RBF-FD:
New Computational Opportunities in the Geo-Fluid Modeling

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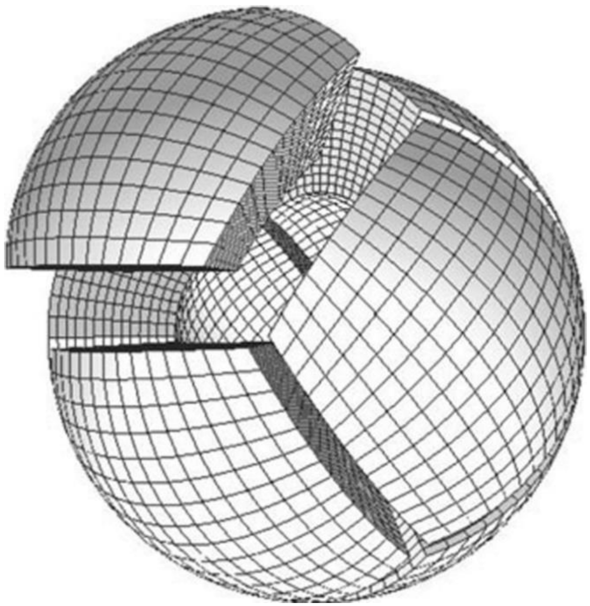
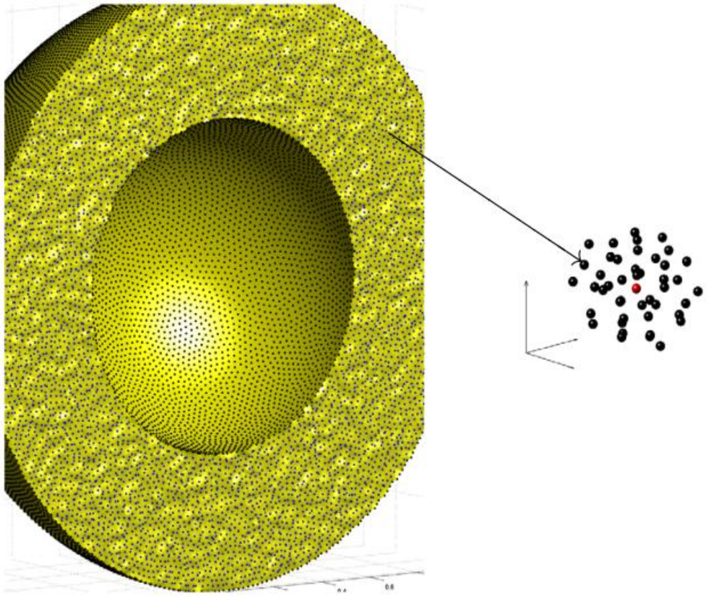
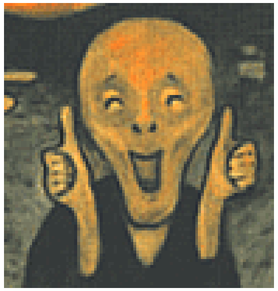
Current vs. Future Spatial Discretization for Modeling PDEs



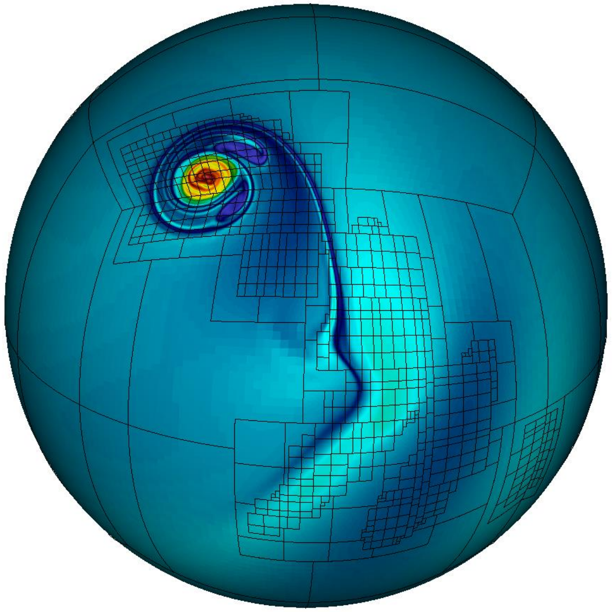


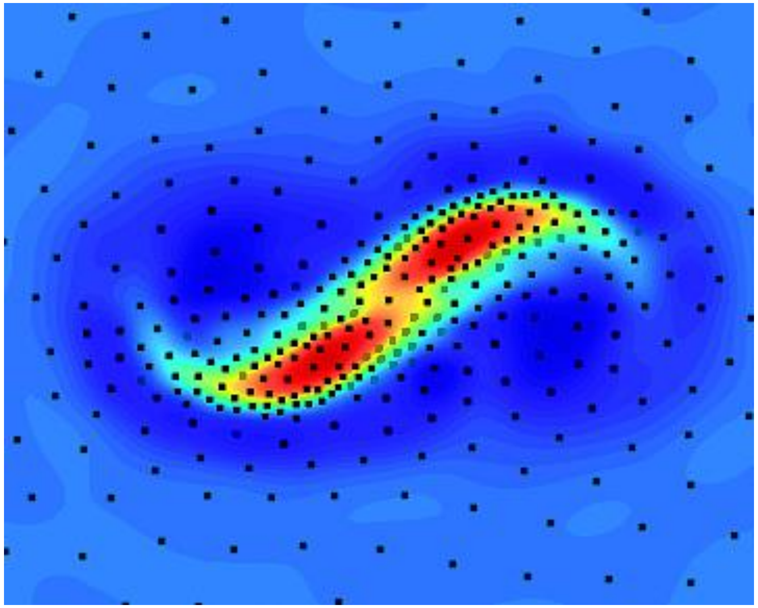
Current: All methods define elements or volumes. Requires mappings/transformations. Easier in 2D, computation in 3D is nightmarish.

Future: Simply scatter nodes in any dimensional space. No connectivites, thus no mappings/transformations
To go from 2D to 3D, changing the code is much more simple.



Current vs. Future Local Refinement

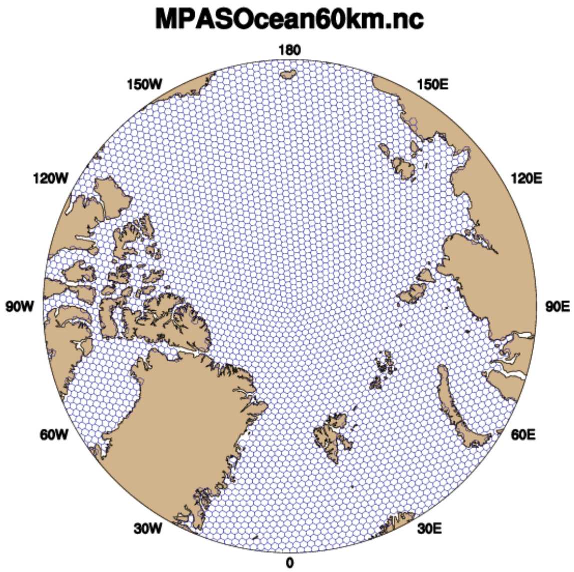


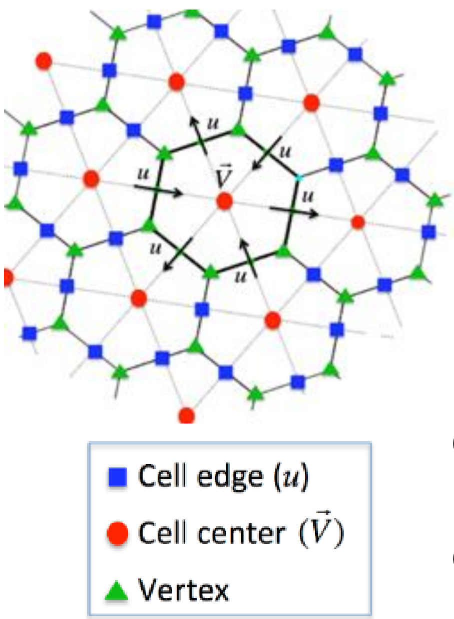


Current: Mesh refinement does not follow the shape of the feature, here, trying to capture a cyclone. Thus less effective in terms of accuracy and computational cost.

Future: Since nodes can be placed wherever needed due to no meshes, refinement occurs where most needed, here according to the gradient of the vorticity. Thus, much less pts. and computation are needed.

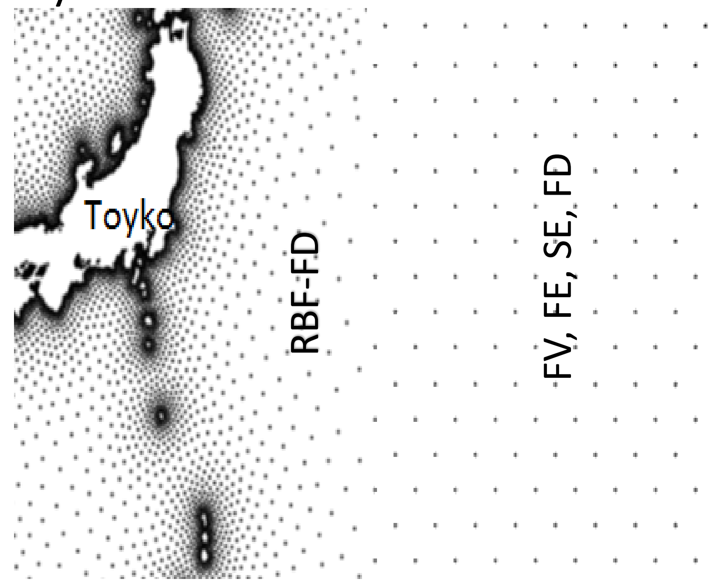
Current vs. Future Treatment of Boundaries, etc.





Current: Uses Voronoi mesh can not cot conform to coastal topography. Need to keep track of hexagon edges, centers, and vertices.

