A New Dynamical Core with Local Mesh Refinement

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Climate, Ocean and Sea-Ice Modeling Project
http://public.lanl.gov/ringler/ringler.html

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Joe Klemp
Lili Ju

Background

Two lines of research have come together to create this dynamical core. This effort started about two years ago.

1. Creating a C-grid staggering that is applicable to a wide class of meshes that conserves energy, conserves potential vorticity and dissipates potential enstrophy with the appropriate time scale. Applicable (without modification) to variable resolution meshes.

- Ringler, T., J. Thuburn, J. Klemp and W. Skamarock, 2009: A unified approach to energy conservation and potential vorticity dynamics on arbitrarily structured C-grids, Journal of Computational Physics, accepted. (pdf).

- Thuburn, J., T. Ringler, J. Klemp and W. Skamarock, 2009: Numerical representation of geostrophic modes on arbitrarily structured C-grids, Journal of Computational Physics, 2009: 228 (22), 8321-8335. doi:10.1016/j.jcp.2009.08.006 (link)

2. The creation of high quality variable resolution meshes that can be used with the above numerical method.

- Ju, L., T. Ringler and M. Gunzburber, 2009, Voronoi Diagrams and their Application in Climate Science, Numerical Techniques for Global Atmospheric Models, Lecture Notes in Computational Science, draft. (pdf).

- Ringler, T., L. Ju and M. Gunzburger, 2008, A multiresolution method for climate system modeling: application of spherical centroidal Voronoi tessellations, Ocean Dynamics, 58 (5-6), 475-498. doi:10.1007/s10236-008-0157-2 (link)

Background (continued)

A one-year infusion of funds from DOE Office of Science has allowed us to make a strong push to move this from a set of good ideas to a prototype ocean (and atmosphere) dynamical core.

Examples include:

1. Implementing high-order transport (Lowerie and Buoni)
2. Sub-grid closures for variable resolution meshes (Carlson)
3. Full implementation of immersed boundary method (Mohd-Yosuf)
4. Dynamical core formulation and implementation (Ringler)
5. Implementation of method as a option for the CCSM CAM (coupling to CCSM led by Mirin et. al at LLNL, model formulation led by Skamarock et. al at NCAR MMM. NCAR MMM is an un-funded partner for this one-year effort.)

Cutting to the chase on the numerical method ....

Analytic results for the nonlinear shallow-water equations:

(includes full ocean models based on isopycnal coordinates)

1. Stationary geostrophic mode is recovered.

2. Total energy is conserved to within time truncation.
   a. Coriolis force is energetically-neutral
   b. Transport of KE is conservative
   c. KE/PE exchange is equal and opposite.

3. Potential vorticity is conserved to round-off. PV is compatible with an underlying thickness equation.

4. Potential enstrophy can be dissipated through the discretization of potential vorticity transport (i.e. monotone transport).

Results hold for a wide class of meshes: Lat/Lon, Stretched Lat/Lon, Voronoi Tessellations, Delaunay Triangulation and Conformally-mapped cubed sphere meshes.

An important aspect of this method is the control over PV dynamics that we can exert while discretizing the momentum equation.

$$\mathbf{k} \cdot \nabla \times \left[\frac{\partial \mathbf{u}}{\partial t} + q(h\mathbf{u}^{\perp}) = -g\nabla\left(h + h_s\right) - \nabla K \right]$$

nonlinear Coriolis force

$$\frac{\partial \eta}{\partial t} + \mathbf{k} \cdot \nabla \times \left[\eta \mathbf{u}^{\perp} \right] = 0$$

$$\frac{\partial \eta}{\partial t} + \nabla \cdot [\eta \mathbf{u}] = 0$$

potential vorticity flux

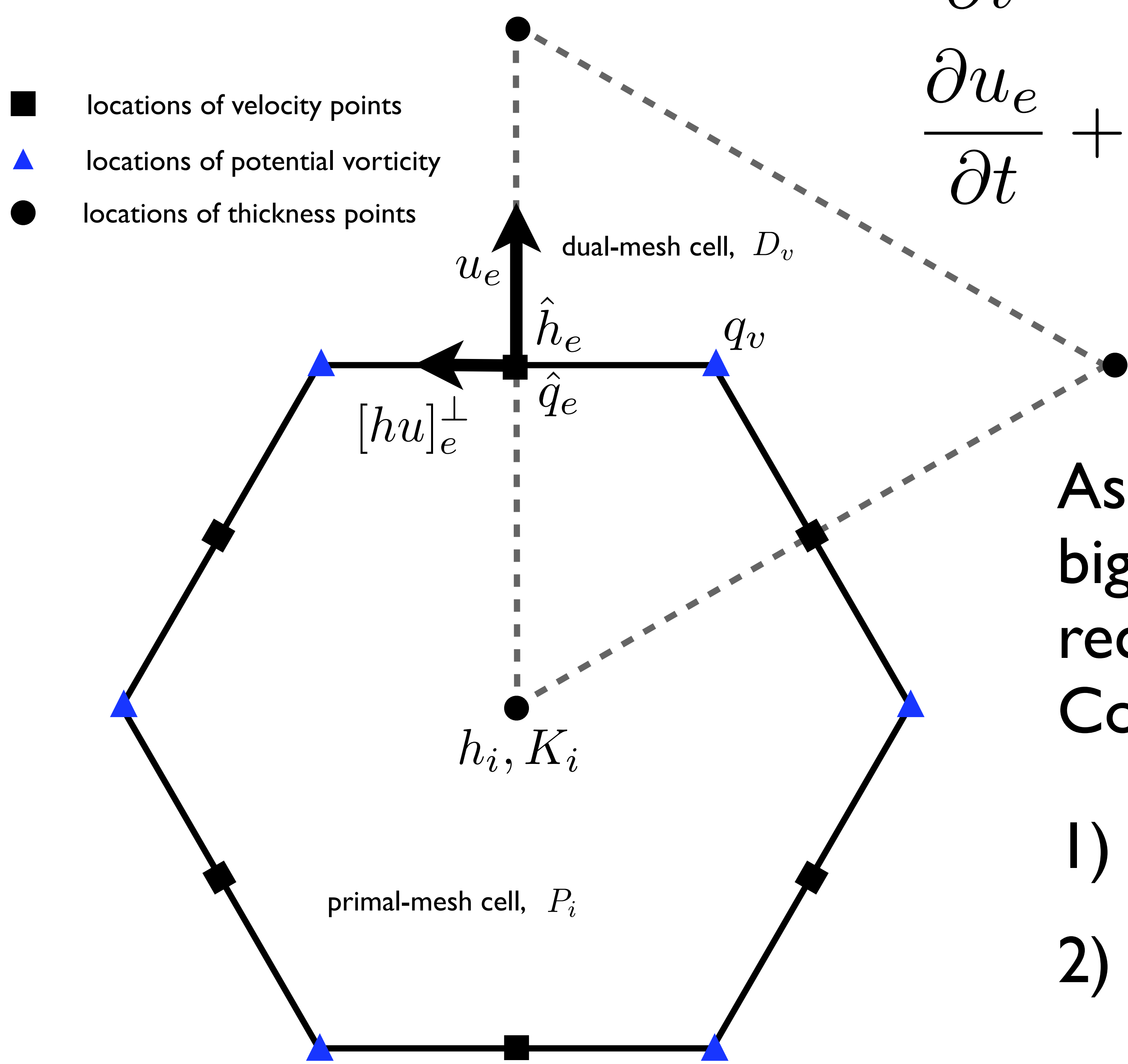
$$\frac{\partial (hq)}{\partial t} + \nabla \cdot [hq\mathbf{u}] = 0$$

The nonlinear Coriolis force IS the PV flux in the direction perpendicular to the velocity. So the evolution of PV is controlled entirely through the discretization of the nonlinear Coriolis force.

This insight was also helpful in the formulation of an extension of GM to include the include the influence of the Bolus velocity on PV transport.

- Ringler, T. and P. Gent, 2009: An eddy closure for potential vorticity, Journal of Physical Oceanography, submitted. (pdf).

Defining the discrete system



$$\frac{\partial h_i}{\partial t} + \left[\nabla \cdot \left(\widehat{h}_e u_e\right)\right]_i = 0$$

$$\frac{\partial u_e}{\partial t} + \widehat{q}_e \left[hu\right]_e^{\perp} = \left[\nabla \left(g h_i + K_i\right)\right]_e$$

