Numerical Noise: The Pros and Cons of Filters, Diffusion and Damping Mechanisms

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Diffusion, Filters and Fixers

- Equations of motion: diabatic effects
- Diffusion
  - Explicit horizontal diffusion (neglecting vertical diffusion)
  - Implicit numerical diffusion
  - Divergence damping
  - Decentering mechanism
- Spatial filters:
  - Polar filters / Fourier filters
  - Digital filters: e.g. Shapiro filters
- Time filters: Asselin-filter
- *a posteriori* Fixers:
  - Mass
  - Energy

The 3D Primitive Equations: diabatic effects

Horizontal momentum equation with $\vec{v}_h = (u, v)$

$$\frac{\partial \vec{v}_h}{\partial t} + \left(\vec{v}_h \vec{\nabla}_z\right)\vec{v}_h + w\frac{\partial \vec{v}_h}{\partial z} + f\vec{k} \times \vec{v}_h = -\frac{1}{\rho}\vec{\nabla}_z p + \boxed{\vec{F}_r}$$

temporal change | horizontal & vertical advection | Coriolis force | pressure gradient | friction

Hydrostatic equation:

$$\frac{\partial p}{\partial z} = -g\rho$$

Equation of state:

$$p = \rho RT$$

The 3D Primitive Equations: diabatic effects

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}_z \bullet \left(\rho \vec{v}\right) = 0$$

Thermodynamic equation:

$$\frac{D\Theta}{Dt} = \frac{\partial \Theta}{\partial t} + (\vec{v}\vec{\nabla})\Theta = \boxed{\frac{1}{c_p}\left(\frac{p_0}{p}\right)^{R_d/c_p} Q}$$

Q: diabatic heating

Conservation of water vapor mixing ratio q:

$$\frac{\partial q}{\partial t} + \vec{v}_h \bullet \nabla_z q + w\frac{\partial q}{\partial z} = \boxed{S_q}$$

S_q: sources/sinks

+ Conservation laws for liquid water + ice

Explicit Horizontal Diffusion

- Diffusion applied to the prognostic variables
  - Regular diffusion ∇^2 - operator
  - Hyper-diffusion ∇^4, ∇^6, ∇^8 - operators: more scale-selective
  - Example: Temperature diffusion, i = 1, 2, 3, …

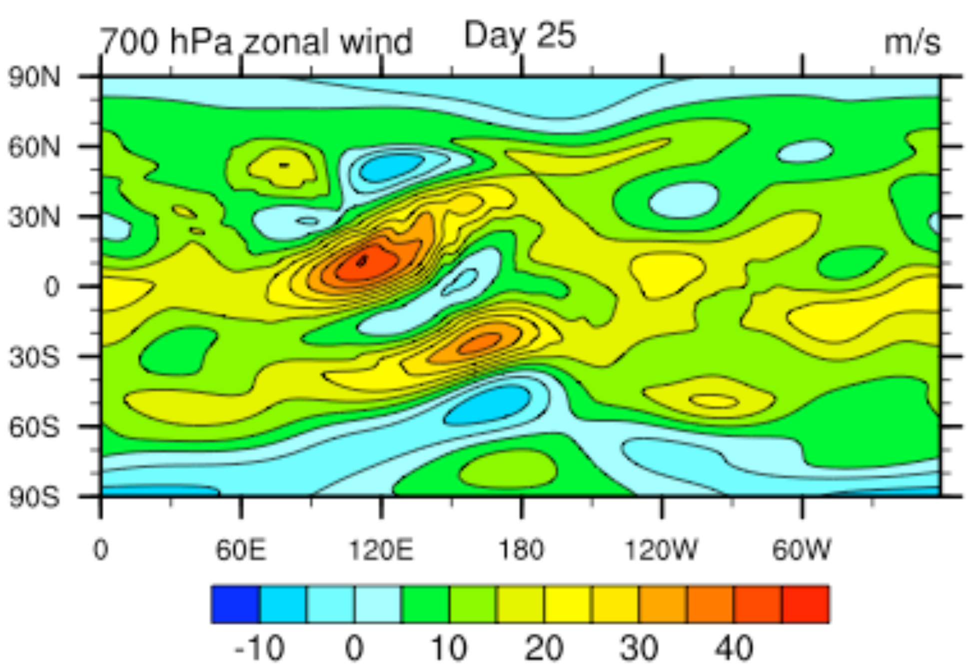
$$\frac{\partial T}{\partial t} = \cdots - (-1)^i \; K^{(2i)} \left(\nabla^{(2i)} \; T \right)$$

  - K: diffusion coefficients, e-folding time dependent on the resolution
  - Choice of the prognostic variables and levels
- Divergence damping

Effects of Horizontal Diffusion

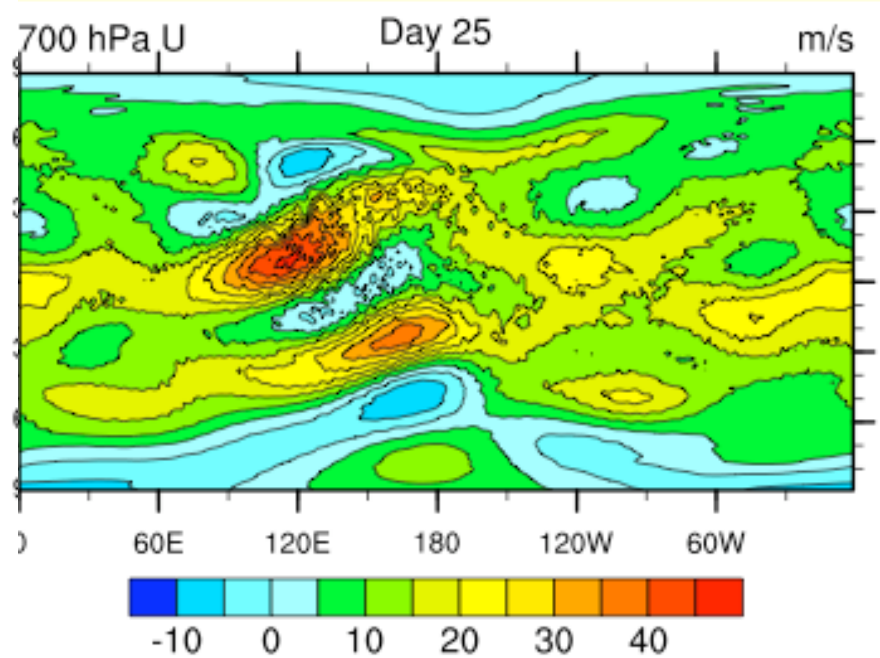
- Comparison of the 700 hPa zonal wind at day 25 in CAM FV and CAM EUL with test 5-0-0

CAM FV 1ºx1ºL26



with monotonicity constraint, divergence damping

CAM EUL T106L26



with standard horizontal diffusion

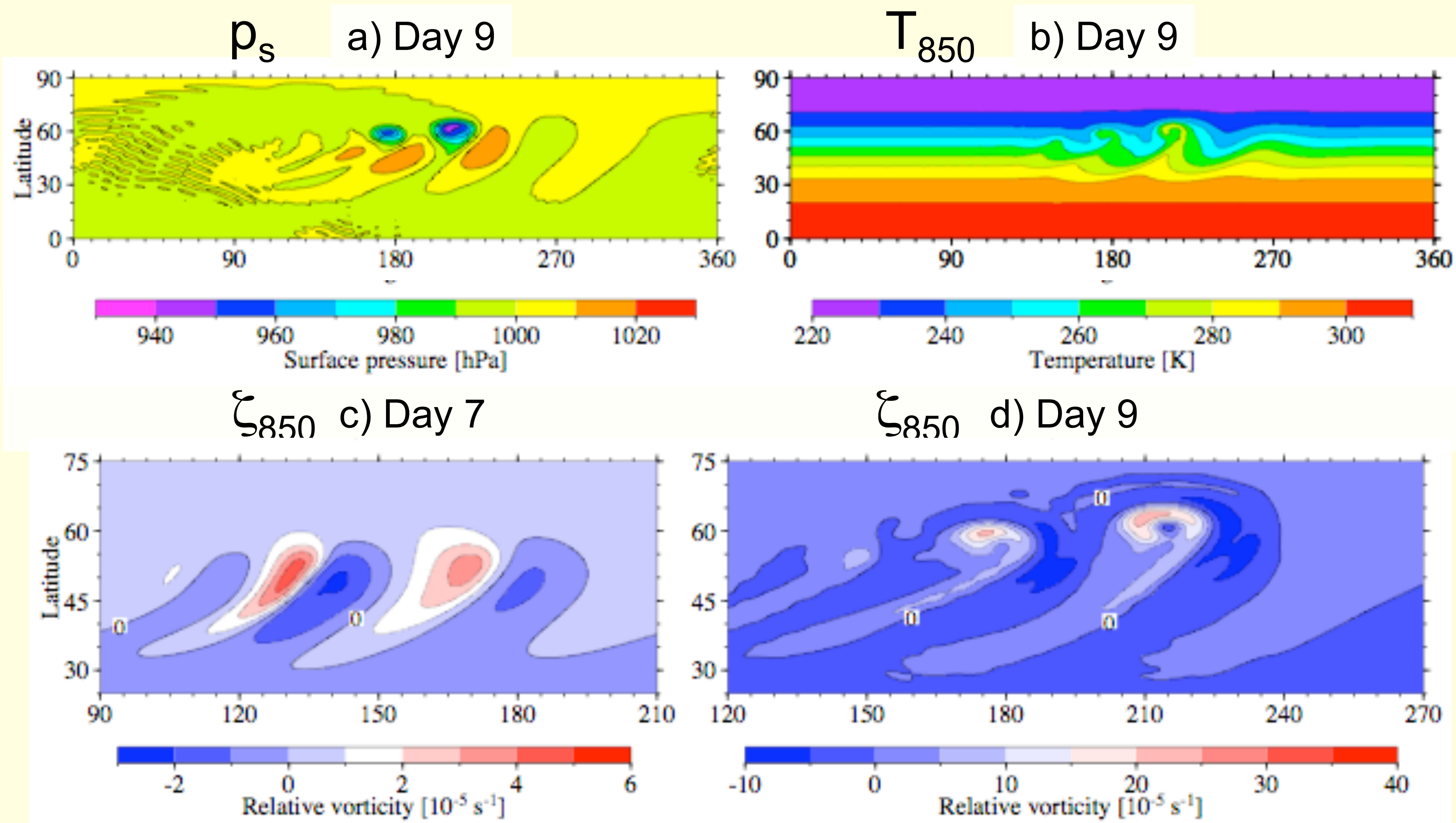
Horizontal Diffusion Coefficients

- Diffusion coefficients are scale-dependent
- Are guided by the so-called e-folding time: How quickly are the fastest waves damped so that their amplitude decrease by a factor of ‘e’?
- Typical 4th-order diffusion coefficients K_4 for CAM EUL

Eulerian spectral transform dynamical core(EUL)				
Spectral Resolution	# Grid points lat × lon	Grid distance at the equator	Time step Δt	Diffusion coefficient K_4 ($m^4\ s^{-1}$)
T21	32 × 64	625 km	2400 s	2.0×10^{16}
T42	64 × 128	313 km	1200 s	1.0×10^{16}
T85	128 × 256	156 km	600 s	1.0×10^{15}
T106	160 × 320	125 km	450 s	0.5×10^{15}
T170	256 × 512	78 km	300 s	1.5×10^{14}
T340	512 × 1024	39 km	150 s	1.5×10^{13}

