An update on model development

Ross Heikes, C.S. Konor and D. Randall

Dept. of Atmospheric Science
Colorado State University

Office of Science

SciDAC
Scientific Discovery through Advanced Computing

CMMAP
Reach for the sky.

Overview of two parts...

PART 1. Some insight into to the 3D elliptic solver and ways to improve convergence

PART 2. A ***new*** sigma coordinate dynamical core.

Possible strategy to improvement the 3D elliptic solver

- The non-hydrostatic model requires the solution to a 3D poisson equation.
- We currently use standard multigrid methods in the horizontal direction coupled with a line relaxation in the vertical direction.
- This approach works ok as shown in previous numerical results.
- However, by examining the characteristics of the system of linear equations we can gain insight to improve the algorithm.

The cells range from very flat to not so flat

Let δx be the average distance between cell centers and δz be the layer thickness.

Define

$$\text{aspect ratio} \equiv \frac{\delta x}{\delta z}$$

The aspect ratio for various configurations

	grd05 δx=239.8(km)	grd06 δx=119.9(km)	grd07 δx=59.96(km)	grd08 δx=29.98(km)	grd09 δx=14.99(km)	grd10 δx=7.495(km)	grd11 δx=3.747(km)	grd12 δx=1.874(km)
km= 32, δz=1000(m)	239.812	119.915	59.9584	29.9793	14.9897	7.49485	3.74742	1.87371
km= 64, δz= 500(m)	479.623	239.829	119.917	59.9587	29.9794	14.9897	7.49485	3.74742
km=128, δz= 250(m)	959.247	479.659	239.834	119.917	59.9588	29.9794	14.9897	7.49485
km=256, δz= 125(m)	1918.49	959.317	479.667	239.835	119.918	59.9588	29.9794	14.9897

There is a considerable range of aspect ratios depending on the simulation:

~400 to 800 for bottom V-cycle multigrid

~100 to 200 for large scale simulations. (Jablonowski, HS)

~1 to 10 for small scale simulations. (bubble tests)

Wish to design the solver that can adapt to any particular problem

The Poisson equation with constant coefficients

Continuous form:

$$\nabla_H^2 \alpha + \frac{\partial^2 \alpha}{\partial z^2} = \beta$$

Discrete form:

k = 1

$$\frac{1}{A_i}\sum_{i'}\frac{\alpha_{i+i',k}-\alpha_{i,k}}{L_{i;i+i'}}l_{i;i+i'} + \frac{1}{(\delta z)_k}\frac{\alpha_{i,k+1}-\alpha_{i,k}}{(\delta z)_{k+1/2}} = \beta_{i,k}$$

$$\frac{1}{A_i}\sum_{i'}\frac{l_{i;i+i'}}{L_{i;i+i'}}\alpha_{i+i',k} + \frac{1}{(\delta z)_k(\delta z)_{k+1/2}}\alpha_{i,k+1} - \left(\frac{1}{A_i}\sum_{i'}\frac{l_{i;i+i'}}{L_{i;i+i'}} + \frac{1}{(\delta z)_k(\delta z)_{k+1/2}}\right)\alpha_{i,k} = \beta_{i,k}$$

k = 2,…, km - 1

$$\frac{1}{A_i}\sum_{i'}\frac{\alpha_{i+i',k}-\alpha_{i,k}}{L_{i;i+i'}}l_{i;i+i'} + \frac{1}{(\delta z)_k}\left[\frac{\alpha_{i,k+1}-\alpha_{i,k}}{(\delta z)_{k+1/2}} - \frac{\alpha_{i,k}-\alpha_{i,k-1}}{(\delta z)_{k-1/2}}\right] = \beta_{i,k}$$

$$\frac{1}{A_i}\sum_{i'}\frac{l_{i;i+i'}}{L_{i;i+i'}}\alpha_{i+i',k} + \frac{1}{(\delta z)_k(\delta z)_{k+1/2}}\alpha_{i,k+1} - \left(\frac{1}{A_i}\sum_{i'}\frac{l_{i;i+i'}}{L_{i;i+i'}} + \frac{1}{(\delta z)_k(\delta z)_{k+1/2}} + \frac{1}{(\delta z)_k(\delta z)_{k-1/2}}\right)\alpha_{i,k} + \frac{1}{(\delta z)_k(\delta z)_{k-1/2}}\alpha_{i,k-1} = \beta_{i,k}$$

k = km

$$\frac{1}{A_i}\sum_{i'}\frac{\alpha_{i+i',k}-\alpha_{i,k}}{L_{i;i+i'}}l_{i;i+i'} - \frac{1}{(\delta z)_k}\frac{\alpha_{i,k}-\alpha_{i,k-1}}{(\delta z)_{k-1/2}} = \beta_{i,k}$$

$$\frac{1}{A_i}\sum_{i'}\frac{l_{i;i+i'}}{L_{i;i+i'}}\alpha_{i+i',k} - \left(\frac{1}{A_i}\sum_{i'}\frac{l_{i;i+i'}}{L_{i;i+i'}} + \frac{1}{(\delta z)_k(\delta z)_{k-1/2}}\right)\alpha_{i,k} + \frac{1}{(\delta z)_k(\delta z)_{k-1/2}}\alpha_{i,k-1} = \beta_{i,k}$$

When the area of the cells is large, the coefficients linking grid points in the horizontal direction become very small.

The Poisson equation written in matrix form. Multigrid nutshell.

The Poisson equation written in matrix form

$$\mathbf{A}\boldsymbol{\alpha} = \boldsymbol{\beta}$$

Suppose there exists a sequence of approximate solutions which converges to the true solution

$$\left\{\boldsymbol{\alpha}^{(1)}, \boldsymbol{\alpha}^{(2)}, \boldsymbol{\alpha}^{(3)}, \ldots, \boldsymbol{\alpha}^{(\kappa-1)}, \boldsymbol{\alpha}^{(\kappa)}, \ldots\right\}$$

The residual $\mathbf{r}^{(\kappa)}$ for an approximate solution $\boldsymbol{\alpha}^{(\kappa)}$ is given by

$$\mathbf{r}^{(\kappa)} = \boldsymbol{\beta} - \mathbf{A}\boldsymbol{\alpha}^{(\kappa)} = \mathbf{A}\boldsymbol{\alpha} - \mathbf{A}\boldsymbol{\alpha}^{(\kappa)} = \mathbf{A}\mathbf{e}^{(\kappa)}$$

where the error $\mathbf{e}^{(\kappa)}$ is the difference between the true solution $\boldsymbol{\alpha}$ and the current approximation $\boldsymbol{\alpha}^{(\kappa)}$

$$\mathbf{e}^{(\kappa)} = \boldsymbol{\alpha} - \boldsymbol{\alpha}^{(\kappa)}$$

If the error is smooth it can be solved for on a coarser grid with little computational effort.

Definitions and concepts

- Borrowed *liberally* from Falgout -- An Introduction to Algebraic Multigrid (2006)
- The two main components of multigrid are **smoothing** and **coarse-grid correction**.
- The **smoother** on the icosahedral grid is a simple pointwise Jacobi method.
- An error not eliminated by the smoother is called a **smooth error**.

> The key to designing an effective (AMG) algorithm is to have a good smooth error characterization.
>
> Smooth error corresponds to eigenvectors of $\mathbf{A}$ associated with small eigenvalues. These are called small eigenmodes.
>
> Smoothing damps large eigenmodes. Coarse-grid correction eliminates the remaining small eigenmodes of $\mathbf{A}$.

- The **near-null space** of $\mathbf{A}$ consists of vectors that are almost linear when plotted on the grid. These vectors are geometrically smooth. Eigenvectors with small associated eigenvalues are such vectors.

> We want to coarsen the grid in the direction of geometric smoothness.
> We can use the eigenvectors to guide the coarse-grid correction process.

