Dynamical core development considerations

An experience report

→ Grids

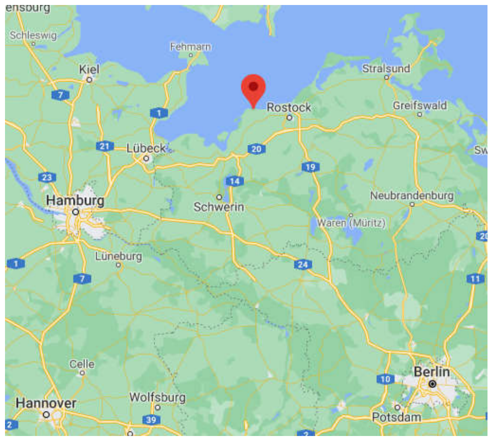
→ Conservation properties

→ Accuracy

→ Physics as inherent part of PDEs

LEIBNIZ-INSTITUT FÜR ATMOSPHÄREN PHYSIK IAP

Almut Gassmann,
Institute of Atmospheric Physics,
Kühlungsborn, Germany



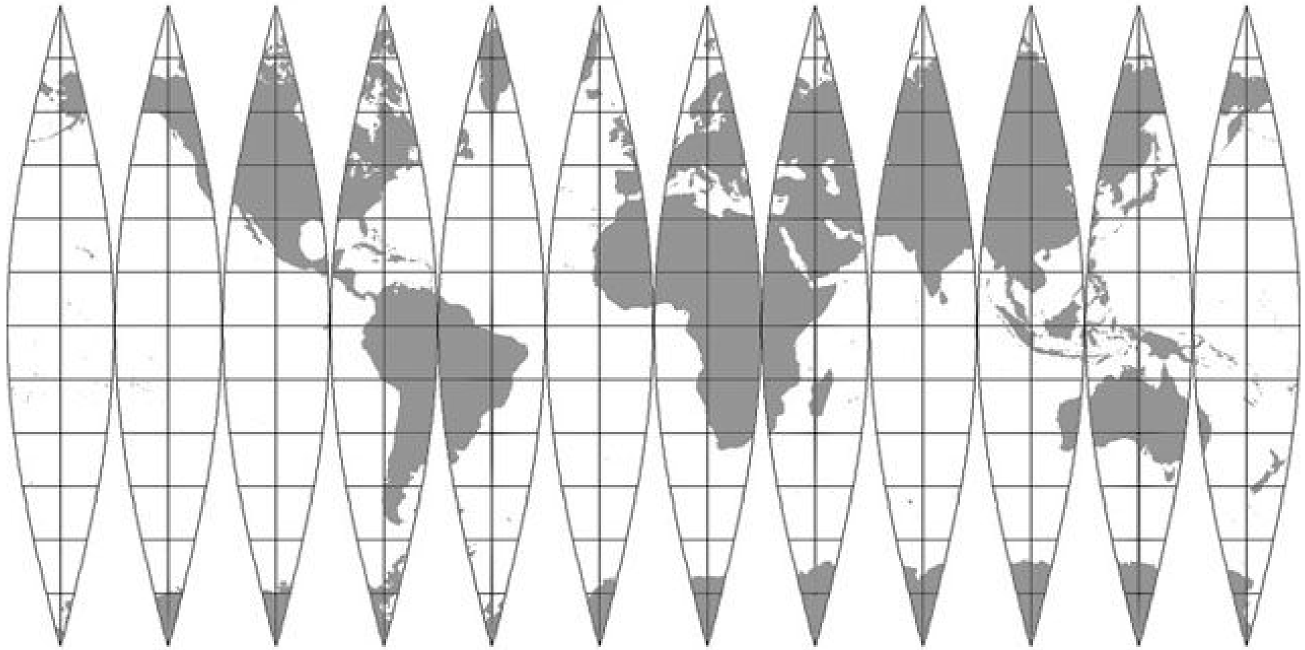
My background

Until 2006: limited area modelling with COSMO at DWD and Uni Bonn: work on the dynamical core and cloud physics