Allows for hybridization with other numerical methods



Future: RBF-FD can easily conform to coastlines and only needs: 1) point locations and 2) the distances between them. Then in open ocean, one can use whatever (FV, FE, SE, FD).

Shallow water wave equations

Simplest equations to describe the evolution of the horizontal structure of a fluid in response to forcings, such as gravity and rotation.

Basic Properties

- Set of nonlinear hyperbolic equations derived from physical conservation laws
- Horizontal scales of motion >> Vertical scales of motion
- Vertical velocity and all derivatives in vertical not present
- It is a 2D model.

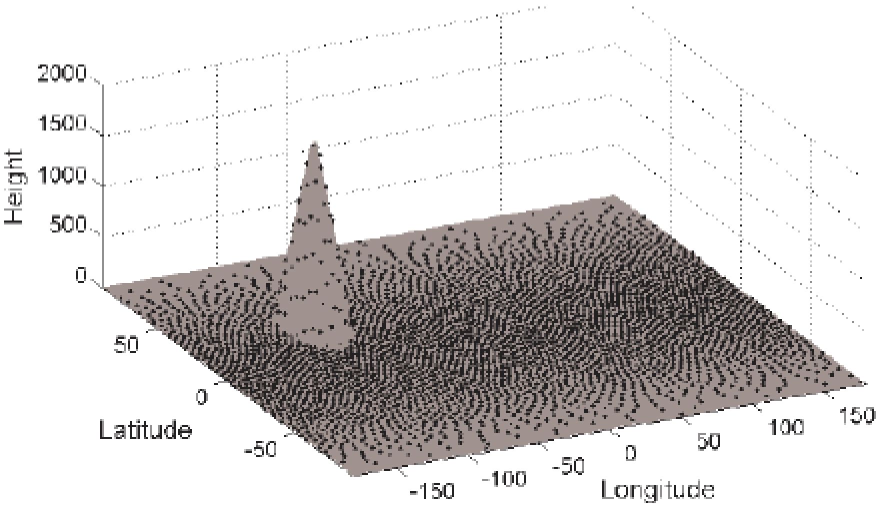
Areas of Application

- Atmospheric flows
- Tsunami prediction
- Planetary flows
- Storm surge
- Dam breaking

Netherlands Overflowing

Jupiter’s atmosphere

Flow over a C^0 Cone Mountain with RBF-FD (Flyer et al., *JCP*, 2012)



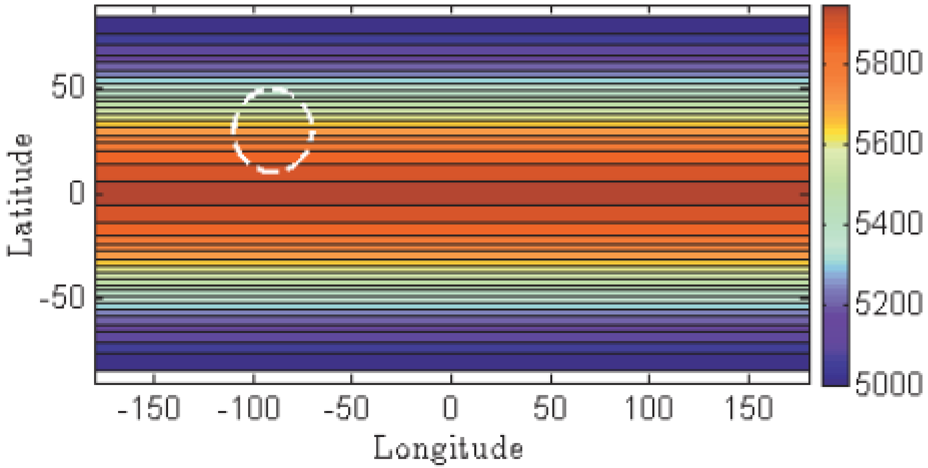
Shallow Water Equations

$$\frac{\partial \boldsymbol{u}}{\partial t} = -(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} - f(\boldsymbol{x}\times\boldsymbol{u}) - g\nabla h$$

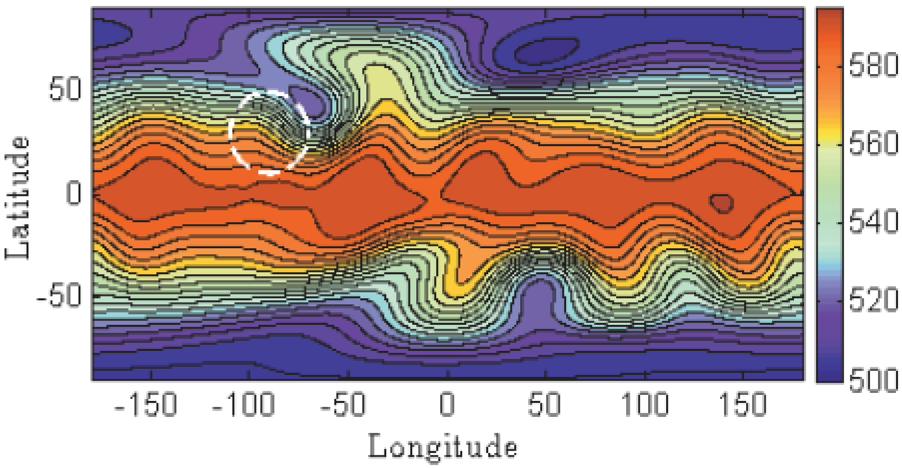
$$\frac{\partial h}{\partial t} = -\nabla\cdot(h\boldsymbol{u})$$

Cone Mountain

GA RBFs
stencil size = 31

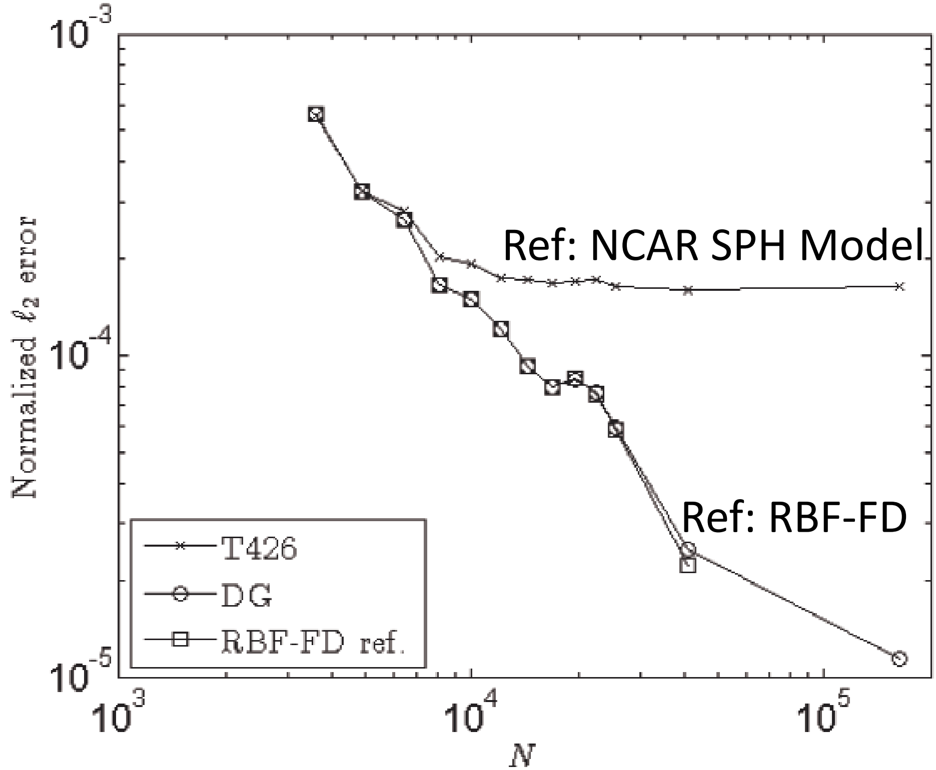


h, t = 0 days

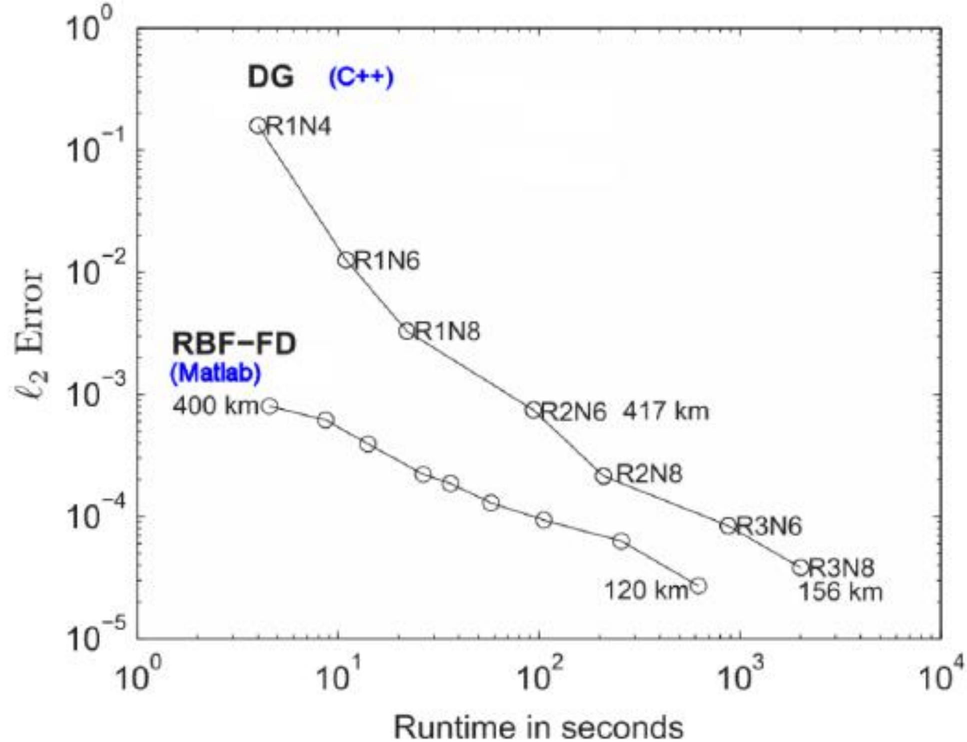


h, t = 15 days

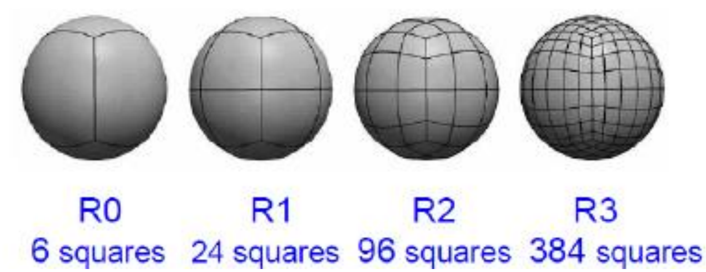
Convergence and Cost Efficiency of RBF-FD



Perfomance on Intel i7 CPU



NCAR SPH Model: 182,329 SPH bases (30km)
RBF-FD gave first evidence that this model, the standard of comparison, was not so accurate.