Definitions and concepts

- Pointwise relaxation geometrically smooths the error in each direction only if the given problem is essentially isotropic.
- In anisotropic problems smoothing is only in the direction of strong couplings. (Stuben (1999))

Eigenvalues for an example matrix

- For a grid with 642 cells horizontal and 16 layers vertical we can calculate all the eigenvalues and eigenvectors. Earth is smaller. Aspect ratio ~120.

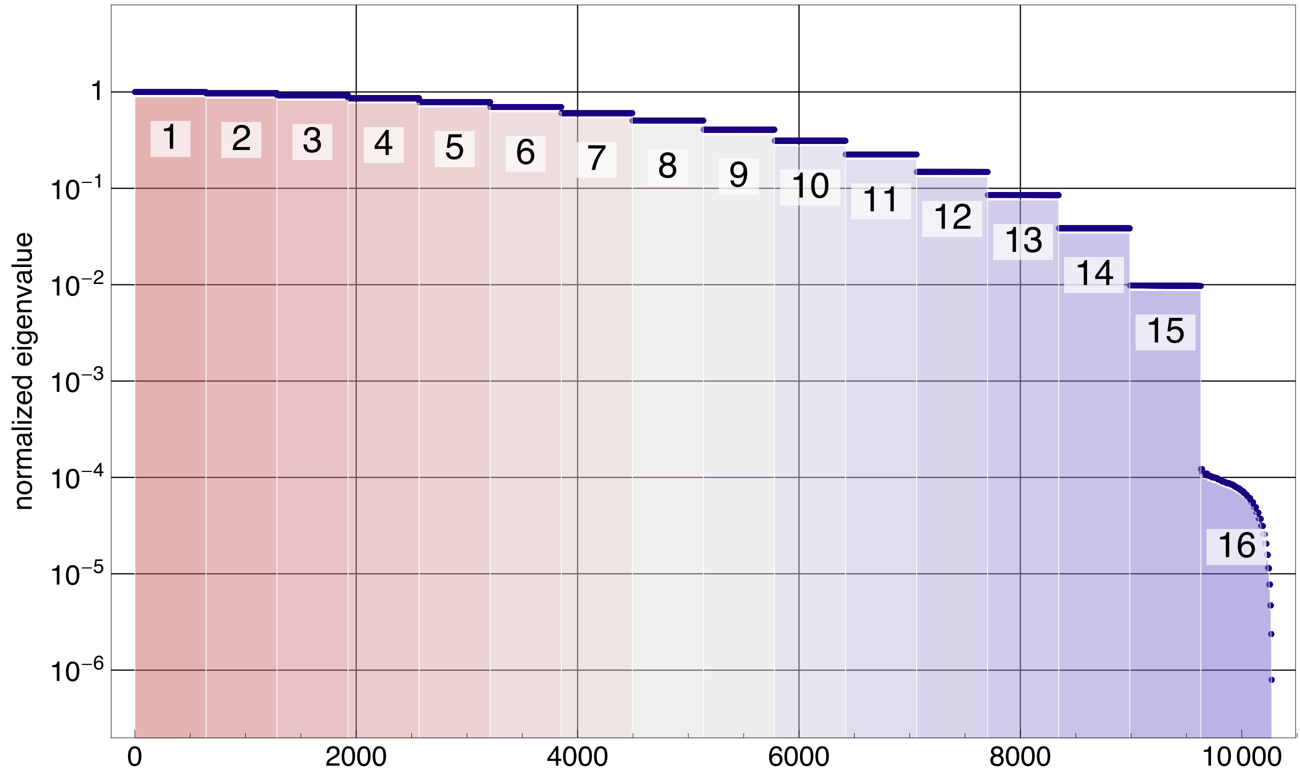
- This plot shows normalized eigenvalues.

- Logarithmic scale

- The ratio

$$\frac{\lambda_{min}}{\lambda_{max}} \approx 10^{-7}$$

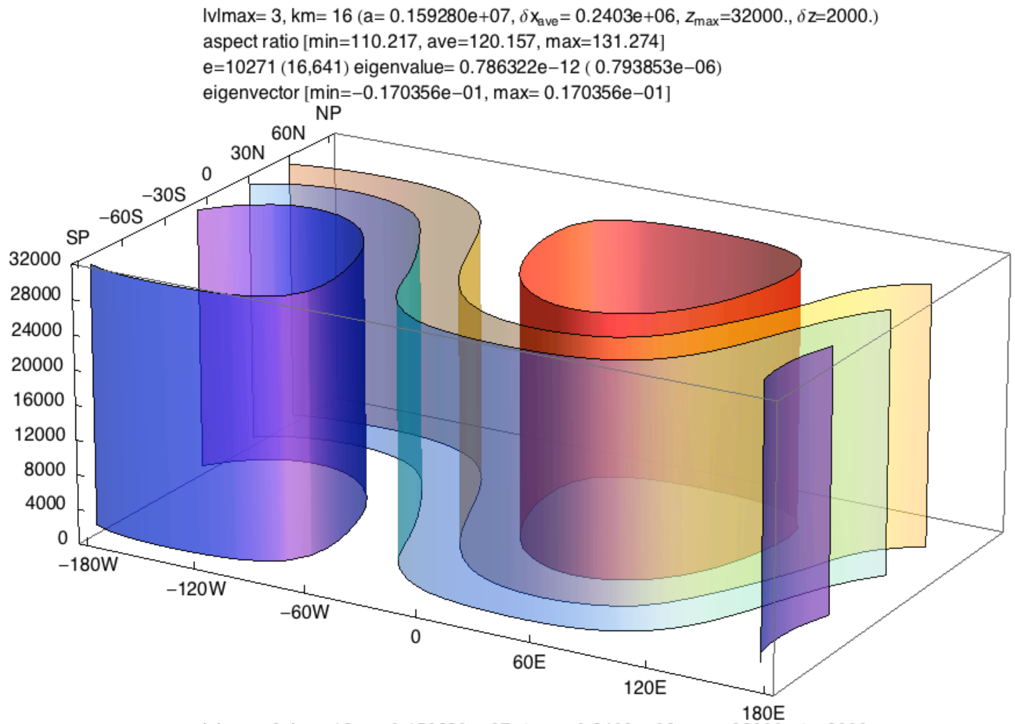
- The ratio is larger when the cell aspect ratio is ≈1