Starting from 2007: global modelling in the ICON group at MPI in Hamburg

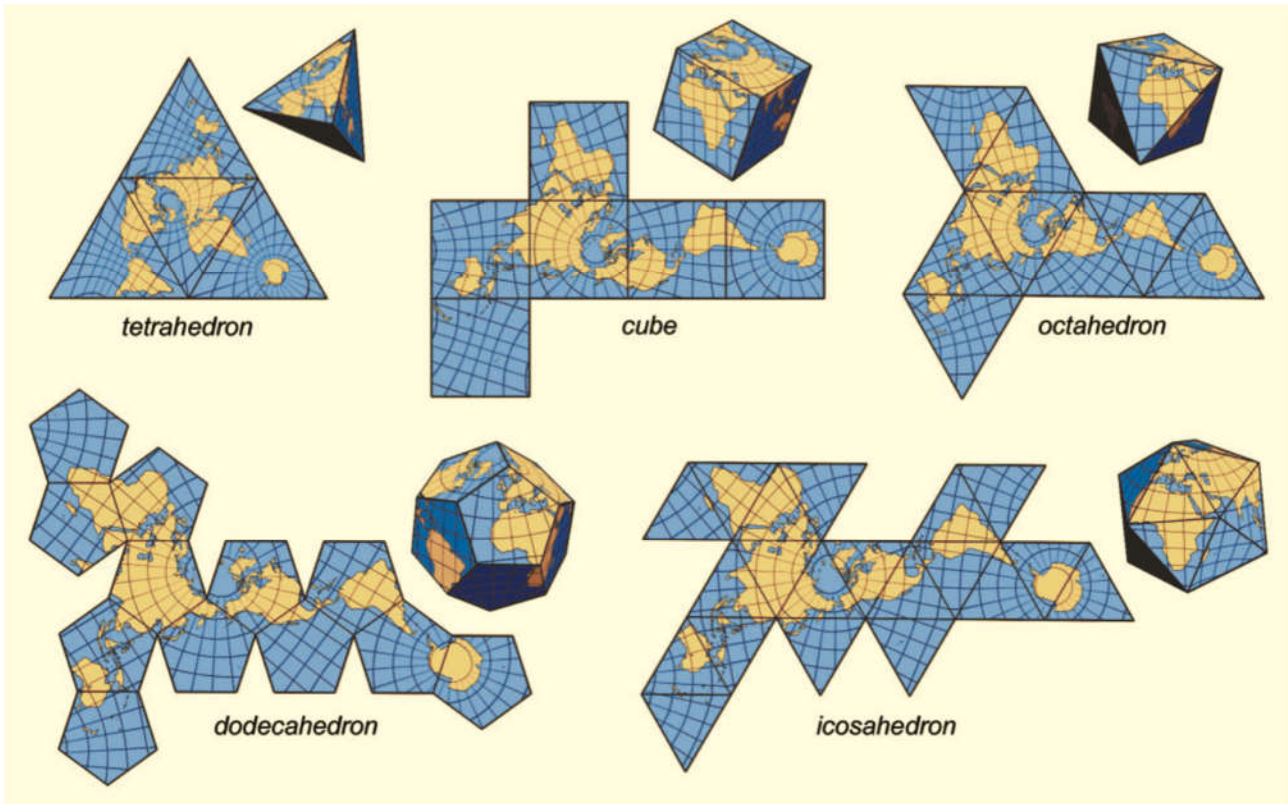
Since 2011: finalizing ICON-IAP model, thoughts about irreversible physics and dissipation in numerical models at IAP Kühlungsborn