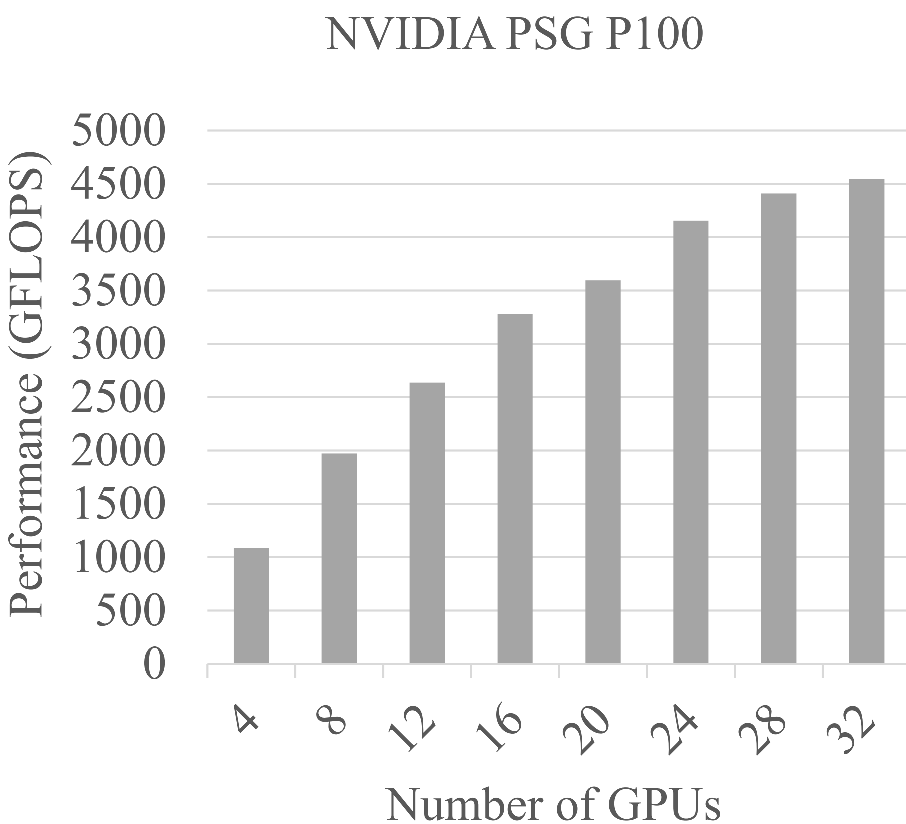


R = Number of subdivisions of each cube face
N = Degree of Legendre poly. in each square

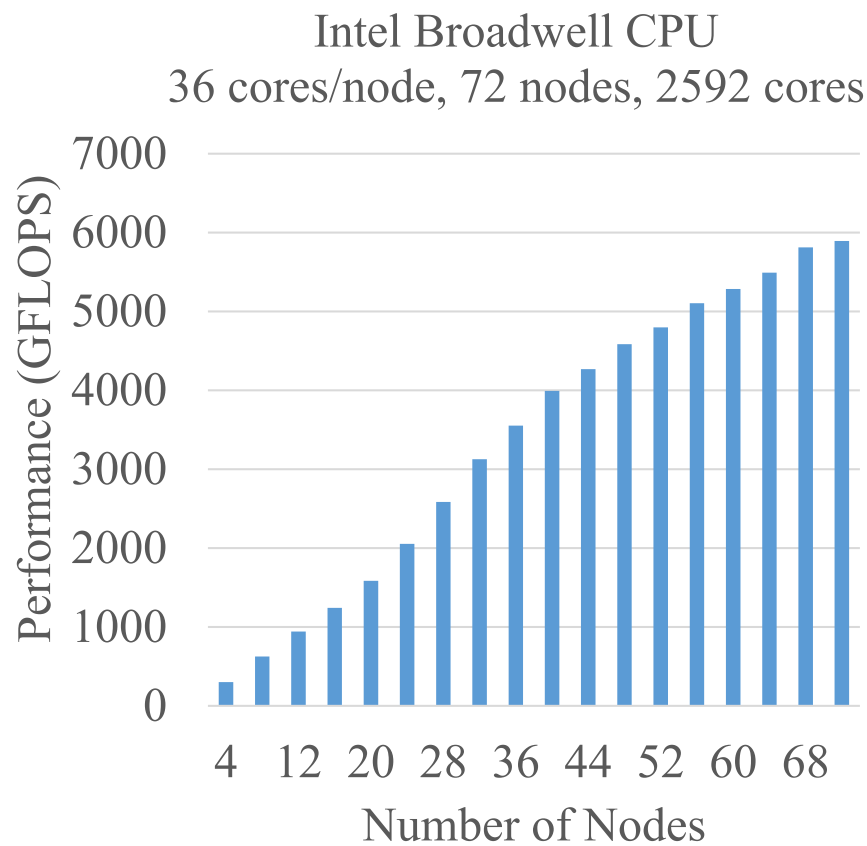
Multi – CPU and Multi – GPU performance: 2.6M nodes on sphere (15km)

(Elliott et al., 2017)

Latest GPU and CPU architectures for HPC



4.5 Teraflops

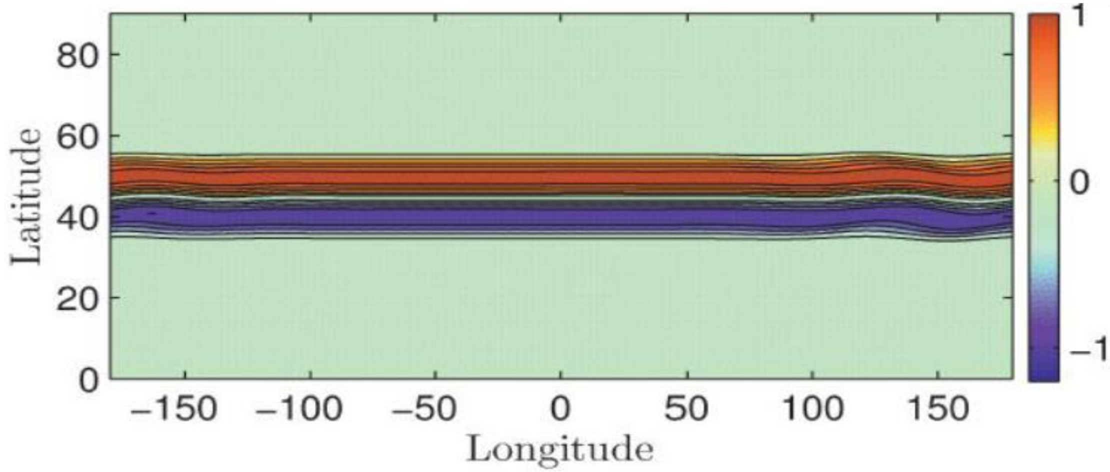


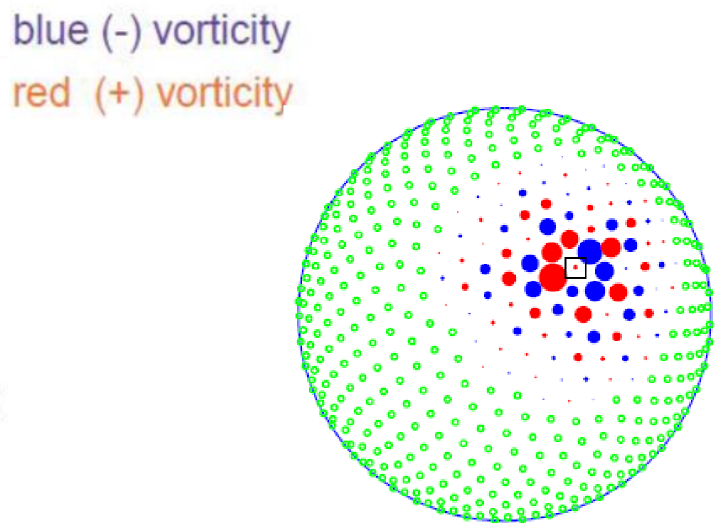
6 Teraflops

Both are $> \mathbf{100X}$ speedups over the highest achieved performance by the previous single device GPU implementation.