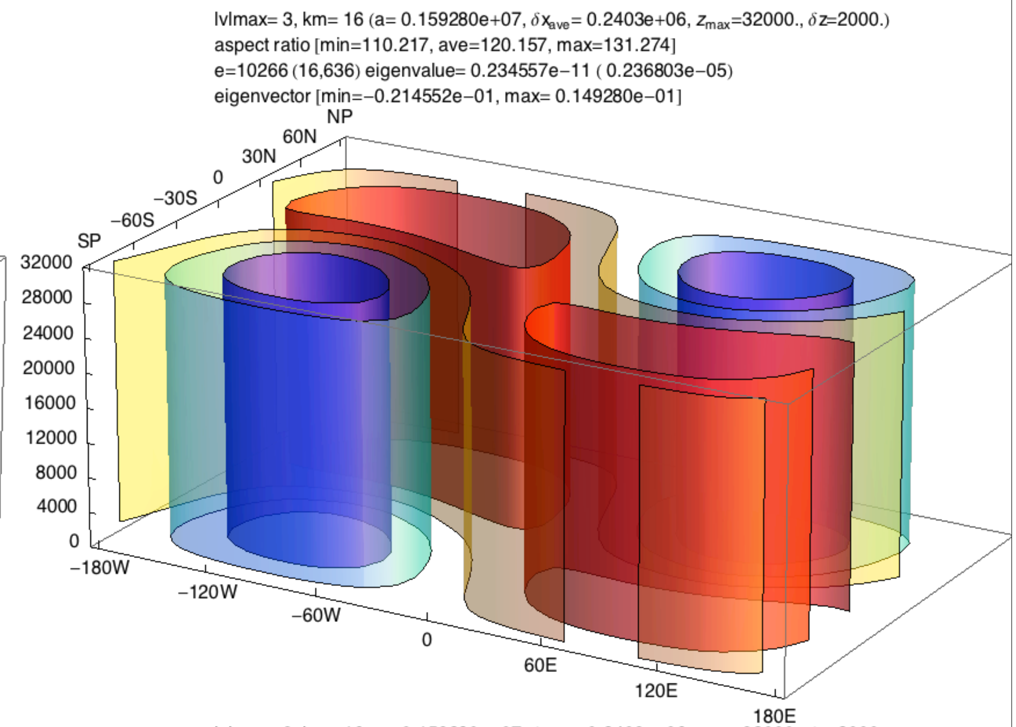


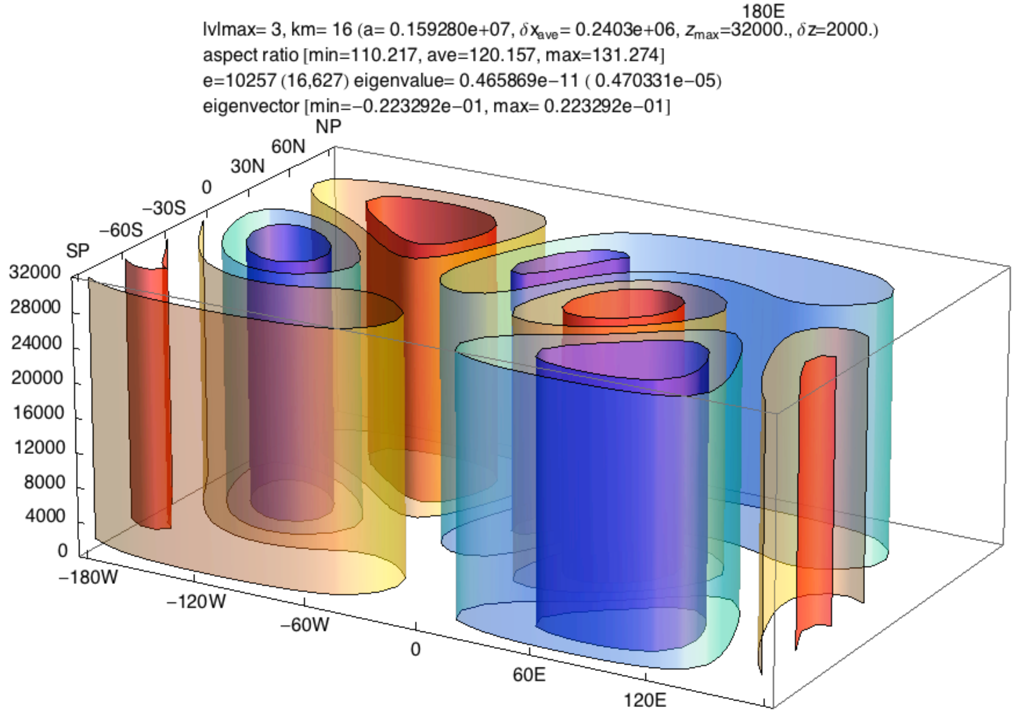
lvlmax= 3, km= 16 (a= 0.159280e+07, δx_{ave}= 0.2403e+06, z_{max}=32000., δz=2000.)
aspect ratio [min=110.217, ave=120.157, max=131.274]
eigenvalue [min= 0.786322e−12, max= 0.990513e−06, ratio= 0.793853e−06] (bliss,3103)

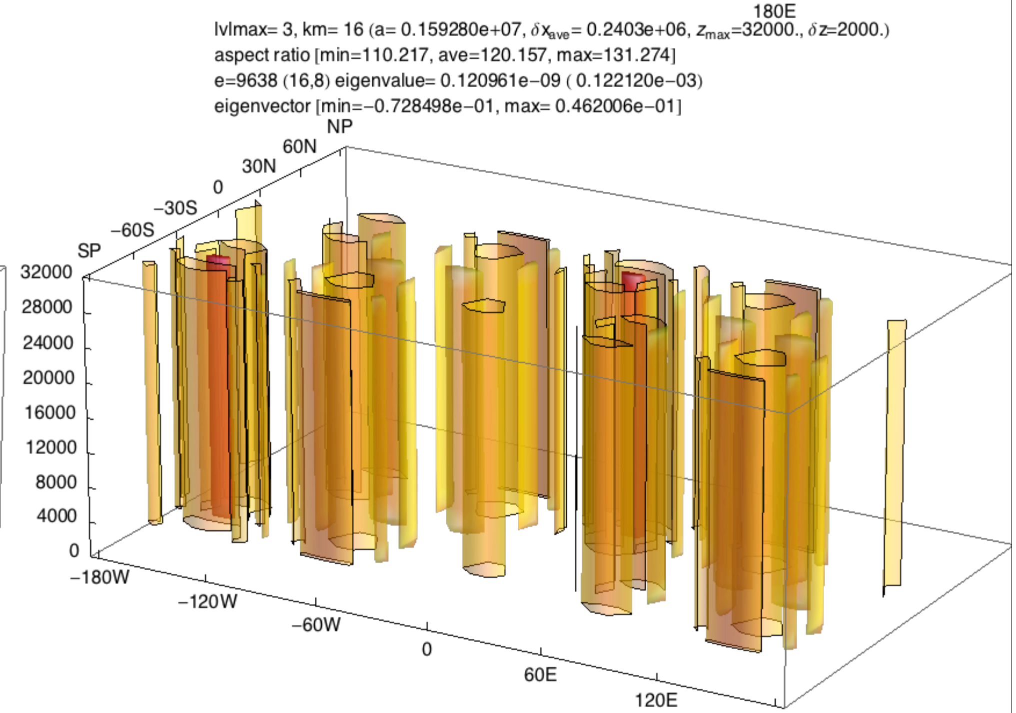
- The group (labeled 16) of eigenvalues is much smaller than the rest.

Eigenvectors from group 16. Smallest eigenvalues have to vertical structure.

