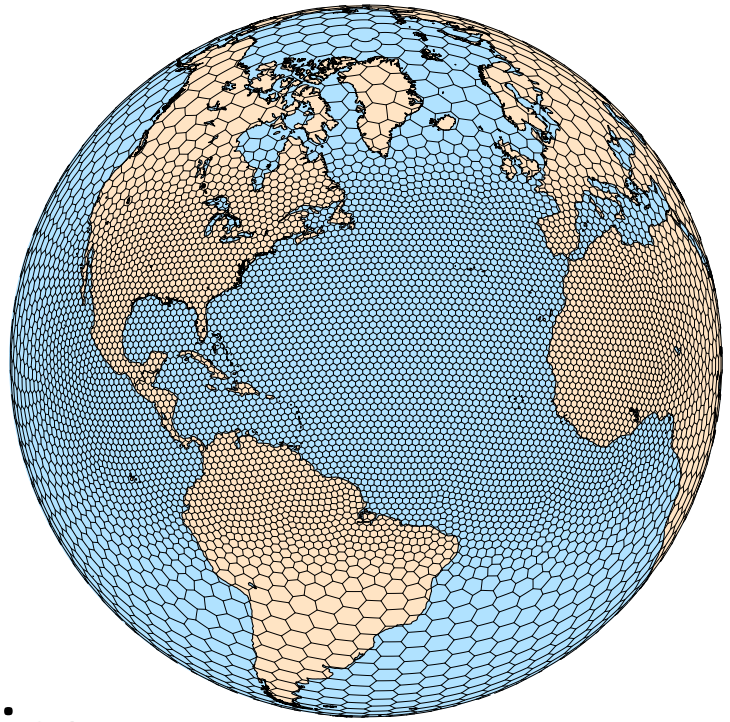
MPAS

Model for Prediction Across Scales



- Overview
- *Meshes*
- Atmospheric solver, physics
- Compiling and running MPAS
- Summary
- Practical session

Los Alamos NATIONAL LABORATORY EST. 1943

U.S. DEPARTMENT OF ENERGY | Office of Science

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NCAR NATIONAL CENTER FOR ATMOSPHERIC RESEARCH

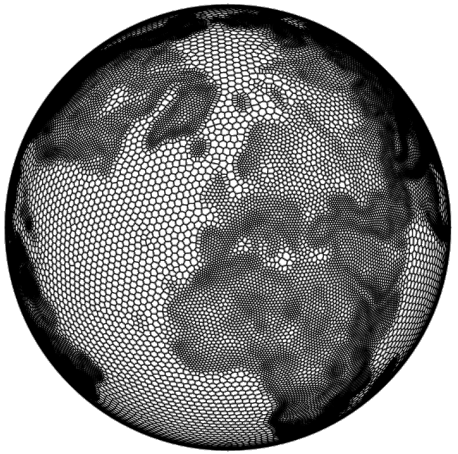
OUTLINE

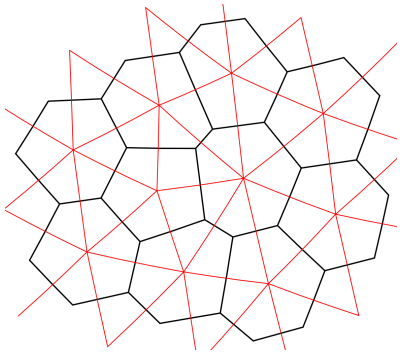
1. Introduction to MPAS meshes
   - What are centroidal Voronoi Tessellations, and how do we represent them in MPAS?

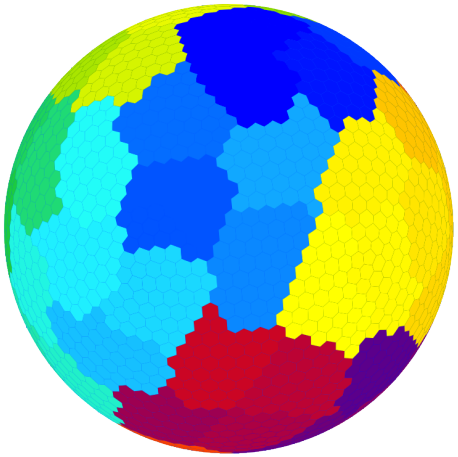
2. Considerations for handling unstructured meshes
   - In an unstructured mesh, how do we define the “positive” flow direction?

3. Mesh partitioning
   - How are meshes divided among processors?

4. Mesh generation
   - How do we achieve variable-resolution in an MPAS mesh?







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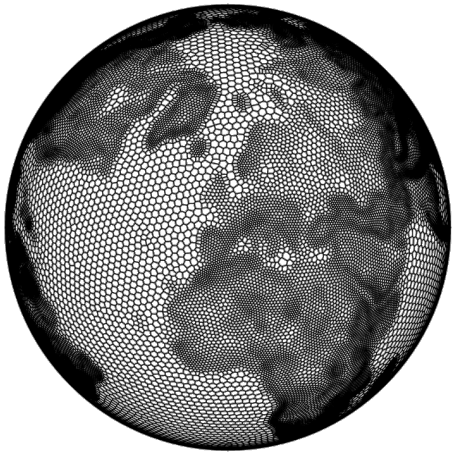
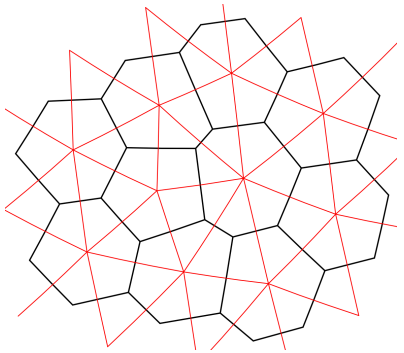
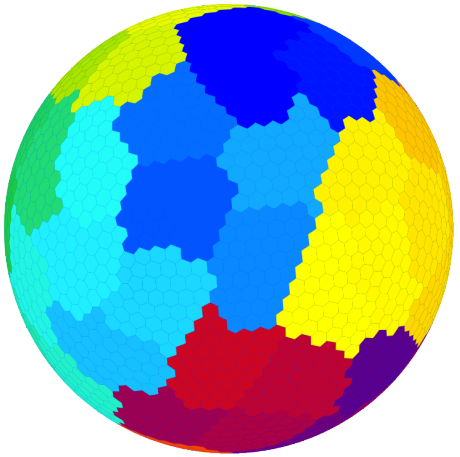






A defining feature of MPAS models is their use of **centroidal Voronoi tessellations** (CVTs) with a C-grid staggering

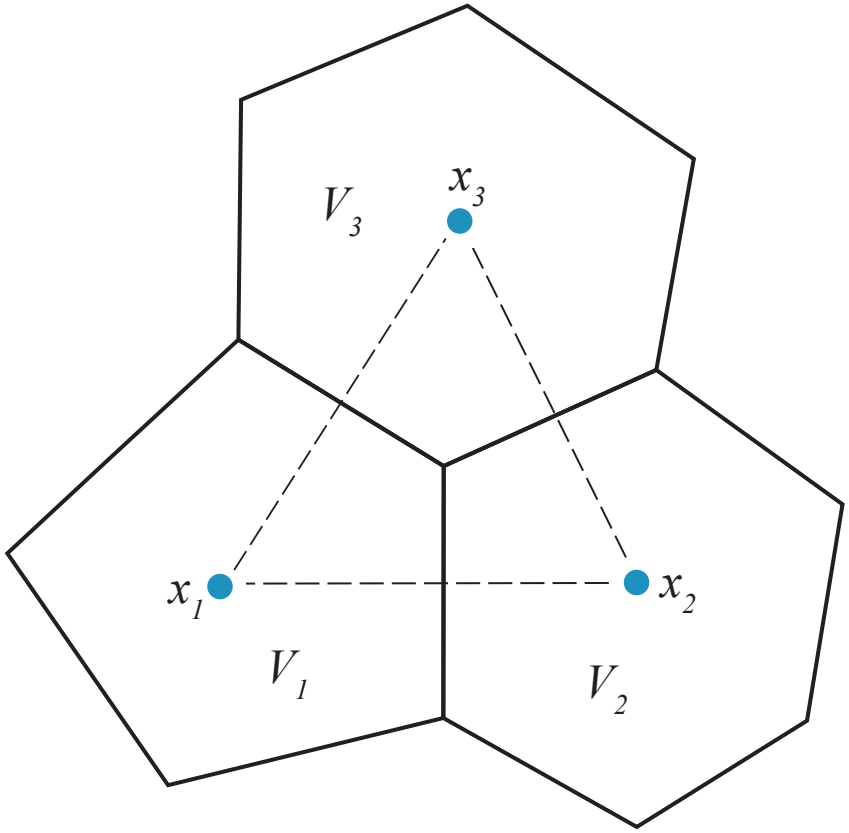
– When constrained to lie on the surface of a sphere, we often call them spherical centroidal Voronoi tessellations (SCVTs)

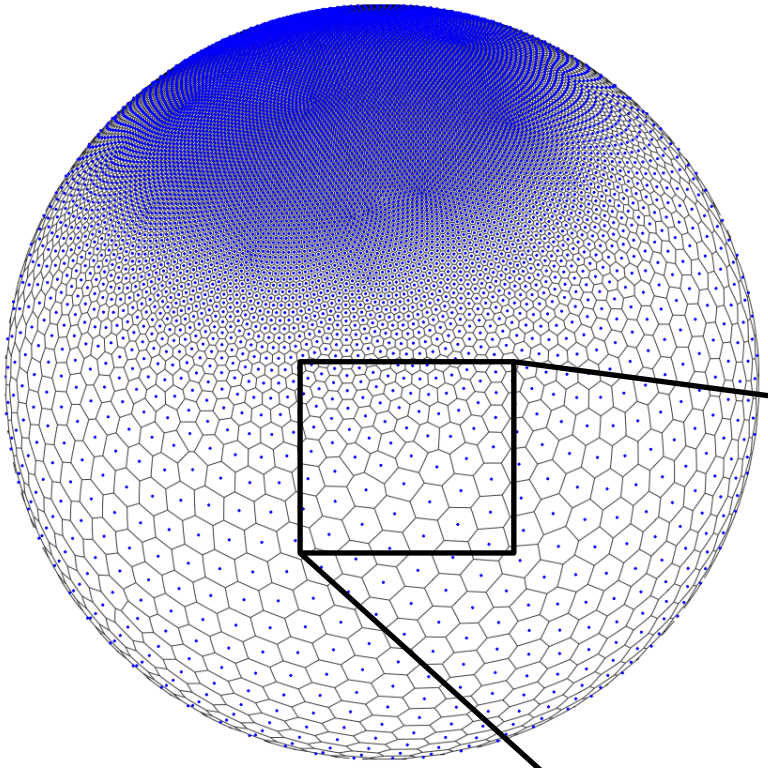
Voronoi = each grid volume (cell) V_i is uniquely associated with a *generating point* $\boldsymbol{x}_i$ such that all points within V_i are closer to $\boldsymbol{x}_i$ than to any other $\boldsymbol{x}_j$

- Lines joining generating points of adjacent cells are

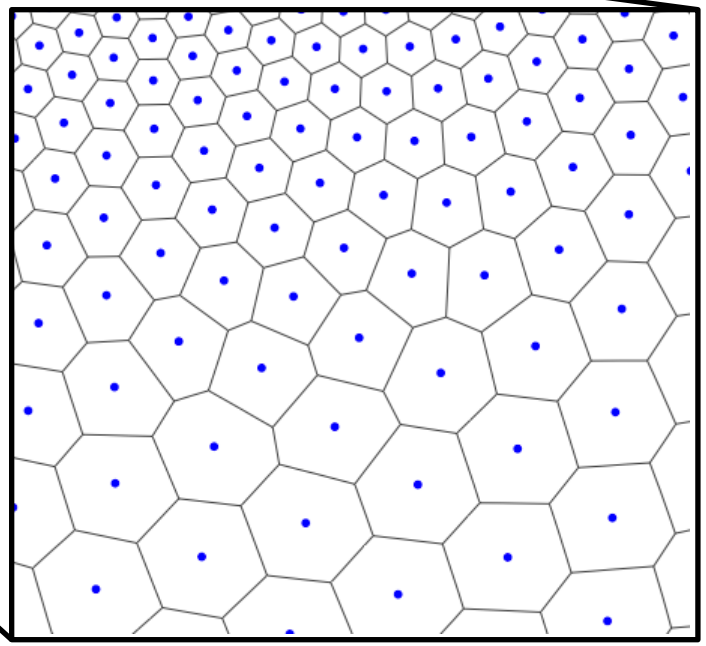
1. bisected by the shared cell face; and
2. intersect the shared cell face at a right angle.