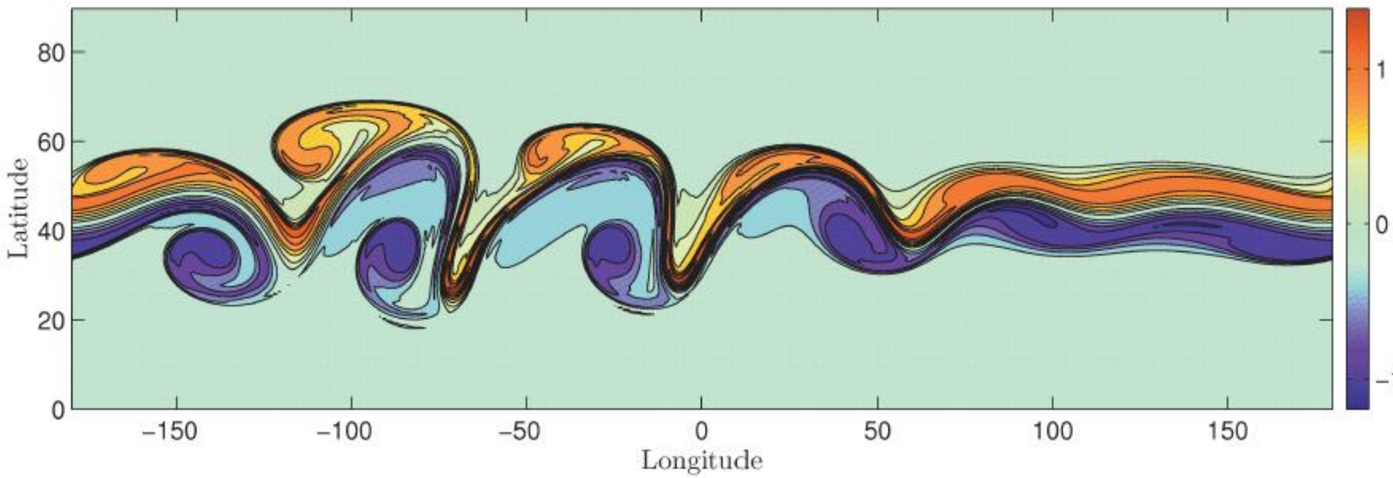
Shallow water wave equations on the sphere: Evolution of a highly unstable wave

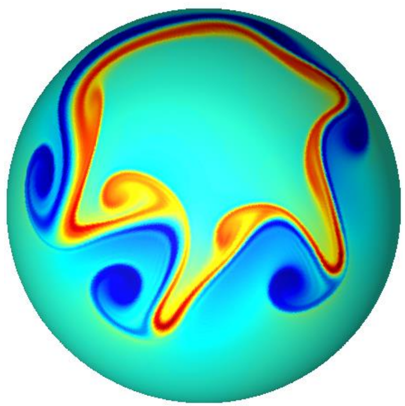
Day 3: Initial Signs of Instability



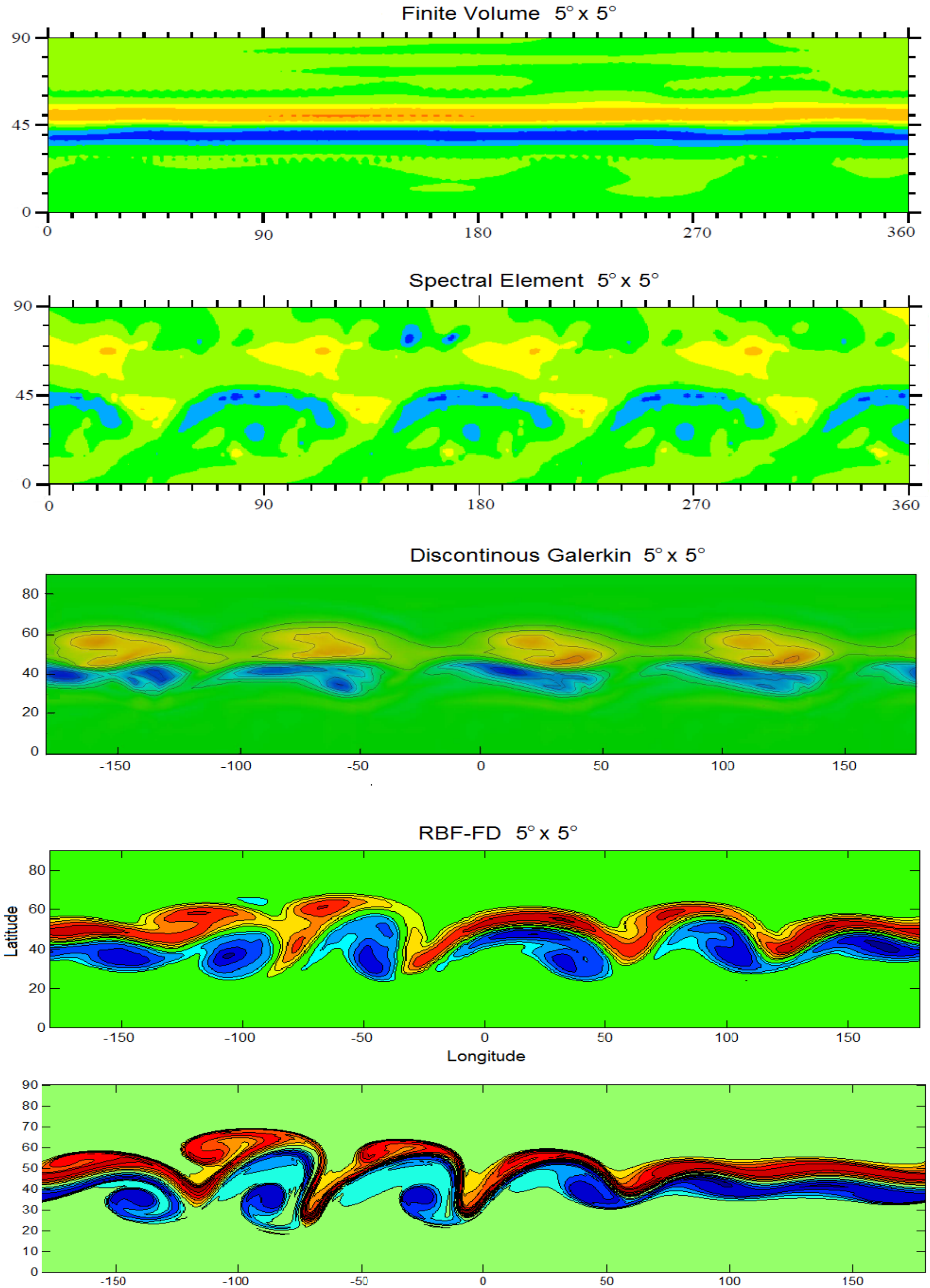


Day 6: Unstable vortex dynamics

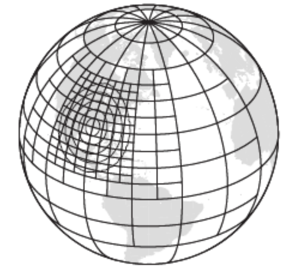




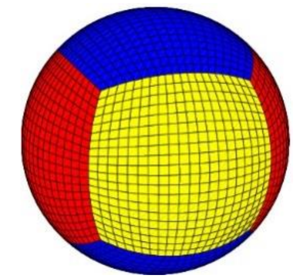
Vorticity at 5° x 5°



Finite Volume

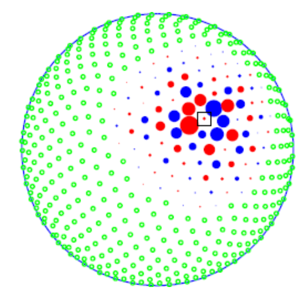


Spectral Element



Discontinuous Galerkin

RBF-FD



“ Truth” 0.35° x 0.35°

DG, SE, RBF-FD

2D Compressible Navier-Stokes (Flyer, Barnett, Wicker, *JCP,* 2016)

First paper in literature to consider using polyharmonic spline (PHS) RBF with high-order polynomials.

WHY? Possible explanation:

From a historical perspective, before RBF-FD, applications of RBFs were global.

1. If PHS RBFs were used, they were used in conjunction with low-order polynomials.
   Role of polynomials → guarantee non-singularity of RBF interpolation matrix for unusual node layouts.
   The role of capturing the physics was the left to the RBFs.

2. Using high-order polynomials on a global scale can be dangerous
   → Runge phenomena near boundaries.
   RBF-FD gives the approximation at the center of the stencil and not at the edges.

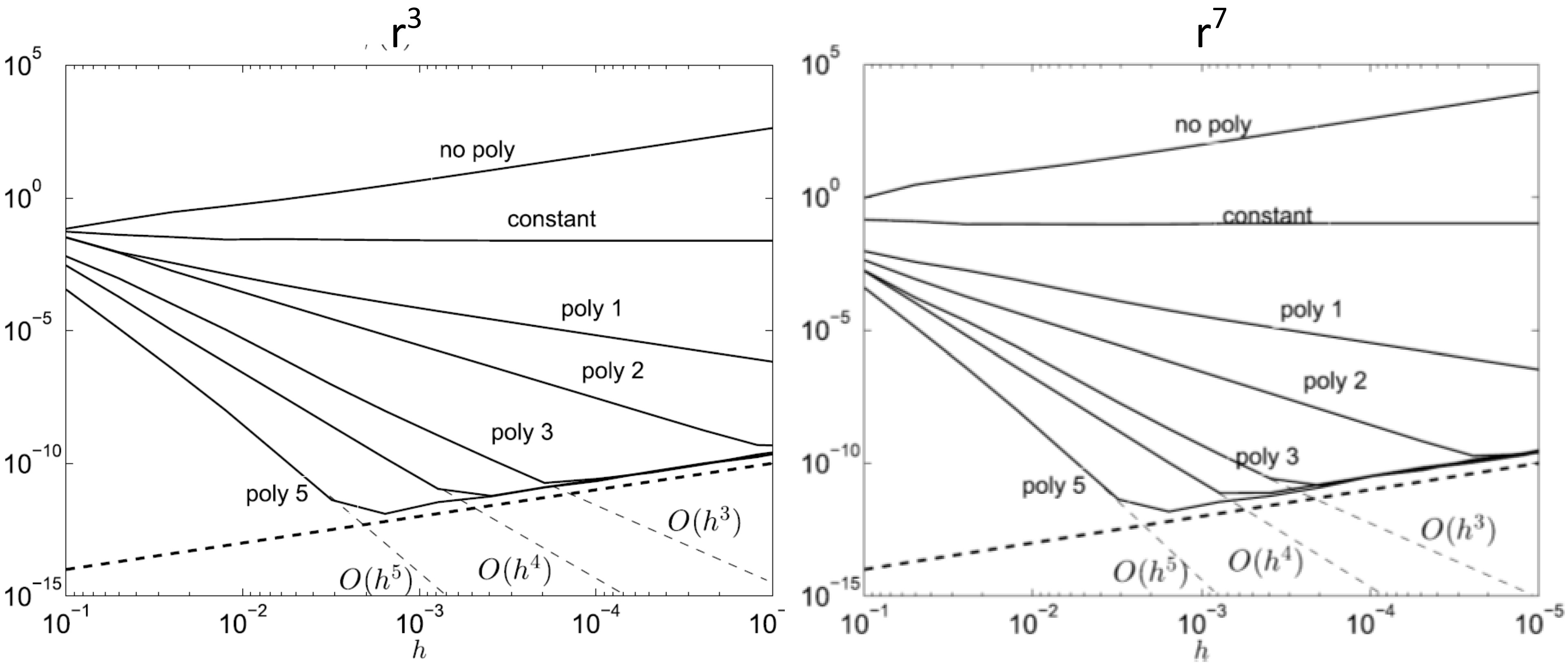
3. PHS RBFs were not as nearly as popular as infinitely smooth RBFs for PDEs.
   For the high computation price of global RBFs, you want the fast convergence and accuracy.