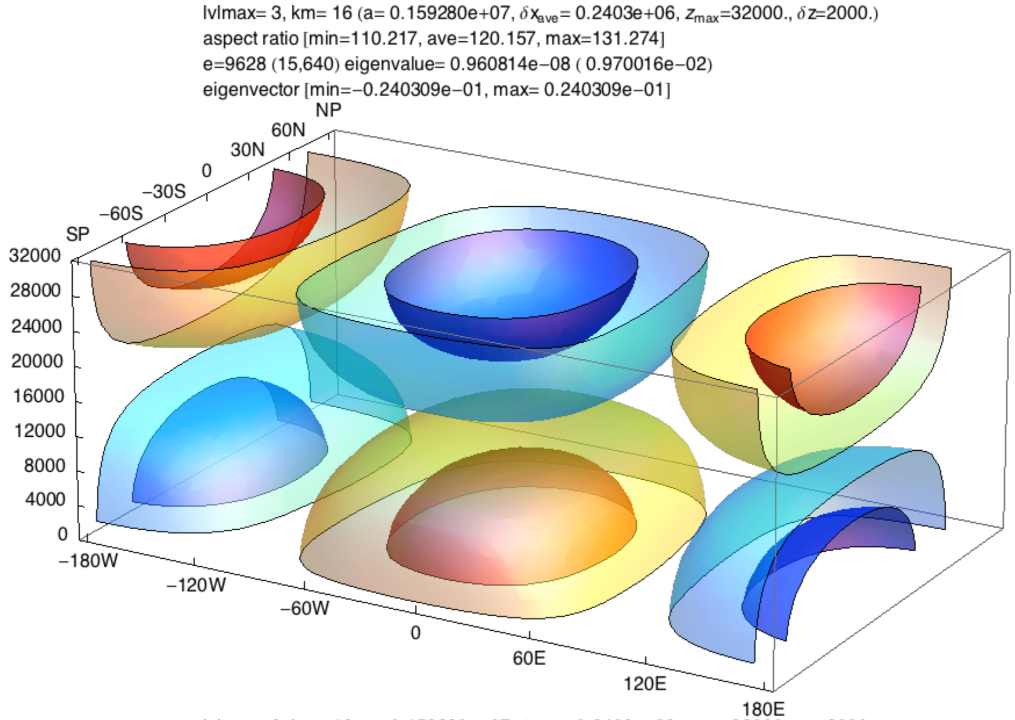


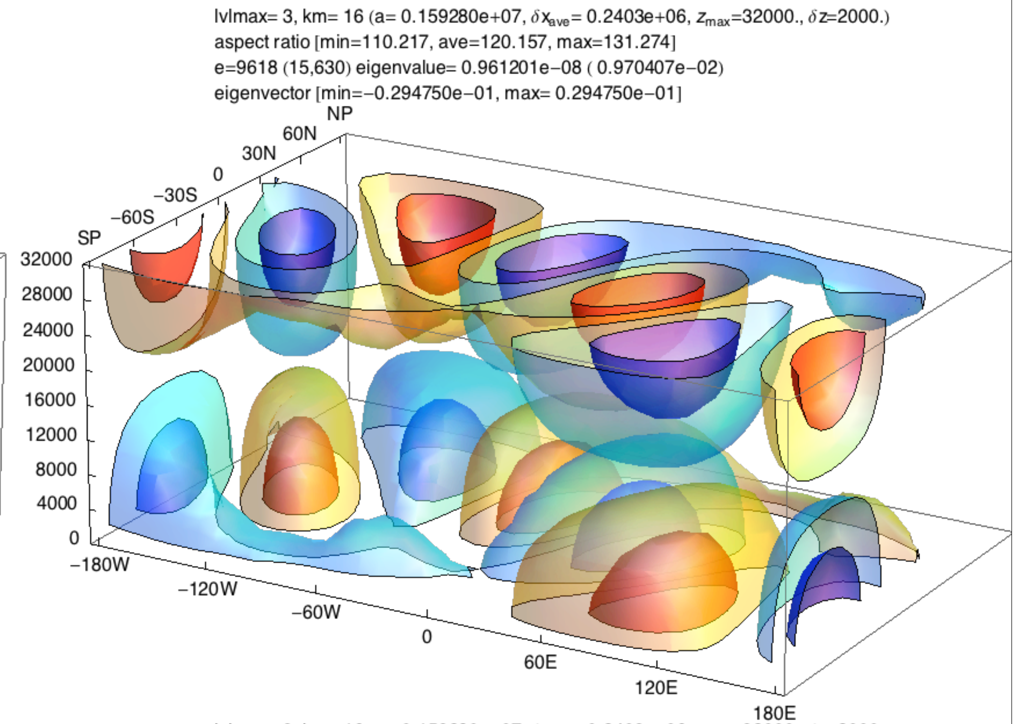


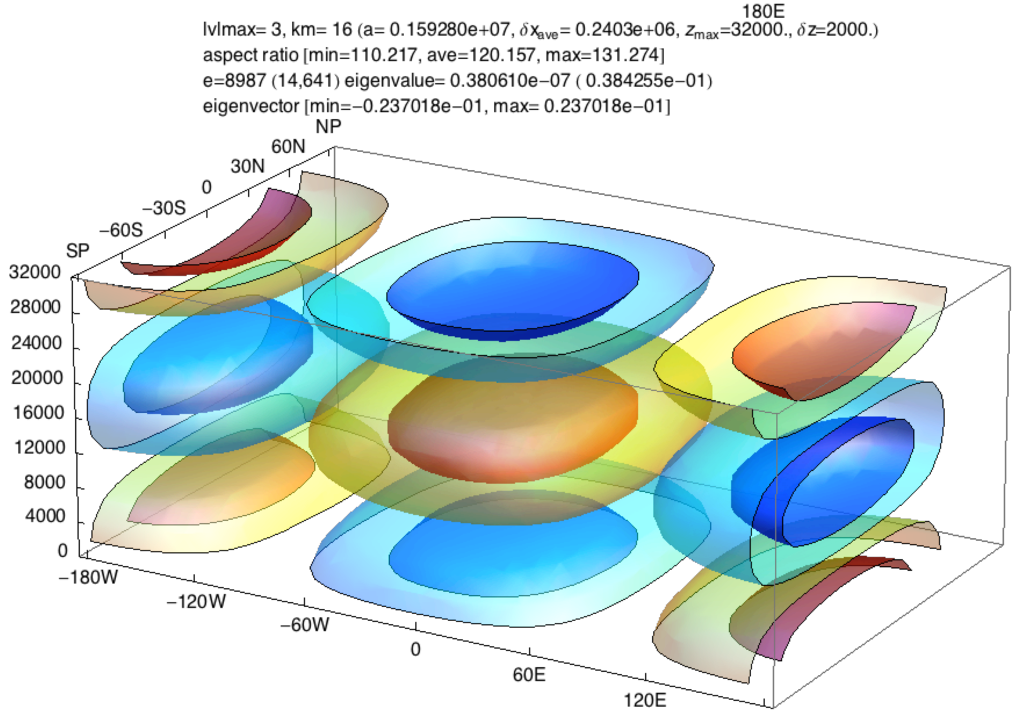


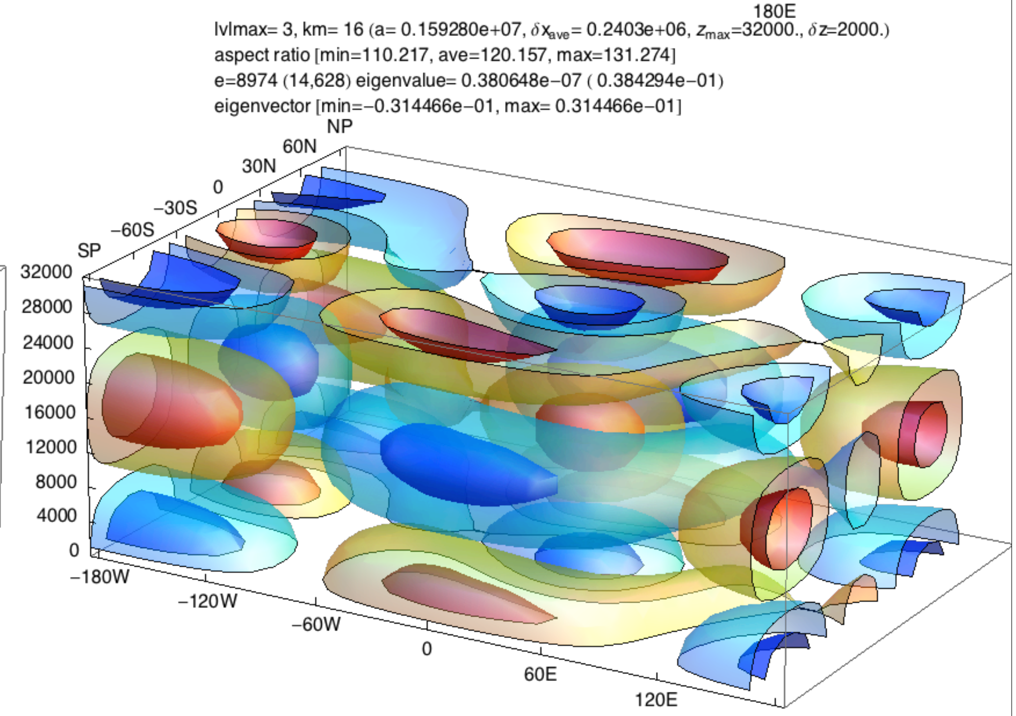


Eigenvectors from group 15 and 14









Conclusions and future work

- By examining the characteristics of the system of linear equations in light of AMG we can gain insight to improve the algorithm.
- It should be possible to tailor the grid coarsening for a given problem. In particular, coarsen in the vertical or horizontal direction.
- Our current approach with vertical line relaxation and horizontal coarsening results in very flat cells which might be causing difficulty.
- Currently modifying the code to allow greater flexibility for coarsening.