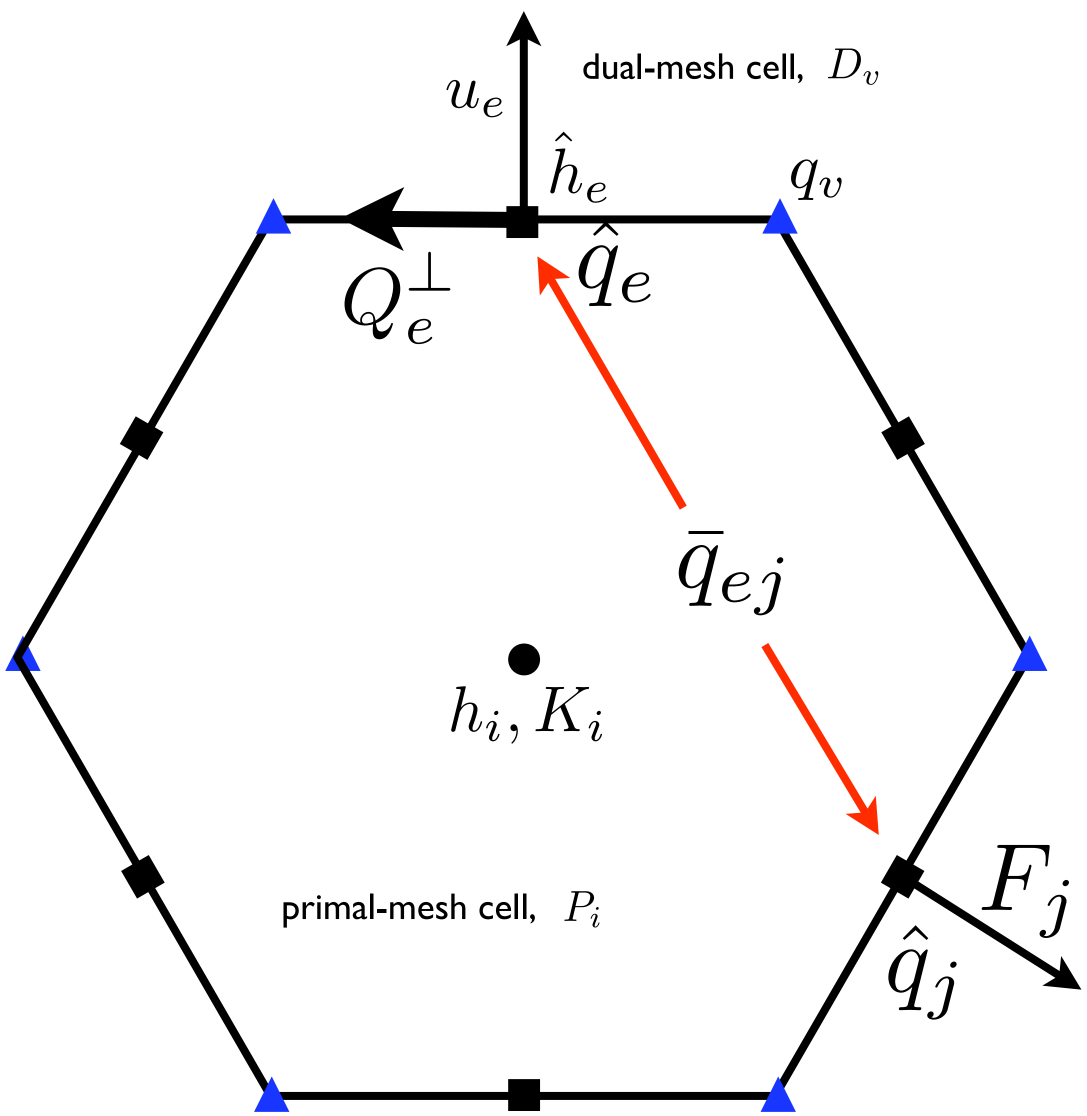
As with all C-grid methods, the biggest challenge is how to reconstruct the nonlinear Coriolis force.

1) How to compute $[hu]_e^{\perp}$?

2) How to compute $\widehat{q}$?

Reconstructing the nonlinear Coriolis force

(recall that the nonlinear Coriolis force is the the PV-flux perpendicular to the velocity)



$$\frac{\partial u_e}{\partial t} + \widehat{q}_e \left[hu\right]_e^{\perp} = \left[\nabla\left(gh_i + K_i\right)\right]_e$$

$$\frac{\partial u_e}{\partial t} + Q_e^{\perp} = \left[\nabla\left(gh_i + K_i\right)\right]_e$$

$$d_e\, Q_e^{\perp} = \sum_j w_e^j\, l_j\, F_j\, \bar{q}_{ej}$$

$$F_j = \hat{h}_j u_j$$ thickness flux

$$w_e^j = -w_j^e$$ weights are equal and opposite

$$\bar{q}_{ej} = \bar{q}_{je}$$ PV is symmetric

The nonlinear Coriolis force will be energetically neutral for any $\bar{q}_{ej}$.
This is an extension to what Sadourny (1975) showed for regular meshes.

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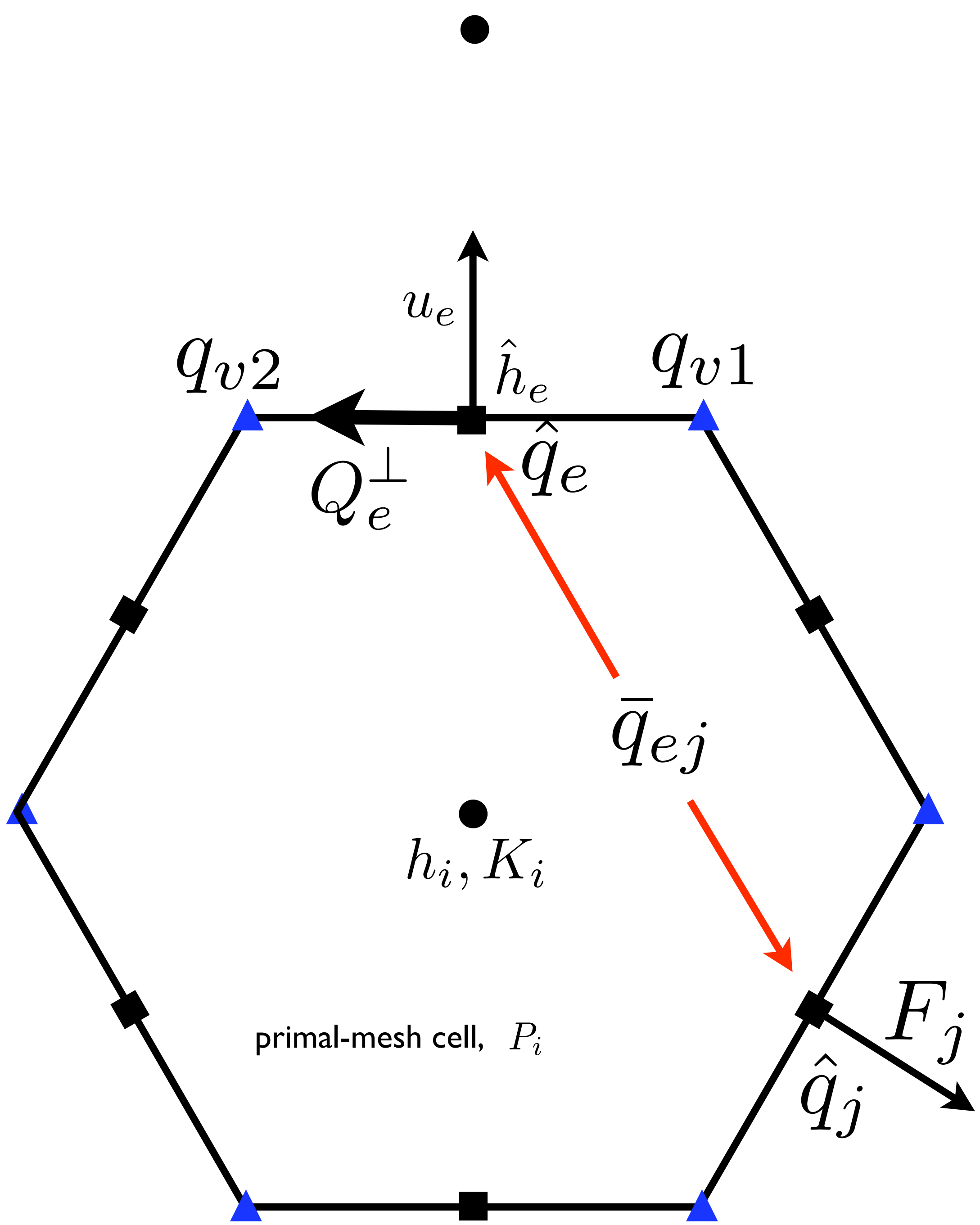

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Energy conservation is obtained by:

$$\bar{q}_{ej} = \bar{q}_{je} = \frac{1}{2}\left(\widehat{q}_e + \widehat{q}_j\right)$$

Energy is conserved for any $\widehat{q}_e$ and any $\widehat{q}_j$!

The APVM is obtained by:

$$\widehat{q}_e = \frac{1}{2}\left(q_{v1} + q_{v2}\right) - \underbrace{\frac{dt}{2}\mathbf{u}\cdot\nabla q}$$

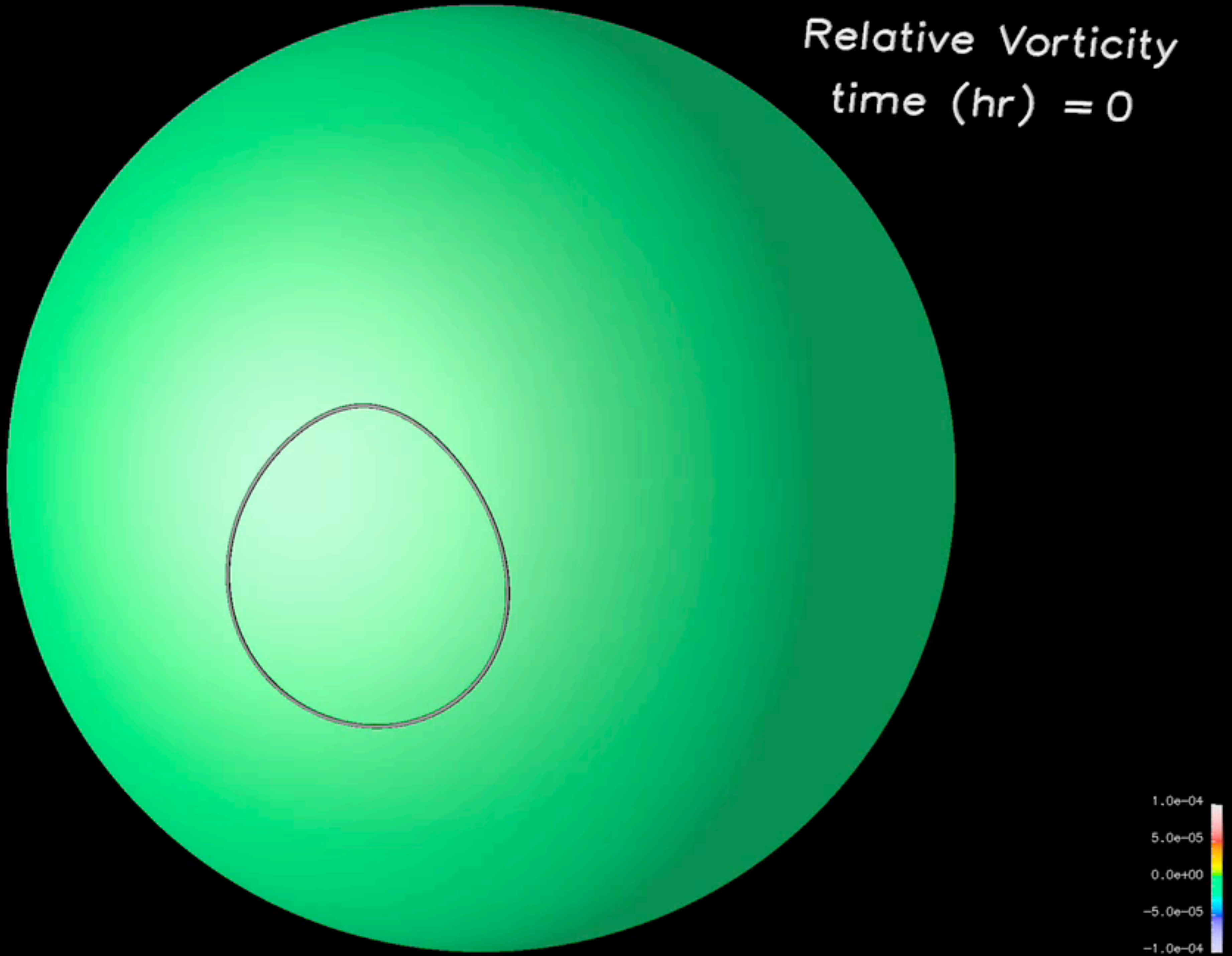
This is the upstream bias that leads to dissipation of potential enstrophy.