Let's briefly explore PHS RBF-FD convergence and accuracy before test cases.

Polynomials in Control (Flyer, Barnett, Wicker, *JCP,* 2016)

L_2 error in approximating d/dx of $f(x, y) = 1 + \sin(4x) + \cos(3x) + \sin(2y)$

near the center of a 37 node hex. stencil, using r^3 and r^7 with corresponding polynomials

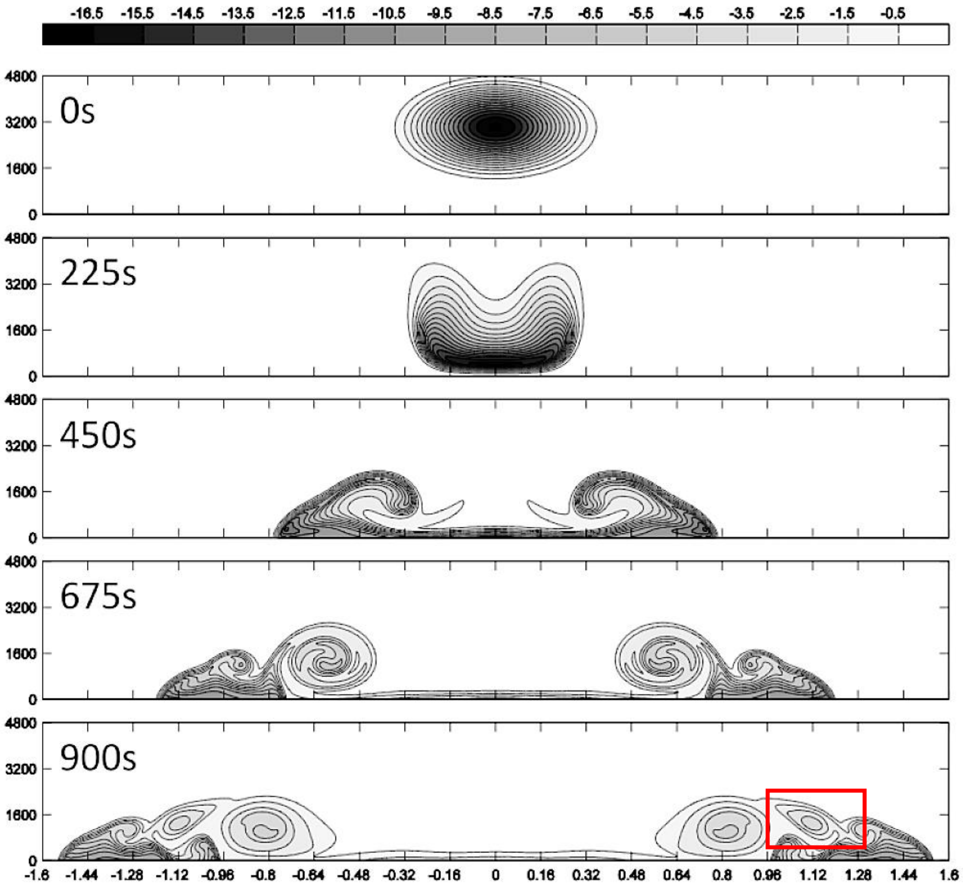


Dashed line machine round-off error of $10^{-15}/h$

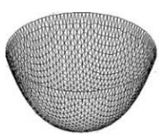
2D Compressible Navier-Stokes

$$\frac{\partial \mathbf{u}}{\partial t} = -\left(\mathbf{u}\cdot\nabla\right)\mathbf{u} - c_p\theta\nabla P - g\mathbf{k} + \mu\Delta\mathbf{u},$$
$$\frac{\partial \theta}{\partial t} = -\left(\mathbf{u}\cdot\nabla\right)\theta + \mu\Delta\theta,$$
$$\frac{\partial P}{\partial t} = -\left(\mathbf{u}\cdot\nabla\right)P - \frac{R}{c_v}\left(\nabla\cdot\mathbf{u}\right)P,$$

Accurate time evolution of Temperature



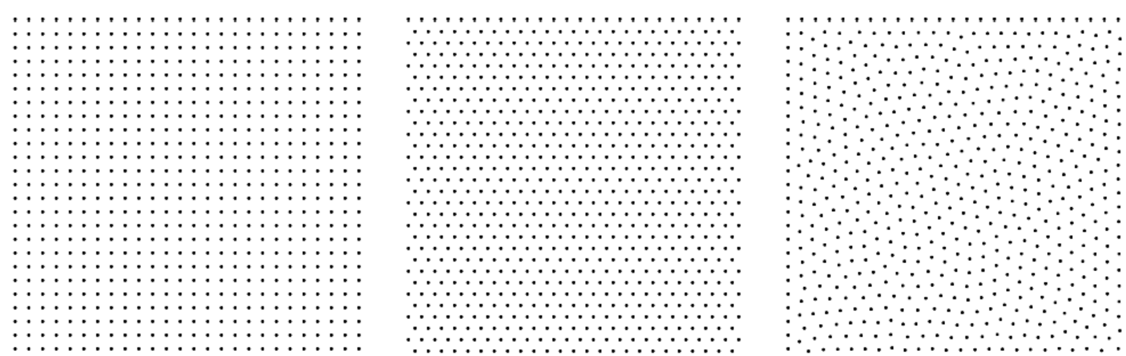
Basis functions used:

RBF r^5  + Up to **4th** degree polys.

Hyperviscosity use GA-based or PHS-based

With RBF-FD, easy to explore the intrinsic capabilities of different layouts. Same Code.

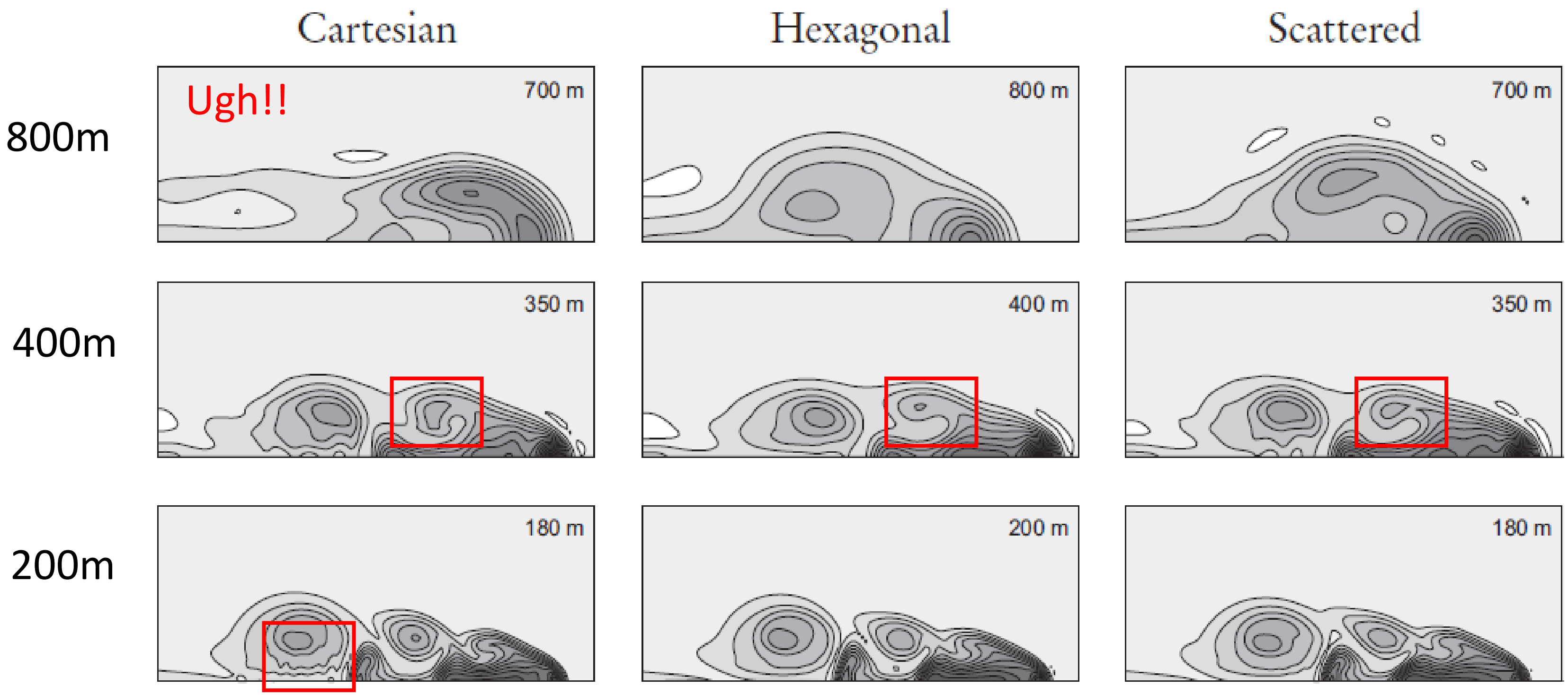
Hexagonal have a long history, never became 'mainstream' due to implementation complexities.