Centroidal = the generating point for each Voronoi cell is also the mass centroid of that cell (**w.r.t. some density function**)



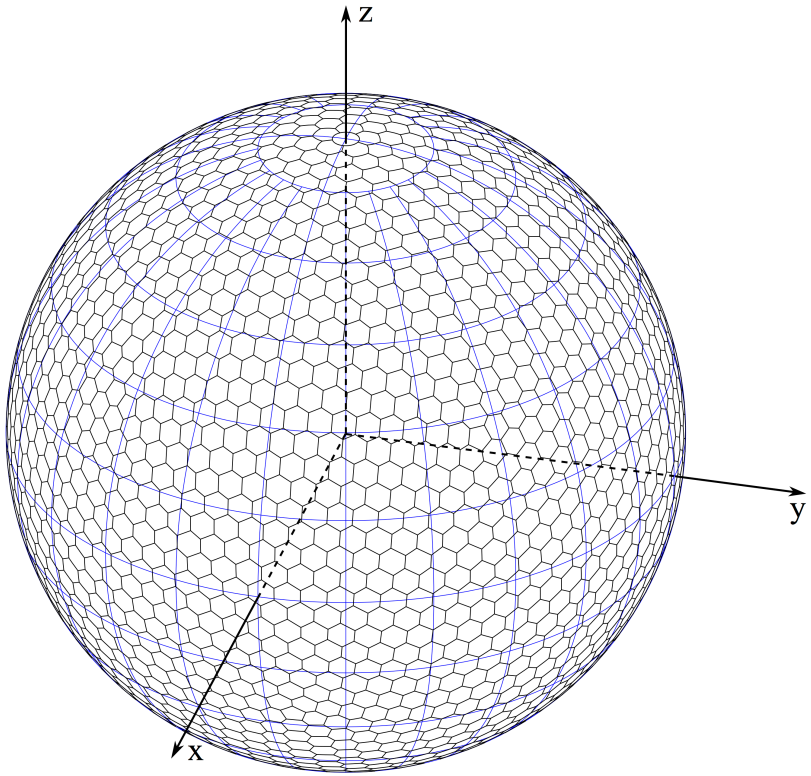


- Given a set of generating points, the primal mesh (finite volume mesh) in MPAS is defined by the Voronoi tessellation induced by this set
- The centroidal aspect of CVTs is used to produce meshes with smoothly-varying resolution



Observe that we have a fully unstructured horizontal mesh, not just a deformation of the icosahedral mesh! ***Cells may have 5, 6, 7, or more sides****.*

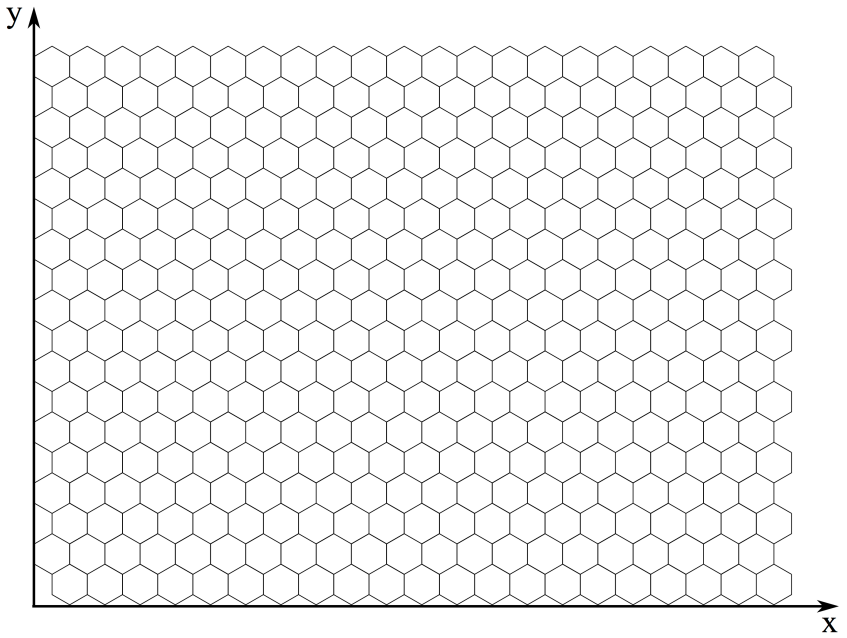
MPAS-Atmosphere supports meshes in two geometries:



On the surface of the sphere: all distances and areas are computed in spherical geometry.

$$x = r\cos(\lambda)\cos(\phi)$$
$$y = r\sin(\lambda)\cos(\phi)$$
$$z = r\sin(\phi)$$

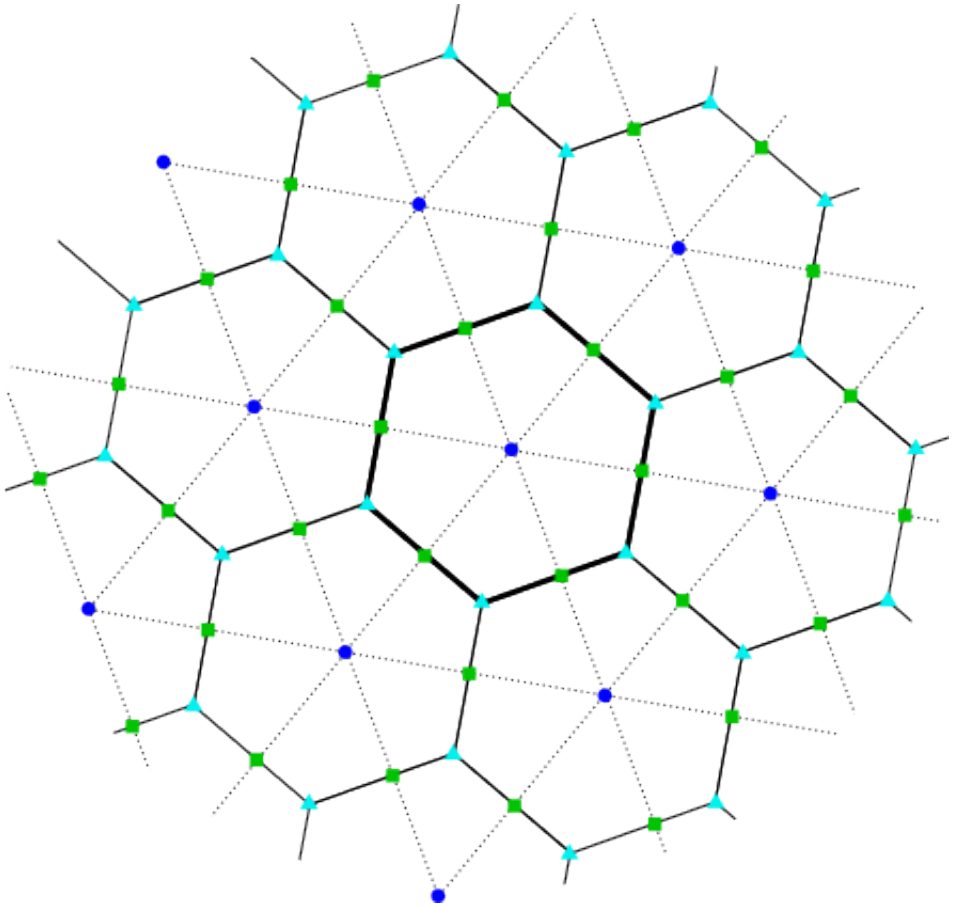
$$\phi = \arcsin\left(\frac{z}{r}\right)$$
$$\lambda = \arctan\left(\left|\frac{y}{x}\right|\right)$$



In the Cartesian plane: all distances and areas are computed in Euclidean geometry.

In the plane, only doubly periodic boundaries are currently supported.

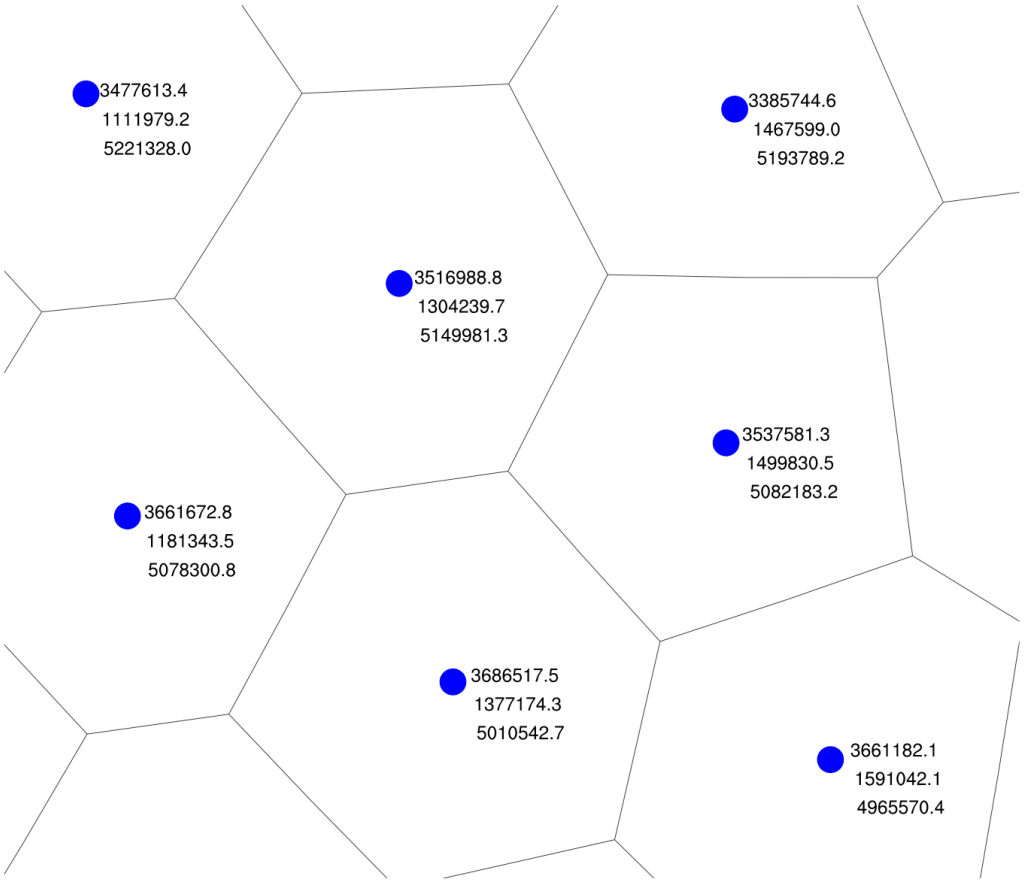
MPAS MESHES



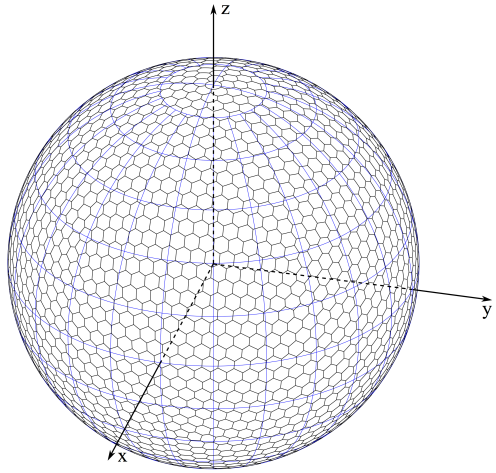
MPAS infrastructure recognizes fields defined at three locations:

- **Cells** (blue circles) - the generating points of the Voronoi mesh
- **Edges** (green squares) - the points where the dual mesh edges intersect the primal mesh edges
- **Vertices** (cyan triangles) - the corners of primal mesh cells

In MPAS-A, these locations are used to implement a C-staggered grid based on the Voronoi tessellation: prognosed normal velocities are located at *edges*, and other prognosed quantities are nominally located at *cells*.