(In terms of computational cost, this closure is essentially free.)

SWTC#5, 100 day integration, quasi-uniform mesh

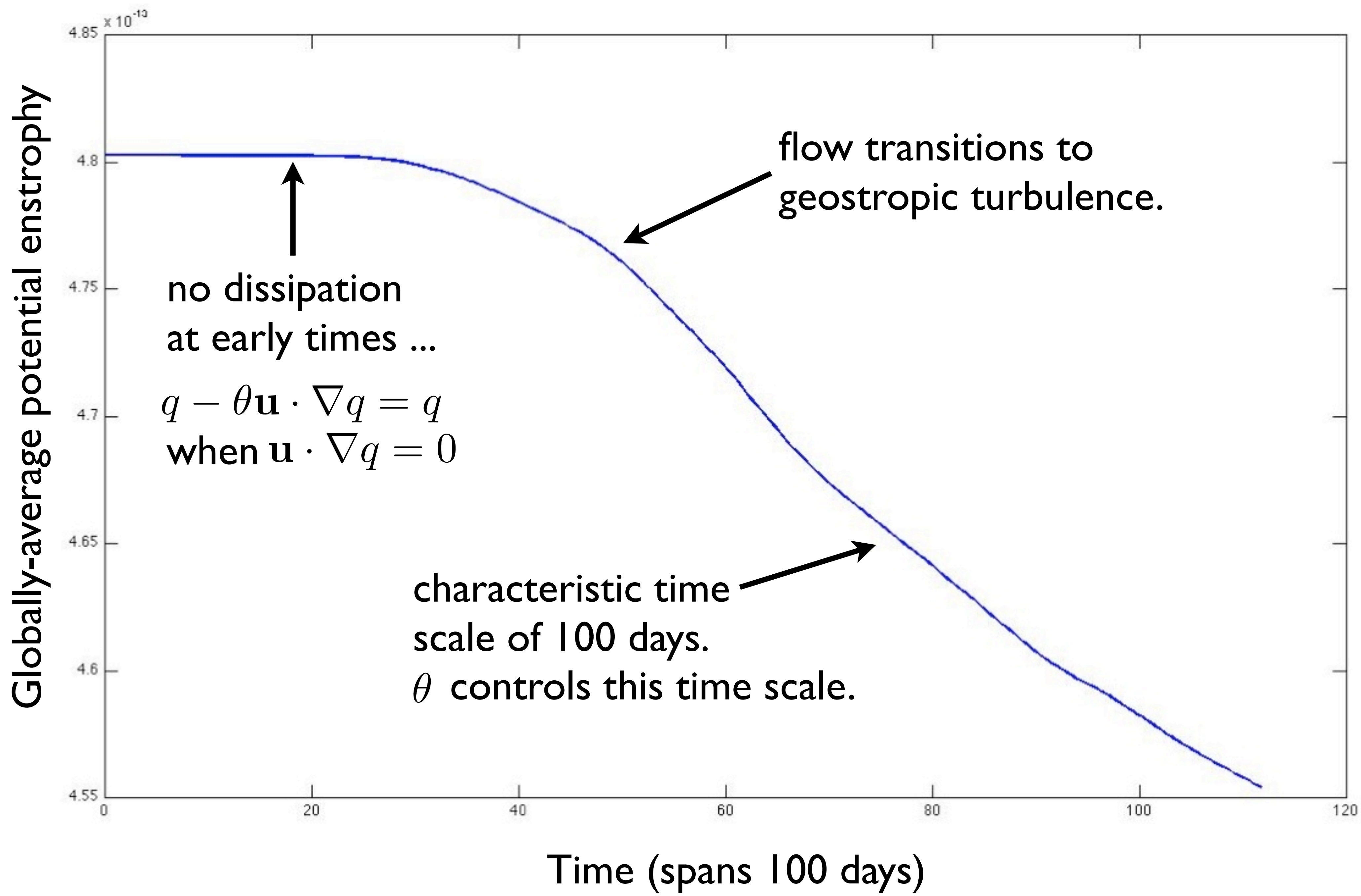
potential enstrophy dissipation with 100 day time scale

energy conserved to 1e-8



http://public.lanl.gov/ringler/movies/2009/APVM.mov

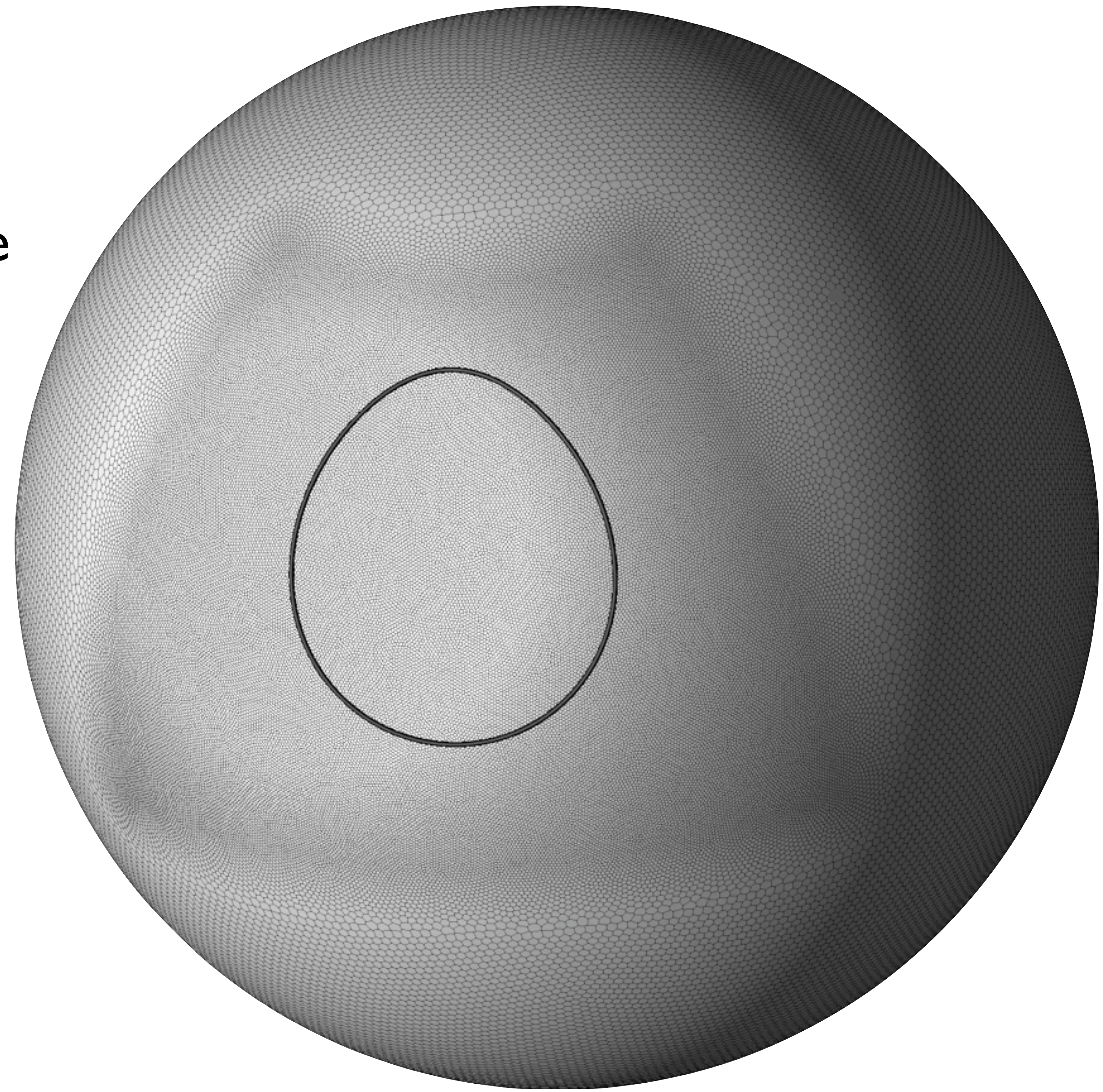
Globally-average potential enstrophy when using the APVM