Cartesian Hexagonal Scattered

Comparisons on different node layouts: change 1 line of code

Only showing half of domain due to symmetry



Comparison:

Cartesian: Most unphysical artifacts (`wiggles'), 1^{st} rotor not formed at 800m

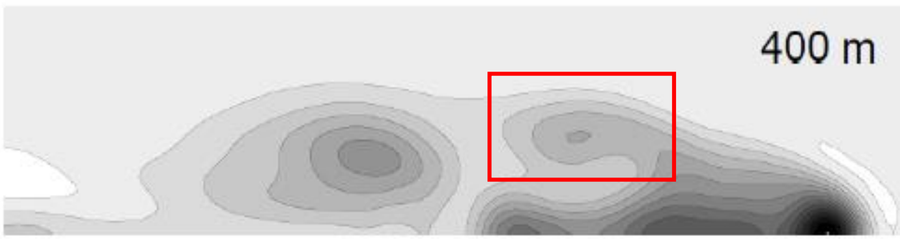
Hexagonal: Excellent results; now easy to implement opposed to past

Scattered: Little performance penalty but one gains greatly geometric flexibility

Comparisons to other numerical methods

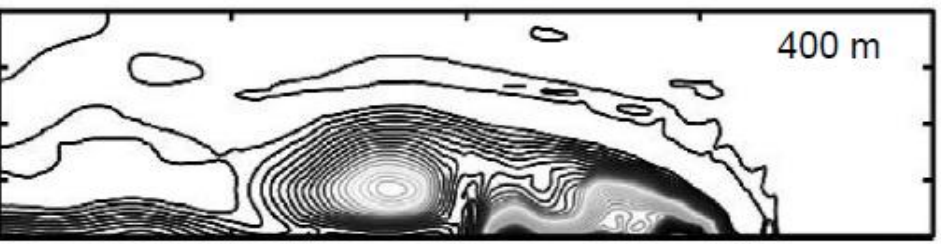
At high resolutions, 100m and under, most methods perform well.
Key issue: Data-based initialization of weather prediction models > 500m
Below: Comparisons from the literature, at 400m resolution?

RBF – FD 37 node stencil

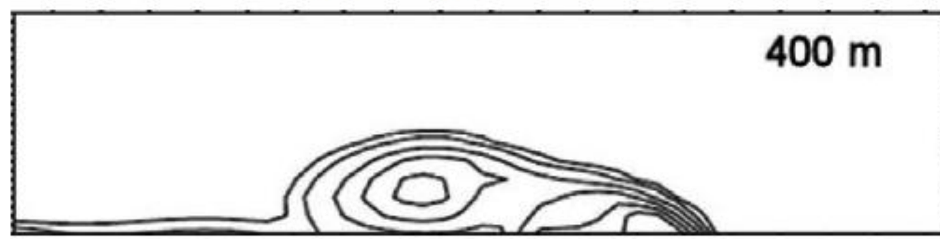


5^{th} – order upwind advection

8^{th} – order DG and SE



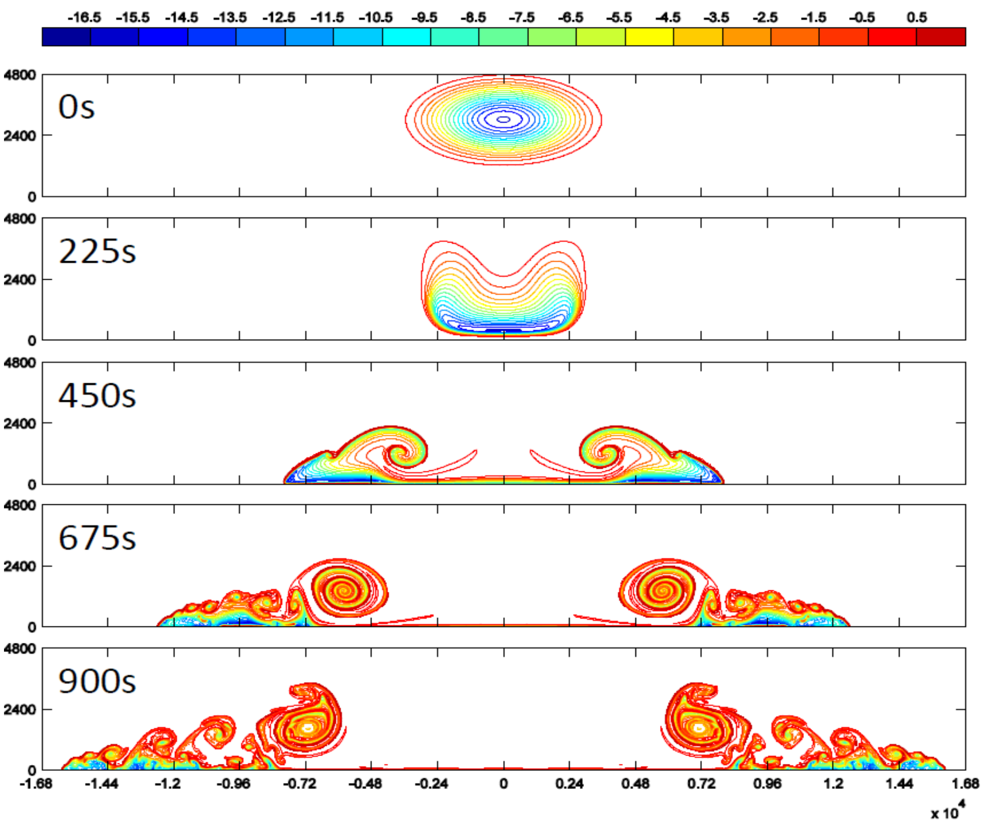
4^{th} – order finite volume



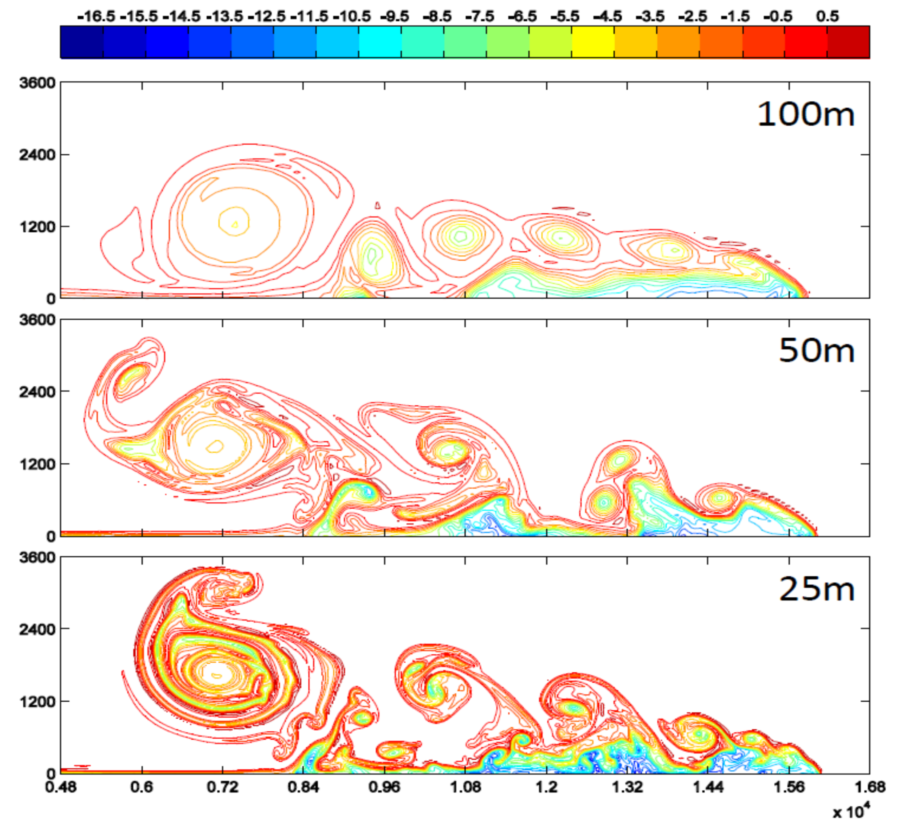
At this coarse resolution, only the RBF-FD calculations shows the beginning of second rotor (does it on Cartesian, hexagonal, and scattered node sets) and can perform at 800m.

Same test problem, but with no physical viscosity

25m resolution (RBF-FD, hex nodes)



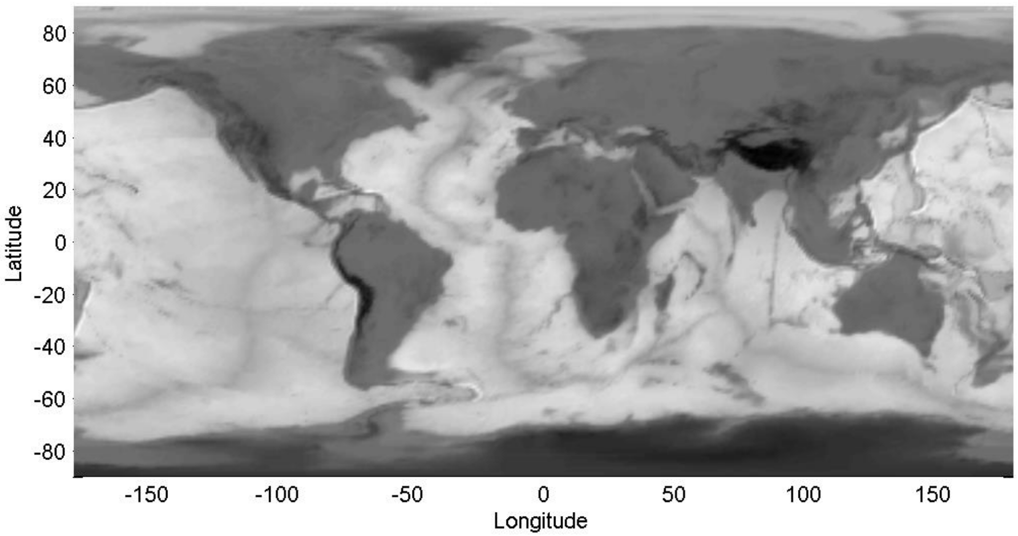
Details when using different resolutions