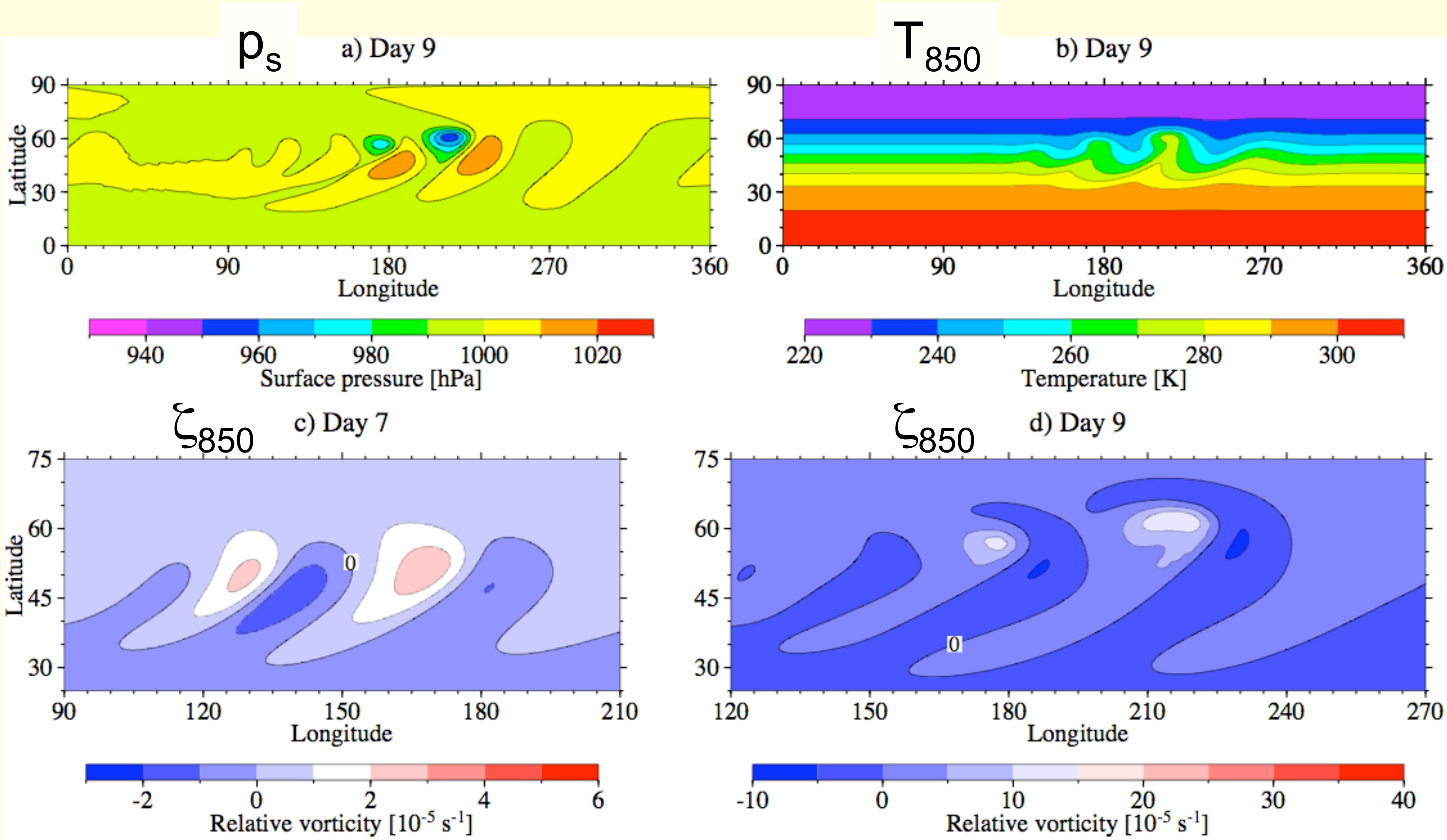
Impact of Explicit Diffusion: Baroclinic Waves

- EUL T85L26 with **standard** $K_4 = 10^{15}$ m^4/s diffusion coefficient
- Spectral noise (Gibb's oscillations), test 2-0-0



Impact of Explicit Diffusion: Baroclinic Waves

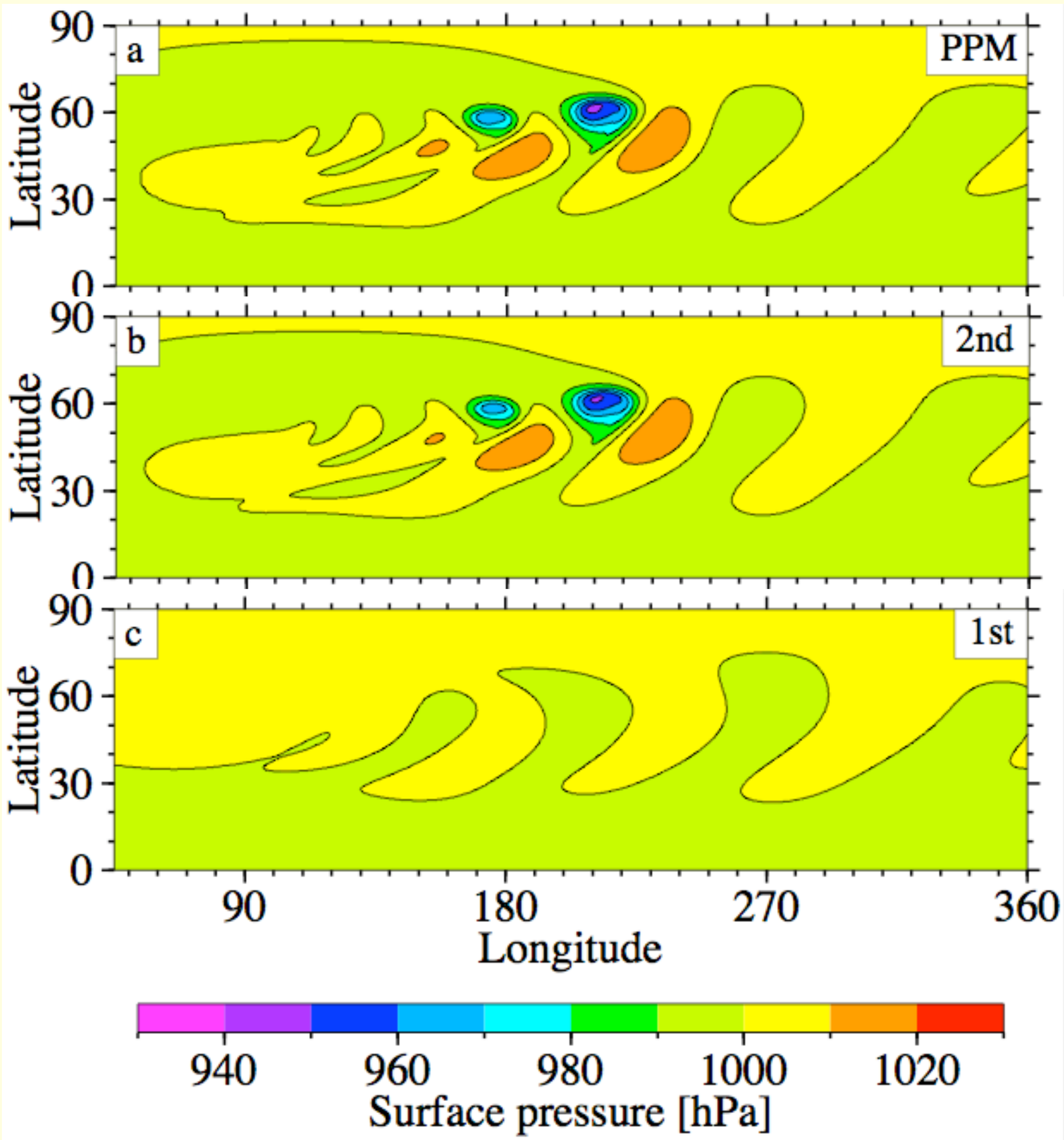
- EUL T85L26 with K_4 **increased** by a factor of 10 (10^{16} m^4/s)
- No spectral noise, but **severe damping** of the circulation



Implicit / Numerical Diffusion

- Implicit diffusion: diffusion that is inherent in the numerical scheme
- Sources of implicit / numerical diffusion:
  - Order of accuracy: 1st order, 2nd order, 3rd order, …, higher order schemes
  - The higher the order, the less diffusive
  - Monotonicity constraints
  - Decentering parameters in semi-implicit time-stepping schemes

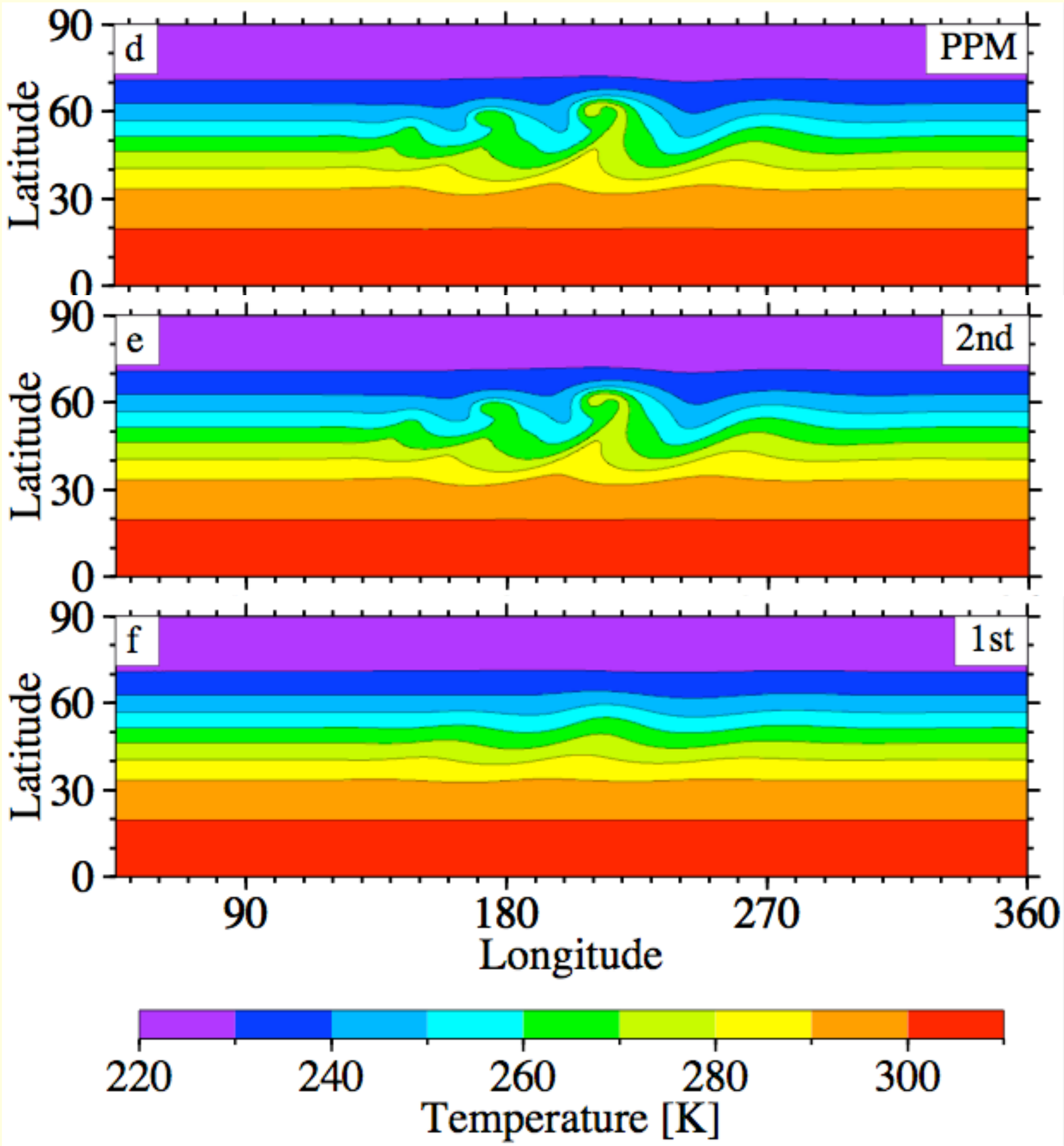
Implicit diffusion: Order of accuracy



- Third order (PPM)
- Second order (van Leer)
- First order upwind scheme

Test 2-0-0
CAM FV 1°x 1.25° L26
p_s at day 9

Implicit diffusion: Order of accuracy

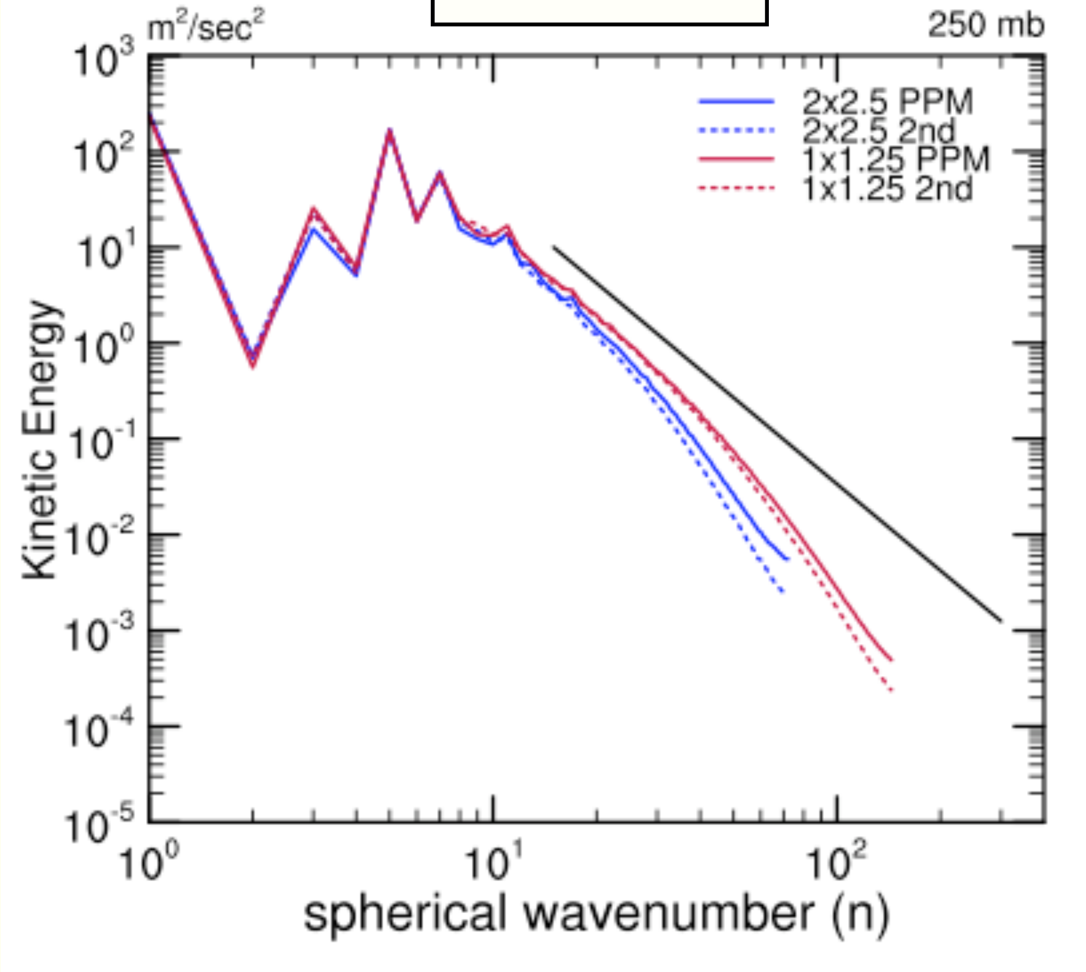


- Third order (PPM)
- Second order (van Leer)
- First order upwind scheme

Test 2-0-0
CAM FV 1°x 1.25° L26
$T_{850\ hPa}$ at day 9

Implicit diffusion: Order of accuracy

Test 2-0-0
CAM FV



- Time-averaged kinetic energy spectrum at two different horizontal resolutions
- Third order (PPM)
- Second order (van Leer scheme)
- Tail of 2nd order scheme drops faster

provided by
D. Williamson (NCAR)