Variable-resolution simulations

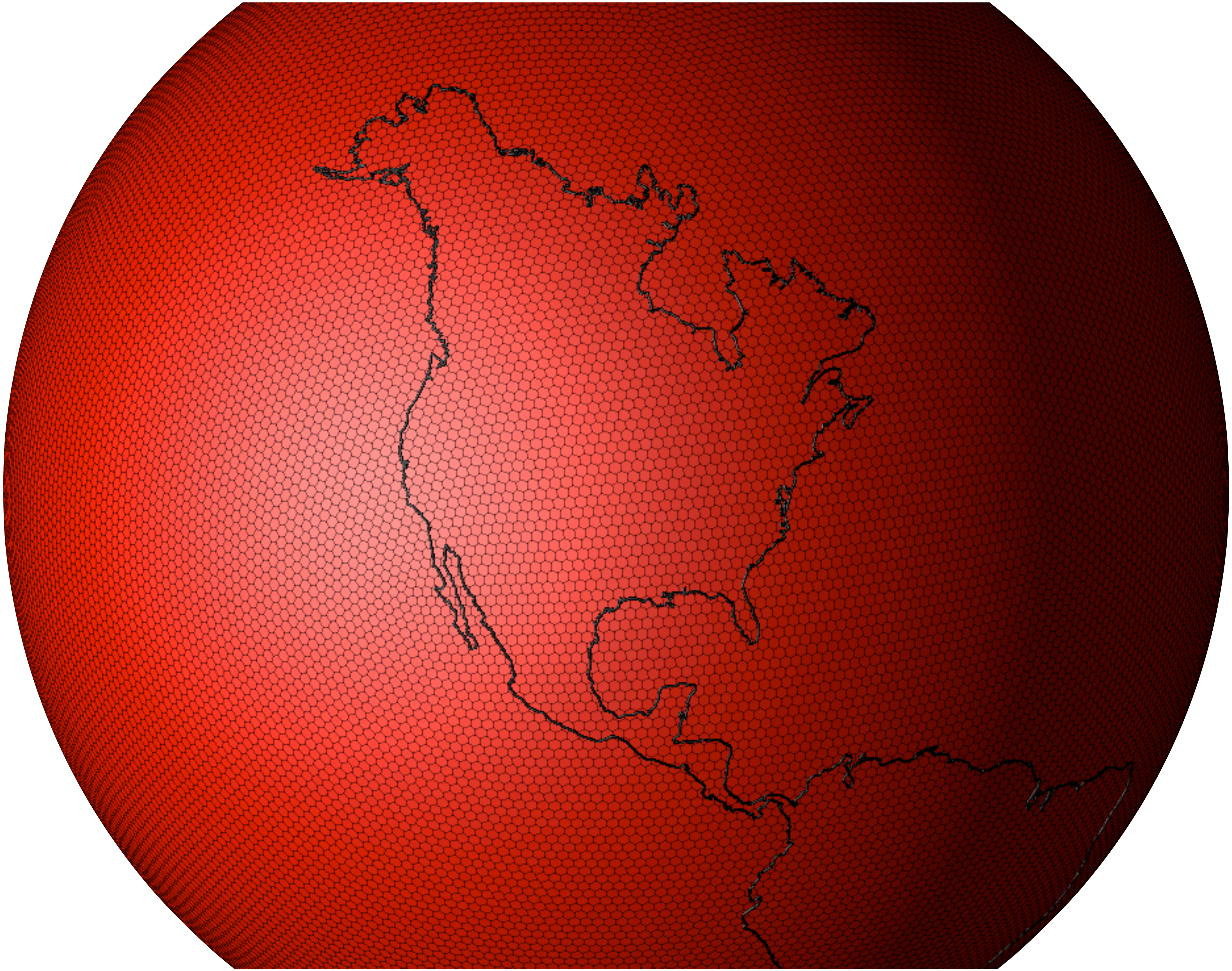
We would like to have the ability to statically refine the mesh in order to improve the local (and global?) simulation.

This improvement arises primarily from the regional improvement of specific physical processes (e.g. cloud-process in the atmosphere and geostrophic-eddy processes in the ocean.)



Variable Resolution Mesh

(oceanographers: please shift mesh ~120 degrees to the east!)



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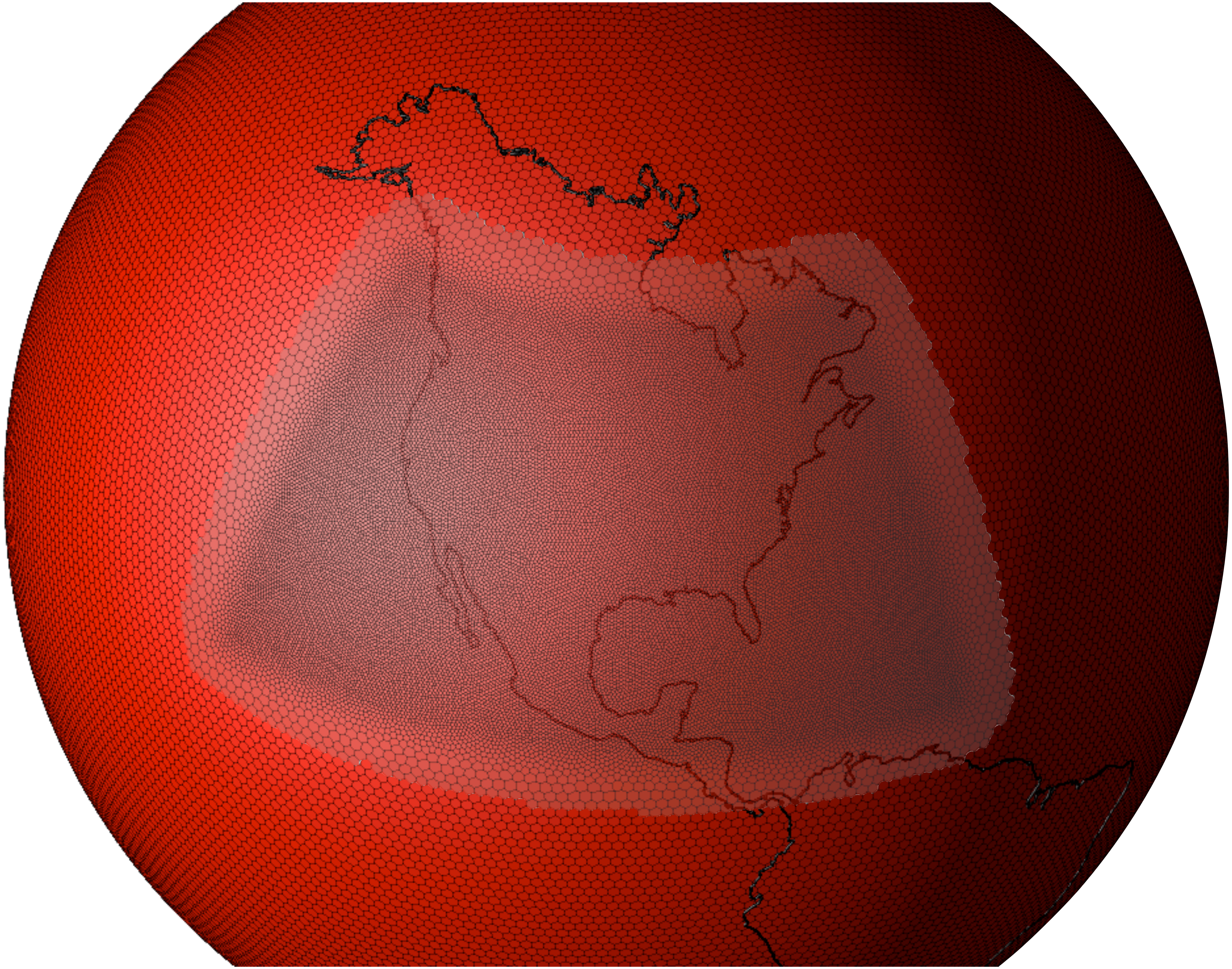
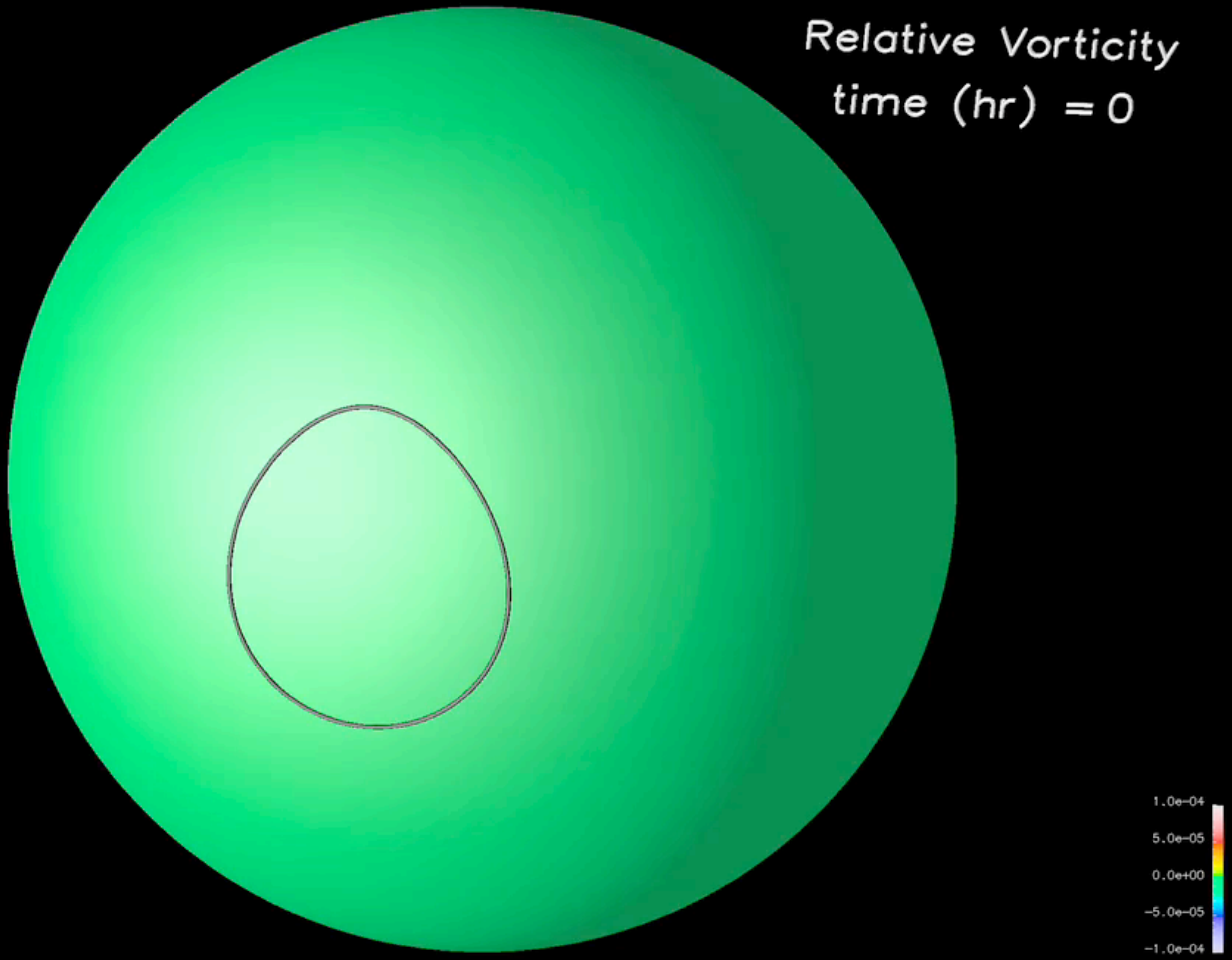