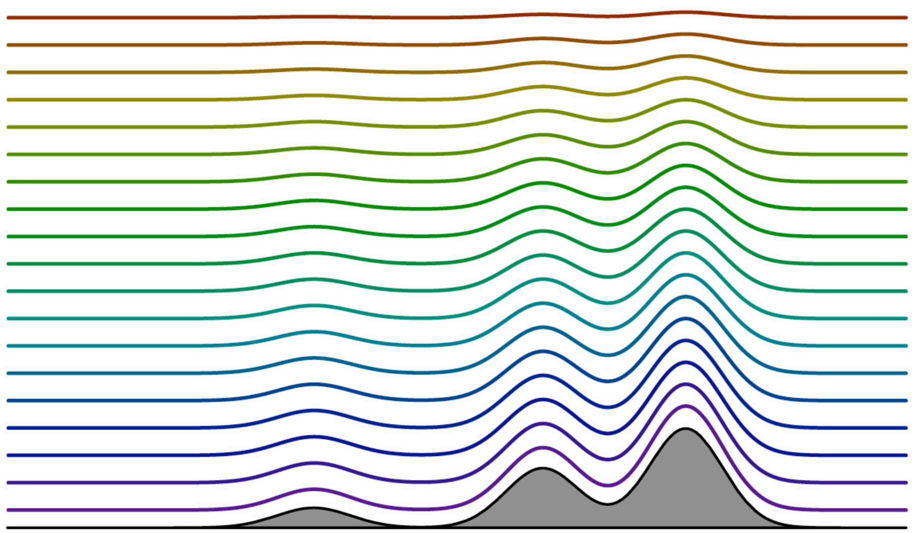
A new sigma coordinate model

- We need to include topography in the model.

- A straightforward way to do this is to use sigma coordinates.

- Defined in the usual way: $$\sigma_{k+1/2} \equiv \frac{\left(p_{qs}\right)_{k+1/2} - \left(p_{qs}\right)_T}{\left(p_{qs}\right)_S - \left(p_{qs}\right)_T}$$

- The surface topography is coincident with the lowest a coordinate surface.



Sigma coordinate model prognostic equations

mass

$$\frac{\partial m}{\partial t} = -\int_0^1 \nabla \bullet \left(m\mathbf{v} \right) d\sigma \quad \text{where} \quad m \equiv \left(p_{qs} \right)_S - \left(p_{qs} \right)_T$$

potential temperature

$$\frac{\partial}{\partial t}\left(m\theta \right) + \nabla \bullet \left(m\theta\mathbf{v} \right) + \frac{\partial}{\partial \sigma}\left(m\theta\dot{\sigma} \right) = \frac{mQ}{c_p \pi_{qs}}$$

vorticity

$$\frac{\partial \eta}{\partial t} + \nabla \bullet \left(\eta\mathbf{v} \right) + \mathbf{k} \bullet \nabla_\sigma \times \left(\dot{\sigma}\frac{\partial \mathbf{v}}{\partial \sigma} \right) = -\mathbf{k} \bullet \nabla_\sigma \times \left[\frac{g}{m}\left(\boldsymbol{\nabla}_\sigma \left(mz \right) - \frac{\partial}{\partial \sigma}\left(z\boldsymbol{\nabla}_\sigma p_{qs} \right) \right) \right] + \mathbf{k} \bullet \nabla_\sigma \times \mathbf{F}$$

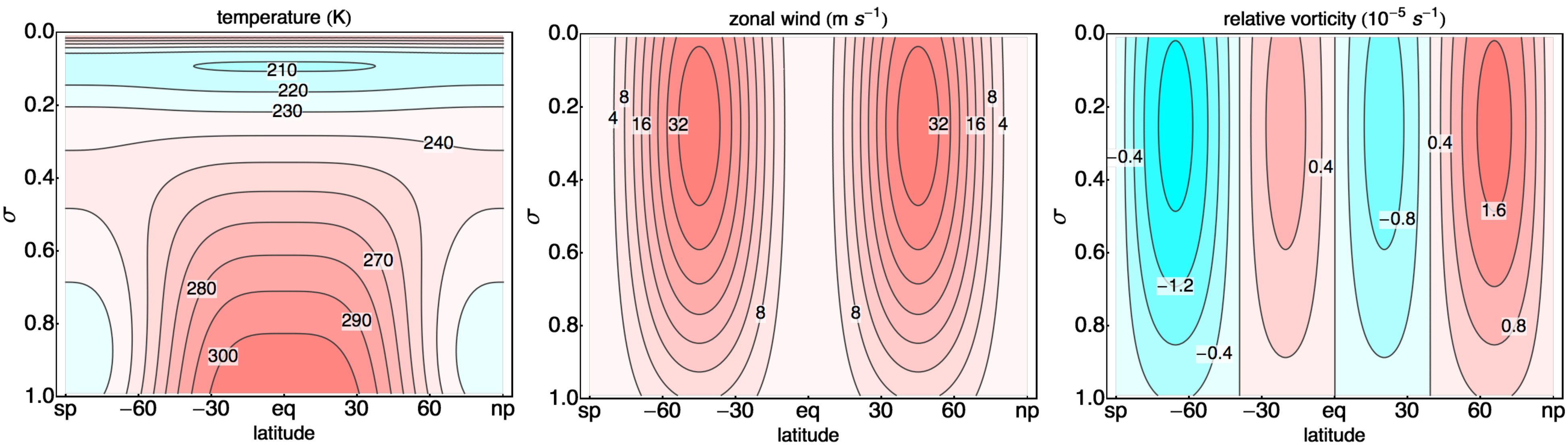
divergence

$$\frac{\partial D}{\partial t} + J(\eta, \chi) - \nabla_\sigma \bullet \left(\eta \nabla \psi \right) + \nabla^2 K + \nabla_\sigma \bullet \left(\dot{\sigma}\frac{\partial \mathbf{v}}{\partial \sigma} \right)$$

$$= -\nabla_\sigma \bullet \left[\frac{g}{m}\left(\boldsymbol{\nabla}_\sigma \left(mz \right) - \frac{\partial}{\partial \sigma}\left(z\boldsymbol{\nabla}_\sigma p_{qs} \right) \right) \right] + \nabla_\sigma \bullet \mathbf{F}$$

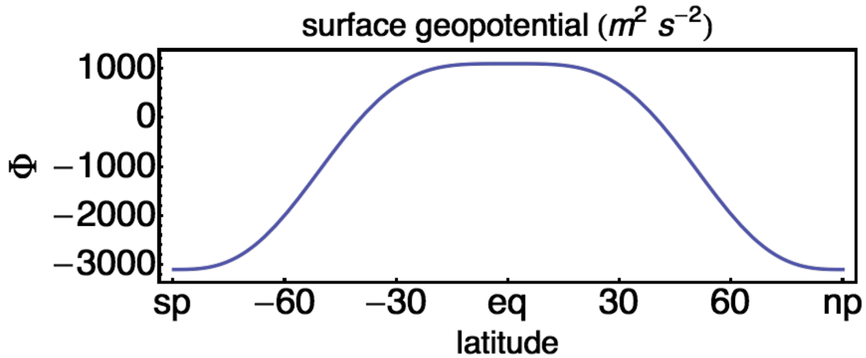
Extratropical cyclone

- Jablonowski and Williamson (2006) *Quart. J. Roy. Meteor. Soc.*, **132,** 2943-2975
- 40962 cells (125 km). 32 layers.
- Prescribed analytic formulas for initial prognostic variables:

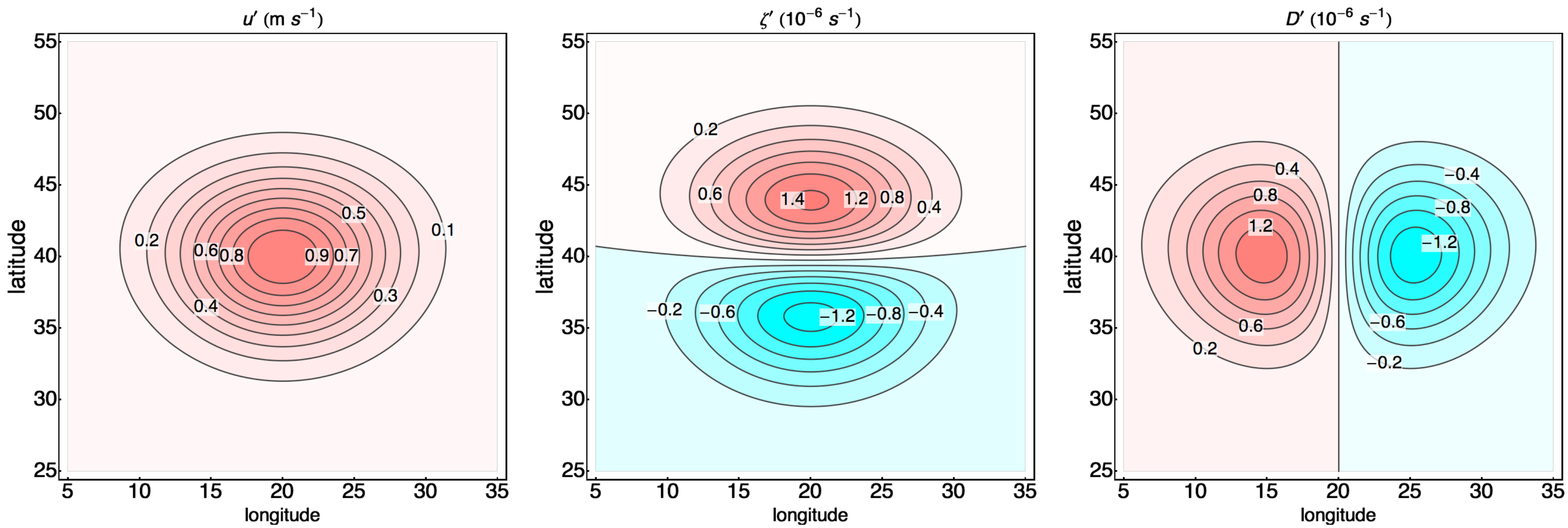


Extratropical cyclone

- The topography balances the non-zero zonal wind at the surface.

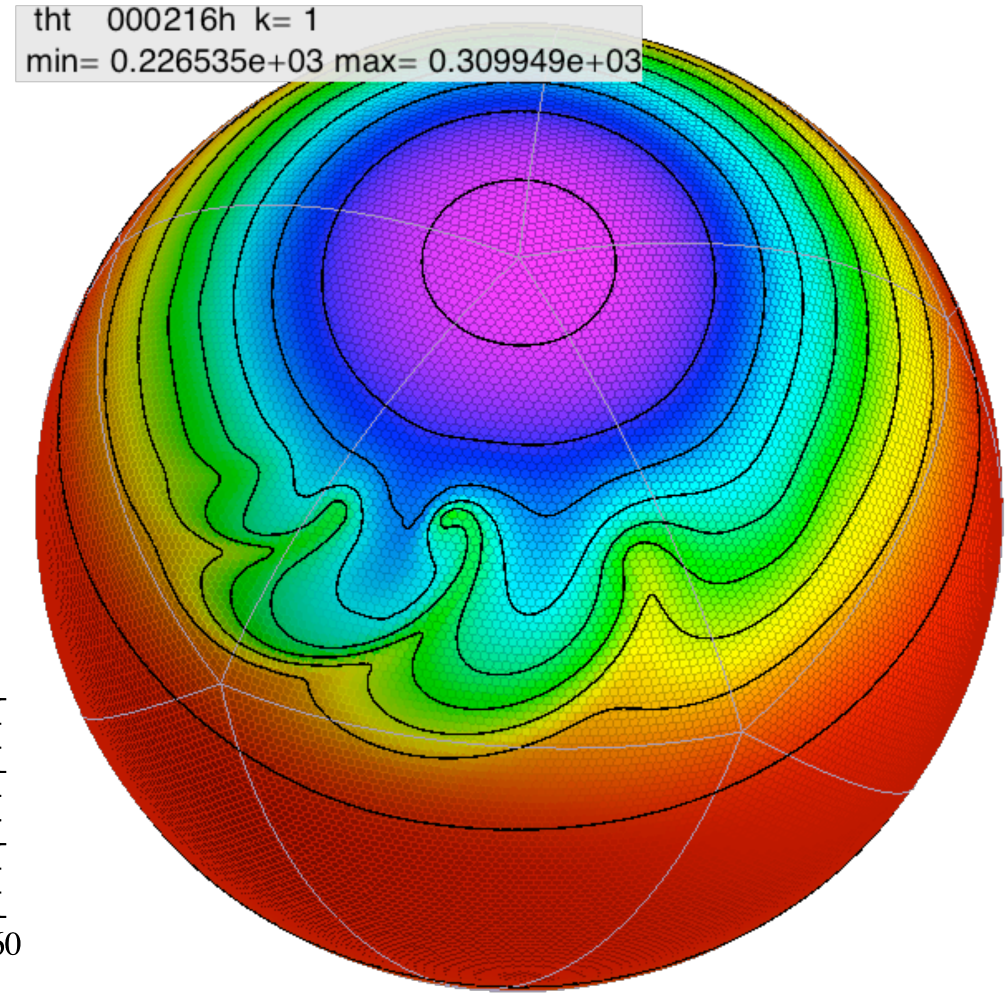


- A baroclinic wave is triggered in the balanced initial conditions by superimposing a perturbation (1 m s^{-1}) in zonal wind at each model level.

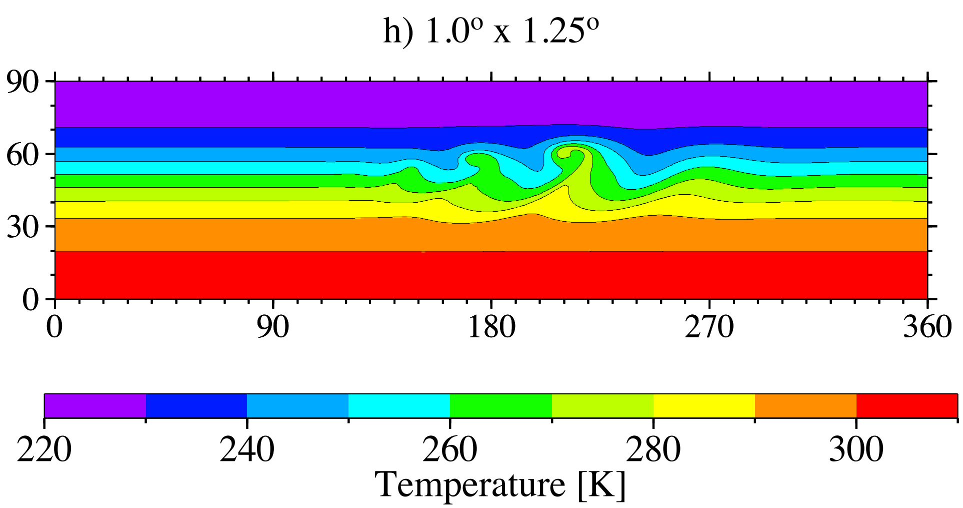


Extratropical cyclone

- Surface Theta. Day 9.
  Contours are 10 K.
  Shape is approximately ok.