Above: Cartesian coordiantes for cell locations near (52.9°N lat, 20.8°E lon) in a variable-resolution spherical mesh with radius 6371229 m.



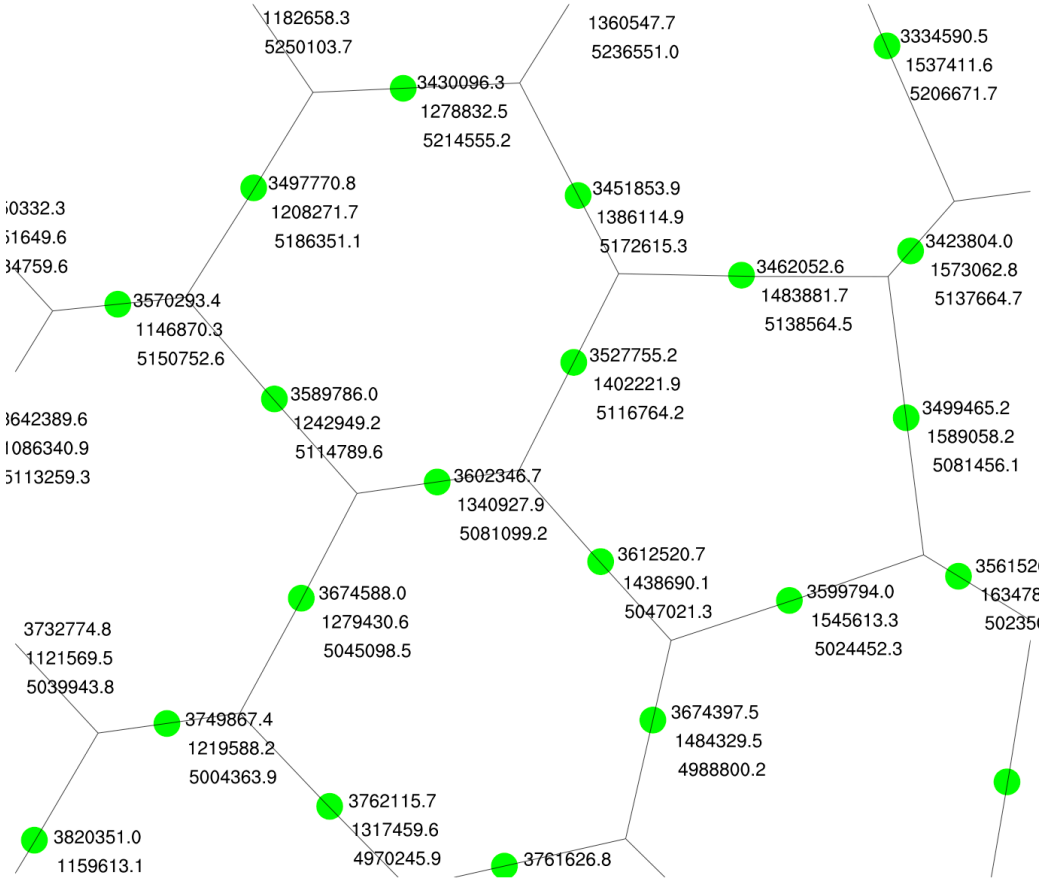
Global Cartesian coordinates are computed for each element

- For planar meshes, coordinates lie in the plane z=0
- For spherical meshes, coordinates lie on the surface of the sphere

For cells: **xCell**, **yCell**, **zCell**

Latitudes and longitudes are computed from Cartesian coordinates as described earlier

- positive x-axis through 0° longitude
- positive y-axis through 90° longitude
- positive z-asix through 90° latitude



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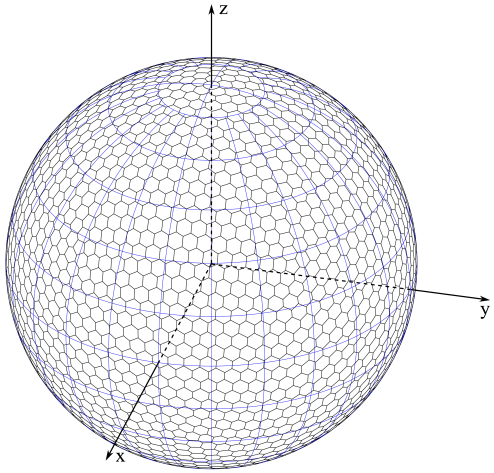

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- For planar meshes, coordinates lie in the plane z=0
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For cells: **xEdge**, **yEdge**, **zEdge**

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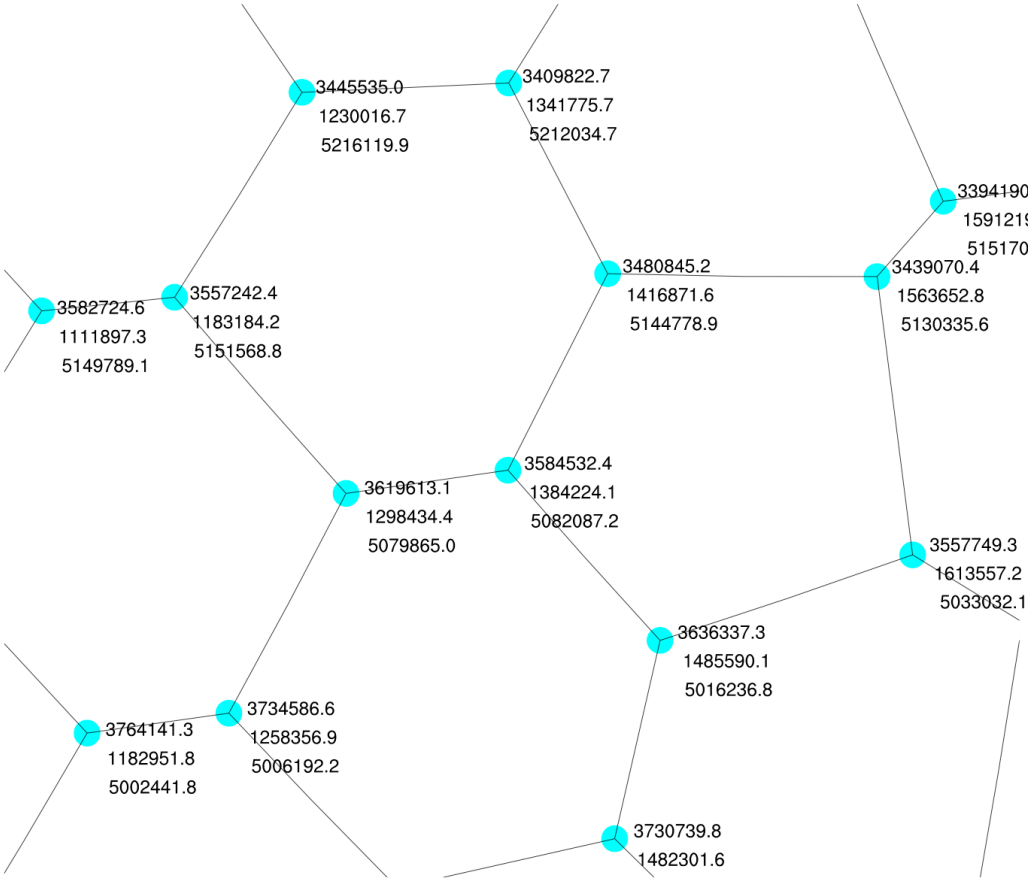

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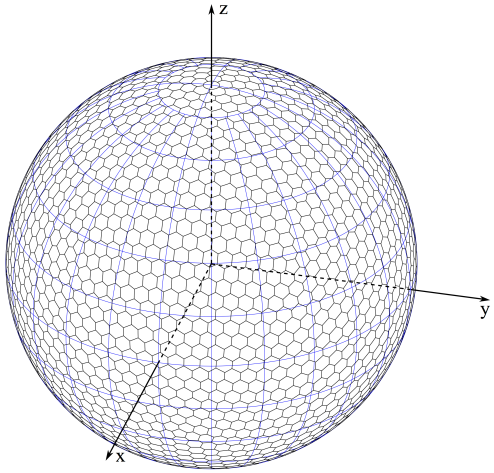

Global Cartesian coordinates are computed for each element

- For planar meshes, coordinates lie in the plane z=0
- For spherical meshes, coordinates lie on the surface of the sphere

For cells: **xVertex**, **yVertex**, **zVertex**

Latitudes and longitudes are computed from Cartesian coordinates as described earlier

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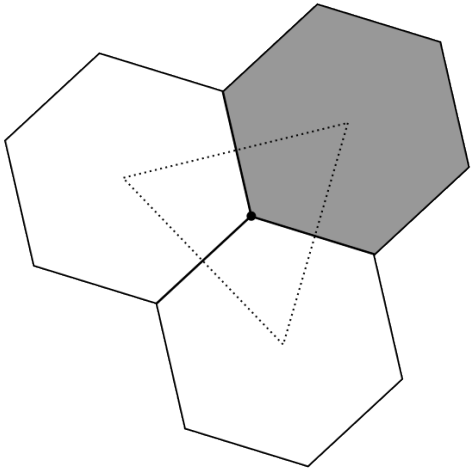
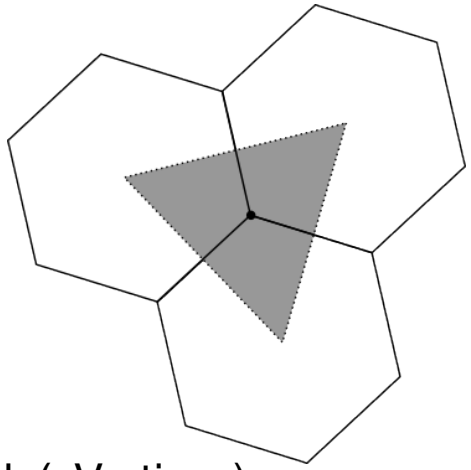
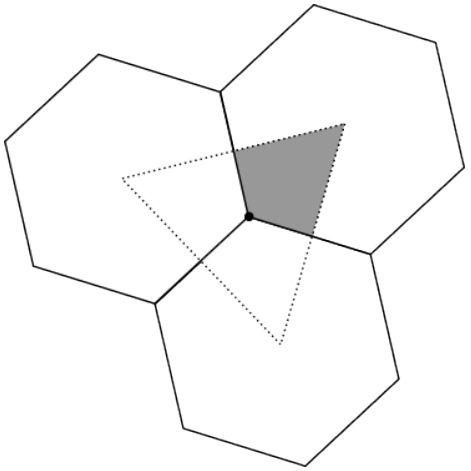
Given cell, edge, and vertex locations, we can compute some useful fields:



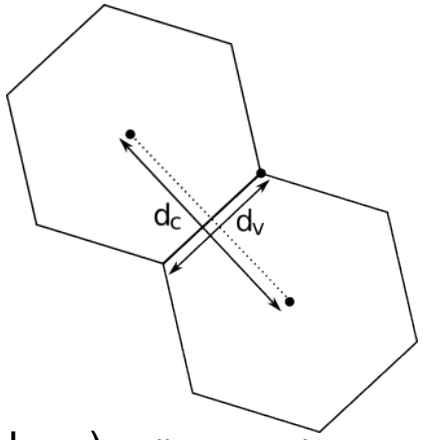
areaCell(nCells) – area of each cell



areaTriangle(nVertices) – area of each dual-grid cell



kiteAreasOnVertex(3,nVertices) – area of intersection between dual- and primal-mesh cells



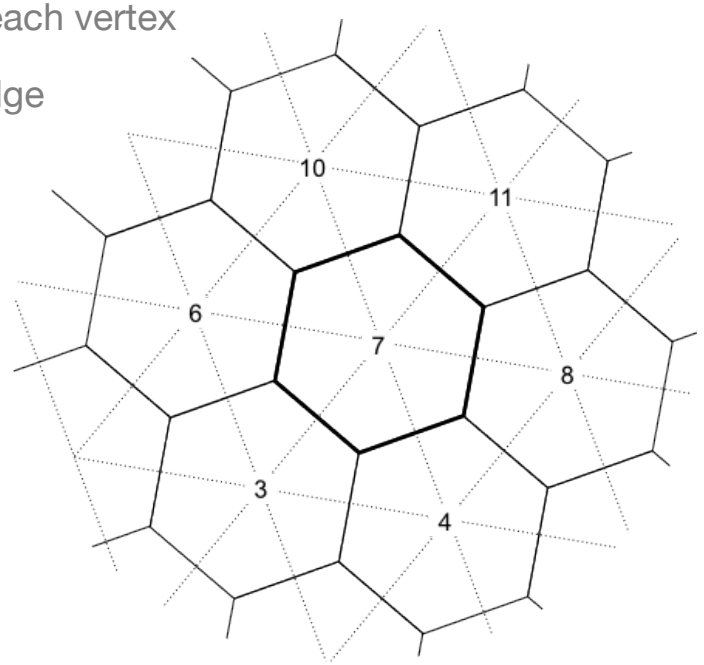
dcEdge(nEdges) – distances between cell centers

dvEdge(nEdges) – length of each edge

Meshes are explicitly described in MPAS by a set of connectivity arrays:

- nEdgesOnCell(nCells) – the number of neighbors for each cell
- cellsOnCell(maxEdges, nCells) – the indices of neighboring cells for each cell
- edgesOnCell(maxEdges, nCells) – the indices of bounding edges for each cell
- verticesOnCell(maxEdges, nCells) – the indices of corner vertices for each cell
- edgesOnVertex(3,nVertices) – the indices of edges incident with each vertex
- verticesOnEdge(2,nEdges) – the indices of endpoint vertices for each edge
- cellsOnVertex(3,nVertices) – the indices of cells meeting at each vertex
- cellsOnEdge(2,nEdges) – the indices of cells split by each edge

```
nEdgesOnCell(7)=6    cellsOnCell(1,7)=8
                     cellsOnCell(2,7)=11
                     cellsOnCell(3,7)=10
                     cellsOnCell(4,7)=6
                     cellsOnCell(5,7)=3
                     cellsOnCell(6,7)=4
```



At model start-up, all cell, edge, and vertex indices are re-numbered to a contiguous range.

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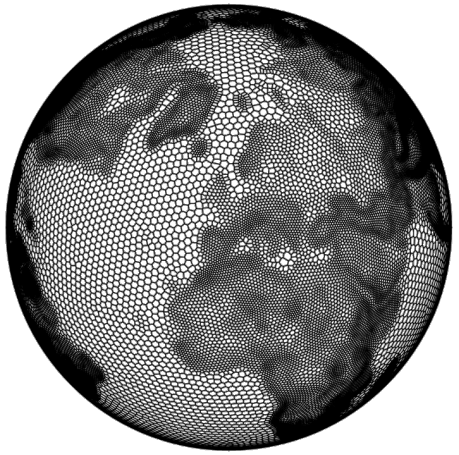
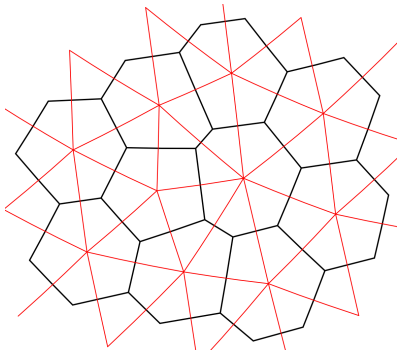
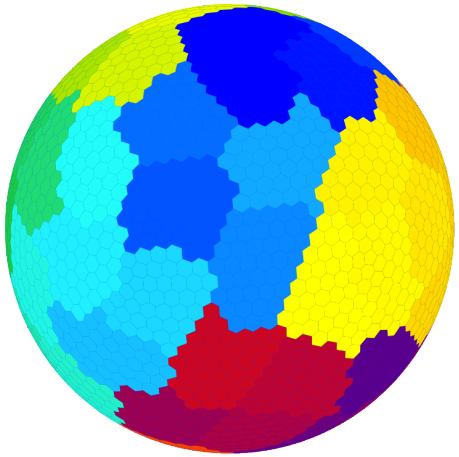
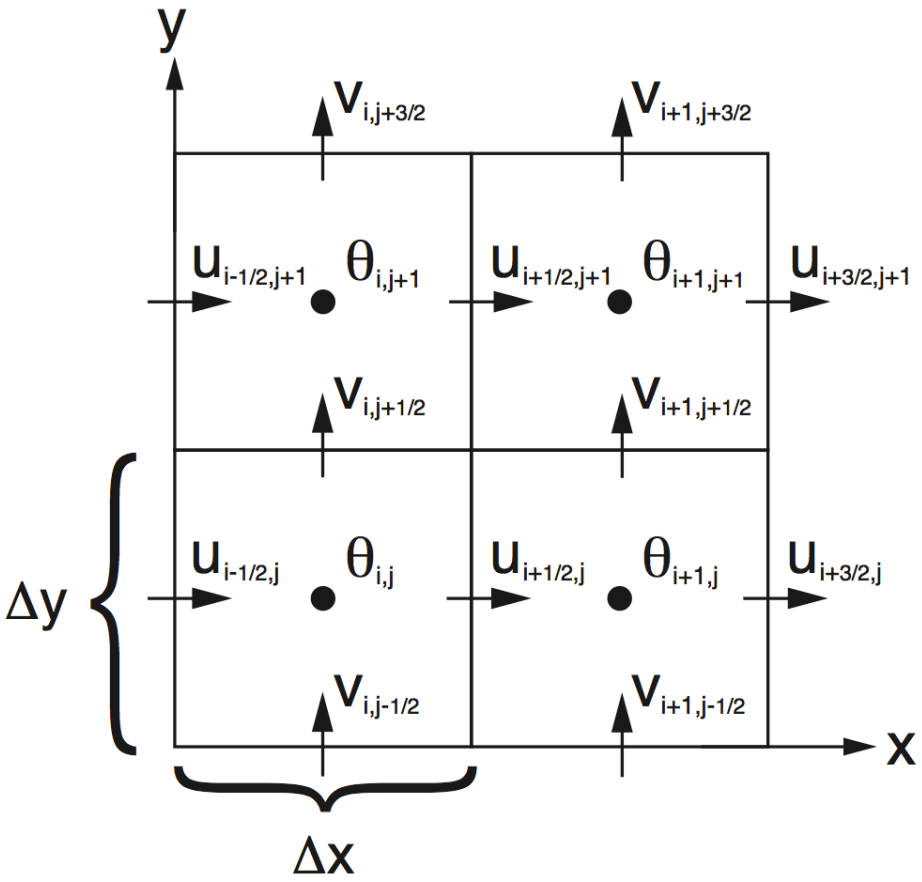


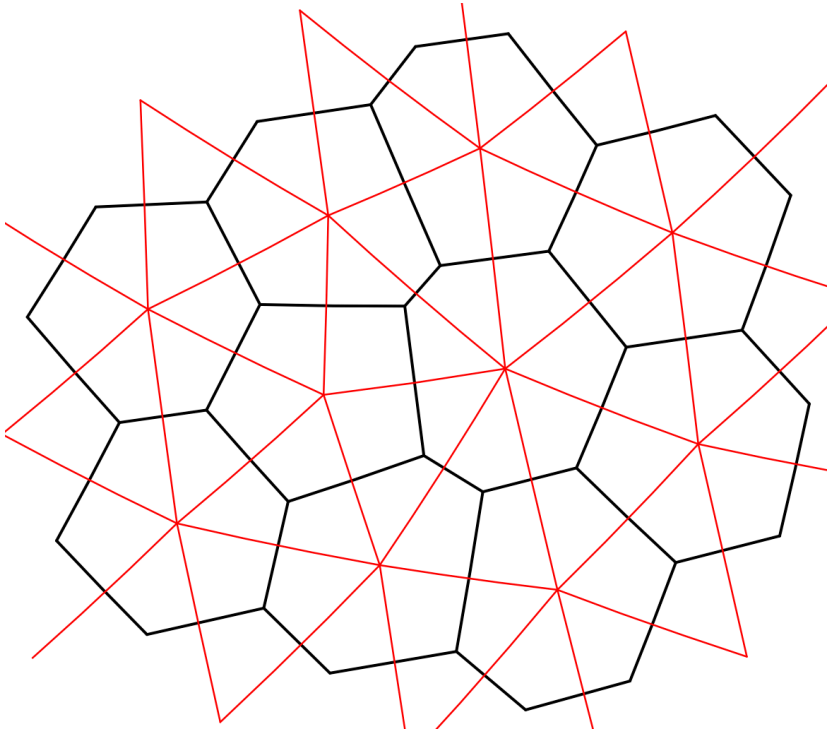




HORIZONTAL WIND VECTORS

In a rectangular C-grid, which directions represent positive U and positive V?



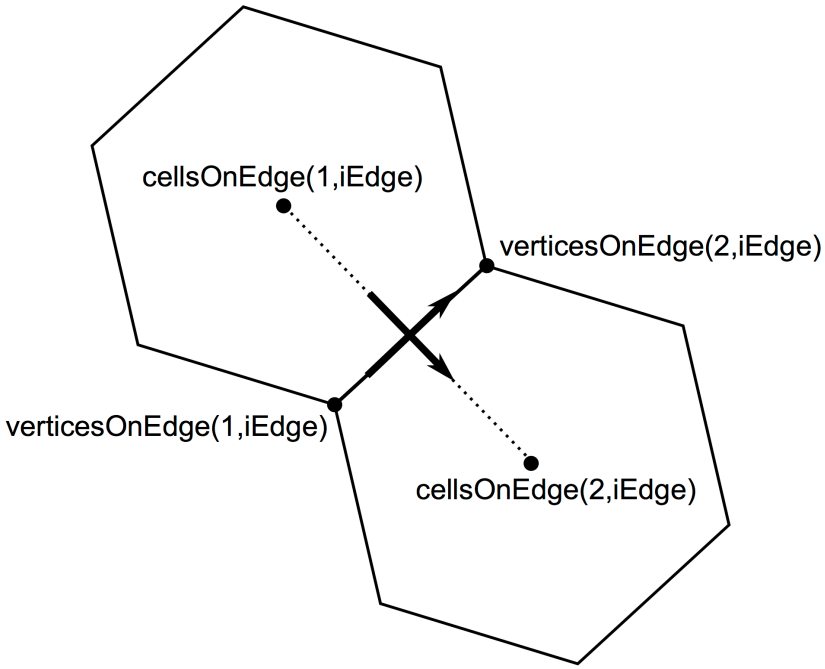


On a rectangular grid, one might say that positive U flows from left to right, and positive V flows from bottom to top when looking down on the xy-plane.