well known
pole problem



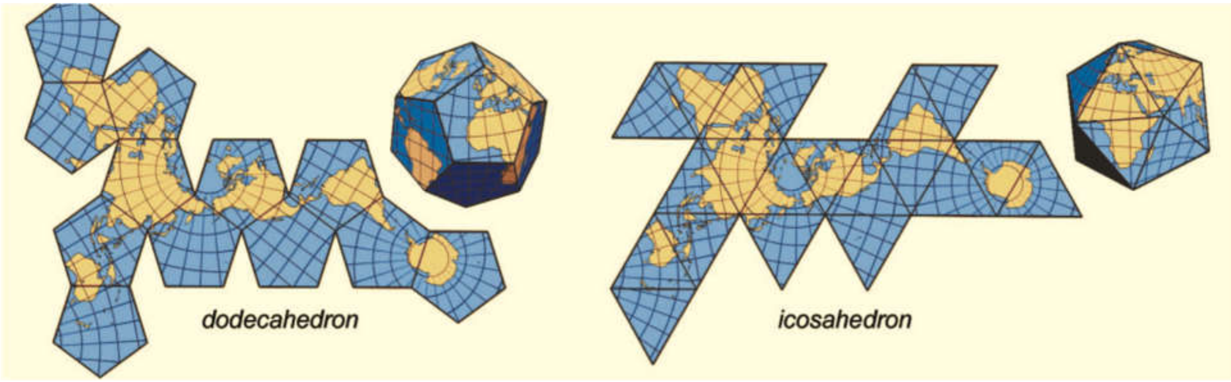
From papercrafting a globe to …

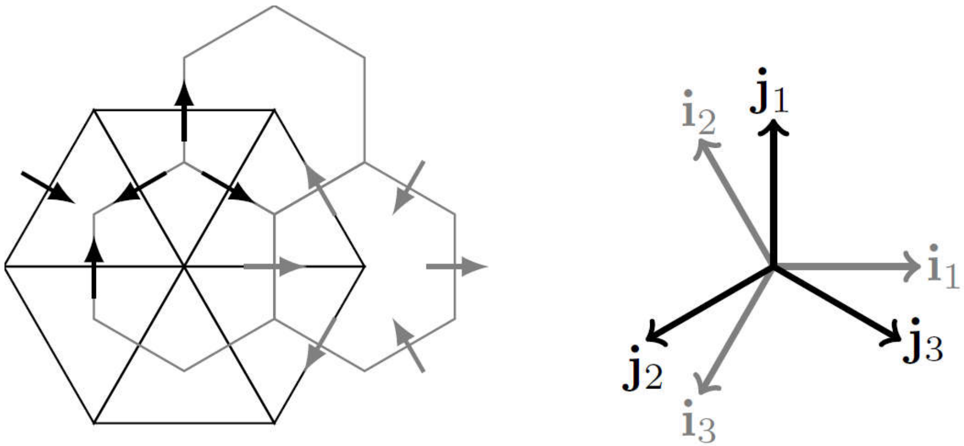
… a dynamical core on the globe



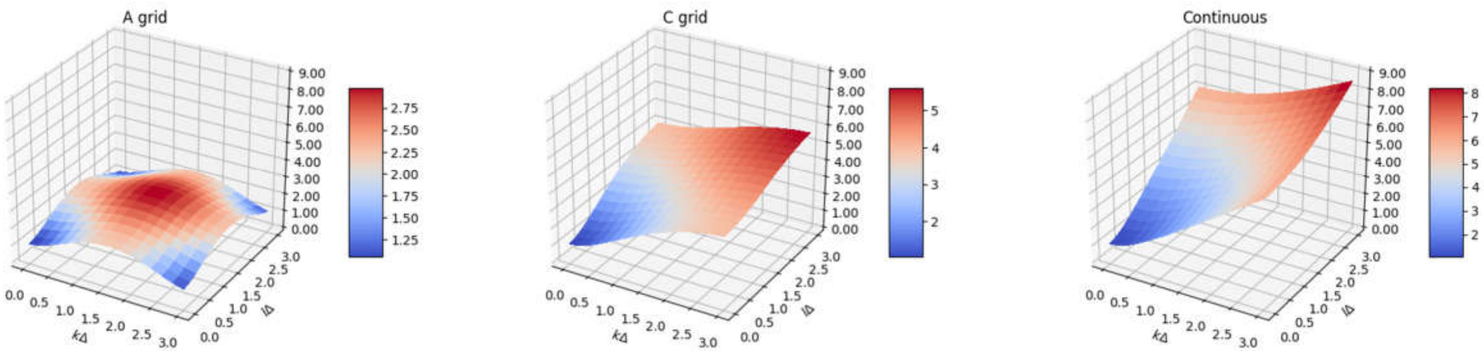
unknown problems which have eventually been solved

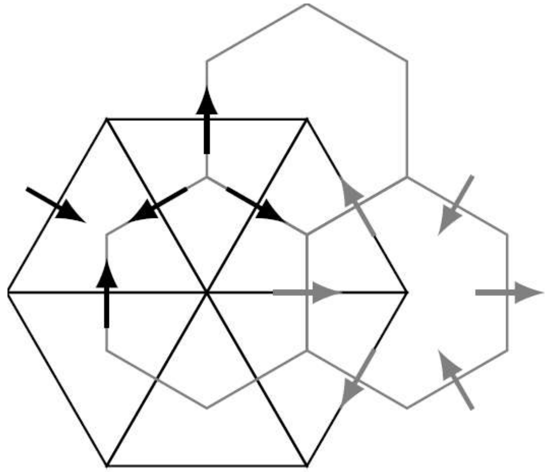
Which is the most promising grid structure?
Hexagons/pentagons or triangles?

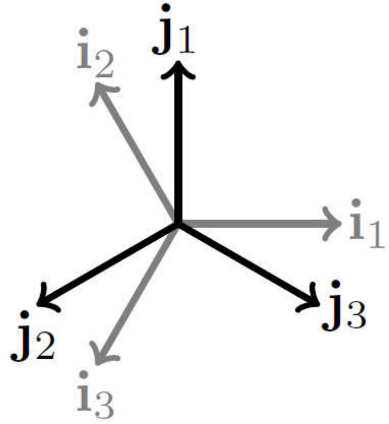


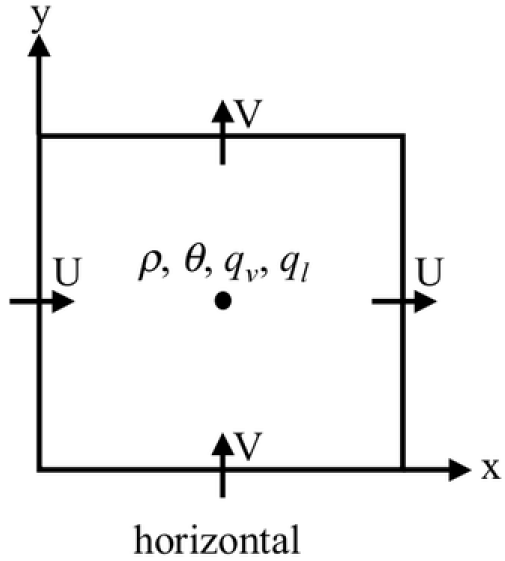


Fixed choice: **C-grid**, because it is good for wave propagation







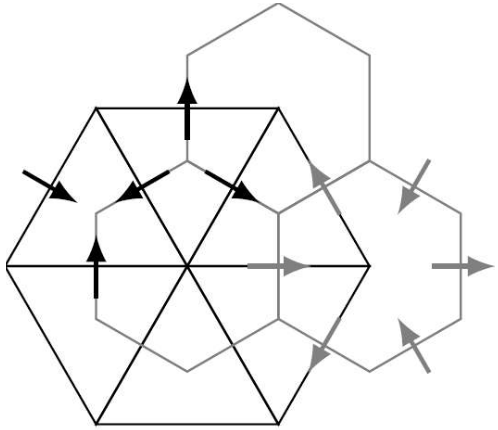


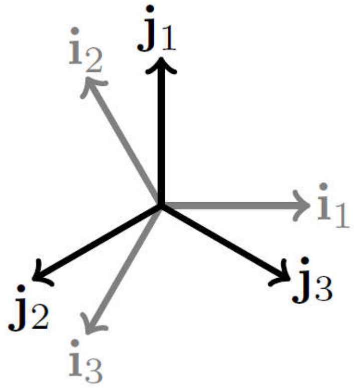
Whatever we choose as grid boxes:

There are three instead of two degrees of freedom in the horizontal velocity.

	unit vectors	***cont.*** velocity components (also the tendencies to those components)	***discrete*** velocity components (also the tendencies to those components)
Hexagons:	$\boldsymbol{i_1} + \boldsymbol{i_2} + \boldsymbol{i_3} = 0$	$u_1 + u_2 + u_3 = 0$	$\widetilde{u_1}^1 + \widetilde{u_2}^2 + \widetilde{u_3}^3 = 0$
Triangles:	$\boldsymbol{j_1} + \boldsymbol{j_2} + \boldsymbol{j_3} = 0$	$v_1 + v_2 + v_3 = 0$	$\widetilde{v_1}^1 + \widetilde{v_2}^2 + \widetilde{v_3}^3 = 0$

Tilde averaging rules (Thuburn, 2008)
make the linear dependency to hold on centers of hexagons