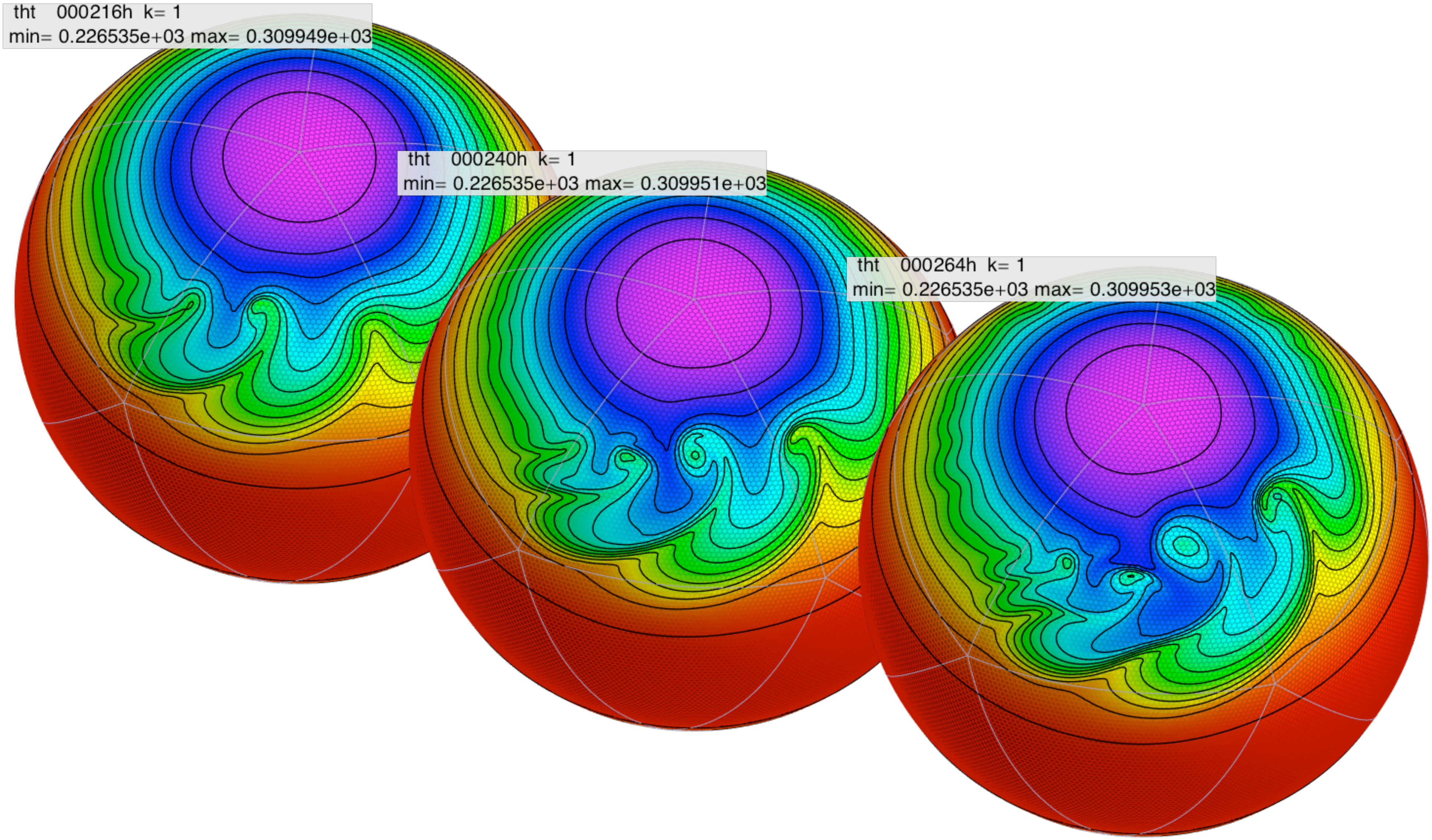


- FV NCAR dynamical core
  of similar resolution.



Extratropical cyclone

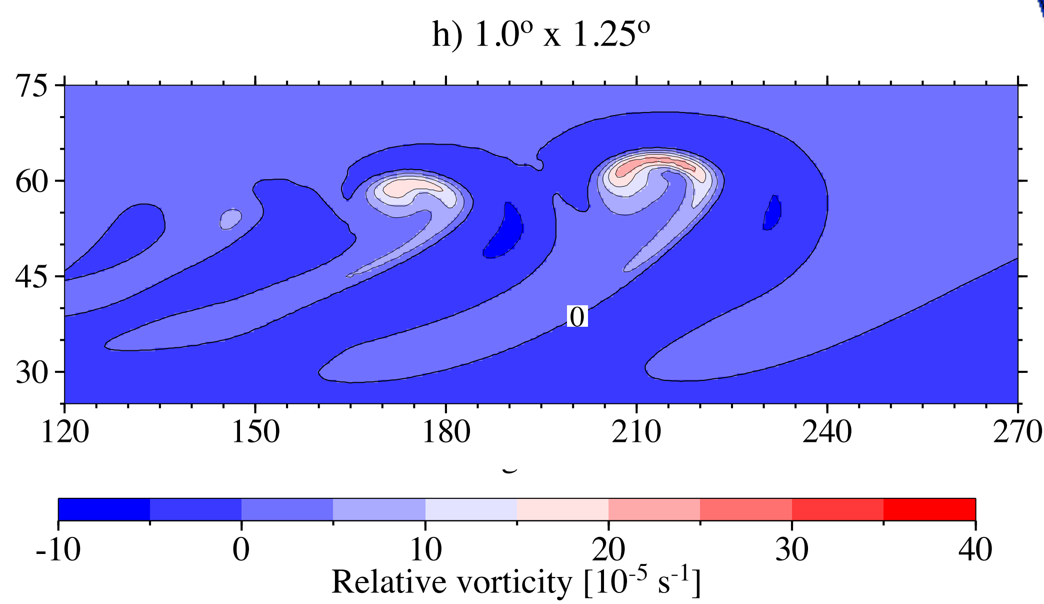
- Evolution of surface theta. Day 9, 10 and 11. Contours are 6 K.