Implicit diffusion: Monotonicity constraints in Finite Volume Methods

- Linear subgrid distribution (van Leer scheme)

Reconstruction: $h(x,y) = \bar{h} + \Delta a^x\, x + \Delta a^y\, y$

Slopes:

$$\Delta a^x = \frac{1}{2}\left(h_{i+1,j} - h_{i-1,j}\right)$$

$$\Delta a^y = \frac{1}{2}\left(h_{i,j+1} - h_{i,j-1}\right)$$

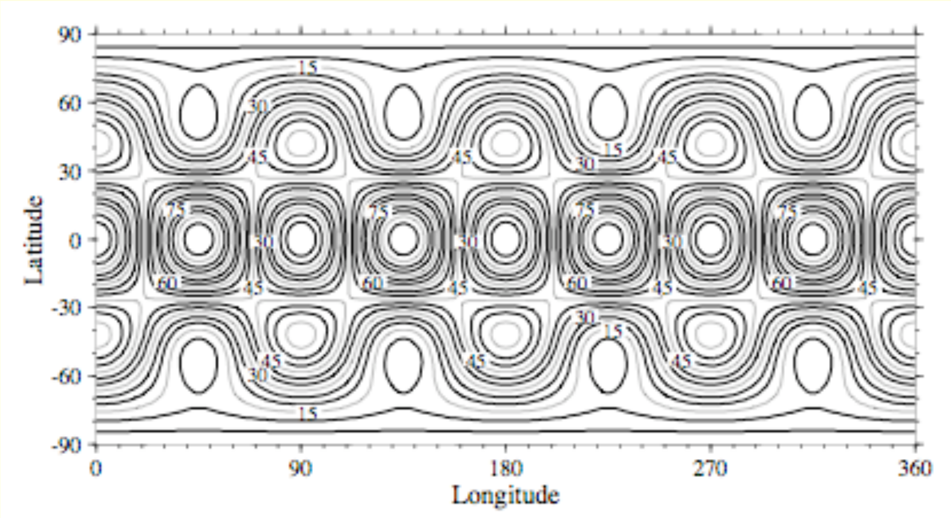
Slope limiter:

$$\begin{aligned}\Delta a^x &= min\left(|\Delta a^x|, 2|h_{i+1,j} - h_{i,j}|, 2|h_{i,j} - h_{i-1,j}|\right)\, sgn(\Delta a^x) \\ &\qquad \text{if } (h_{i+1,j} - h_{i,j})(h_{i,j} - h_{i-1,j}) > 0 \\ &= 0 \quad \text{otherwise}\end{aligned}$$

- Parabolic subgrid distribution (PPM) with cross terms

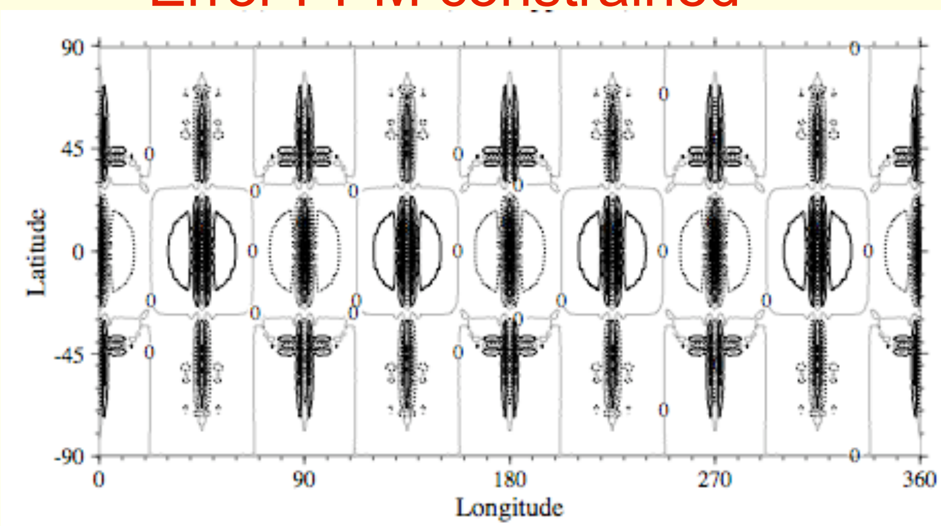
$$h(x,y) = \bar{h} + \delta a^x\, x + b^x \left(\frac{1}{12} - x^2\right) + \delta a^y\, y + b^y \left(\frac{1}{12} - y^2\right) + \frac{1}{2}(c^{xy} + c^{yx})\, x\, y$$

Implicit diffusion: Monotonicity constraint



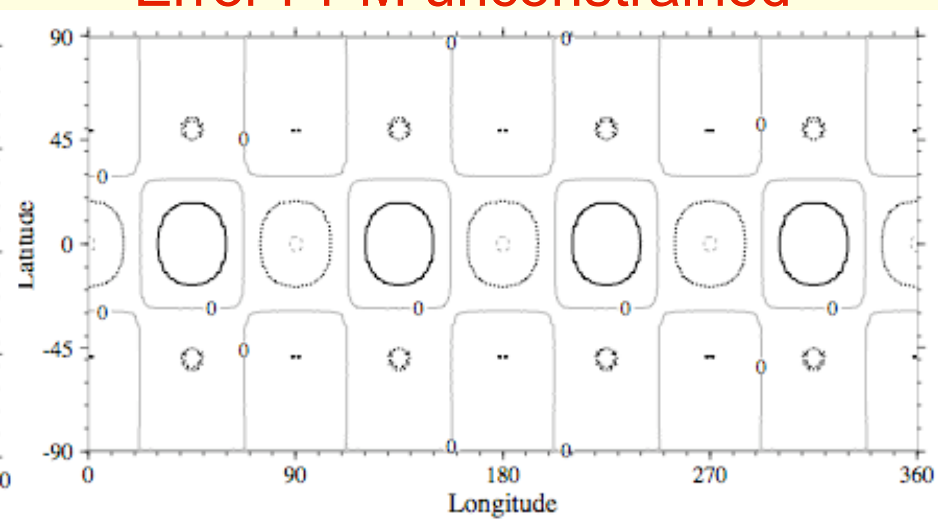
- SW Rossby-Haurwitz wave
- Initial u field at 2°x 2.5°
- Split cells to 1°x 1.25° grid and interpolate via a PPM reconstruction, compare to analytical solution (error)

Error PPM constrained



Errors cluster near the extrema where the monotonicity constraint is strongest

Error PPM unconstrained

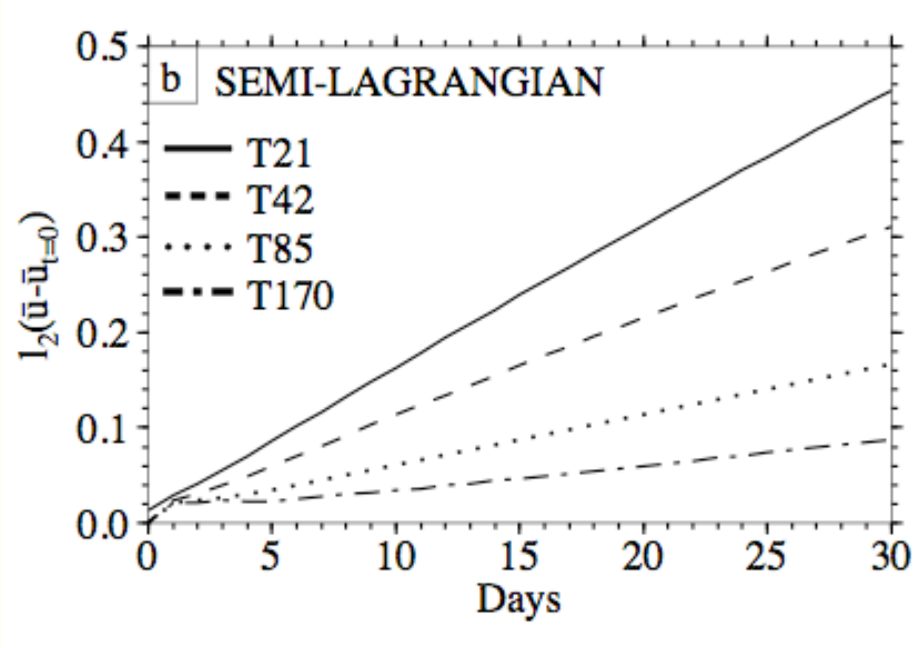


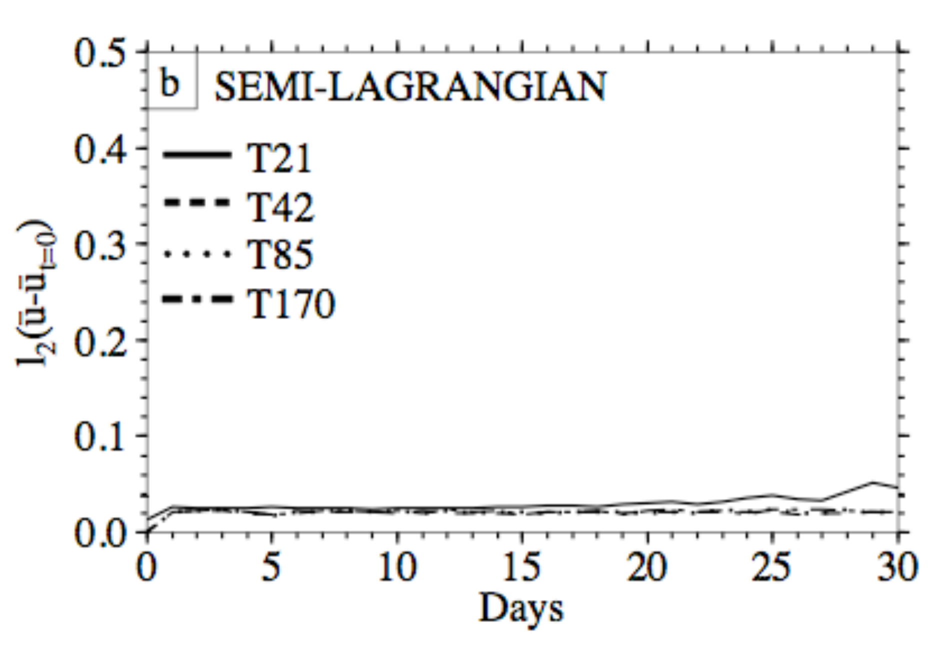
Errors are reduced, but over- or undershoots are possible

Decentering mechanism (semi-implicit)

- Decentering mechanism is used in the semi-implicit semi-Langrangian model CAM SLD, parameter ε
- Decentering technique damps noise induced by orographic resonance, ε needed in real simulations
- Damping clearly shown in test 1-0-0, l_2 error (Eqn. 18)

$\varepsilon = 0.2$ $\varepsilon = 0$





Divergence damping

- Example: 2D shallow water momentum equation

coefficient

Momentum equation:

$$\frac{\partial \vec{v}}{\partial t} = -\Omega_a \vec{k} \times \vec{v} - \nabla \Big(\Phi + \mathcal{K} - c\, D \Big)$$

Horizontal divergence:

$$\begin{aligned} D &= \frac{1}{a\,\cos\varphi}\left[\frac{\partial u}{\partial \lambda} + \frac{\partial}{\partial \varphi}(v\cos\varphi)\right] \\ &\approx \frac{1}{a\,\cos\varphi}\left[\frac{\Delta u}{\Delta \lambda} + \frac{\Delta(v\cos\varphi)}{\Delta \varphi}\right] \end{aligned}$$