SWTC#5, 100 day integration, variable-res mesh

potential enstrophy dissipation with 100 day time scale

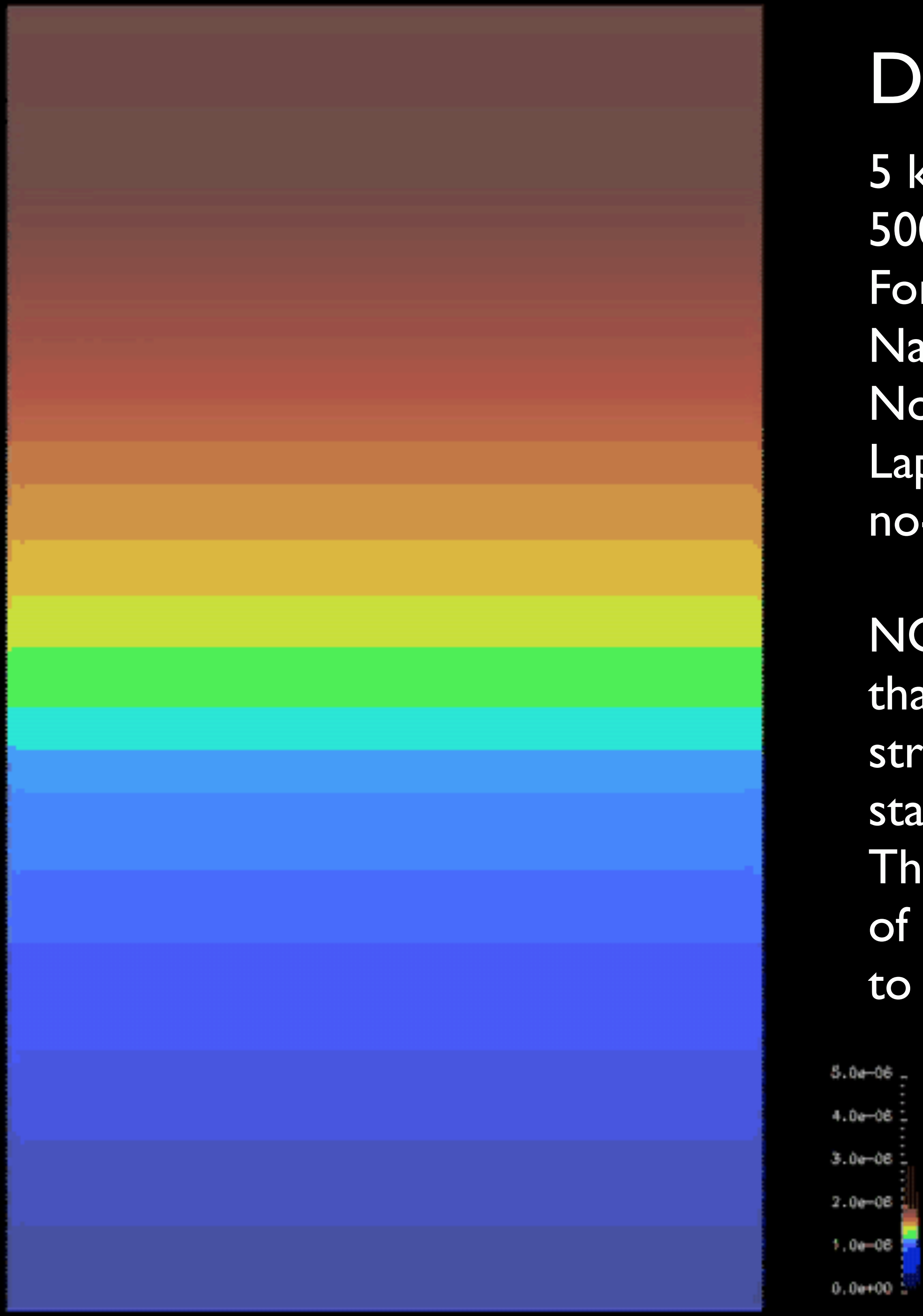
energy conserved to 1e-8



NOTE: The grid-scale phenomena at t=0 is due to geostrophic adjustment, i.e. the numerical model responding to imperfect balance at t=0. As appropriate, this results in gravity and Rossby waves that disperse as the flow attains geostrophic balance.

NOTE: Each grid cell is drawn as polygon and shaded with a single color. Thus, data is shown without interpolation. No dissipation or other "closure" is used, including in the mesh transition zone.

http://public.lanl.gov/ringler/movies/2009/APVM_var.mov



Potential Vorticity: one frame per day

http://public.lanl.gov/ringler/movies/2009/eddies_18.mov

Double-Gyre Problem

5 km mesh
5000 km x 2500 km domain
Forcing consistent with Greatbatch and Nadiga (2000).
No bottom drag
Laplacian mixing on velocity at 1.0 m^2/s
no-slip boundary conditions

NOTE: The purpose here is to confirm that the numerical scheme can handle strong eddy activity without the need for stabilization through ad hoc dissipation. The scheme is stable for a very wide range of dissipations, even those that clearly lead to an underdamped system.

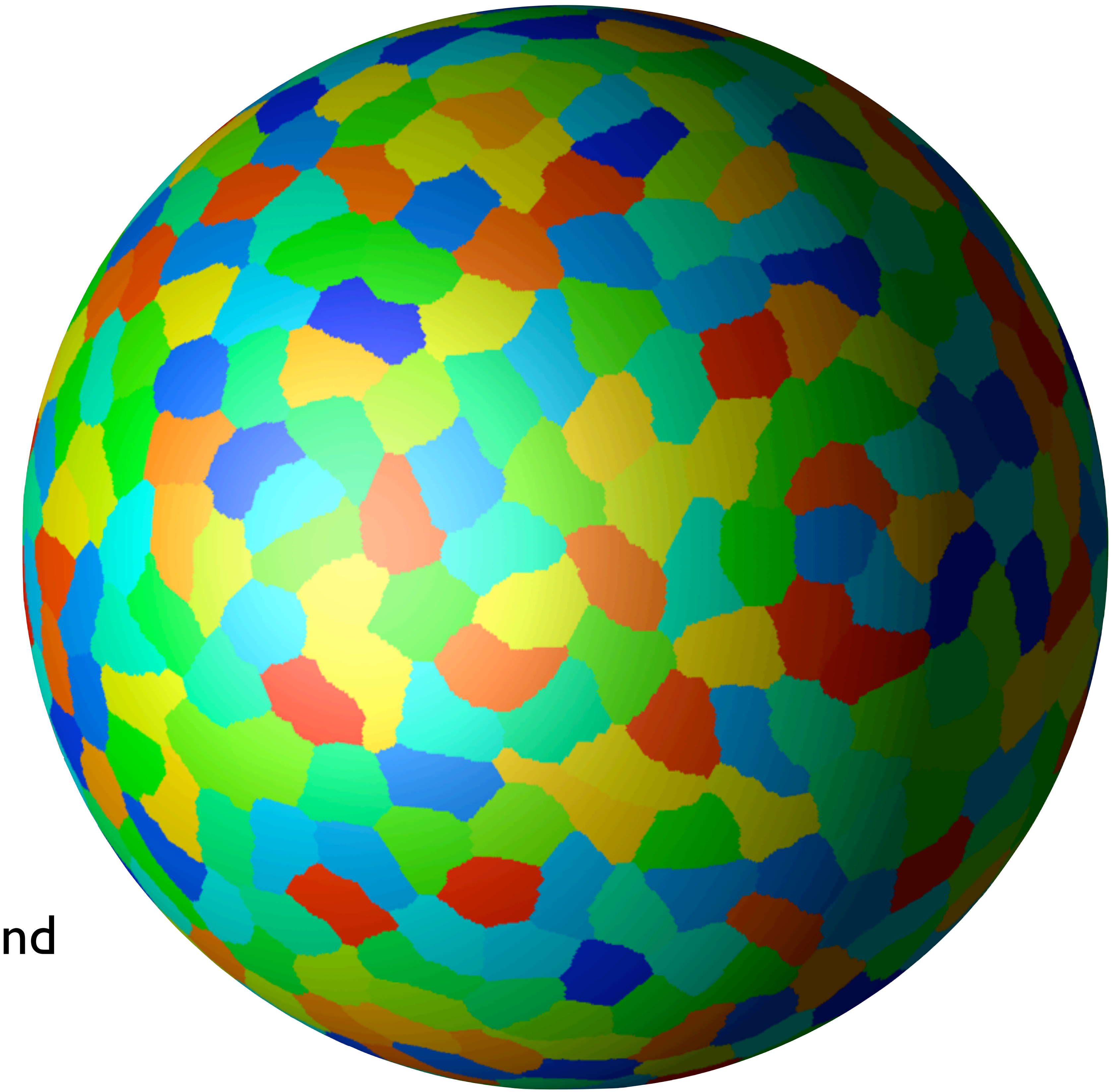
How is this implemented into a high-performance computing environment?

Decomposition for implementation on MPPs.