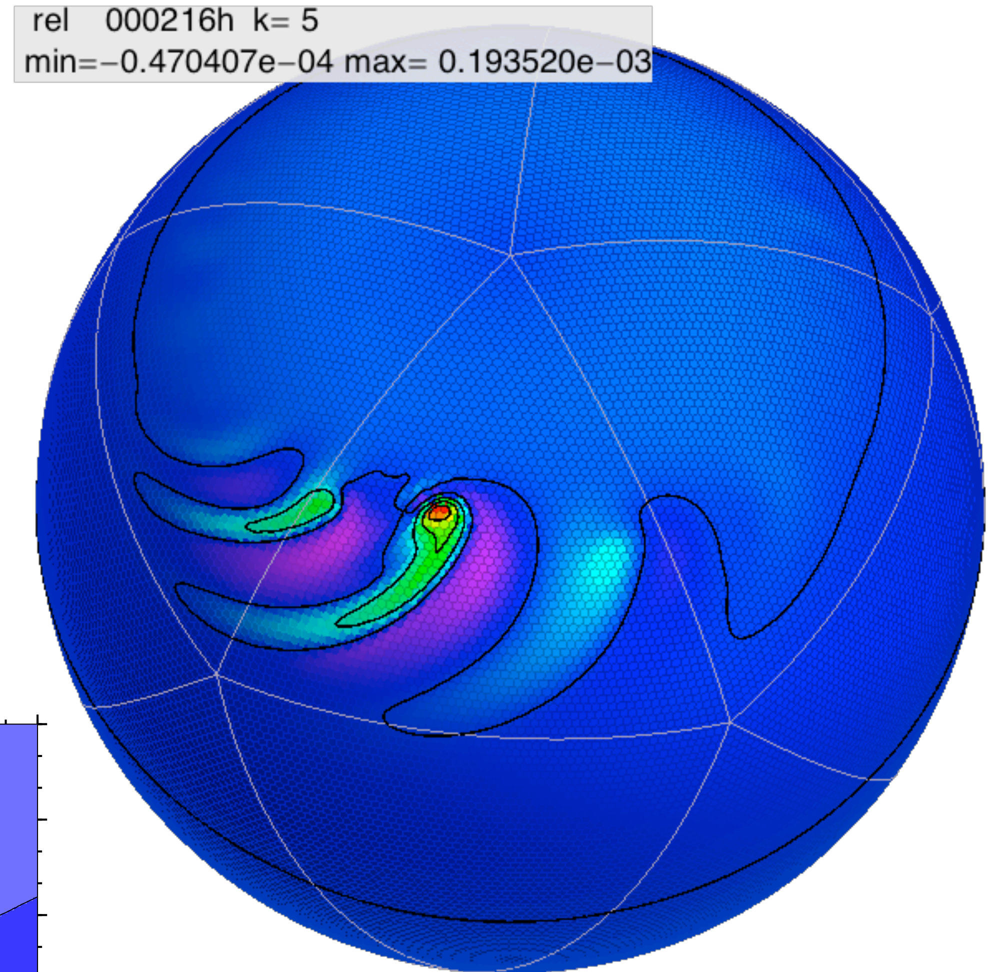


Extratropical cyclone

- 850 hPa relative vorticity. Day 9.
  Contours are 5 X 10^{-5} s^{-1}.
  Maximum is 19 X 10^{-5} s^{-1}.
  Shape is a little off, but it is difficult to tell with this resolution.

- FV NCAR dynamical core.
  Maximum = 22 X 10^{-5} s^{-1}

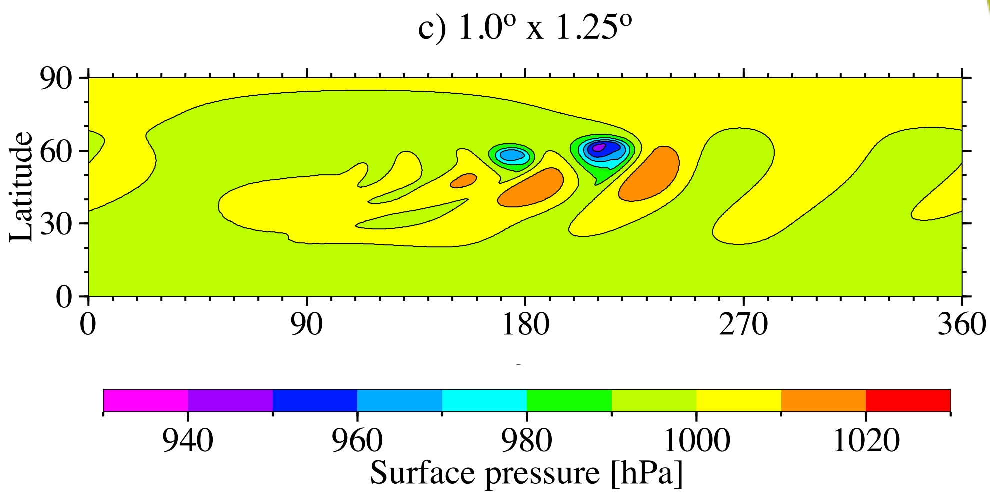


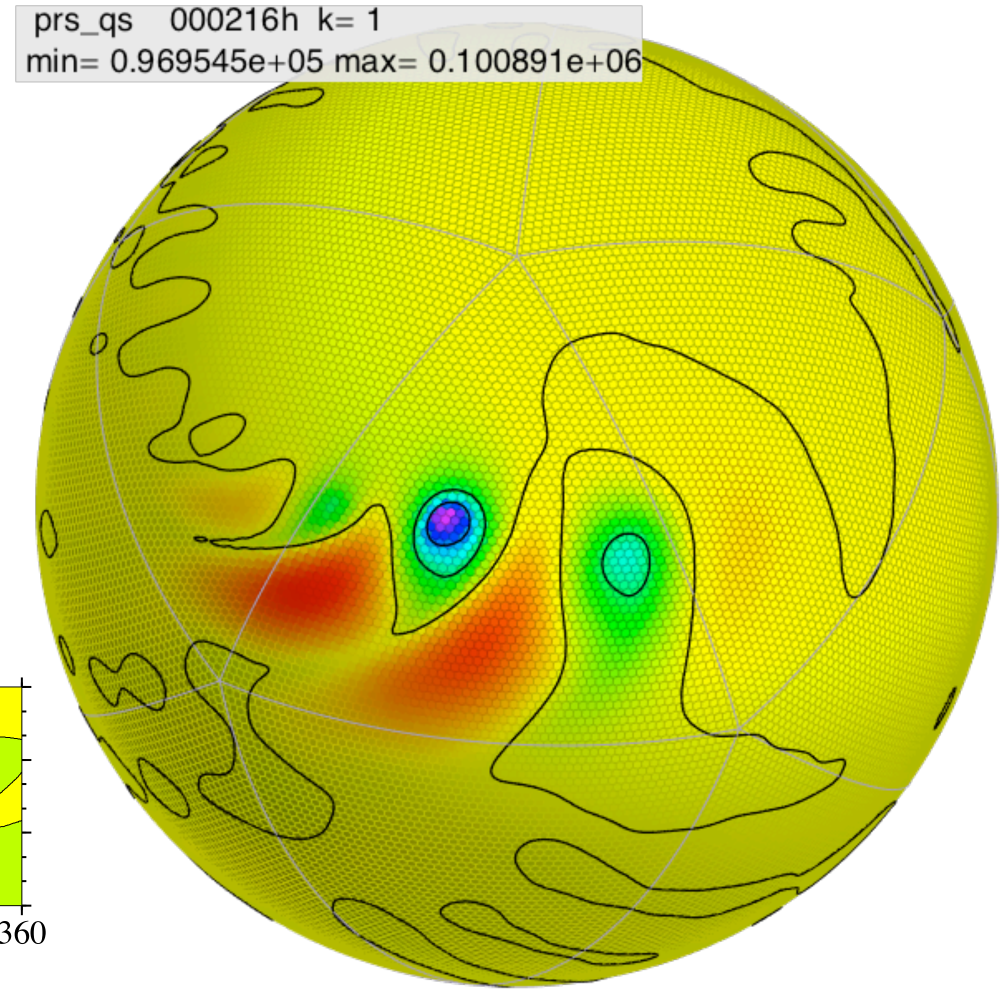


Extratropical cyclone

- Surface pressure. Day 9.
  (min, max) = (969hPa, 1009hPa)

- FV NCAR dynamical core
  (min, max) = (949hPa, 1012hPa)





Progress, conclusions and future work.

- A sigma coordinates dynamical core has been written and debugged.
- The results are *ballpark* ok but pretty dull. The code still needs a careful inspection.
- Experiment with test cases involving more challenging topography.

Interpolation and Restriction

Borrowed *liberally* from Falgout -- An Introduction to Algebraic Multigrid (2006)

Coarse-grid correction involves operators that transfer information between fine and coarse grids.

Fine and coarse grids are denoted in linear algebra terms as a higher-dimensional (fine) vector space $\Re^n$ and the lower-dimensional (coarse) vector space $\Re^{n_c}$.

Interpolation (prolongation) maps the coarse grid to the fine grid.
It is the $n \times n_c$ matrix $\mathbf{P}$: $\Re^{n_c} \rightarrow \Re^n$.

Restriction maps the fine grid to the coarse grid.
It is the transpose of interpolation ($\mathbf{P}^T$).

Definitions

Borrowed *liberally* from Falgout -- An Introduction to Algebraic Multigrid (2006)

The **near-null space** of $\mathbf{A}$ consists of any vector that is almost linear when plotted on the grid.

The classical AMG algorithm (C-AMG) is based on the assumption that geometrically smooth functions are in the near-null space of $\mathbf{A}$.

Let $\mathbf{e}$ be a small normalized eigenmode of $\mathbf{A}$. $\mathbf{Ae} = \lambda\mathbf{e}$

$$\mathbf{e}^T\mathbf{Ae} = \lambda \ll 1$$