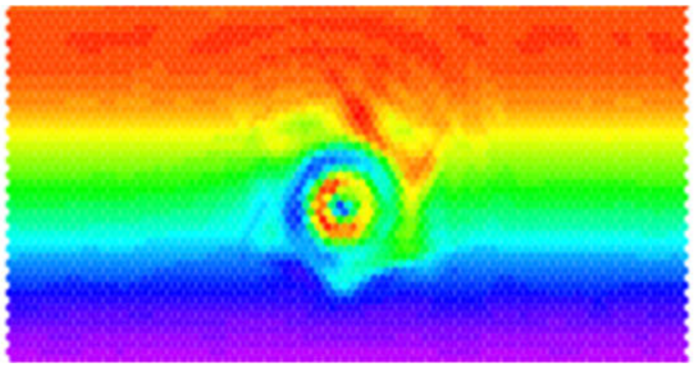


$$\partial_t \widetilde{u_1}^1 + \partial_t \widetilde{u_2}^2 + \partial_t \widetilde{u_3}^3 = 0$$

$$\partial_t \widetilde{v_1}^1 + \partial_t \widetilde{v_2}^2 + \partial_t \widetilde{v_3}^3 = 0$$

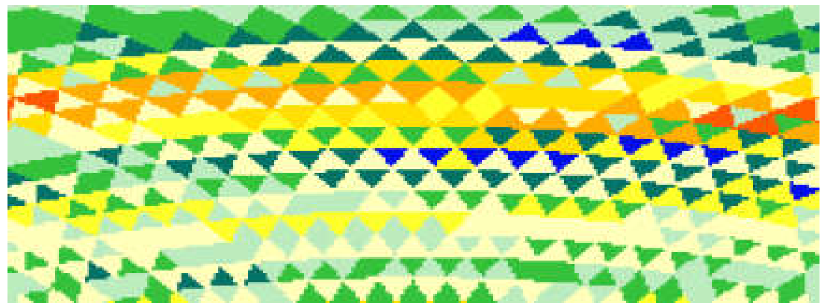
Gassmann (2011, 2018): If the **tilde averaging is not maintained** by the tendencies a **checkerboard pattern** will evolve in that measure, which is naturally defined on triangles.

Hexagons: problematic vorticity
Geostrophic balance disturbed



Coriolis, nonlinear advection of momentum:
Problem can be solved
C-grid staggering idea remains valid
TRSK papers (2009/2010), Gassmann (2018)

Triangles: problematic divergence
Gravity wave propagation disturbed, checkerboard in divergence



Pressure gradient:
Problem cannot be solved
Curing with divergence averaging questions C-grid staggering idea

Conclusion:

Under the premise of the C-grid staggering, hexagons must be chosen as grid boxes

C-grid staggering in the general nonlinear context:

The Dynamics of Finite-Difference Models of the Shallow-Water Equations

ROBERT SADOURNY

Laboratoire de Météorologie Dynamique du C.N.R.S., Paris, France

(Manuscript received 15 January 1974, in revised form 9 December 1974)

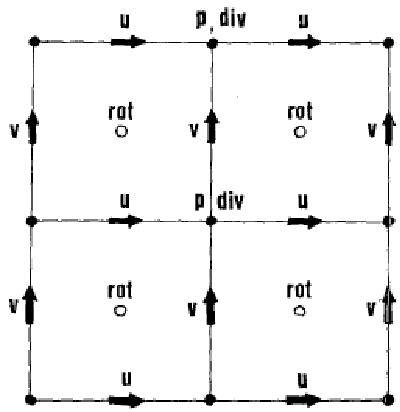


FIG. 1. Staggered arrays for the finite-difference models.

- supports correct energy conversions, and therefore energy conservation

$$\left.\begin{aligned}
&\frac{\partial u}{\partial t}-\eta\overline{\overline{V}^{x}}^{y}+\delta_x H=0\\
&\frac{\partial v}{\partial t}+\eta\overline{\overline{U}^{y}}^{x}+\delta_y H=0\\
&\frac{\partial P}{\partial t}+\delta_x U+\delta_y V=0
\end{aligned}\right\},$$

$$\begin{aligned}
\frac{dE}{dt}&+\sum\left(V\eta\overline{\overline{U}^{y}}^{x}-U\eta\overline{\overline{V}^{x}}^{y}\right)\\
&+\sum\left(U\delta_x H+H\delta_x U\right)\\
&+\sum\left(V\delta_y H+H\delta_y V\right)=0,
\end{aligned}$$

$$\left.\begin{aligned}
&\sum a\overline{b}^{x}=\sum b\overline{a}^{x}\\
&\sum a\delta_x b=-\sum b\delta_x a
\end{aligned}\right\}$$

C-grid staggering generalized

Sadourny (1975)

$$\left.\begin{aligned}\sum a\overline{b}^{x} &= \sum b\overline{a}^{x}\\ \sum a\delta_x b &= -\sum b\delta_x a\end{aligned}\right\}$$

Formalize such relations with the help of knowledge from theoretical physics: namely Poisson brackets

A General Method for Conserving Energy and Potential Enstrophy in Shallow-Water Models

RICK SALMON (JAS, 2007)

$$\frac{dF}{dt} = \{F, H\} \qquad \frac{dH}{dt} = \{H, H\} = 0$$

$$\{F, H\} = \iint d\mathbf{x}\,[q(F_u H_v - H_u F_v) - F_{\mathbf{u}} \cdot \nabla H_h + H_{\mathbf{u}} \cdot \nabla F_h]$$

$$H[u, v, h] = \frac{1}{2}\iint d\mathbf{x}\,(hu^2 + hv^2 + gh^2).$$

- H: Hamiltonian= energy functional
- Formulation needs functional derivatives
- F: arbitrary functional = for instance the Hamiltonian or the delta functional which selects just one variable at a selected position. Individual prognostic equations can be formulated with selected delta functionals.