Semi-discretized:

$$\frac{\partial \vec{v}}{\partial t} = -\Omega_a \vec{k} \times \vec{v} - \nabla \Big(\Phi + \mathcal{K} - \left[c_u\, \Delta u + c_v\, \Delta(v\cos\varphi)\right] \Big)$$

Divergence damping coefficients divided by metric terms, different in both directions

Divergence damping

- Divergence damping diffuses the divergent part of the flow

$$\frac{\partial \vec{v}_h}{\partial t} = -\Omega_a \vec{k} \times \vec{v}_h - \nabla\left(\Phi + K - cD\right) \qquad \text{(SW equation)}$$

$$\Rightarrow \frac{\partial \vec{v}_h}{\partial t} = \cdots + \nabla\left(cD\right)$$

$$\Rightarrow \nabla \bullet \frac{\partial \vec{v}_h}{\partial t} = \cdots + \nabla \bullet \nabla\left(cD\right) \qquad \text{Apply divergence operator}$$

$$\Leftrightarrow \frac{\partial D}{\partial t} = \cdots + \nabla^2\left(cD\right) \qquad \text{with D : horizontal divergence}$$

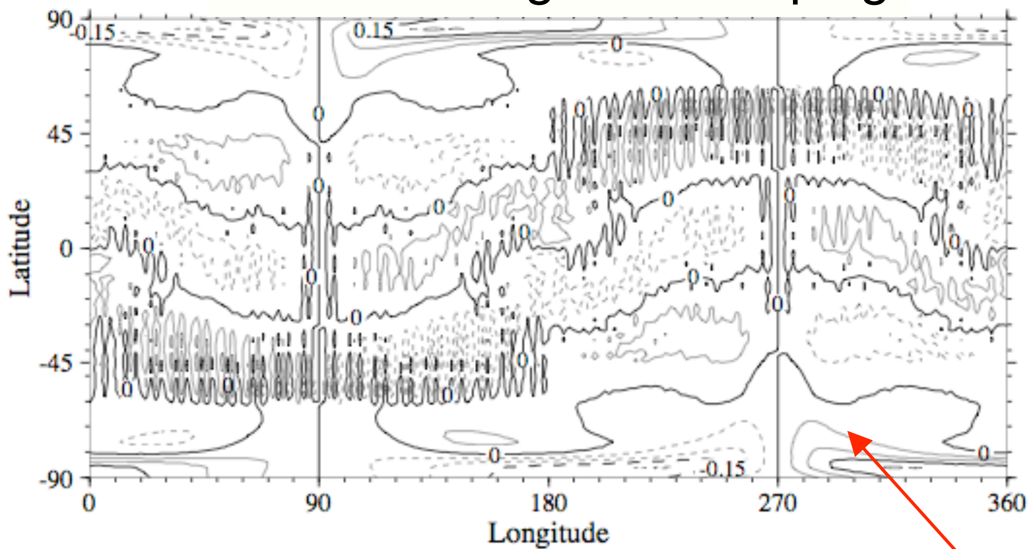
2nd order diffusion

Spatially variant divergence damping coefficient, units m^2/s

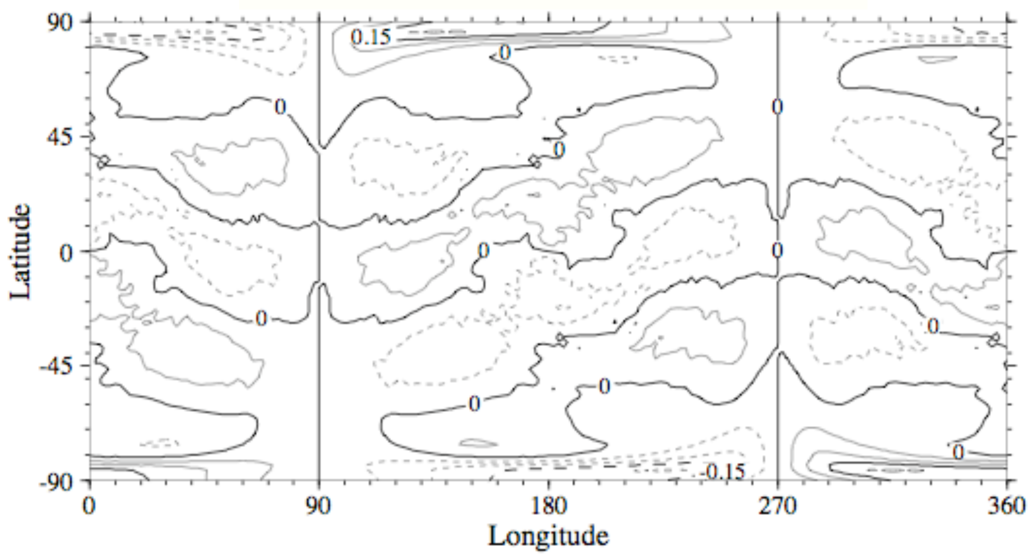
- Can you select any coefficient c? Selection criterion?

Divergence damping

without divergence damping

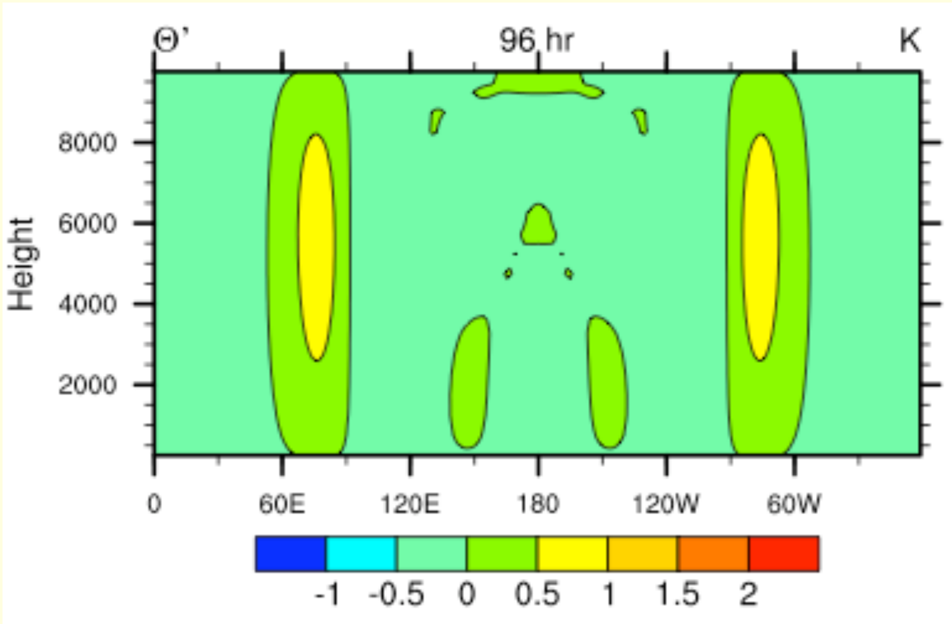


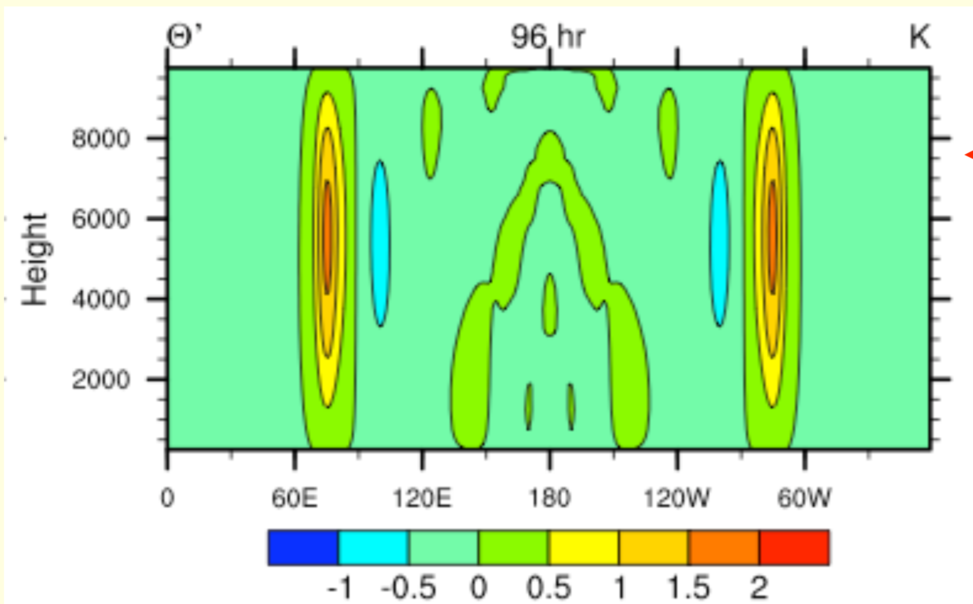
with divergence damping



- Example: 2D SW steady state test case with α=90°, model FV
- Difference field at day 10 compared to analytical solution
- Contour interval is 0.05 m/s
- Why is the polar region always smooth? Because of other filters (here polar Fourier filter)