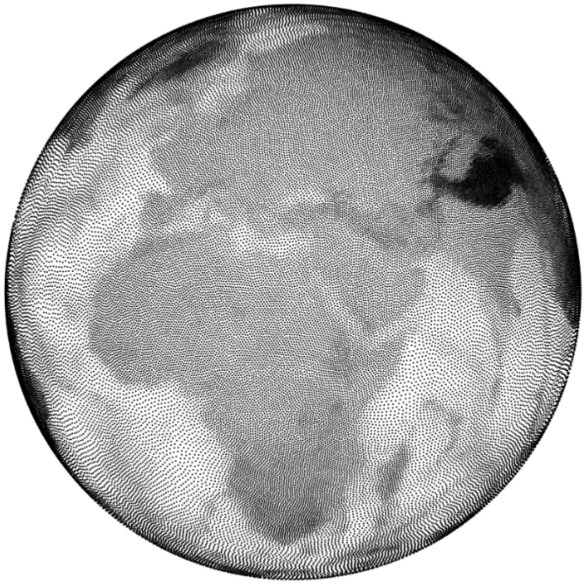


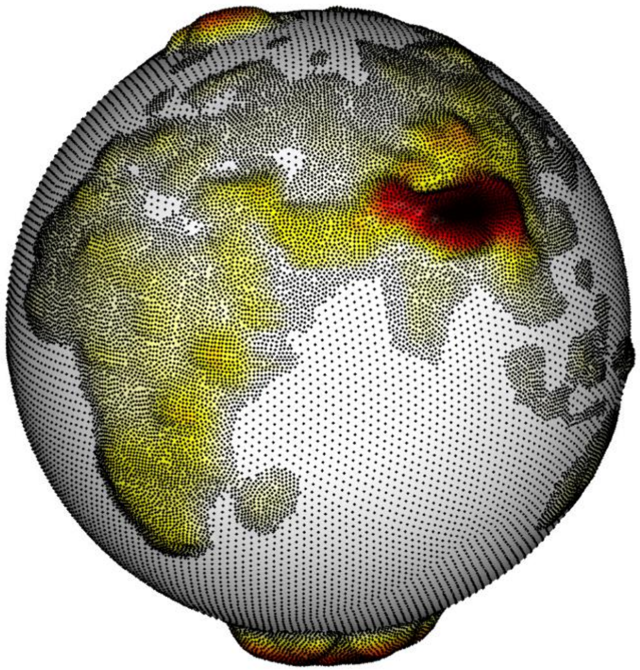
Distributing variable node density on sphere

(Fornberg and Flyer, 2015)

Below: Gray scale rendering of the file topo.mat in Matlab's Mapping toolbox







Top right:

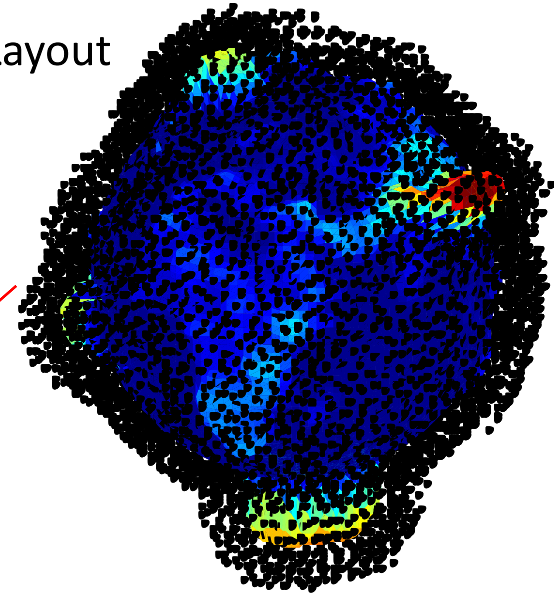
N = 105,419 nodes rendering of the topo map above
Computational speed in MATLAB still around
11,000 nodes per second.

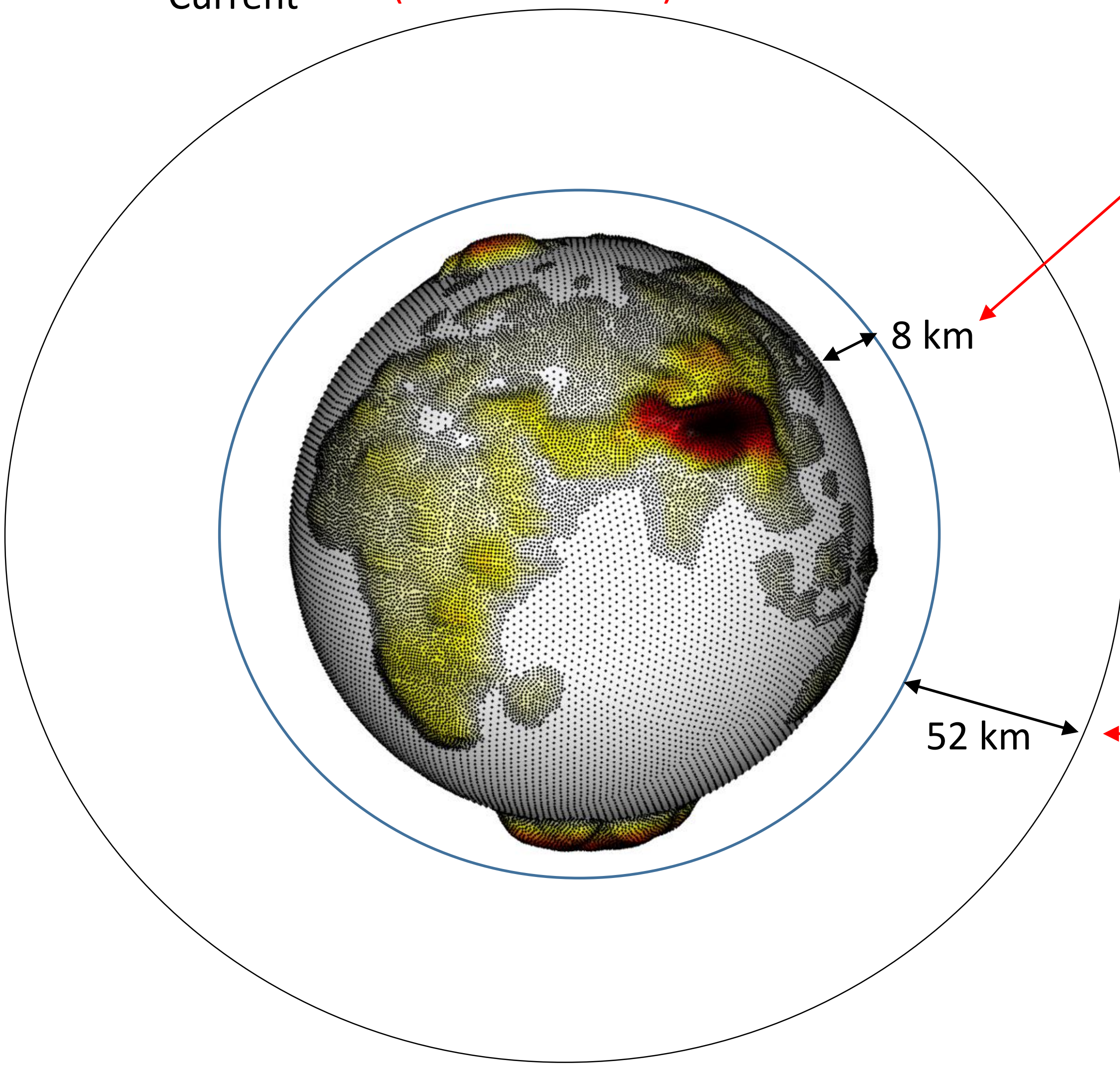
Next step in modeling (Bayona et al. 2015) :
Take elevation physically taken into account

3D Elliptic PDE: Modeling Electrical Currents in the Atmosphere

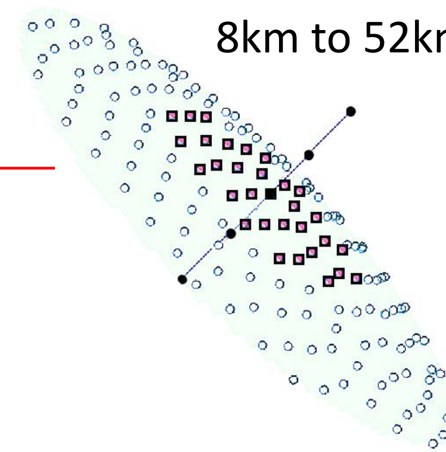
$$\nabla_{3D} \cdot \underbrace{\vec{J}\left(\vec{x}\right)}_{\text{Electric Current}} = \underbrace{F\left(\vec{x}\right)}_{\substack{\text{Thunderstorms} \\ \text{(measured data)}}}$$