On a CVT mesh, one could introduce a similar definition, but we have only U, not V, so such a definition becomes more complicated...

HORIZONTAL WIND VECTORS (2)

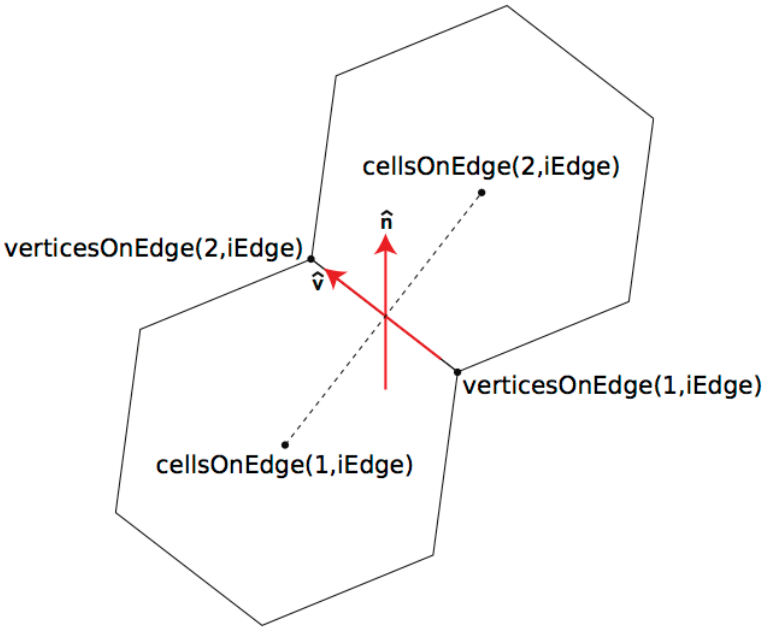
Without grid cells arranged in rows and columns, we need some simple rules to unambiguously define the positive directions for velocities



- Positive u (normal) velocity is always defined as flow from **cellsOnEdge(1,iEdge)** to **cellsOnEdge(2,iEdge)** for an edge iEdge
- Positive v (tangential) velocity is always defined as flow from **verticesOnEdge(1,iEdge)** to **verticesOnEdge(2,iEdge)** for an edge iEdge
- The cross product of the positive *u* and *v* vectors always points upward (out of the plane)

HORIZONTAL WIND VECTORS (3)

The absolute geographic orientation of each edge is specified with the field *angleEdge*, which gives the angle between local north and the positive tangential direction for an edge



angleEdge(nEdges) – angle of edge w.r.t. true north

$$\text{angleEdge} = \arcsin \left\| \hat{\mathbf{n}} \times \hat{\mathbf{v}} \right\|$$

Earth-relative horizontal winds, u_{zonal} and $u_{meridional}$, can be calculated using u and v:

$$\begin{bmatrix} u_\lambda \\ u_\phi \end{bmatrix} = \begin{bmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix}$$

where α is angleEdge.

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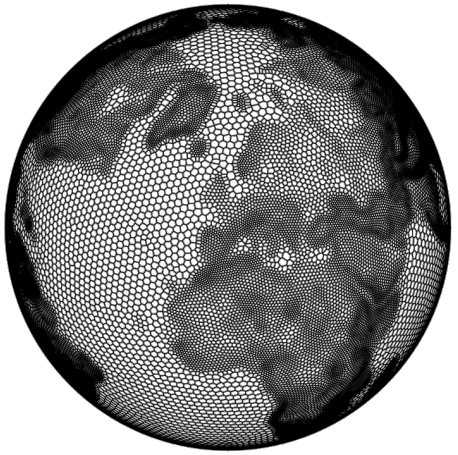
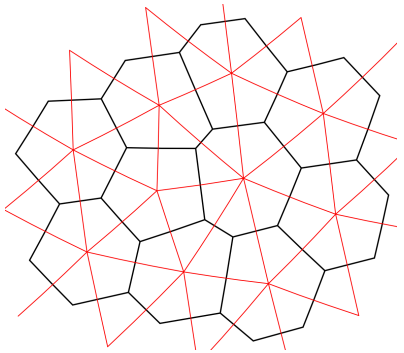
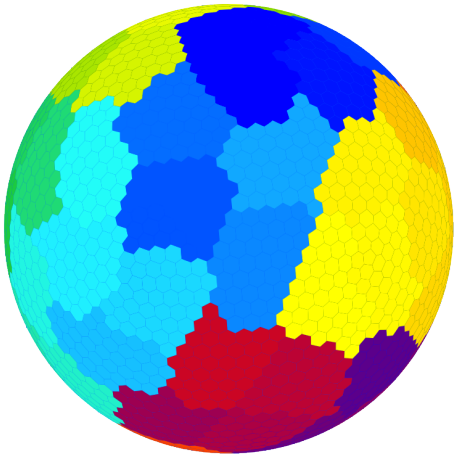
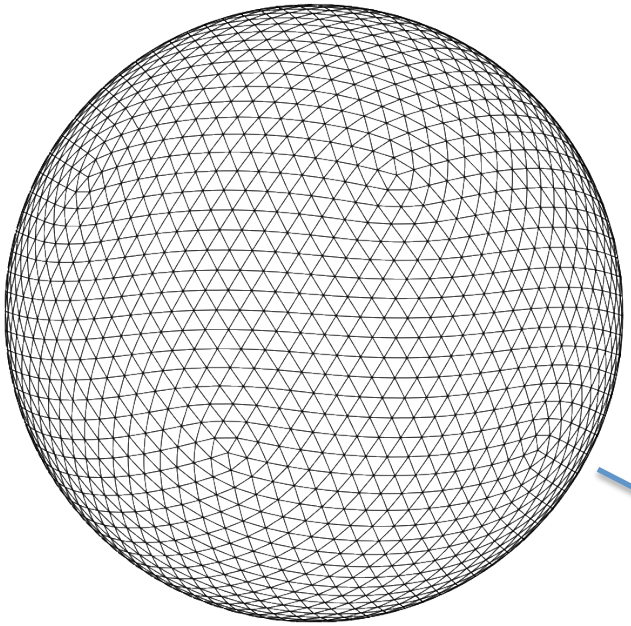






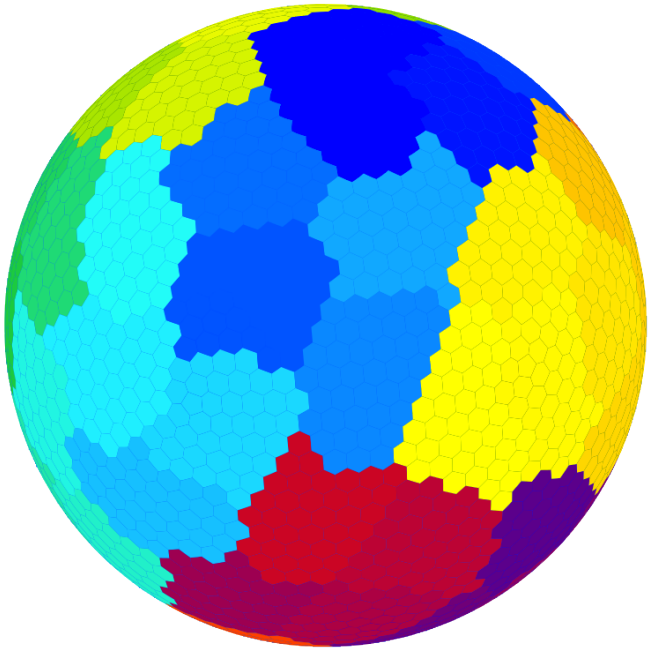
PARALLEL DECOMPOSITION



The *dual* mesh of a Voronoi tessellation is a Delaunay triangulation – essentially the connectivity graph of the cells

Parallel decomposition of an MPAS mesh then becomes a graph partitioning problem***: equally distribute nodes among partitions (give each process equal work) while minimizing the edge cut (minimizing parallel communication)***

Graph partitioning



We use the Metis package for parallel graph decomposition

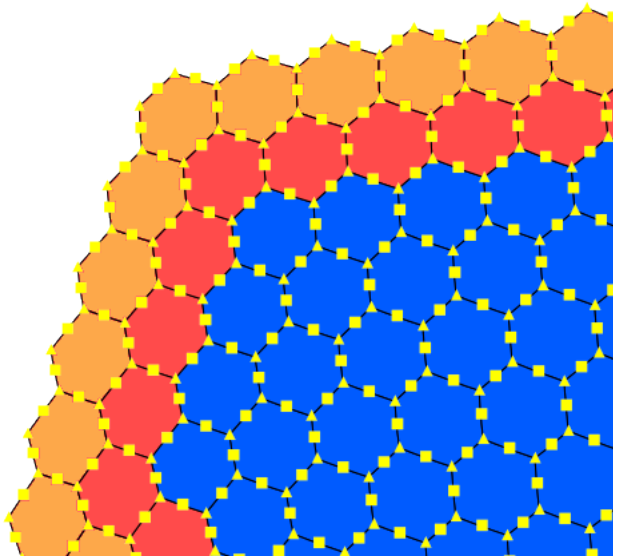
- Currently done as a pre-processing step, but could be done “on-line”

Metis also handles weighted graph partitioning

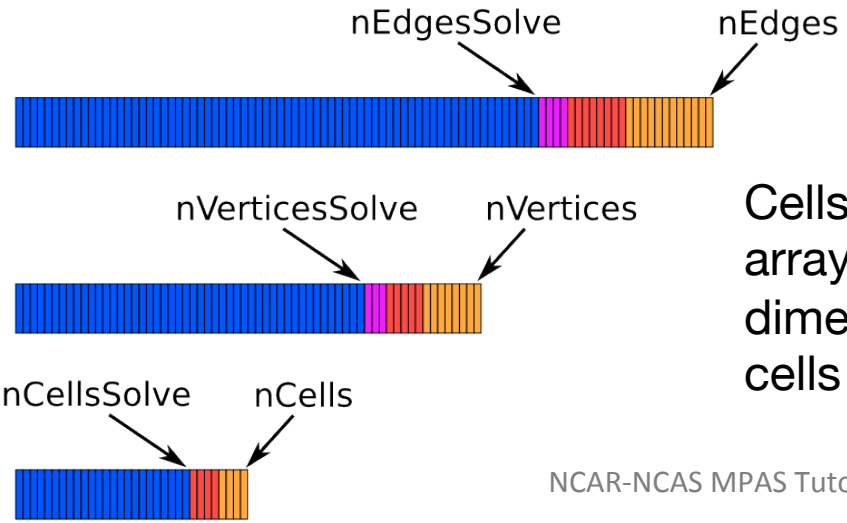
- Given *a priori* estimates for the computational costs of each grid cell, we can better balance the load among processes

PARALLEL DECOMPOSITION (2)

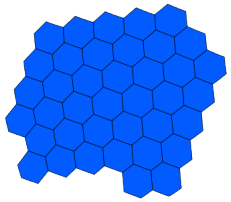
Given an assignment of cells to a process, any number of layers of halo (ghost) cells may be added



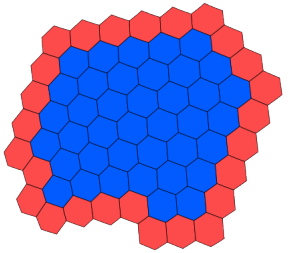
With a complete list of cells stored in a block, adjacent edge and vertex locations can be found; we apply a simple rule to determine ownership of edges and vertices adjacent to real cells in different blocks