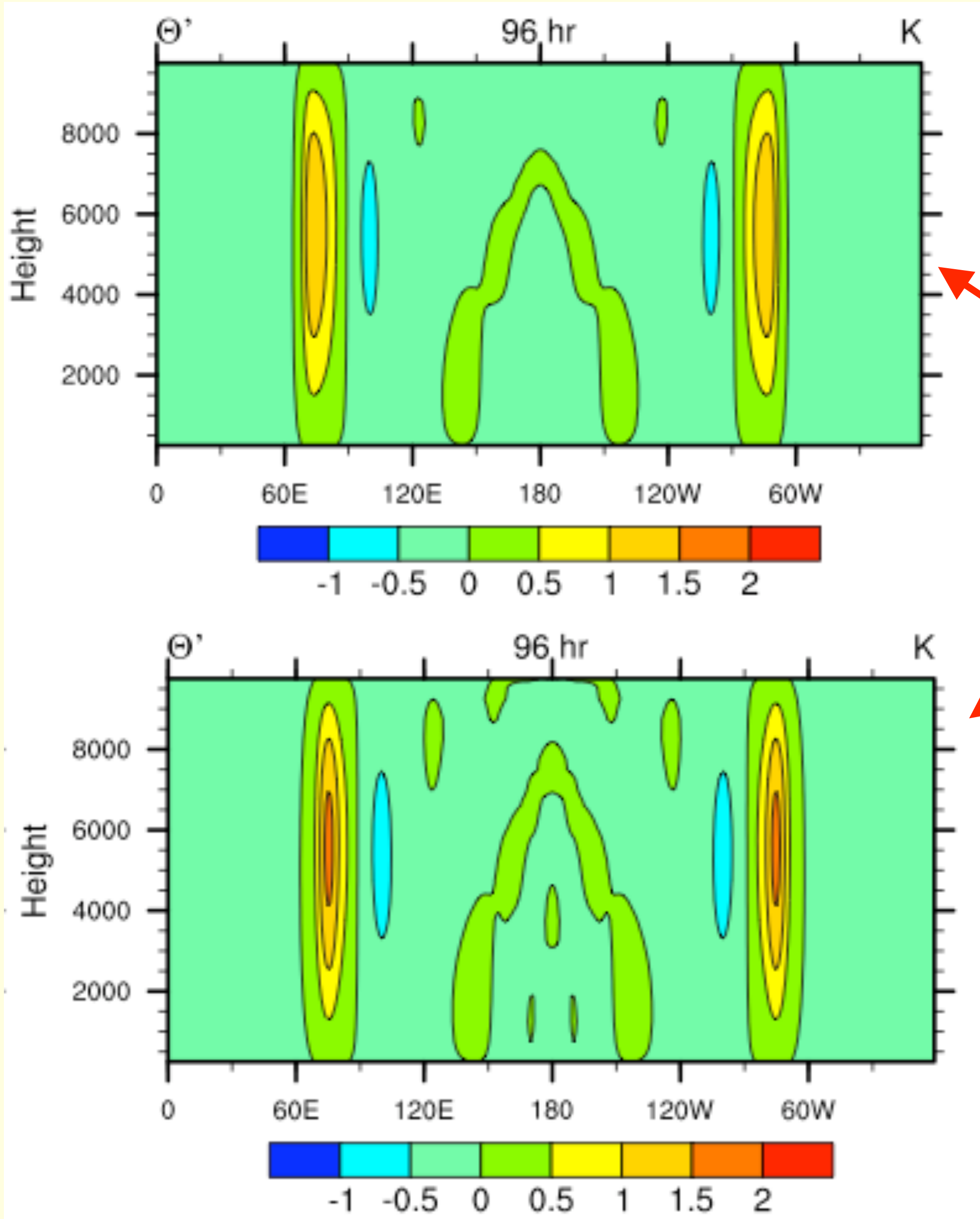
Divergence damping: Effects





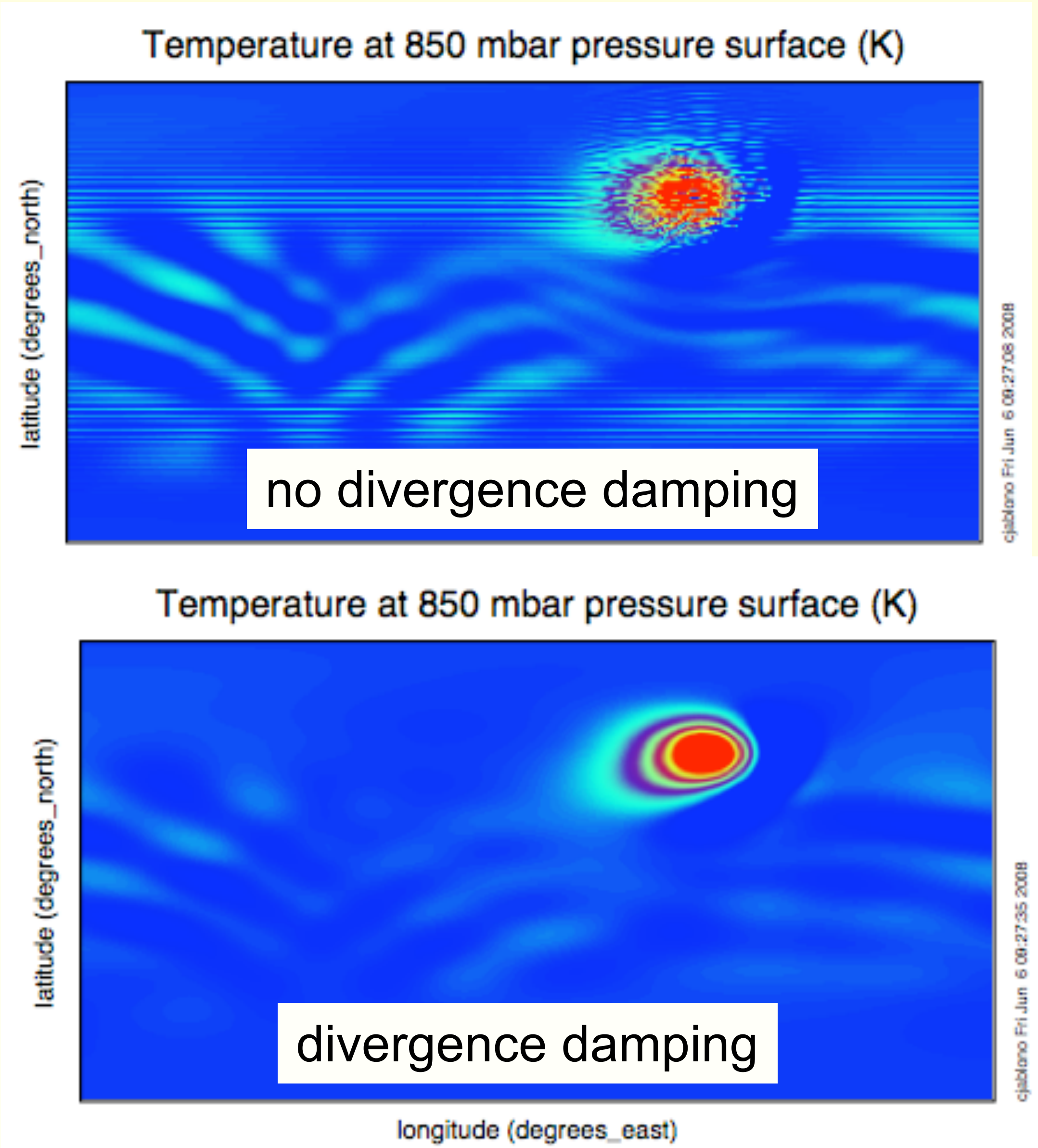
- Example: 3D gravity wave test 6-0-0
- Model CAM FV 1°x 1° L20 at day 4, cross section at equator
- with standard divergence damping coefficients (top)
- without divergence damping (bottom)
- Clear difference in the amplitudes of the gravity wave

All types of diffusion change the solution



- Example: 3D gravity wave test 6-0-0, cross section at the equator at day 4
- Model CAM EUL T106L20 with explicit ∇^4 diffusion (top)
- Model CAM FV 1°x 1° L20, no divergence damping (bottom)
- Clear difference in the shape of the potential temperature perturbation
- Check sharpness of leading edge

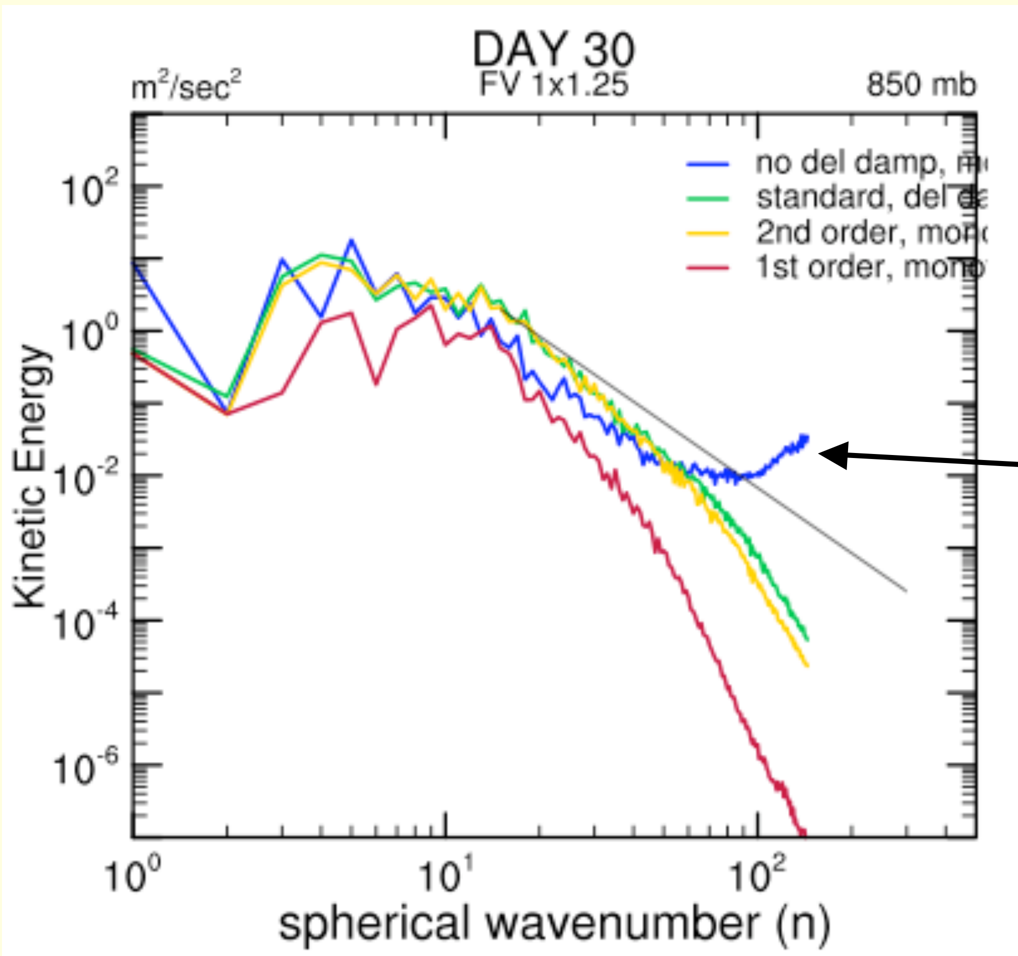
Divergence damping: Needed for stability ?



- Example: alternative 3D inertio-gravity wave test with background flow
- Model CAM FV 1°x 1° L20 at day 5.5, lat-lon cross section at 850 hPa
- Numerical stability of CAM FV depends on the resolution- and time step dependent choice of the divergence damping coefficient c

Divergence Damping

- Effects of the divergence damping and order of accuracy on the Kinetic Energy spectrum (test 2-0-0)



Blue: PPM, **no** divergence damping

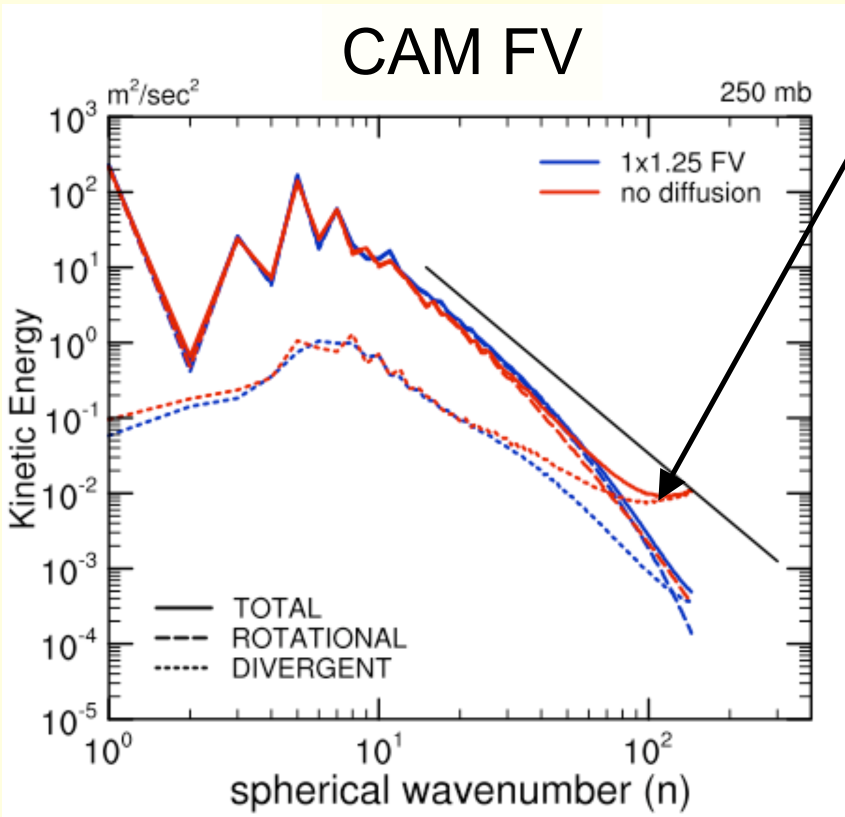
Green: PPM, standard divergence damping

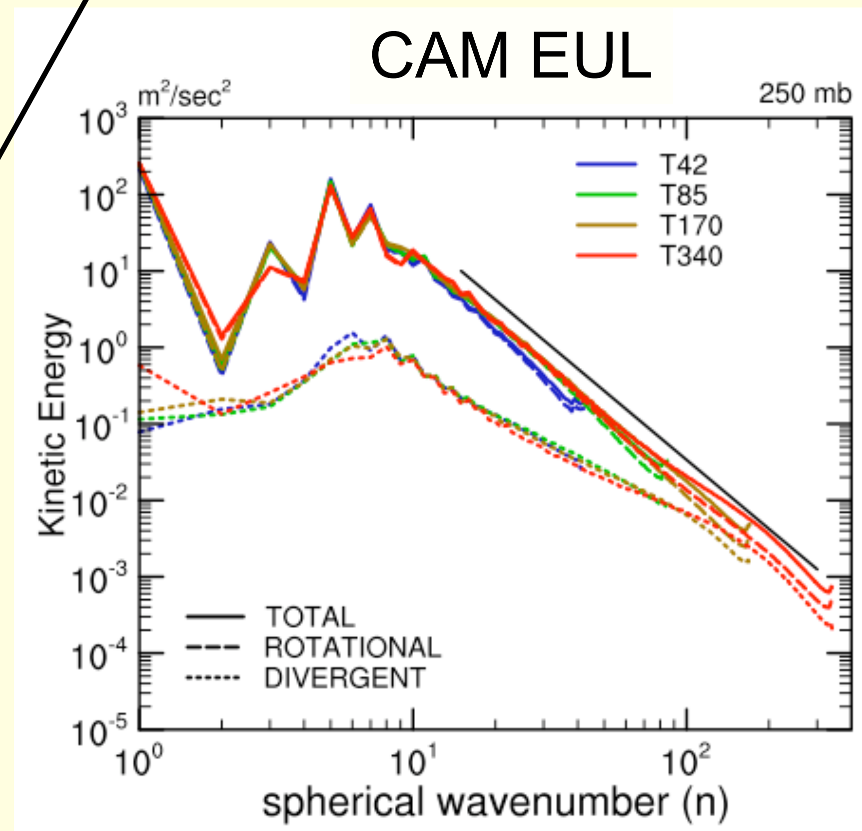
Accumulation of energy at small scales without divergence damping

Model: CAM FV,
plot provided by
D. Williamson (NCAR)