3D Node Layout
to 8km

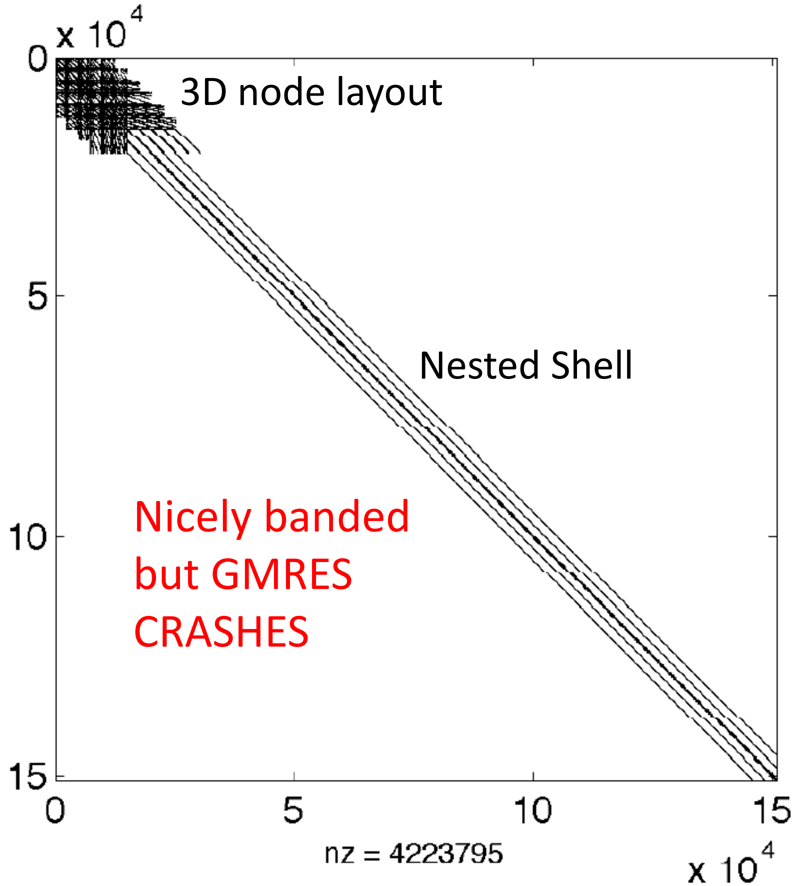




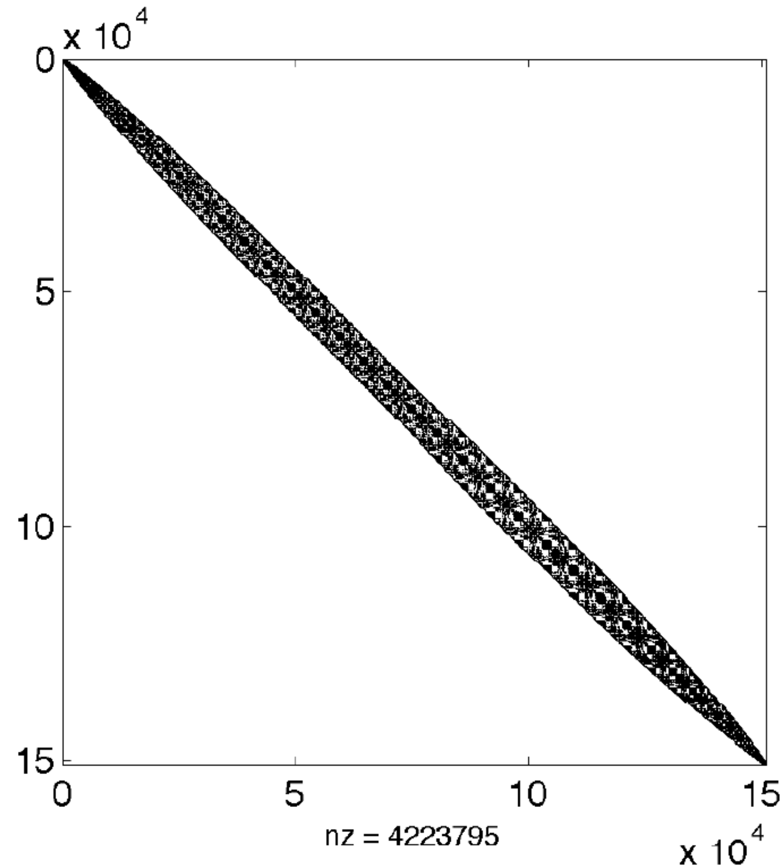
Nested shells
8km to 52km



Sparsity pattern of 3D elliptic operator (99.998% zeros)



Before any node reordering



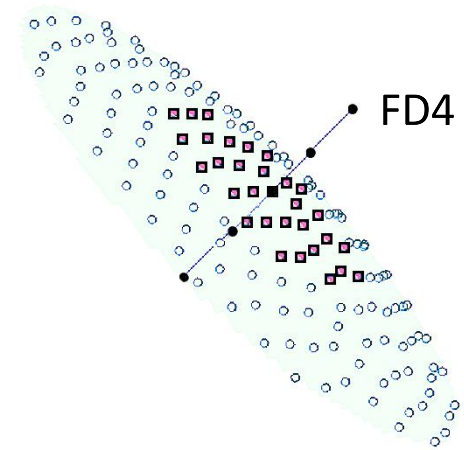
After using reverse Cuthill- McKee

Result: Testing with data, 4.2M nodes
100 km. lat. – long. By 600m vertical, 31 mins on laptop using GMRES

GitHub Open Source Code: Bayona et al. , A 3-D RBF-FD solver for modelling the atmospheric Global Electric Circuit with topography (GEC-RBFFD v1.0), Geosci. Model Dev. 2015.

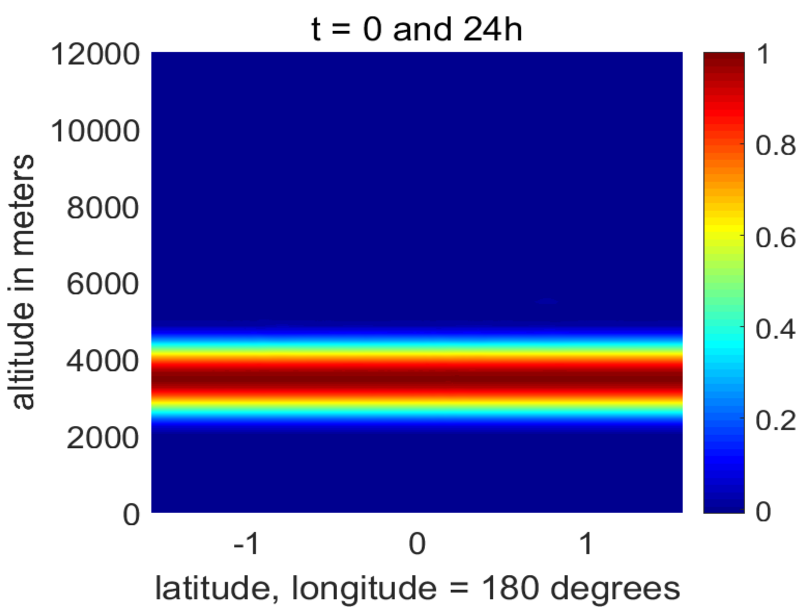
Tracer Transport in 3D Spherical Shell

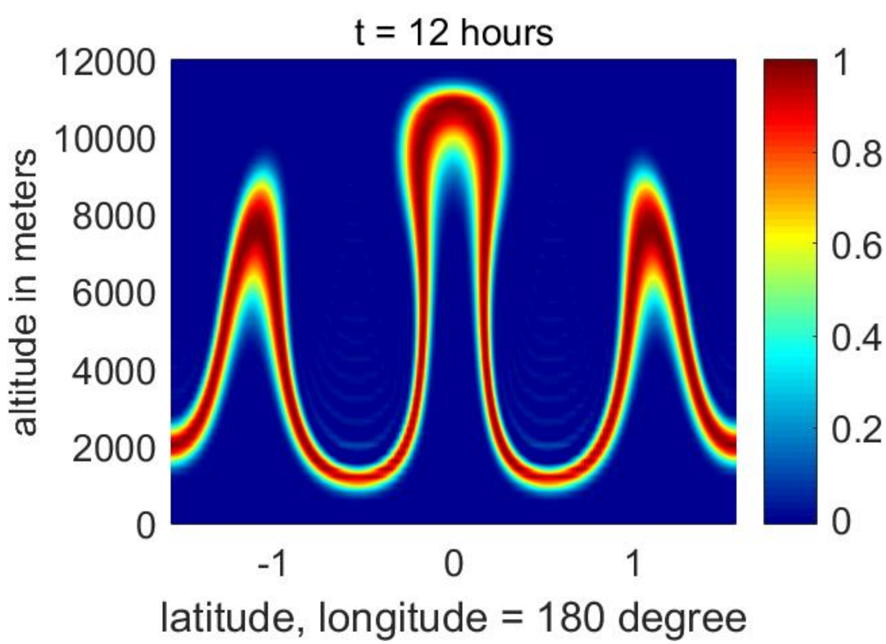
$$\partial q / \partial t + \mathbf{v}(x,y,z,t) \cdot \nabla_{3D}\, q = 0$$



Specs:
Nodes: Icosahedral on nested spheres
RBF: r^3 with up to 5^{th}-order polynomials on sphere
FD4: In vertical
Stencil: n = 55
No Hyperviscosity Needed!

Concentration of tracer q plotted





Comparison to other community models based on finite volume

Numbers represent error in L_2

	2° by 300m (N = 360K)	1° by 200m (N = 2.45M)	$1/2^\circ$ by 100m (N = 19.6M)
CAM-FV	0.20	0.05	0.02
Mcore(FV)	0.17	0.05	0.01
RBF-FD	0.03	0.003	0.0005

FV is used for its conservation properties, but sacrifice is accuracy and convergence.

Comment: The need for hyperviscosity depends on how long it takes for the spurious eignmodes that are close to machine rounding to grow.

Conclusions

Established:

- RBF-FD latches onto the physics at much coarser resolutions than other numerical methods, giving higher accuracy and convergence
- RBF-FD have shown strong linear scaling on on the latest HPC platforms
- Startup cost for modeling with RBF-FD is cheap due to their algorithmic simplicity

Some recent review material

1. N. Flyer, G.B. Wright, and B. Fornberg, 2014. *Radial basis function-generated finite differences: A mesh-free method for computational geosciences*, Handbook of Geomathematics, Springer-Verlag

2. B. Fornberg and N. Flyer, 2015 *Solving PDEs with Radial Basis Functions*, Acta Numerica.

3. B. Fornberg and N. Flyer, 2015 *A Primer on Radial Basis Functions with Applications to the Geosciences*, SIAM Press.