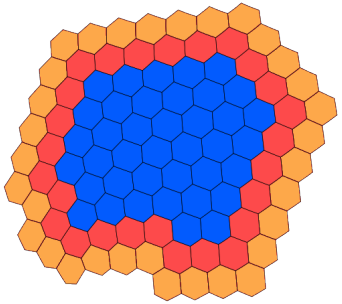
Cells are stored in a 1d array (2d with vertical dimension, etc.), with halo cells at the end of the array



Block of cells owned by a process



Block plus one layer of halo/ghost cells

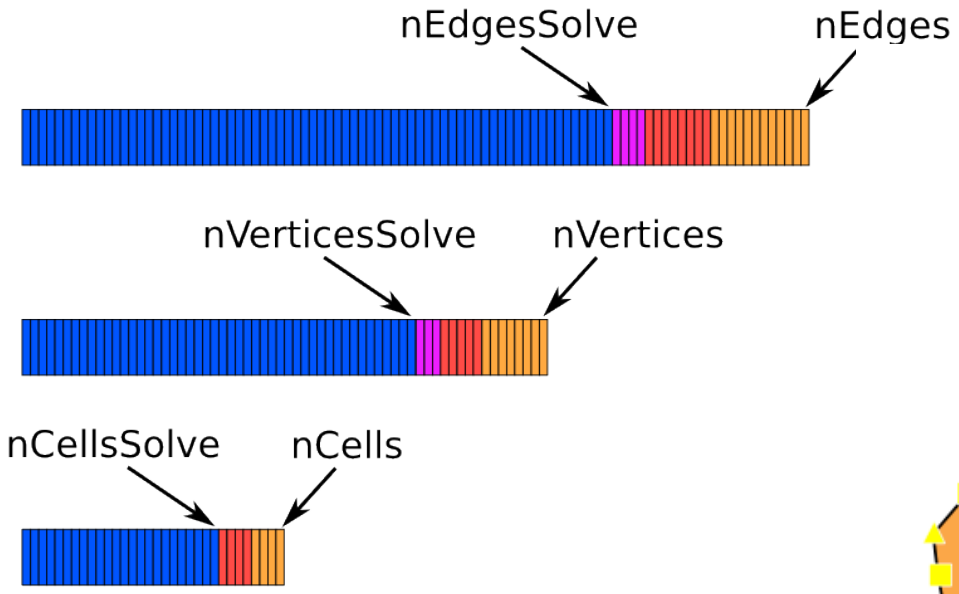


Block plus two layers of halo/ghost cells

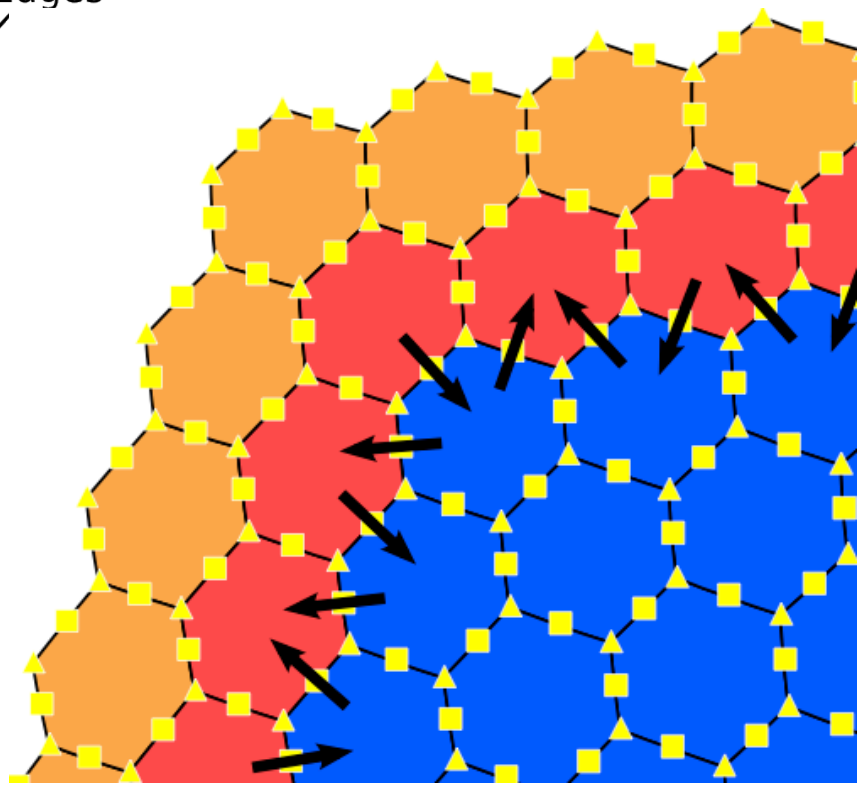
PARALLEL DECOMPOSITION (3)

An edge *E* is an owned edge **iff** cellsOnEdge(1,*E*) is an owned cell

A vertex *V* is an owned vertex **iff** cellsOnVertex(1,*V*) is an owned cell

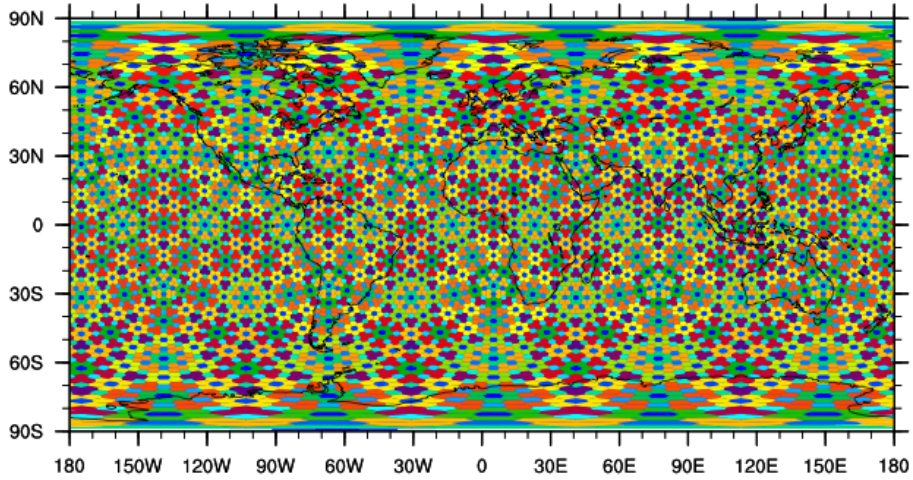


For *n* layers of ghost cells, we have *n+1* layers of ghost edges and ghost vertices.

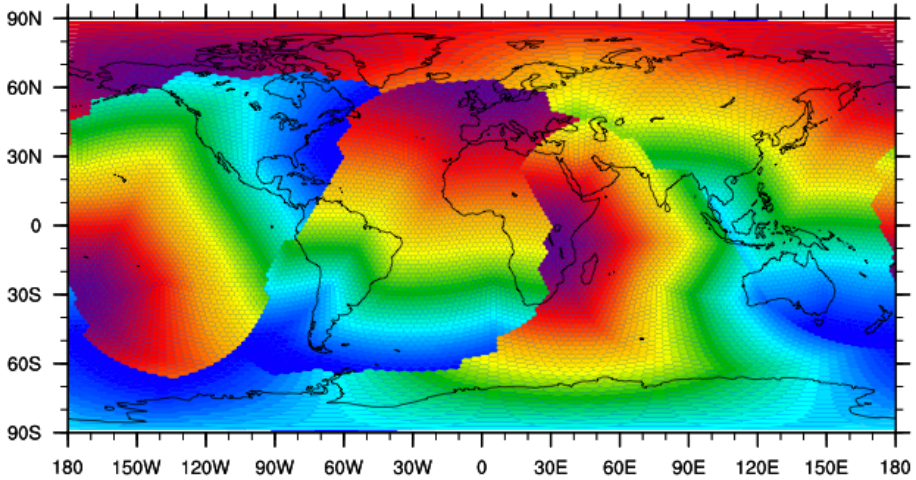


MISCELLANEOUS NOTES ON GRID INDEXING

- Vertical dimension inner-most (fastest varying in Fortran)
  - E.g., **`theta(nVertLevels,nCells)`**
- We do not perform any sort of local cell re-ordering, e.g., in an attempt to improve cache reuse



Cells of a 10242 mesh colored according to their global index



Cells of a 10242 mesh decomposed across 4 MPI tasks and colored according to their re-ordered local index

- Indices exist that allow a solver to process just the “owned”, any individual halo layers, or all cells/edges/vertices
  - Allows us to reduce redundant computation as much as possible
  - Provides fine granularity for trading computation and communication

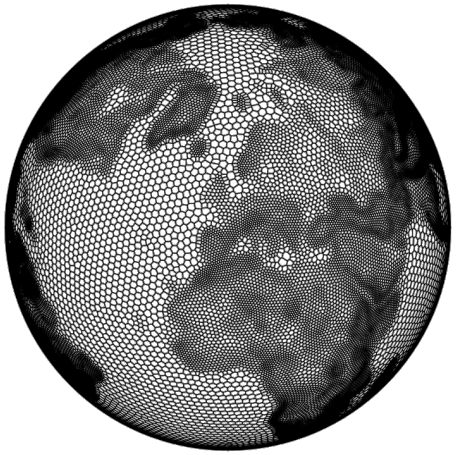
OUTLINE

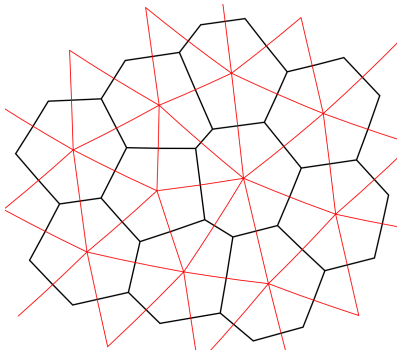
1. Introduction to MPAS meshes
   - What are centroidal Voronoi Tessellations, and how do we represent them in MPAS?

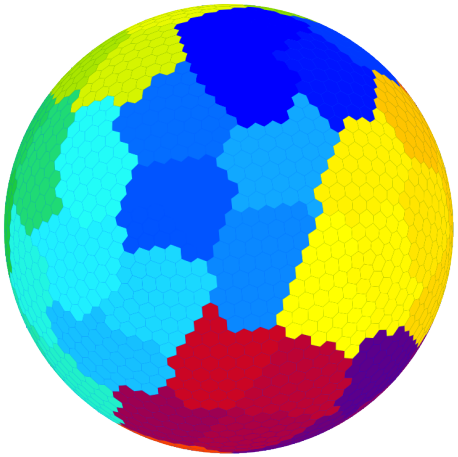
2. Considerations for handling unstructured meshes
   - In an unstructured mesh, how do we define the “positive” flow direction?