Trick: Don't discretize individual prognostic equations.
Discretize the bracket → convert integral into a sum over grid points, define averaging operator, define gradient **or** divergence on the grid

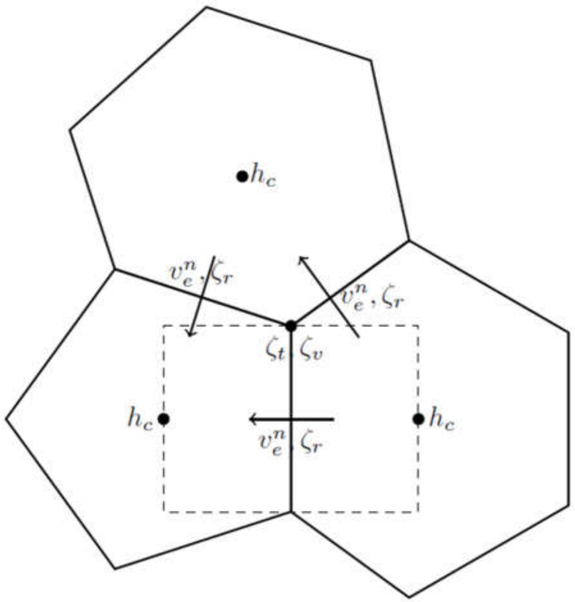
The C-grid is naturally suited here, but other approaches are also possible

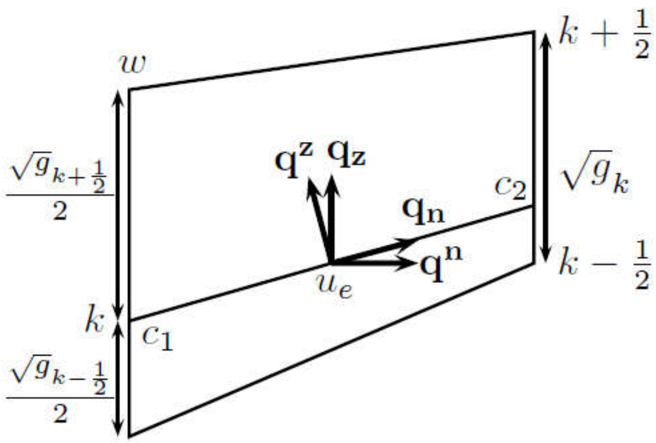
Hexagonal C-grid staggering generalized for nonhydrostatic compressible dynamics on the in terrain-following coordinates: The ICON-IAP model (Gassmann 2013)

$$\frac{\partial \mathcal{F}}{\partial t} = \{\mathcal{F}, \mathcal{H}\} + (\mathcal{F}, \mathbf{f}_r) + (\mathcal{F}, Q) \qquad \mathcal{H}(\mathbf{v}, \varrho, \tilde{\theta}) = \int_V \left(\frac{1}{2}\varrho \mathbf{v}^2 + \varrho g z + \varrho c_v T\right) \mathrm{d}\tau \qquad \tilde{\theta} = \varrho\theta$$

$$\{\mathcal{F}, \mathcal{H}\} = -\int_V \frac{\delta \mathcal{F}}{\delta \mathbf{v}} \cdot \left(\frac{\vec{\omega}_a}{\varrho} \times \frac{\delta \mathcal{H}}{\delta \mathbf{v}}\right) \mathrm{d}\tau - \int_V \left(\frac{\delta \mathcal{F}}{\delta \varrho} \nabla \cdot \frac{\delta \mathcal{H}}{\delta \mathbf{v}} - \frac{\delta \mathcal{H}}{\delta \varrho} \nabla \cdot \frac{\delta \mathcal{F}}{\delta \mathbf{v}}\right) \mathrm{d}\tau - \int_V \left(\frac{\delta \mathcal{F}}{\delta \tilde{\theta}} \nabla \cdot (\theta \frac{\delta \mathcal{H}}{\partial \mathbf{v}}) - \frac{\delta \mathcal{H}}{\delta \tilde{\theta}} \nabla \cdot (\theta \frac{\delta \mathcal{F}}{\delta \mathbf{v}})\right) \mathrm{d}\tau$$

- nonlinear Coriolis term $-\boldsymbol{\omega}_a \times \mathbf{v}$
- gradients of potential terms ($\phi + E_{kin}$) **and** mass continuity equation
- pressure gradient **and** transport of potential temperature





Main advantage

Consistent view on metric terms in terrain-following coordinates.

Pressure gradient term is related to the contravariant θ-flux term in steep terrain.

All the formulations so far are second order accurate:

The C-grid is inherently 2nd order accurate for momentum advection and continuity.