Divergence Damping

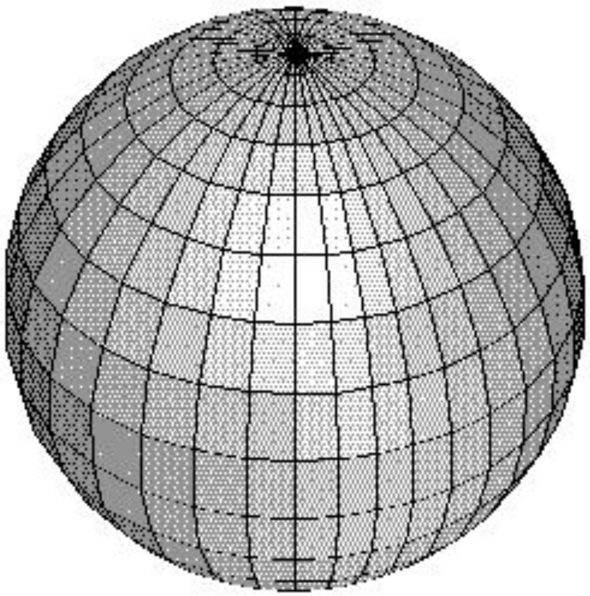
- Without diffusion (here divergence damping): divergent part of the flow responsible for the hook





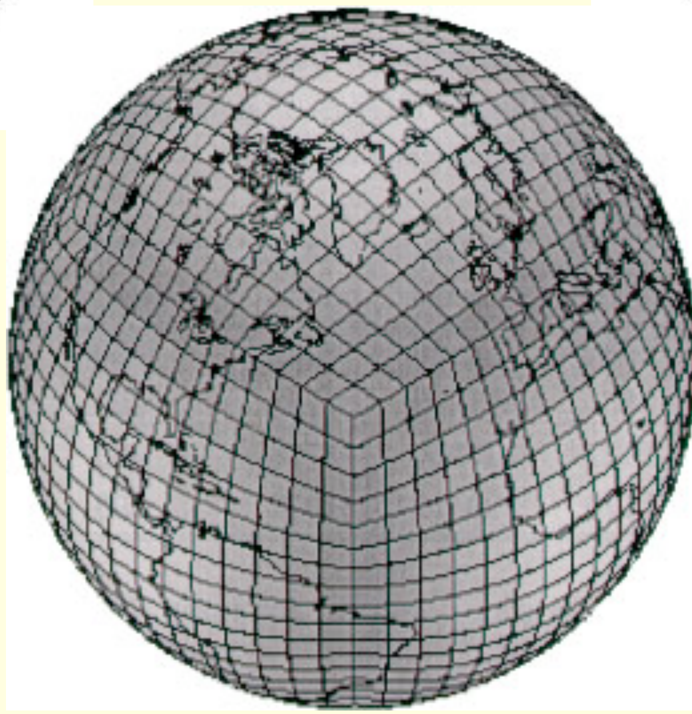
plots provided by D. Williamson (NCAR)

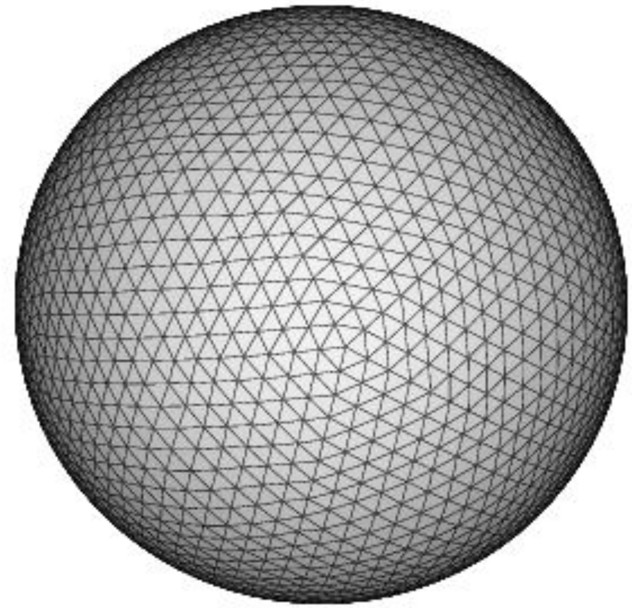
Computational grids (horizontal)



Latitude-longitude grid: needs polar filtering due to convergence of meridians

Cubed sphere





Icosahedral grid

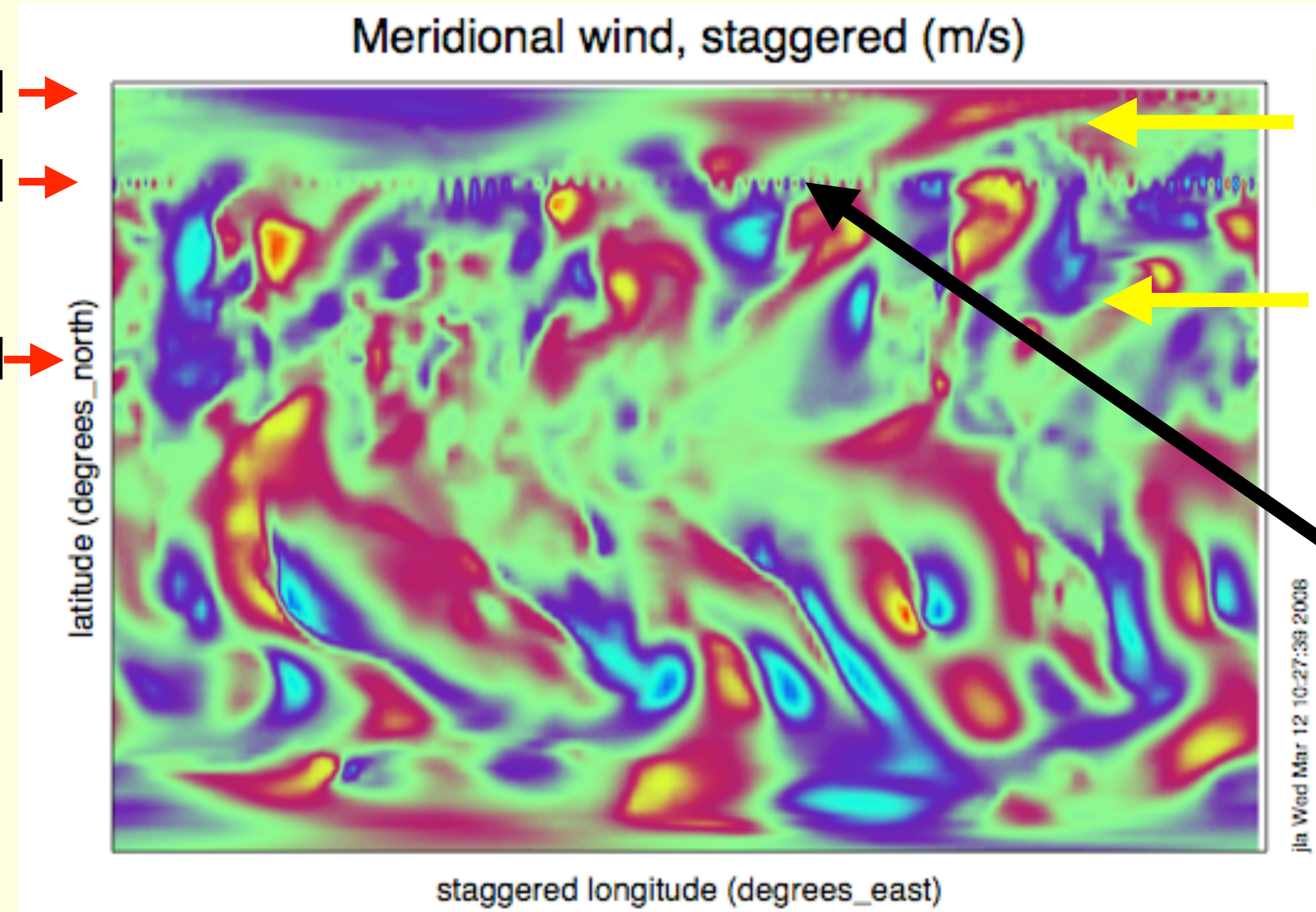
No polar filter requires

Spatial filters

- Most popular and most effective polar filter: 1D Fourier filter (spectral filter), used in the zonal (x) direction
- **Basic idea:**
  - Transform the grid point data into spectral space via Fourier transformations
  - Eliminate or damp high wave numbers (noise) by either setting the spectral coefficients to 0 or multiplying them with a damping coefficient $\in [0,1]$
  - Transform the field back from spectral space into grid point space: result is a filtered data set
- Filter strength is determined by the spectral damping coefficients, can be made very scale-selective and dependent on the latitude (e.g. less strong towards equator)
- Drawback: needs all data along latitude ring (poor scaling)

Spatial filters: Fourier & Digital Filter

- Data assimilation run with CAM FV, D-grid v field at 266 hPa



90° N
67° N
36° N
Fourier filter
Digital filter
Filter change at 67°N

provided by Jeff Anderson, NCAR

Digital filters

- Digital or algebraic filters are local grid-point filters that only take neighboring grid points into account
- Examples are the Shapiro filters (Shapiro, 1975)
- 2nd order Shapiro filter (i is the grid point index):

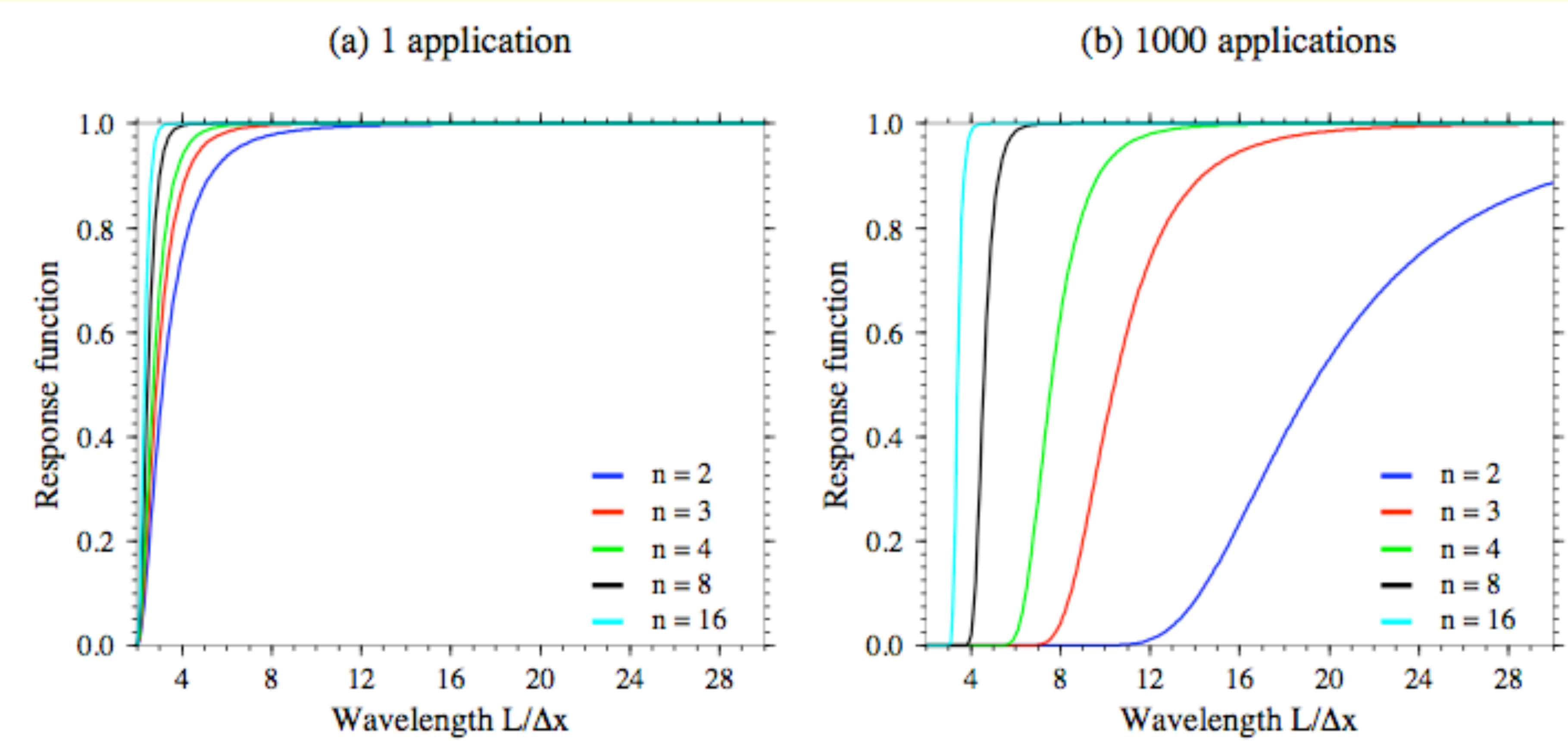
$$\bar{f}_i = \frac{1}{16}\big(- f_{i-2} + 4f_{i-1} + 10f_i + 4f_{i+1} - f_{i+2}\big)$$

- The filter response/damping function is (Shapiro, 1971)

$$\begin{aligned} \rho_n(k) &= 1 - sin^{2n}\left(k\frac{\Delta x}{2}\right) \\ &= 1 - sin^{2n}\left(\pi\frac{\Delta x}{L}\right) \end{aligned}$$