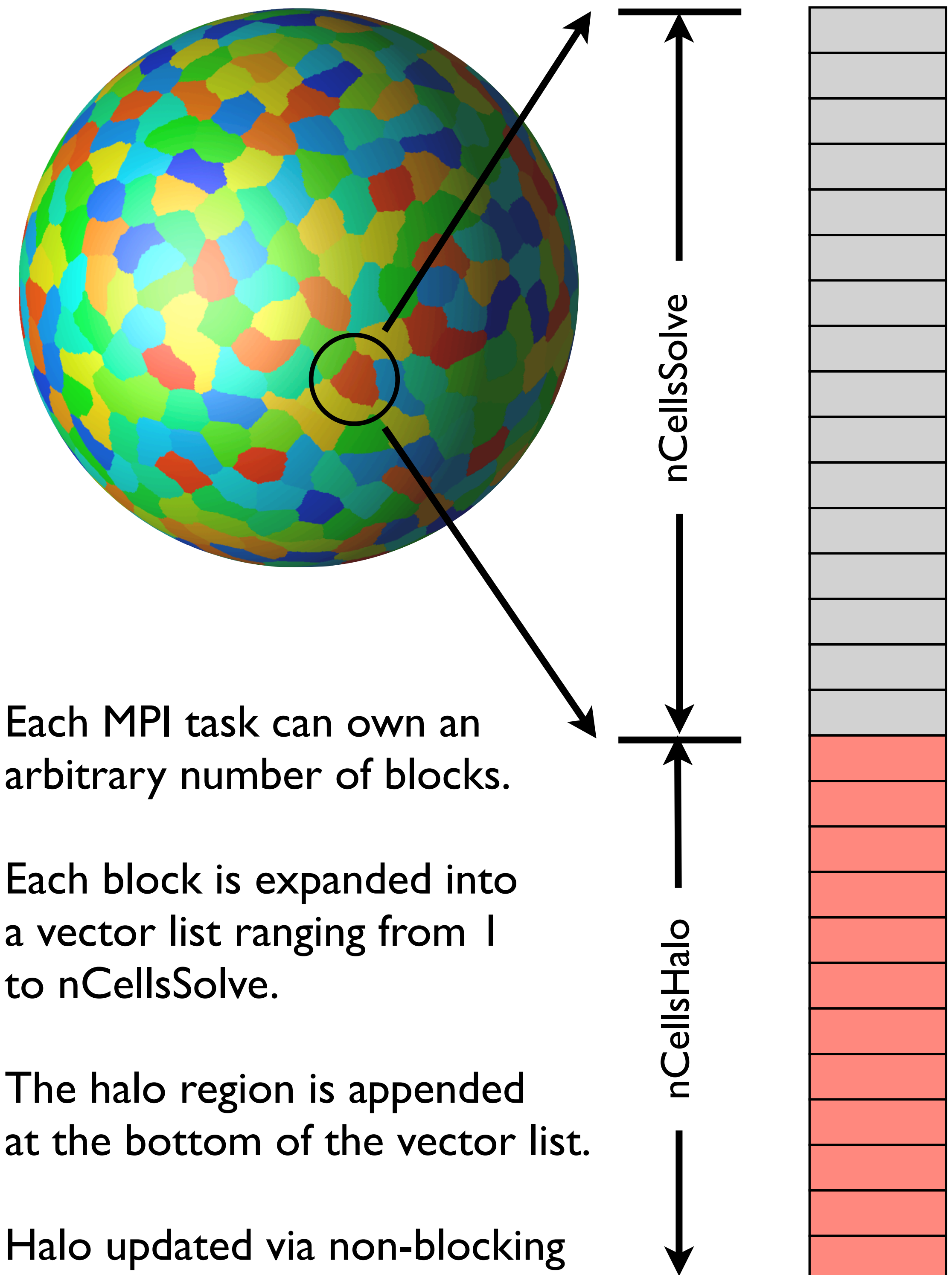
Horizontal decomposition is done with METIS.

At present, each processor gets one block. In the future, each processor will own multiple blocks to improve cache reuse.

We will be supporting multiple climate system model components under this single software frame-work: atmosphere, ocean, and (in all likelihood) ice sheet.



Data Layout: Unstructured in horizontal, structured in vertical: Creating a data structure to exploit hybrid computing architectures.



Each MPI task can own an arbitrary number of blocks.

Each block is expanded into a vector list ranging from 1 to nCellsSolve.

The halo region is appended at the bottom of the vector list.

Halo updated via non-blocking sends.

nCellsTotal = nCellsSolve + nCellsHalo

The ordering of the cells is determined by Reverse Cuthill-McKee (RCM) to maximize cache reuse.

The data access pattern in repeated in the vertical leading to arrays dimensioned as

mass(nVertLevels, nCellsTotal, nBlocks)

Example: sum mass at neighbors cells, each proc executes

```
do iBlock = 1, nBlocks
 do i = 1 , nCellsSolve(iBlock)
   do j=1,nCellsOnCell(i,iBlock)
        coc = cellsOnCell(i,j,iBlock)
        do k=1,nVertLevels
           r(k,i) = r(k,i) + mass(k,coc,iBlock)
        enddo
   enddo
 enddo
enddo
```

The vertical loop is always the inner most loop to vectorize and to limit indirect addressing.

The layout is repeated for variables that live at vertices and at edges.

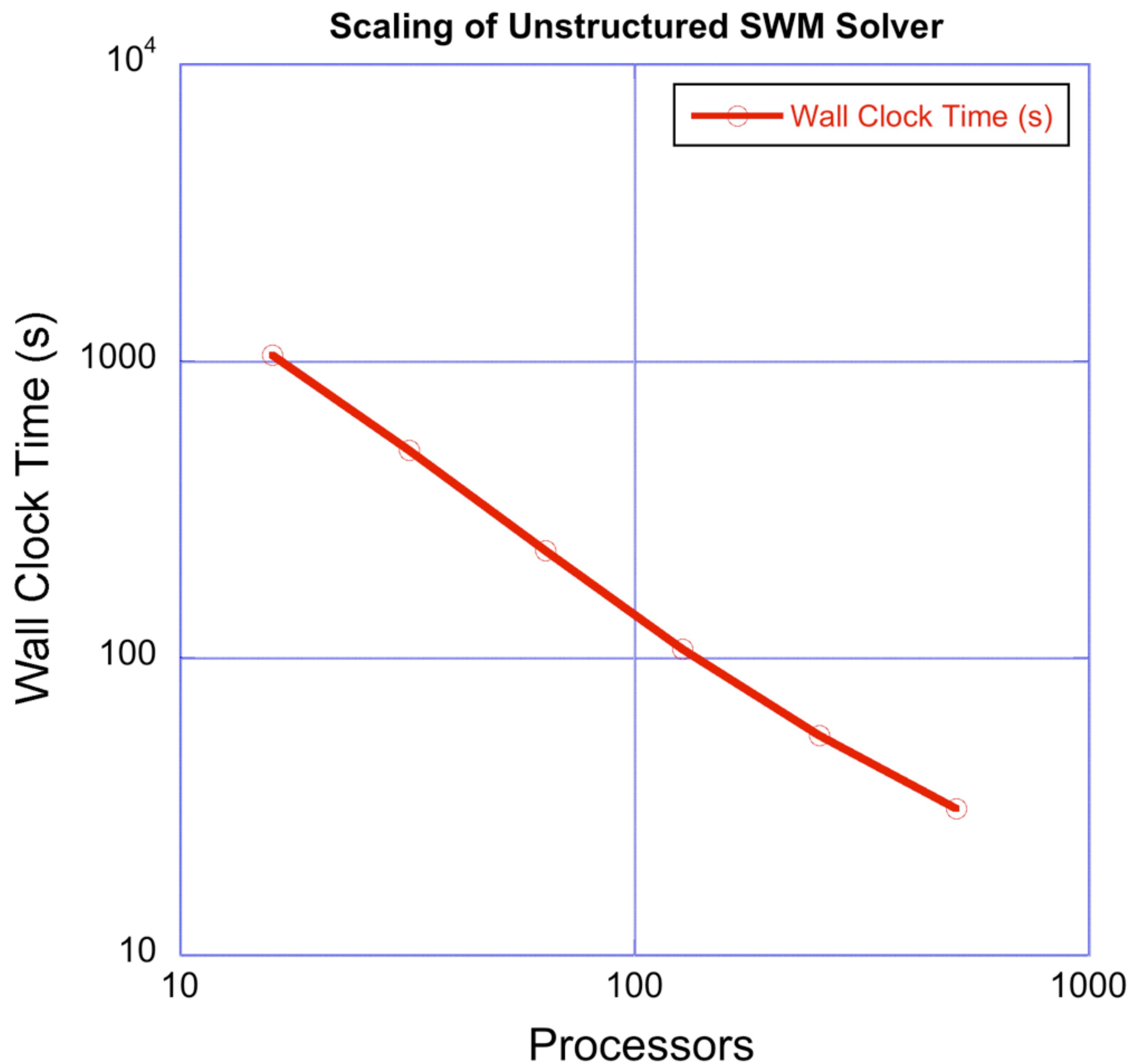
Preliminary scaling results of SWM with global 30 km mesh.

Super-linear scaling out to 512.

This is about 1000 cells per processor. Yet we have not implemented any flop-intensive parts of the model, such as model physics, high-order transport, or 10 to 100 tracer constituents.

Weak scaling at the level observed with POP (200 horizontal cells per processor) seems readily attainable here. Especially since we anticipate no global reductions.