The bracket leaves the degree of freedom for higher order advection for scalars

$$\{\mathcal{F},\mathcal{H}\} = -\int_V \frac{\delta\mathcal{F}}{\delta\mathbf{v}}\cdot\left(\frac{\vec{\omega}_a}{\varrho}\times\frac{\delta\mathcal{H}}{\delta\mathbf{v}}\right)\mathrm{d}\tau - \int_V\left(\frac{\delta\mathcal{F}}{\delta\varrho}\nabla\cdot\frac{\delta\mathcal{H}}{\delta\mathbf{v}} - \frac{\delta\mathcal{H}}{\delta\varrho}\nabla\cdot\frac{\delta\mathcal{F}}{\delta\mathbf{v}}\right)\mathrm{d}\tau - \int_V\left(\frac{\delta\mathcal{F}}{\delta\tilde{\theta}}\nabla\cdot(\theta\frac{\delta\mathcal{H}}{\partial\mathbf{v}}) - \frac{\delta\mathcal{H}}{\delta\tilde{\theta}}\nabla\cdot(\theta\frac{\delta\mathcal{F}}{\delta\mathbf{v}})\right)\mathrm{d}\tau$$

$$\frac{\partial(\rho\psi)}{\partial t} = -\nabla\cdot\mathbf{V}\rho\psi,$$

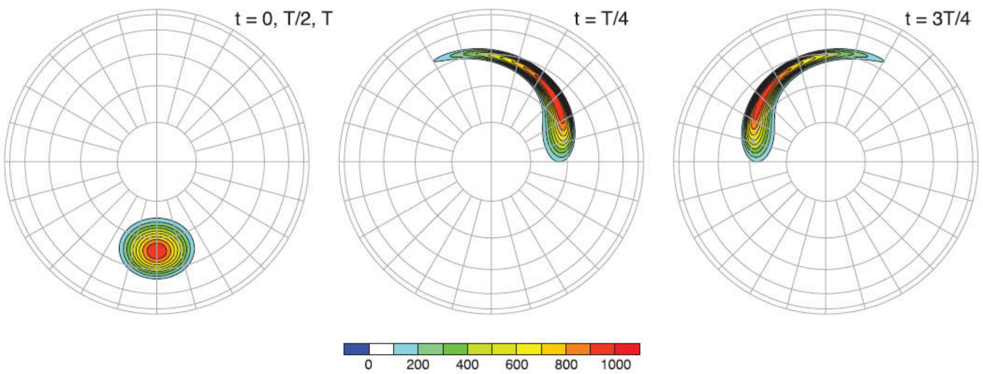


FIG. 5. Exact solution for the Blossey and Durran (deformational flow) test case adapted to the sphere, from Skamarock and Menchaca (2010).

Conservative Transport Schemes for Spherical Geodesic Grids: High-Order Flux Operators for ODE-Based Time Integration

WILLIAM C. SKAMAROCK

National Center for Atmospheric Research, Boulder, Colorado*

ALMUT GASSMANN

Max Planck Institute for Meteorology, Hamburg, Germany

(Manuscript received 30 November 2010, in final form 4 April 2011)

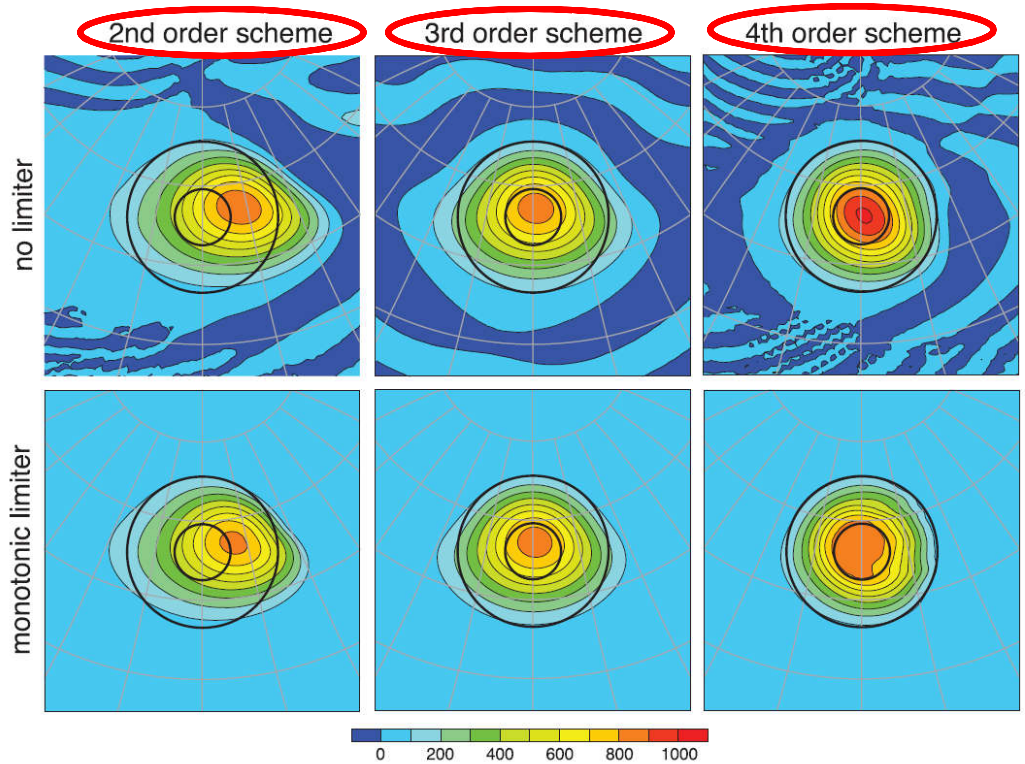
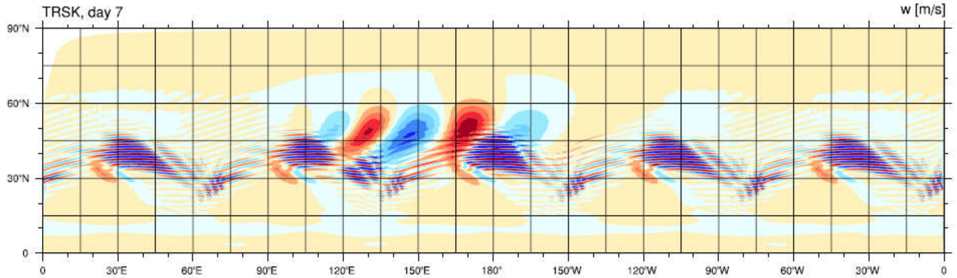


FIG. 6. Deformational flow test case results at time T. The thick contours are the exact solution for $\psi = 100$ and 800. The simulations were performed on the 40 962-cell mesh.

