voronoi Tessellation - Energy

Energy functional (cost function/variance/inertia)

$$\mathcal{E}\left(\{\boldsymbol{z}_{\boldsymbol{i}}\}_{i=1}^{k}, \mathcal{V}\left(\{\boldsymbol{z}_{\boldsymbol{i}}\}_{i=1}^{k}\right)\right) = \sum_{i=1}^{k} \mathcal{E}_{i}\left(\boldsymbol{z}_{\boldsymbol{i}}, \mathcal{V}_{i}(\boldsymbol{z}_{\boldsymbol{i}})\right) = \sum_{i=1}^{k} \int_{V_{i}} \rho(\boldsymbol{x}) |\boldsymbol{x} - \boldsymbol{z}_{\boldsymbol{i}}|^{2} d\boldsymbol{x}$$

- Total energy is equal to the sum of the energies of each region within domain
- $\rho(\mathbf{x}) > 0$ is a differentiable density function defined in $\overline{\Omega}$ (important for MPAS later!)
- "Measure of how well information in Ω is spread out in \mathcal{V} for a given information density $\rho(\mathbf{x})$ "

Centroidal Voronoi Tessellation



In general, the generating point z_i of each Voronoi region is not the same as the mass centroid z_i^* of the region

 $z_i \neq z_i^*, i = 1, ..., k$ $z_i = z_i^*, i = 1, ..., k$

$CVT - Definition through \mathcal{E}$

 CVT = generating points are collocated with centers-ofmass of Voronoi regions:

$$\boldsymbol{z_i} = \frac{\int_{V_i} \boldsymbol{x} \rho(\boldsymbol{x}) d\boldsymbol{x}}{\int_{V_i} \rho(\boldsymbol{x}) d\boldsymbol{x}} = \boldsymbol{z_i^*}$$

• $z_i = z_i^*$ results in a critical point of energy \mathcal{E}

$CVT - Definition through \mathcal{E}$

- Can show by (homework):
- Variational approach
 - Perturb generating point z_i with some small αv , where v is some arbitrary vector in \mathbb{R}^N and let $\alpha \to 0$
- Gradient approach
 - Find z_i such that $\nabla \mathcal{E} = 0$

$$\boldsymbol{z_i} = \frac{\int_{V_i} \boldsymbol{x} \rho(\boldsymbol{x}) d\boldsymbol{x}}{\int_{V_i} \rho(\boldsymbol{x}) d\boldsymbol{x}}$$





Energy functional reaches a critical point with a CVT, but **not necessarily** an absolute minimum

CVT – Uniqueness

More precisely:



For a given set of generating points $Z = \{z_i\}_{i=1}^k$ there is one unique $\mathcal{V} = \{V_i\}_{i=1}^k$

For a given Ω , *k*, and/or ρ , there is no unique **Z** (so no unique \mathcal{V})

CVT – Goal

• Best thing we can do for a given Ω , *k*, and/or ρ :

Find a tessellation ${\mathcal V}$ that minimizes ${\mathcal E}$

- Gersho's conjecture in 2D (1979): for sufficiently large k, the shapes of the Voronoi regions for an optimal tessellation is the hexagon
 - Proved by Newman (1982)
 - No proof for 3D+

Spherical Centroidal Voronoi Tessellation

Goal: Given a spherical region $S^2 = \{x \in \mathbb{R}^3 : |\mathbf{x}| = r\}$, a positive integer *k*, and a differentiable density function ρ , compute a *k*-point CVT of S^2 (with *k* regions V_i , i = 1,...,k)



Both meshes have 2562 regions, but have different density functions.

Applications of (S)CVTs

- Original papers by Gersho (1979) focused on how to cut up a signal fairly (quantization)
- Analog -> Digital stuff
- Useful for electrical engineers

CVTs for Image Compression Original Monte-Carlo (random distribution)



(Du et al. 1999)

CVT + "Dithering"

CVTs in Biology/Zoology

Male tilapia territories (sand pits)



(Du et al. 1999)

CVTs in Geology



https://economictimes.indiatimes.com/magazines/panache/the-40000-odd-basalt-formations-at-the-giants-causeway-in-northern-ireland/articleshow/65454173.cms

Giant's Causeway, Northern Ireland



https://www.ireland.com/en-se/what-is-available/natural-landscapes-and-sights/articles/giants-causeway-myth/

CVTs in Statistics/Data Analysis



https://aws.amazon.com/blogs/machine-learning/k-means-clustering-with-amazon-sagemaker/

Mesh Generation Methods

- All methods are iterative
- Two main methods:
 - Deterministic Methods
 - Next iteration based directly on the locations of generator points/Voronoi regions from previous step
 - Slow, but generally better convergence
 - Probabilistic Methods
 - Next iteration affected by some random process
 - Fast, but generally worse convergence

Mesh Generation Methods

- Most common deterministic method: Lloyd's Method (Lloyd 1982)
- Update generators z_i and Voronoi regions V_i independently from each other
 - Fix generating points, and create Voronoi regions
 - Fix regions, and compute new centroids

Lloyd's Method

Lloyd's Method (currently used by MPAS)

- 1) Populate sphere with generating points **z**_i
- 2) Create Voronoi regions with those points
- 3) Compute centroids of those regions via numerical integration
- 4) Repeat (2) and (3) until change in some criterion (like energy) reaches tolerance (i.e. "converges" to some value)

Lloyd's Method for MPAS

 Ju et al. (2011): for sufficiently many Voronoi cells, the diameters h of the cells on an SCVT are conjectured to be related by:

$$\boxed{\frac{h_i}{h_j} \approx \left(\frac{\rho(\mathbf{z}_j)}{\rho(\mathbf{z}_i)}\right)^{1/4}}$$

 Can use density function to control resolution of mesh at certain points!

Lloyd's Method for MPAS

Jacobsen et al. (2013): 8x difference in resolution between coarse and fine portions of mesh; $max(\rho) = 1$, $min(\rho) = \left(\frac{1}{8}\right)^4$



Lloyd's Method – Convergence for MPAS



http://www2.mmm.ucar.edu/people/duda/files/mpas/talk s/mpas_mesh_generation.pdf



- CVTs and SCVTs have lots of applications in various fields, including weather and climate modelling
- CVTs/SCVTs have more desirable (energy) properties than general VTs
- Many ways to generate an SCVT (but it's a very tough problem)
- MPAS mesh currently uses Lloyd's method to generate an SCVT

Next Time on *Dragon Ball Z....*

$$egin{array}{rll} f(x) &=& f(x_0)+f'(x_0)(x-x_0)+rac{f''(x_0)}{2!}(x-x_0)^2 \ &+rac{f'''(x_0)}{3!}(x-x_0)^3+rac{f'''(x_0)}{4!}(x-x_0)^4+\cdots \ &=& \displaystyle\sum_{n=0}^\infty rac{f^{(n)}(x_0)}{n!}(x-x_0)^n. \end{array}$$

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