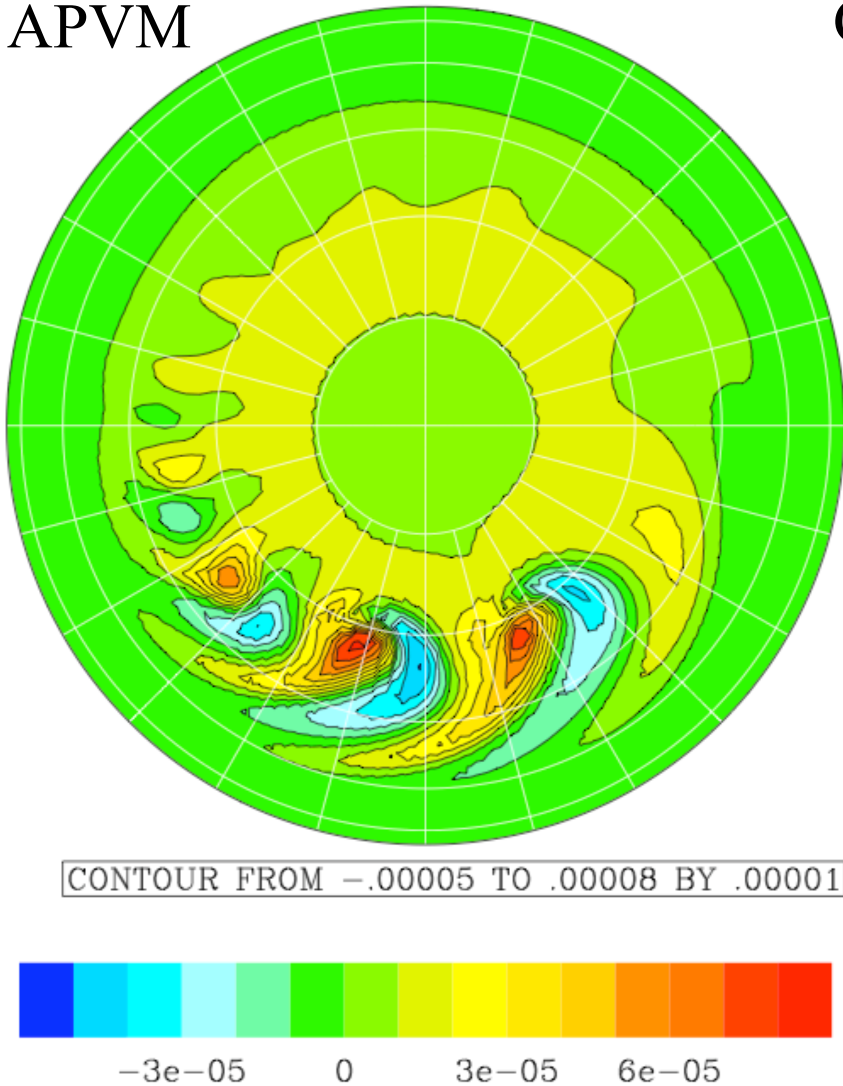
NOTE: Scaling results reproduced up to 1024 processors on Ranger with global 15 km mesh. (Duda)



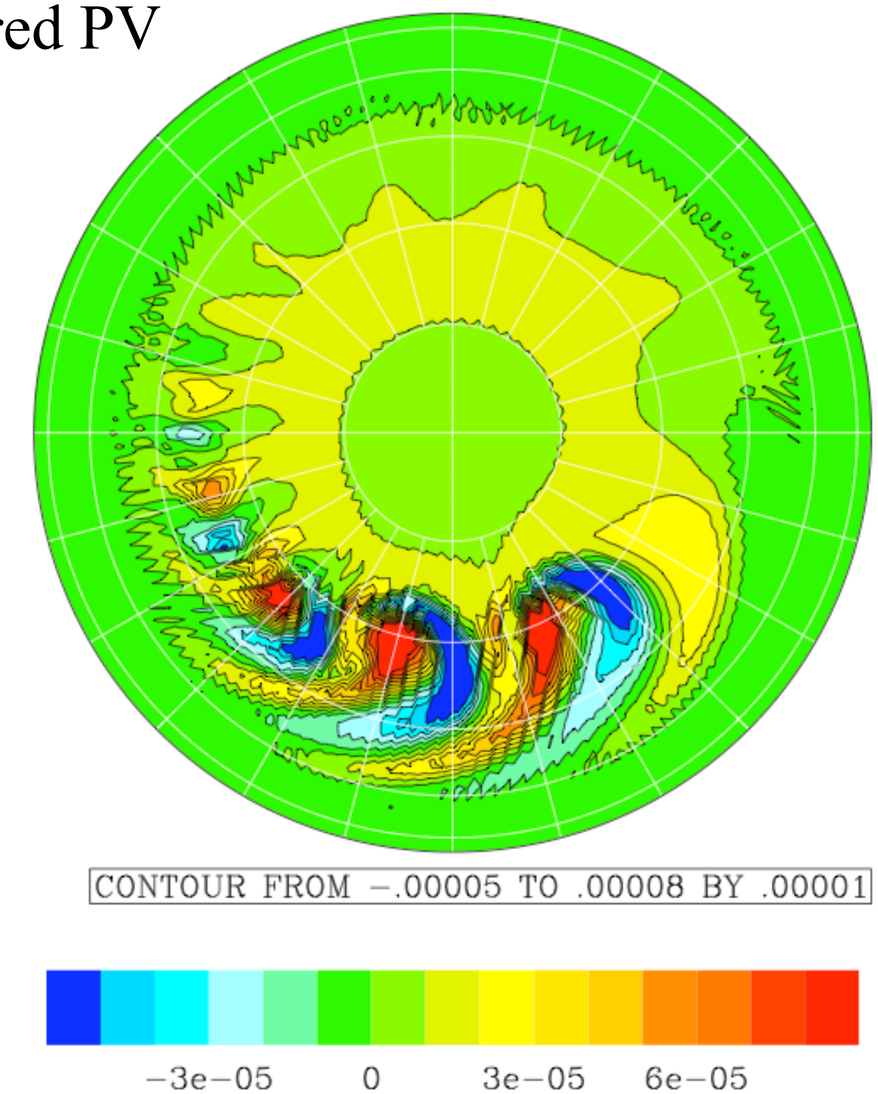
Lobo: AMD Opteron cores for computation, using an Infiniband interconnect. 272x16-core nodes for production capacity computing. Each node has 32 GB of non-uniform-access memory. CPUs run at 2.2 Ghz and have 0.5-MB L2.

Some results from MPI visit - hydrostatic MPAS core

APVM



Centered PV



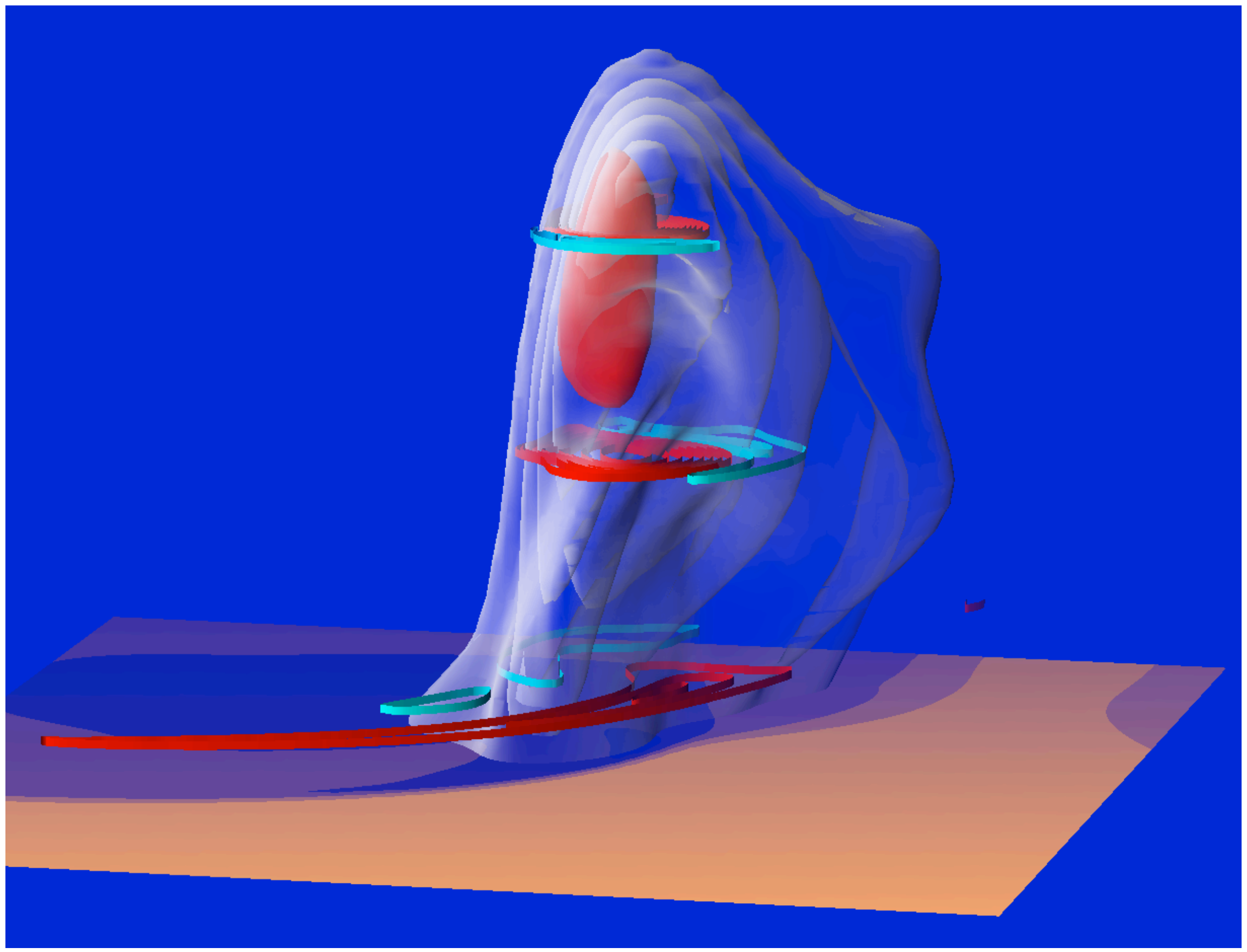
Jablownowski and Williamson baroclinic-wave test case
Relative vorticity (1/s), day 9, at ~850 hPa, 10262 cells