2n: order

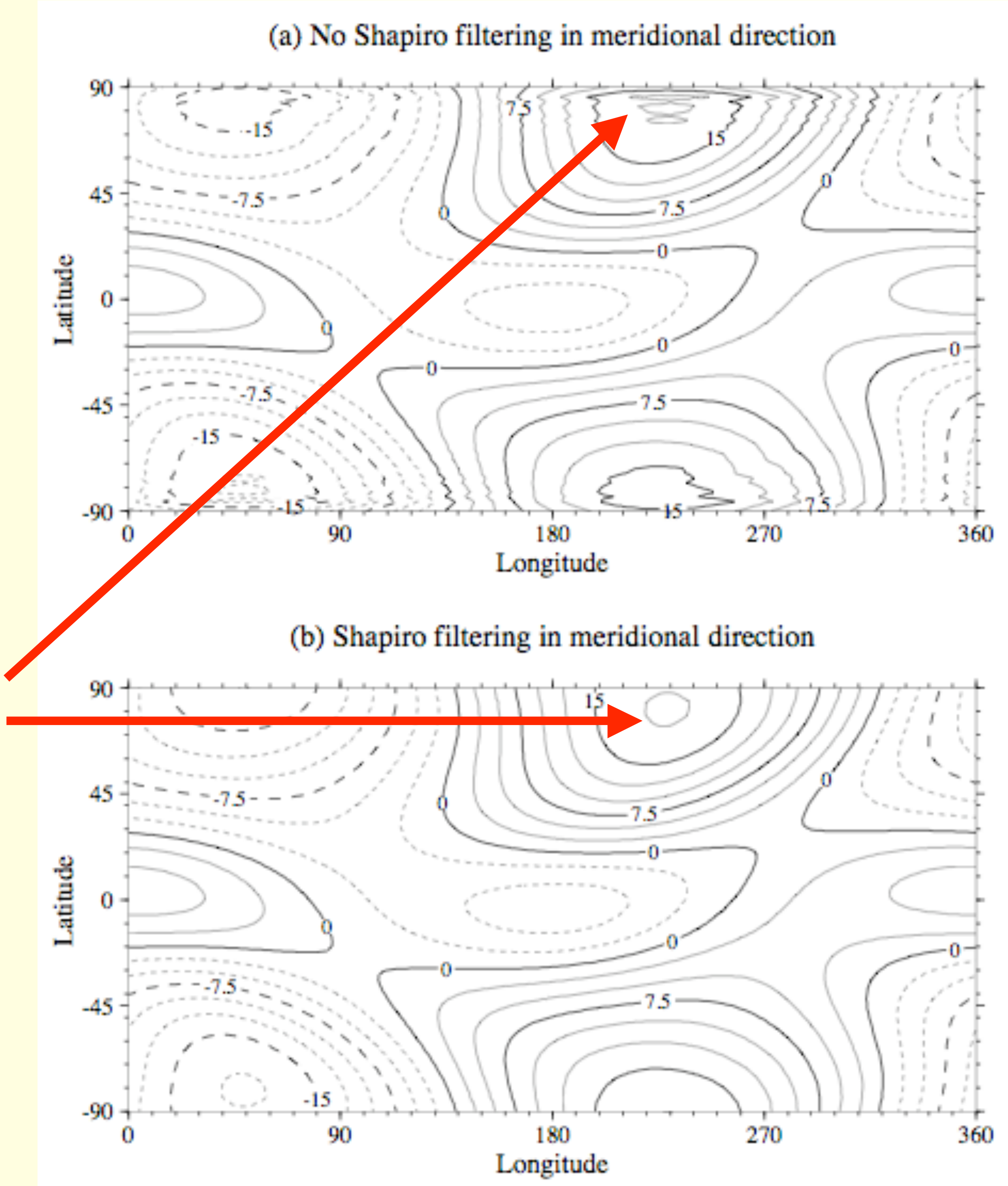
Digital filters: Response function



- Response function of different Shapiro filters after (a) 1 application and (b) 1000 applications. *n* indicates the order of the Shapiro filter. Higher orders need more data points.

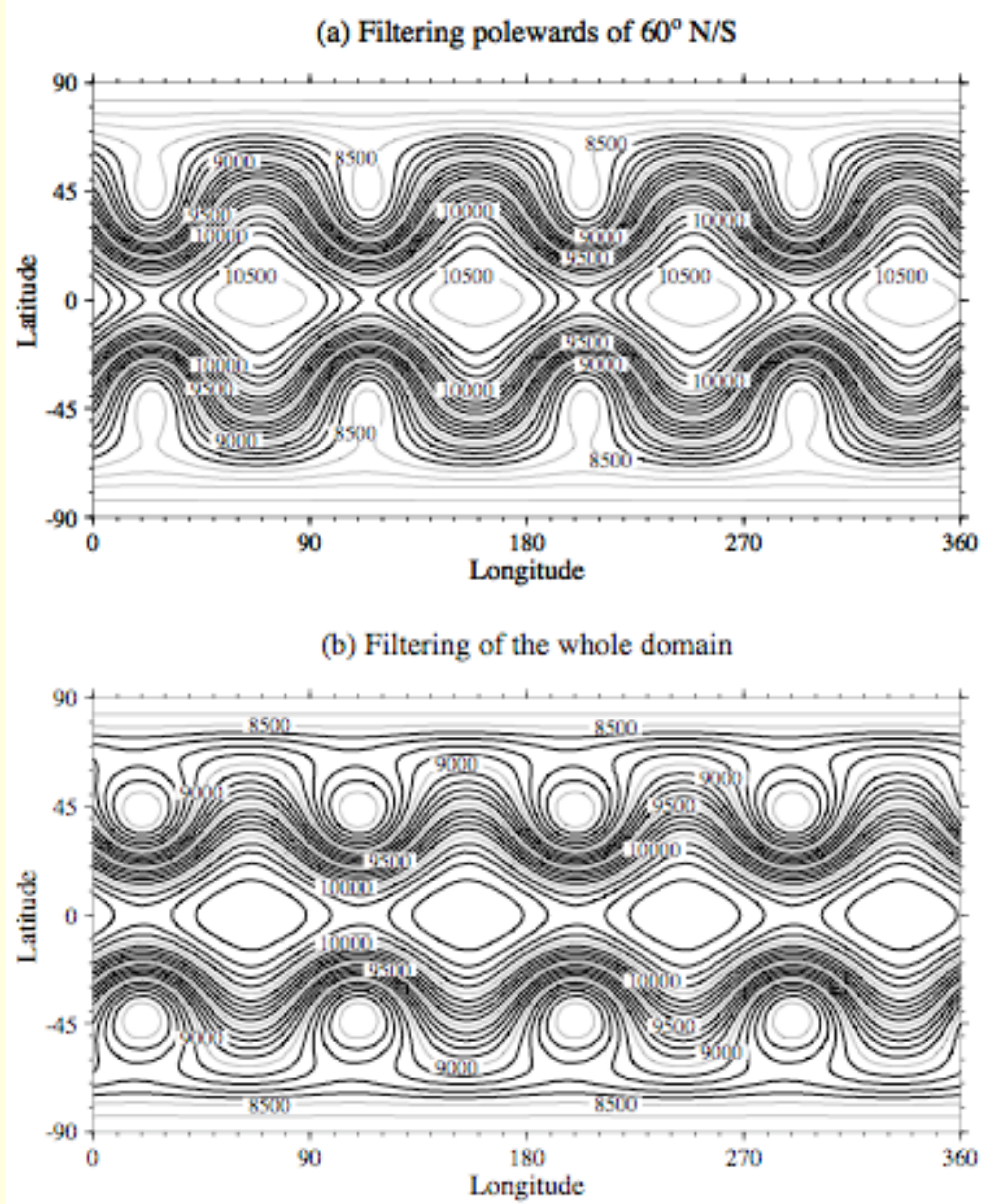
Digital filters

- Can provide a strong damping effect
- Use very selectively
- Example: SW simulation, digital filtering in y-direction applied near the pole points



Spatial Filters

- Can provide a strong damping effect
- Example: Rossby-Haurwitz wave in SW FV model, height at day 14
- (a) Fourier (90º-75º N/S) and digital Shapiro filtering (75º-60º N/S)
- (b) Digital Shapiro filter also applied between 60ºN - 60ºS, very diffusive, not suitable



Time filters

- Used in models with 3-time level schemes
- Most often used: Asselin filter (Asselin, 1972)
- Avoids that the even and odd time steps separate
- Basic idea: Second-order diffusion in time
- Example with time levels n-1, n, n+1:

$$\overline{\psi}^{n} = \psi^{n} + \alpha\left(\overline{\psi}^{n-1} - 2\psi^{n} + \psi^{n+1}\right)$$

- Filter strength is determined by the coefficient α
- Often used $\alpha \approx 0.05$

Conservation of Mass

- Conservation of the (dry) air mass is only guaranteed if the continuity equation equation is written in conservative form:

$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \bullet \left(\rho \vec{v} \right) = 0$$

→ requires the density ρ to be a prognostic variable

- Alternative form for Lagrangian vertical coordinates:

$$\frac{\partial}{\partial t} \int_{\xi_l}^{\xi_u} \frac{\partial p}{\partial \xi} d\xi + \nabla_\xi \cdot \left(\vec{\vec{v}} \int_{\xi_l}^{\xi_u} \frac{\partial p}{\partial \xi} d\xi \right) + \frac{\partial}{\partial \xi} \int_{\xi_l}^{\xi_u} \left(\dot{\xi} \frac{\partial p}{\partial \xi} \right) d\xi = 0$$ Integrate

→ $$\frac{\partial}{\partial t} \delta p + \nabla_\xi \cdot \left(\vec{\vec{v}}\, \delta p \right) = 0$$

Pressure thickness δp is prognostic variable

Conservation of Mass: Mass fixers

- Evaluate mass conservation properties of some models in the colloquium:
  ICON, CAM FV, CAM EUL
- Be careful what you see: Some models, especially climate models, apply *a posteriori* mass fixers
- Conservation of mass is needed in long-term climate simulations, less important in short weather prediction runs
- Basic idea behind the mass fixer: adjust the mean value of p_s after each time step, adjustment modifies all grid points at the surface
- This technique does not alter the pressure gradients
- Ask your modeling mentor!

Conservation of Total Energy

- There are many forms of the Total Energy (TE or E) Equation that depend on the choice of the fluid dynamics equations and the vertical coordinate (see Appendix F)
- An example for hydrostatic models with Cartesian coordinates is

$$
\begin{aligned}
E &= \int_A \int_{z_{top}}^{z_s} \left(\frac{\mathbf{v}^2}{2} + c_v T + g z \right) \rho \, dz \, dA \\
&\approx \int_A \left[\sum_{k=1}^{K_{max}} \left(\frac{u_k^2 + v_k^2}{2} + c_v T_k + g z_k \right) \rho_k \, \Delta z_k \right] dA.
\end{aligned}
$$

- In general: The TE equation is a global integral of the kinetic, thermal and potential energy in the model.
- The global integral is conserved in the continuous equations.

Conservation of Total Energy

- The question is whether TE is a conserved quantity in a dynamical core with numerical discretizations.
- Should we care?
  - in Weather Prediction Models
    - The answer is ‘not necessarily’
  - in Climate Models
    - The answer is ‘yes’
- When running for long times the violation of the total energy conservation leads to artificial drifts in the climate system (e.g. ocean heat fluxes)

Total Energy Fixer

- In nature:
  - conservation of total energy
  - energy lost by molecular diffusion provides heat
- In atmospheric models:
  - Energy is lost due to explicit or implicit (numerical) diffusion processes
  - Molecular diffusion is not represented on the model grid (spatial scale in models in way too big)
  - Numerical scheme might also lead to increase in total energy
- Therefore: some models provide an *a posteriori* energy fixer that restores the conservation of total energy by modifying the temperature

A posteriori Total Energy Fixer

- Goal: Total energy at each time step should be constant
- Compute the residual: $RES = \hat{E}^{+} - E^{-}$
- Compute the total energy before (-) and after (+) each time step

$$\hat{E}^{+} = \int_A \left\{ \left[\sum_{k=1}^{K} \left(\frac{(\hat{\mathbf{v}}_k^{+})^2}{2} + c_p \hat{T}_k^{+} \right) (p_0\, \Delta A_k + \hat{p}_s^{+}\, \Delta B_k) \right] + \Phi_s \hat{p}_s^{+} \right\} dA$$

$$E^{-} = \int_A \left\{ \left[\sum_{k=1}^{K} \left(\frac{(\mathbf{v}_k^{-})^2}{2} + c_p T_k^{-} \right) (p_0\, \Delta A_k + p_s^{-}\, \Delta B_k) \right] + \Phi_s p_s^{-} \right\} dA$$

A posteriori Total Energy Fixer

- **Idea:** Correct the temperature field to achieve the conservation of total energy (mimics heating by molecular diffusion)
- Option: **Fixer 1**, correction proportional to the magnitude of the local change in T at that time step