Baroclinic wave test: w-field on day 7

First shot…



After accounting for linear dependency of tendencies
of the nonlinear momentum advection …

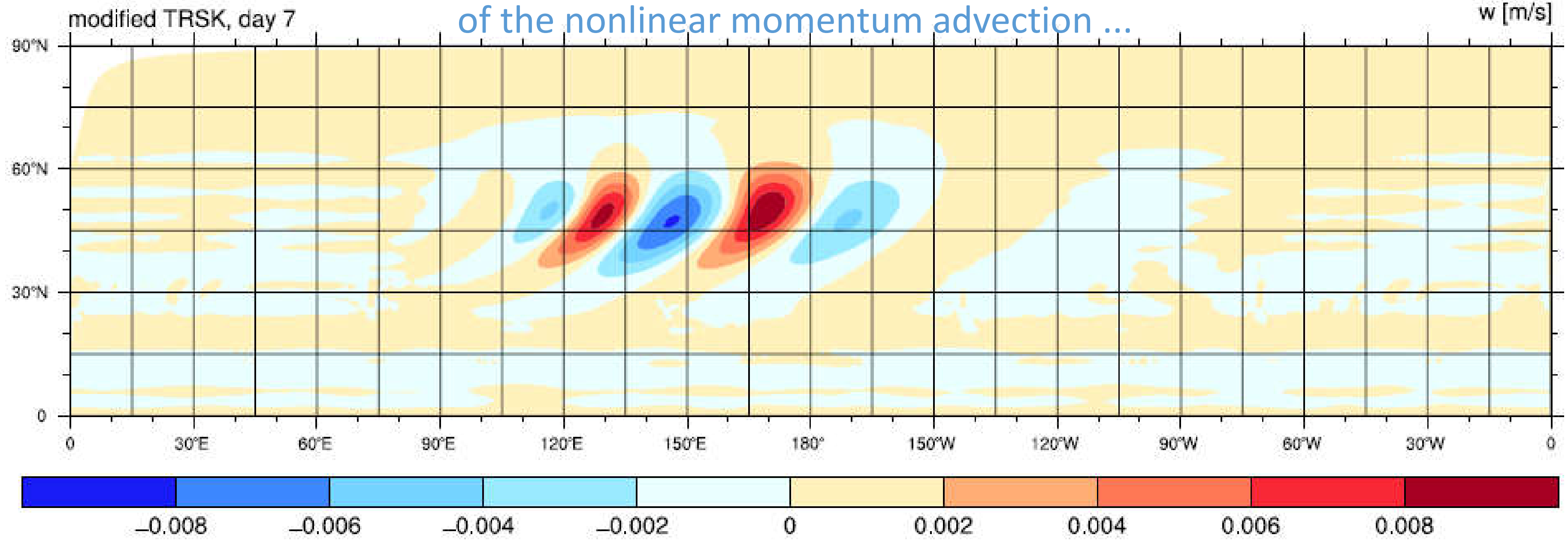
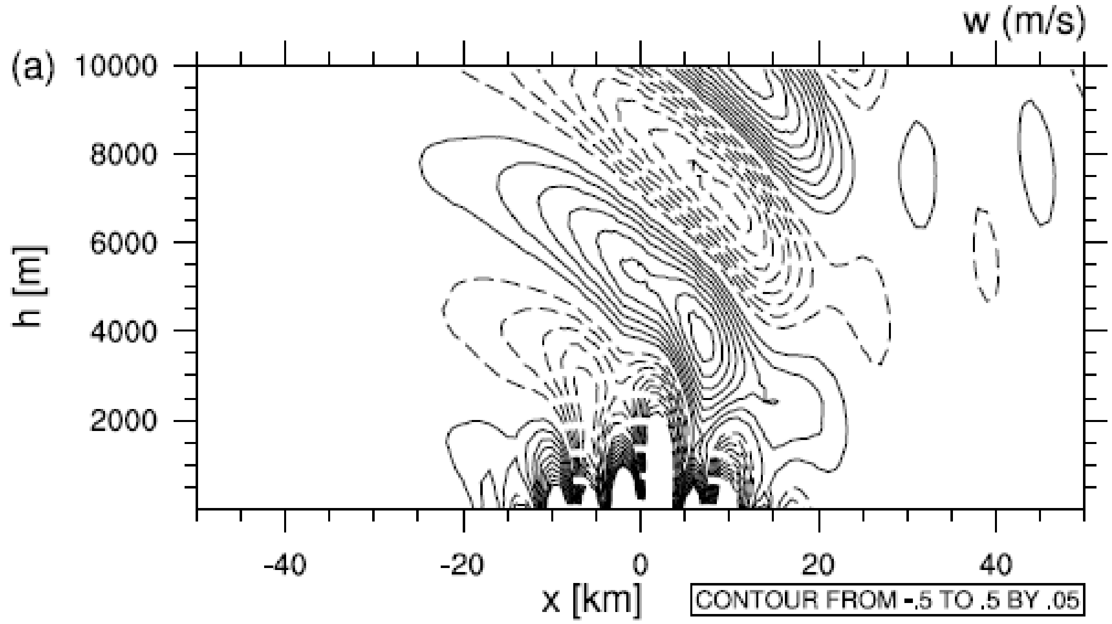