MPI, 10 November 2009

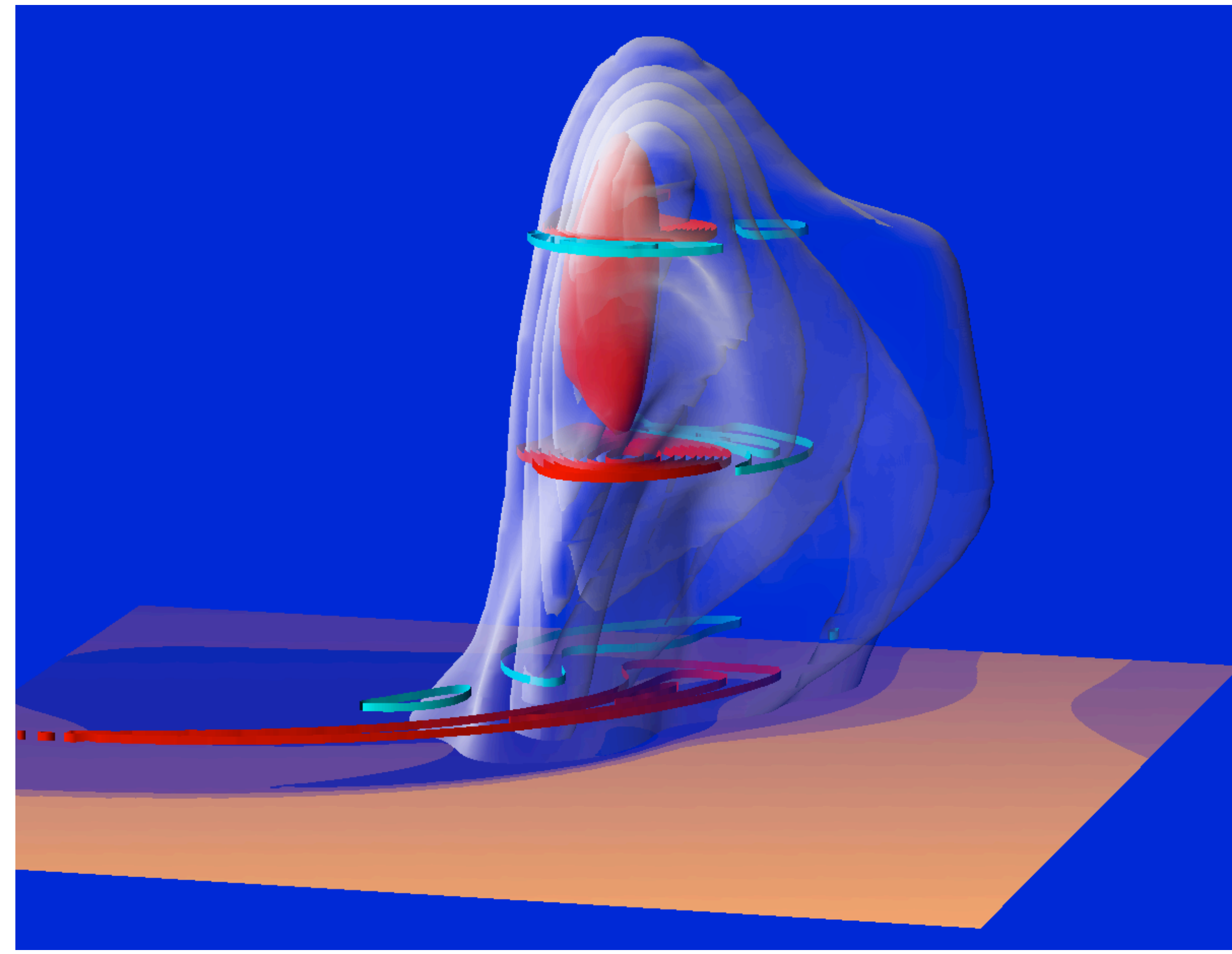
From Skamarock, implementation of numerical scheme as a hydrostatatic atmosphere dynamical core.

3-D Supercell Simulation ~500 m Horizontal Grid

Rectangular Grid



Hexagonal Grid



Vertical velocity contours at 1, 5, and 10 km (c.i. = 3 m/s)

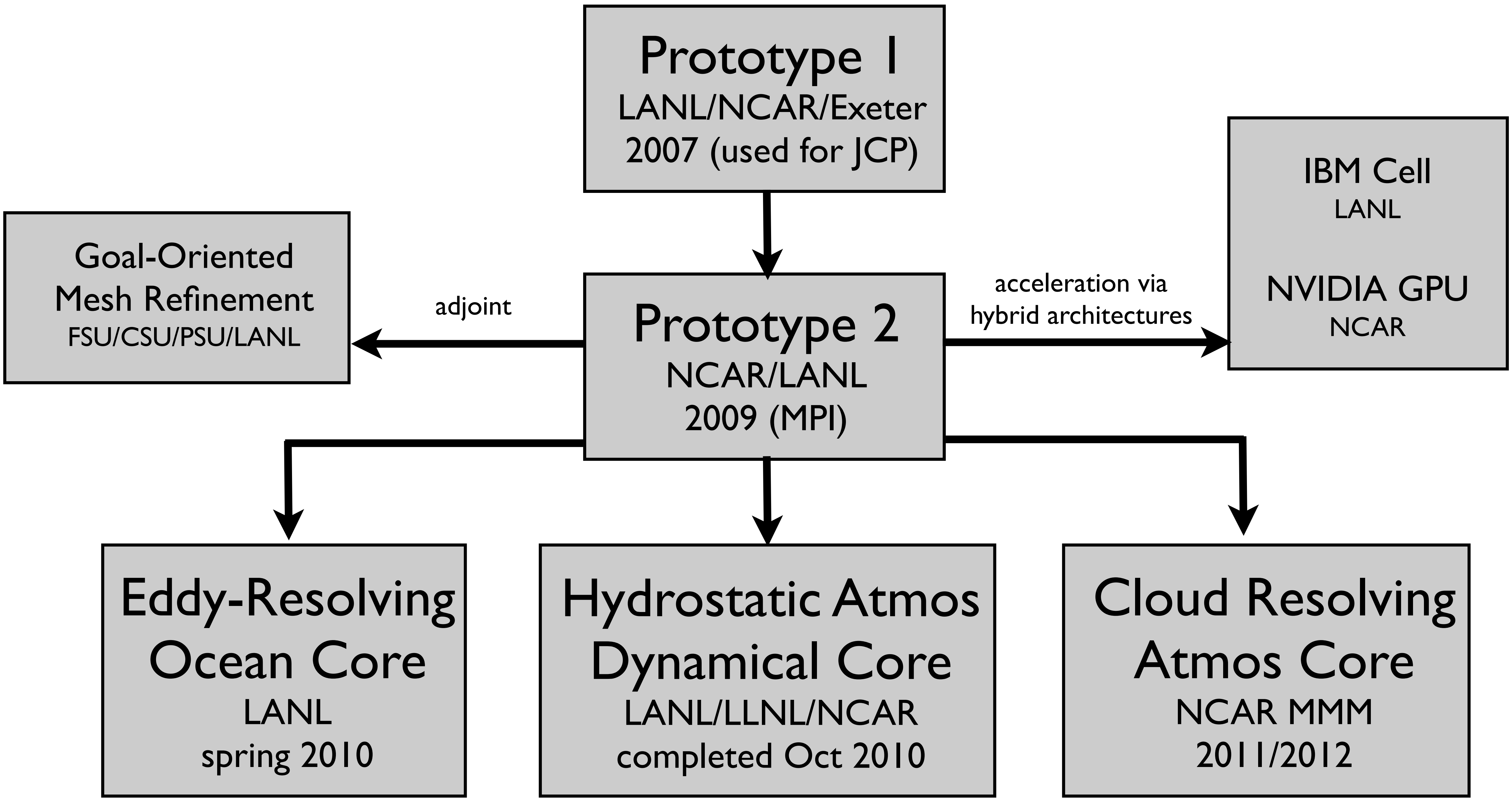
30 m/s vertical velocity surface shaded in red

Rainwater surfaces shaded as transparent shells

Perturbation surface temperature shaded on baseplane

From Klemp, implementation of numerical scheme as a cloud resolving model

Proposed Development Path



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What is the method?

1. The method is a C-grid staggering that conserves total energy and PV. In addition it allows for the direct control over the evolution of PV through the discretization of the nonlinear Coriolis force.

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What are the benefits?

1. The method can be implemented on POP stretched grid with no modification, so backward compatibility in terms of meshes, boundary conditions, etc. is supported.
2. The ability to conduct regionally eddy-resolving simulations within the framework of a global model.
3. The ability to more precisely position degrees of freedom to improve simulation, for example equatorial regions and overflow regions.
4. The opportunity to incorporate (either explicitly or conceptually) a set of forward-looking ideas related to hybrid computing, LANS-alpha sub-grid closure, high-order transport, immersed boundary method, layered modeling and implicit time stepping.
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What are the disadvantages?

1. Getting use to a new software framework.

Manuscripts available ...

http://public.lanl.gov/ringler/publications.html

- Ringler, T., J. Thuburn, J. Klemp and W. Skamarock, 2009: Numerical treatment of energy and potential vorticity on arbitrarily structured C-grids, Journal of Computational Physics, accepted. (pdf).
- Thuburn, J., T. Ringler, J. Klemp and W. Skamarock, 2009: Numerical representation of geostrophic modes on arbitrarily structured C-grids, Journal of Computational Physics, 2009: 228 (22), 8321-8335. doi:10.1016/j.jcp.2009.08.006 (link)
- Ju, L., T. Ringler and M. Gunzburber, 2009, Voronoi Diagrams and their Application in Climate Science, Numerical Techniques for Global Atmospheric Models, Lecture Notes in Computational Science, draft. (pdf).
- Ringler, T., L. Ju and M. Gunzburger, 2008, A multiresolution method for climate system modeling: application of spherical centroidal Voronoi tessellations, Ocean Dynamics, 58 (5-6), 475-498. doi: 10.1007/s10236-008-0157-2 (link)
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extra

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4. The same core numerical algorithm appears appropriate for both eddy-resolving ocean simulations and cloud-resolving atmosphere simulations. (As it should be).