3. Mesh partitioning
   - How are meshes divided among processors?

4. Mesh generation
   - How do we achieve variable-resolution in an MPAS mesh?

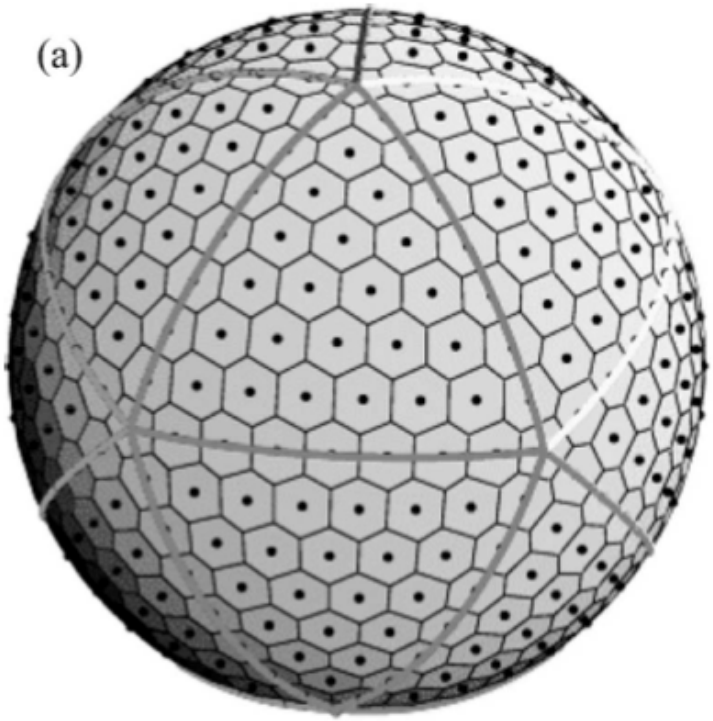


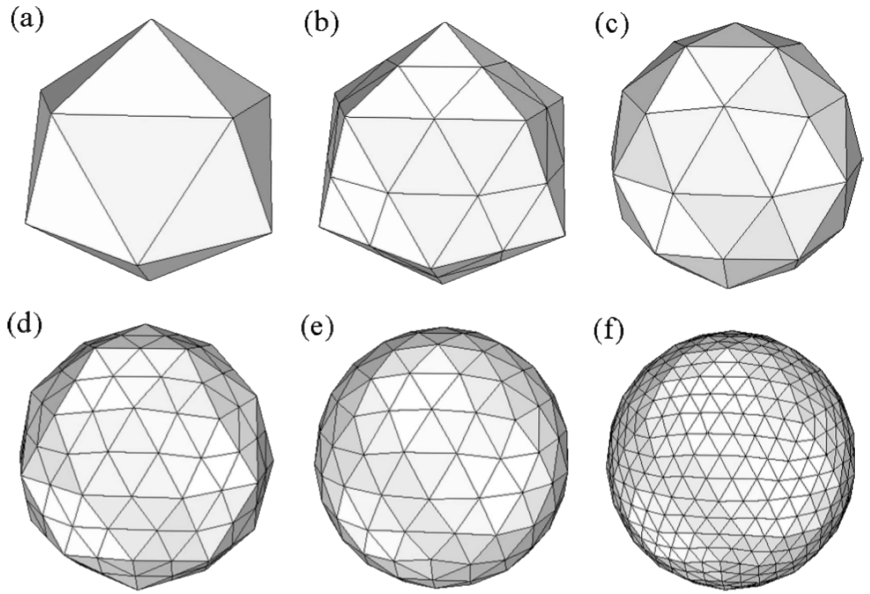




HOW DO WE CREATE MESHES FOR MPAS-ATMOSPHERE?

- For quasi-uniform Voronoi tessellations, we can employ successive subdivision of the icosahedron
  - The vertices of these triangular meshes can be used as the generating points for a spherical Voronoi tessellation
  - To create a spherical ***centroidal*** Voronoi tessellation, some iteration is required

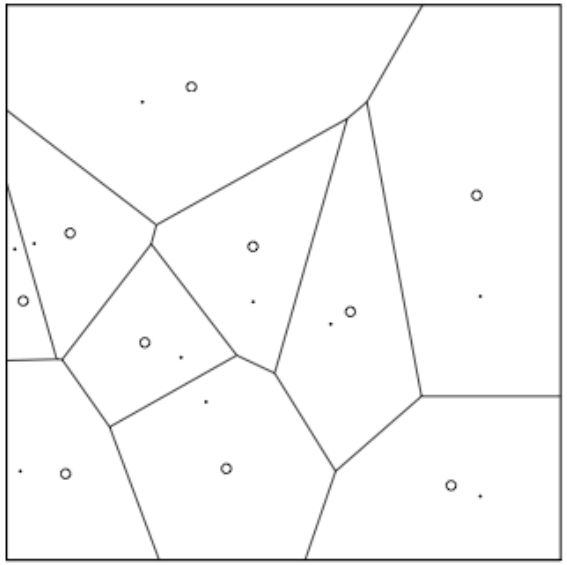


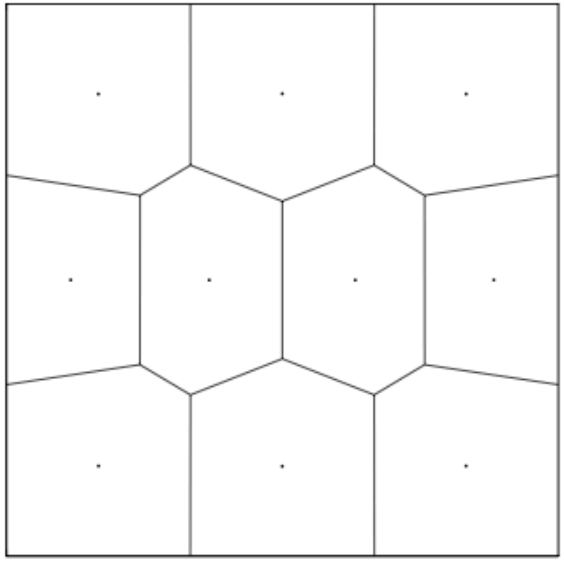


From Lipscomb and Ringler (2005)

Given an initial set of generating points, **Lloyd's method** may be used to arrive at a CVT:

1. Begin with any set of initial points ("generating points")
2. Construct a Voronoi diagram for the point set
3. Locate the mass centroid of each Voronoi cell
4. Move each generating point to the mass centroid of its Voronoi cell
5. Repeat 2-4 to convergence



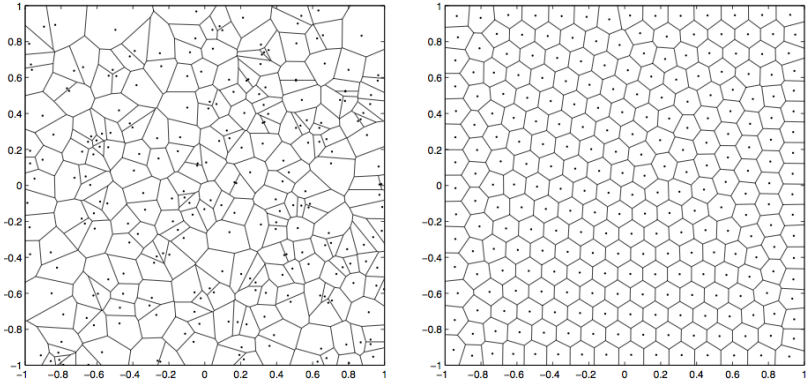


From Du et al. (1999)

MacQueen's method, an randomized alternative to Lloyd's method may also be used; no Voronoi diagrams need to be constructed, but convergence is generally much slower

Lloyd's method can be viewed as the minimization of an energy functional; in the plane, it can be shown that hexagonal Voronoi cells provide the minimum energy configuration *for constant density*

To create regions of grid refinement, we simply define a non-uniform density function over the domain, and use this when computing the mass centroids of Voronoi cells in Lloyd's method



From Du et al. (1999)

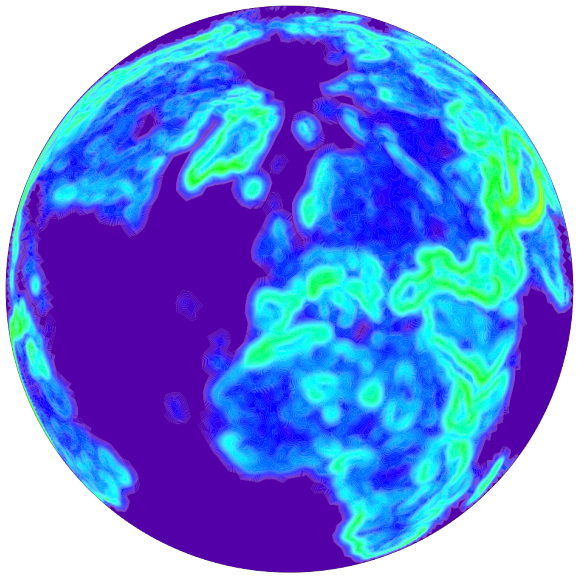
For a density function $\rho(\boldsymbol{x}) > 0$, it is conjectured (Ju et al. (2010)) that, as the number of Voronoi cells increases, the diameters, *h*, of Voronoi cells are related by

$$\frac{h_i}{h_j} \approx \left(\frac{\rho(\mathbf{x}_j)}{\rho(\mathbf{x}_i)} \right)^{1/(d'+2)}$$

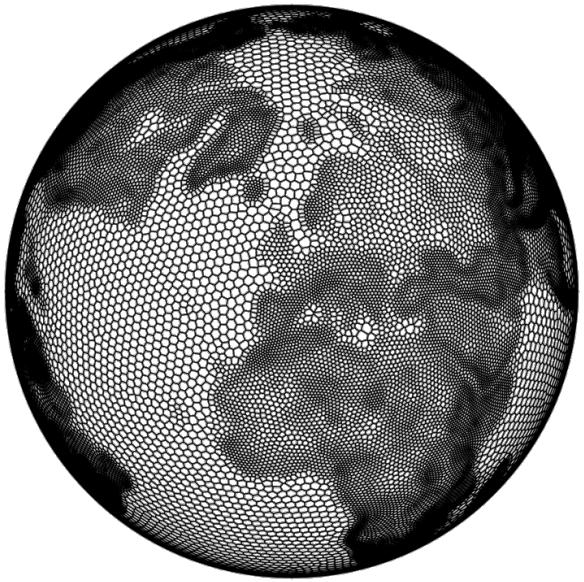
where *d'* is 2.

AN ABSURD EXAMPLE OF MESH REFINEMENT

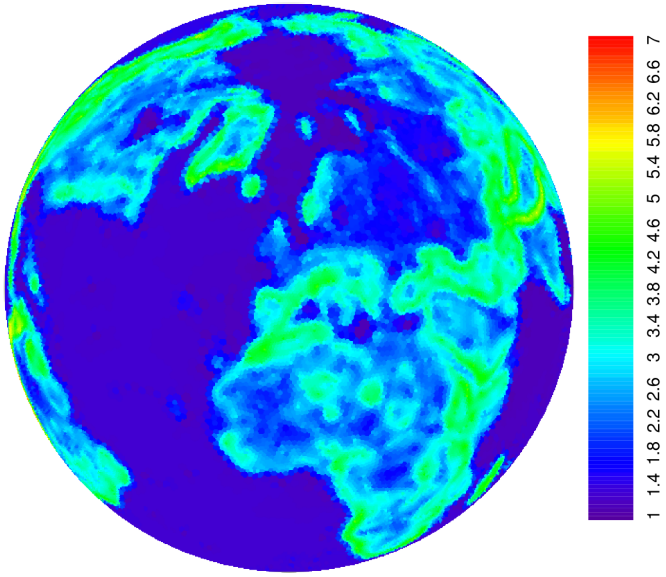
Define ρ(***x***) as a function of the magnitude of the topography gradient, for example:



Fourth root of density function



Resulting SCVT



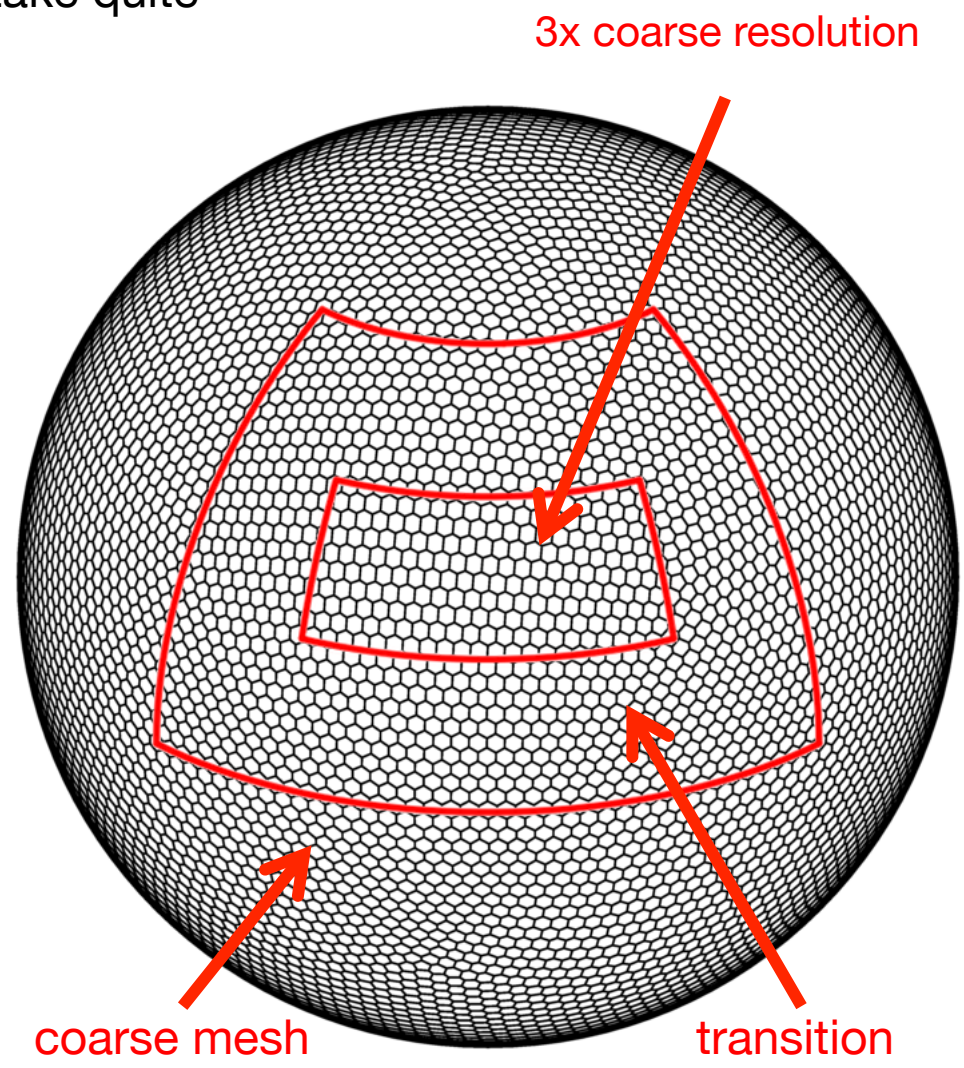
Normalized inverse mean distance of cell centroid from each of its neighboring centroids

Evidence from initial testing of the MPAS non-hydrostatic atmosphere code on multi-resolution meshes on the Cartesian plane suggests that smoother refinement (i.e., less abrupt transitions) produces better results

Meshes with more than $O(10^5)$ cells take quite a while to generate!

Typical procedure:

1. Decide on size/shape of refinement region, mesh resolution
2. Estimate the total number of cells needed in the mesh
3. Work backwards from final number of cells to $O(100)$ cells
   - Coarsening a mesh by a factor of two gives $(n+6)/4$ cells
4. Iterate to convergence, bisect the mesh, repeat



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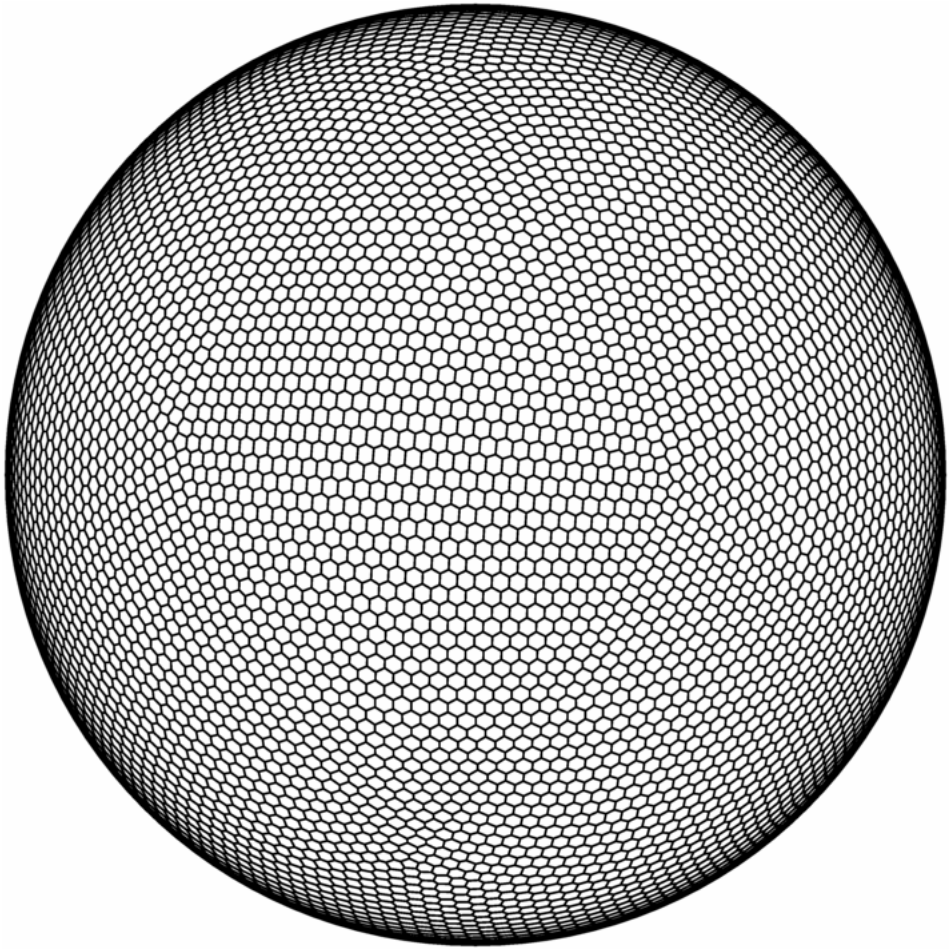


An alternative approach is to add refinement cells in the refinement region, and hold the rest of the mesh fixed

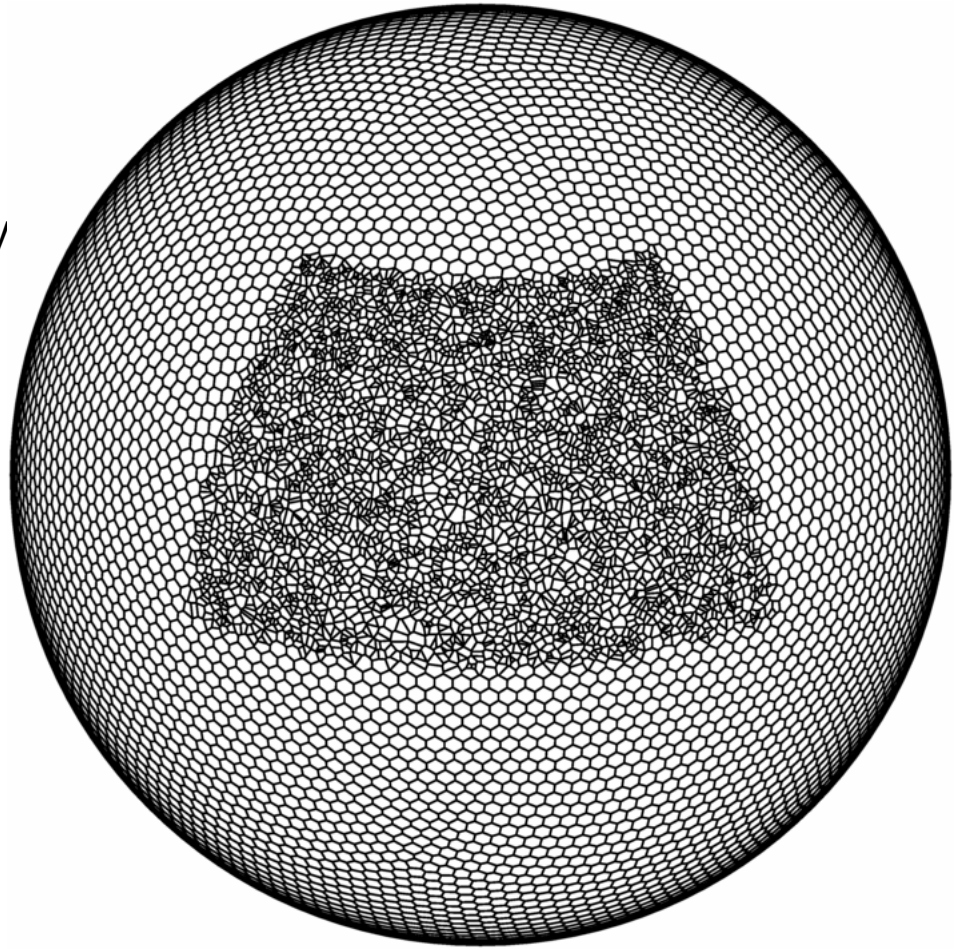
Simple Monte-Carlo method to estimate how many points (nCells) are needed to achieve a specified absolute resolution, given a density function:

ds_{min} = min. desired grid distance in the mesh

N_s = desired # samples

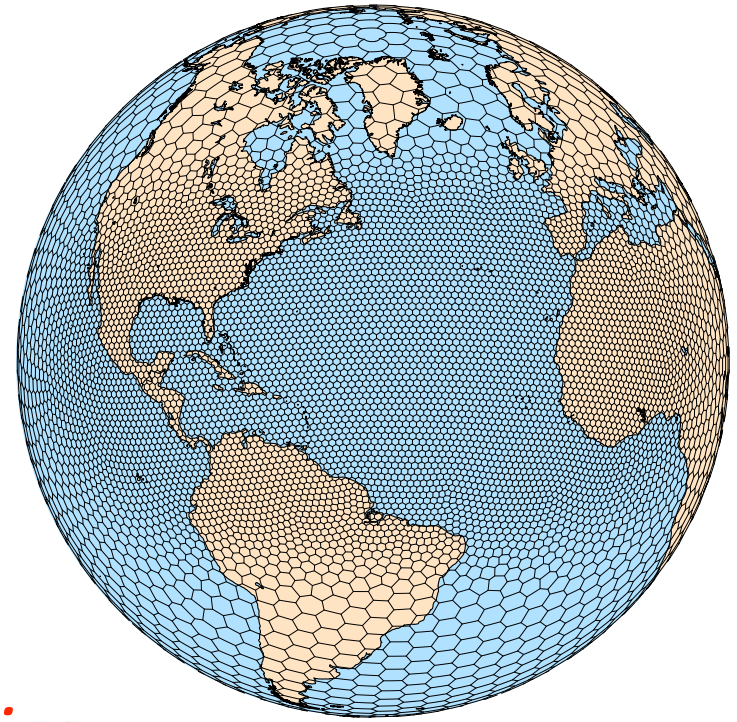
$A_s = 4\pi R^2 / N_s$

for 1 to N_s
    p = random point on sphere
    r = density(p)
    $ds = ds_{min} / r^{0.25}$
    nCells = nCells + A_s / hexagon_area(ds)
end for



MPAS

Model for Prediction Across Scales



- Overview
- Meshes
- *Atmospheric solver, physics*
- Compiling and running MPAS
- Summary
- Practical session

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