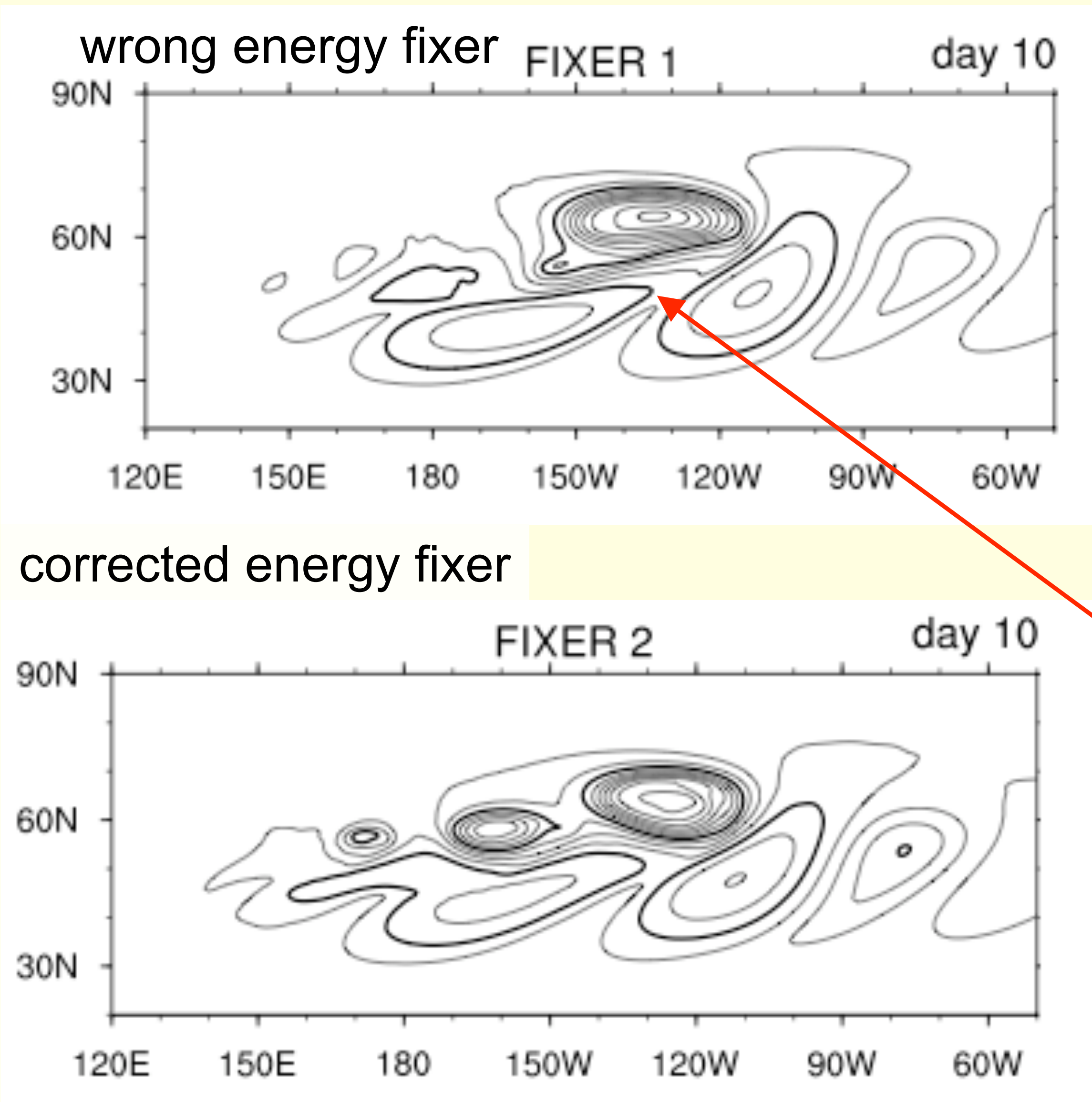
$$T^{+}(\lambda,\varphi,\eta) = \hat{T}^{+}(\lambda,\varphi,\eta) + \beta_1 |\hat{T}^{+}(\lambda,\varphi,\eta) - T^{-}(\lambda,\varphi,\eta)|$$

- Option: **Fixer 2**, correction is constant everywhere

$$T^{+}(\lambda,\varphi,\eta) = \hat{T}^{+}(\lambda,\varphi,\eta) + \beta_2$$

- Fixer 1 looks physical, but leads to wrong results

Energy Fixer: Surprising Consequences

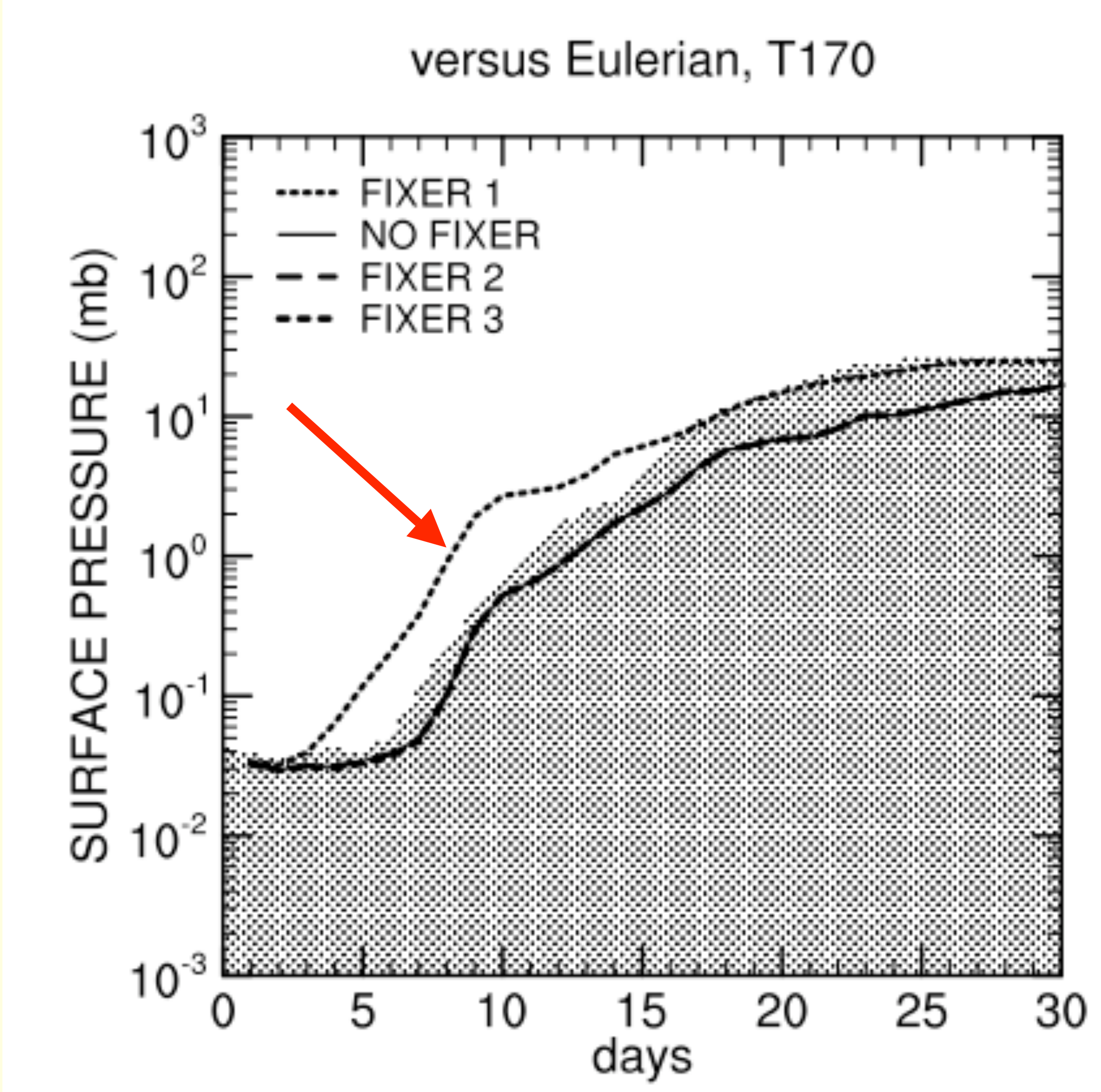


- Baroclinic wave test 2-0-0, p_s at day 10
- CAM SLD with a 'wrong' and 'corrected' choice of an energy fixer
- Wrong choice leads to wrong circulation pattern

Williamson, Olson & Jablonowski, MWR, in review

Energy Fixer: CAM SLD simulations

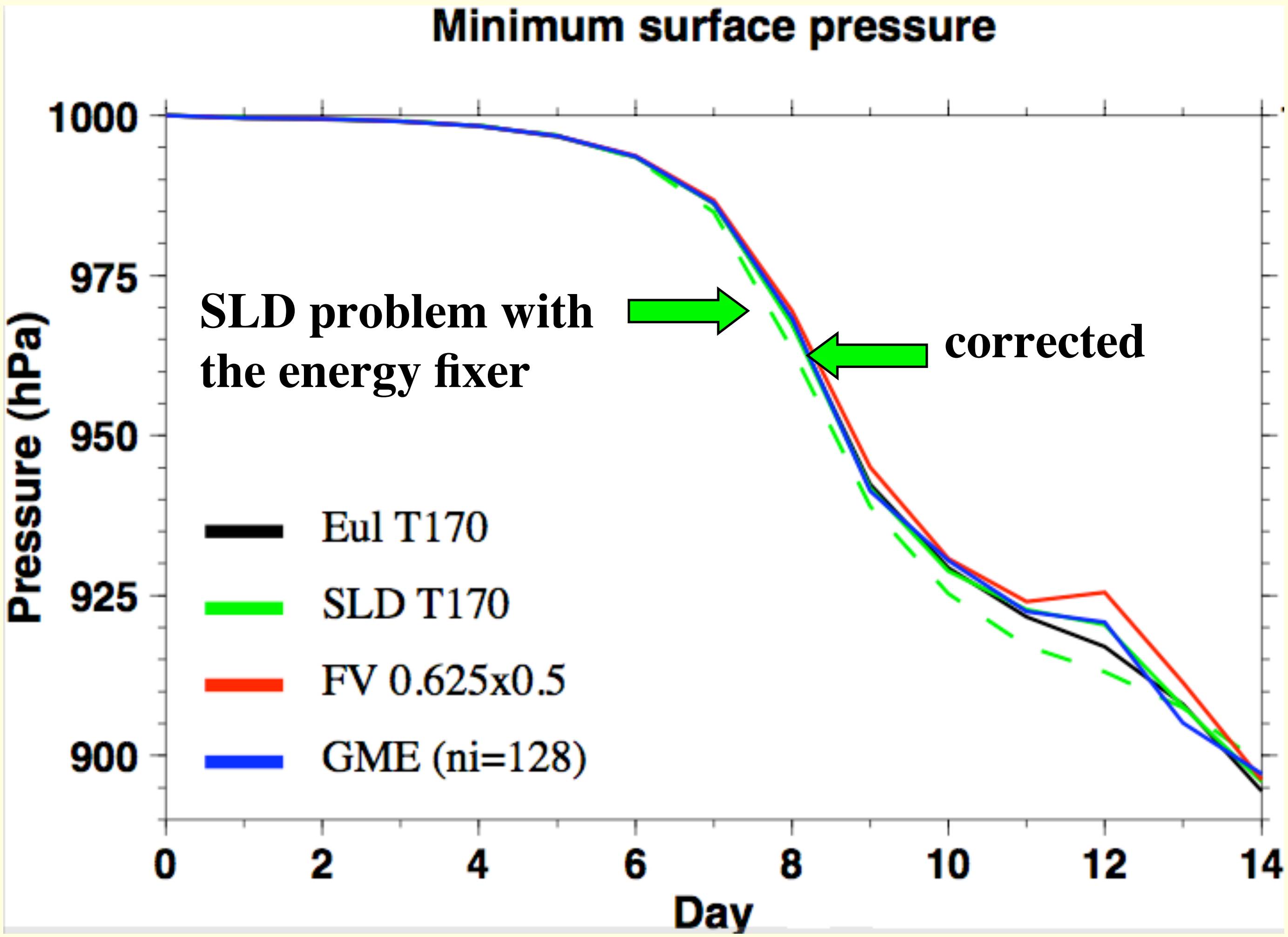
- Wrong choice (Fixer 1) is a clear outlier in the l_2 (p_s) error norm plot
- Lies above the uncertainty of the reference solutions (gray shaded)



Williamson, Olson & Jablonowski, MWR, in review

Energy Fixer: SLD Dynamical Core

- Fixer 1 in the SLD simulation is also an outlier in the time series of the minimum surface pressure



Conclusions

- These are the modeling aspects that nobody will tell you unless you ask.
- Ask your modeling mentor lots of questions !!
- Diffusion and filters help maintain the numerical stability
- Some diffusion (either explicit or implicit) is always needed to prevent a build-up of energy at the smallest scale (due to truncated energy cascade)
- But: Use the techniques selectively and know their consequences.
- It is very easy to compute nice-looking smooth, highly diffusive, but very inaccurate solutions to the equations of motion.