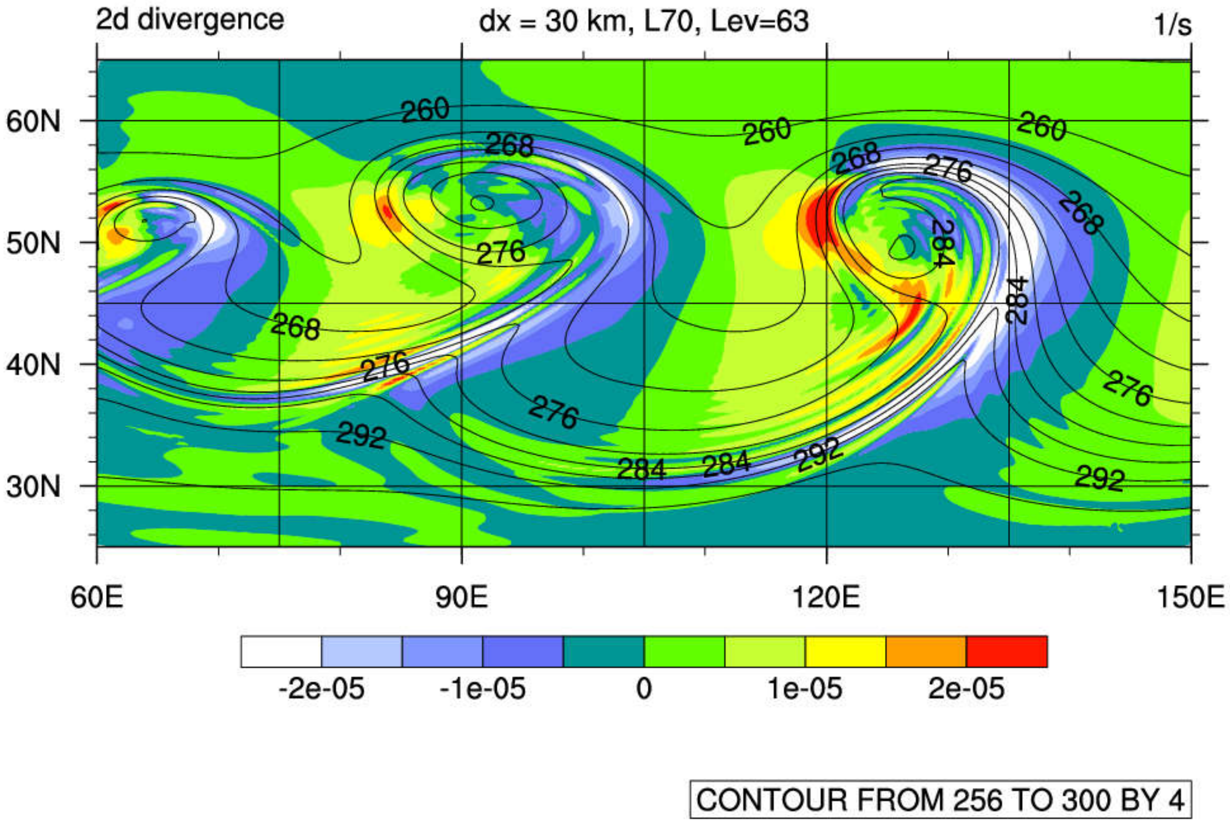
FIGURE 5 Vertical velocity on level 18 at day 7 of the baroclinic wave test displayed for the Northern Hemisphere. Upper panel: TRSK scheme, middle panel: Gassmann (2013) scheme, lower panel: modified TRSK scheme [Colour figure can be viewed at wileyonlinelibrary.com]

Achievements:

- no checkerboard pattern in divergence
- no nonlinear (Hollingsworth) instability due to momentum advection in vector invariant form: $-\boldsymbol{v} \cdot \nabla \boldsymbol{v} = -\nabla K - (\nabla \times \boldsymbol{v}) \times \boldsymbol{v}$
- no further smoothers or artificial dampers are necessary, this runs without diffusion until sharp fronts form which call for a subscale turbulence scheme

Schär mountain testcase





Gravity wave structures generated near fronts are reasonably evolving

→ Grids
→ Conservation properties
→ Accuracy
→ **Physics as inherent part of PDEs**

It is possible to derive an 'internal energy form' of the temperature equation

$$\hat{c}_v \varrho d_t T = \underbrace{-p\nabla \cdot \mathbf{v}}_{\text{work}} \underbrace{+\varepsilon_{fric} \underbrace{- \sum_i (\widetilde{h_{0,i}} + c_{v,i} T) I_i}_{\text{latent heating}} - \nabla \cdot (\mathbf{R} + \mathbf{J}_s + \sum_i c_{p,i} T \mathbf{J}_i) + T \nabla \cdot \sum_i \mathbf{J}_i c_{v,i}}_{\text{diabatic heating: } Q_{c_v T}}$$

or an 'enthalpy form' of the temperature equation

$$\hat{c}_p \varrho d_t T = \underbrace{\omega}_{\text{work}} \underbrace{+\varepsilon_{fric} \underbrace{- \sum_i (\widetilde{h_{0,i}} + c_{p,i} T) I_i}_{\text{latent heating}} - \nabla \cdot (\mathbf{R} + \mathbf{J}_s + \sum_i c_{p,i} T \mathbf{J}_i) + T \nabla \cdot \sum_i \mathbf{J}_i c_{p,i}}_{\text{diabatic heating: } Q_{c_p T}}$$

Physics terms that enter the PDEs have to be energetically consistent.

- mass weighted heat capacities
- frictional heating
- temperature dependent latent heats
- accounting for turbulent/sedimentation fluxes in all respects

→ Grids
→ Conservation properties
→ Accuracy
→ **Physics as inherent part of PDEs**

The miracle behind the brackets is the duality between the divergence and gradient

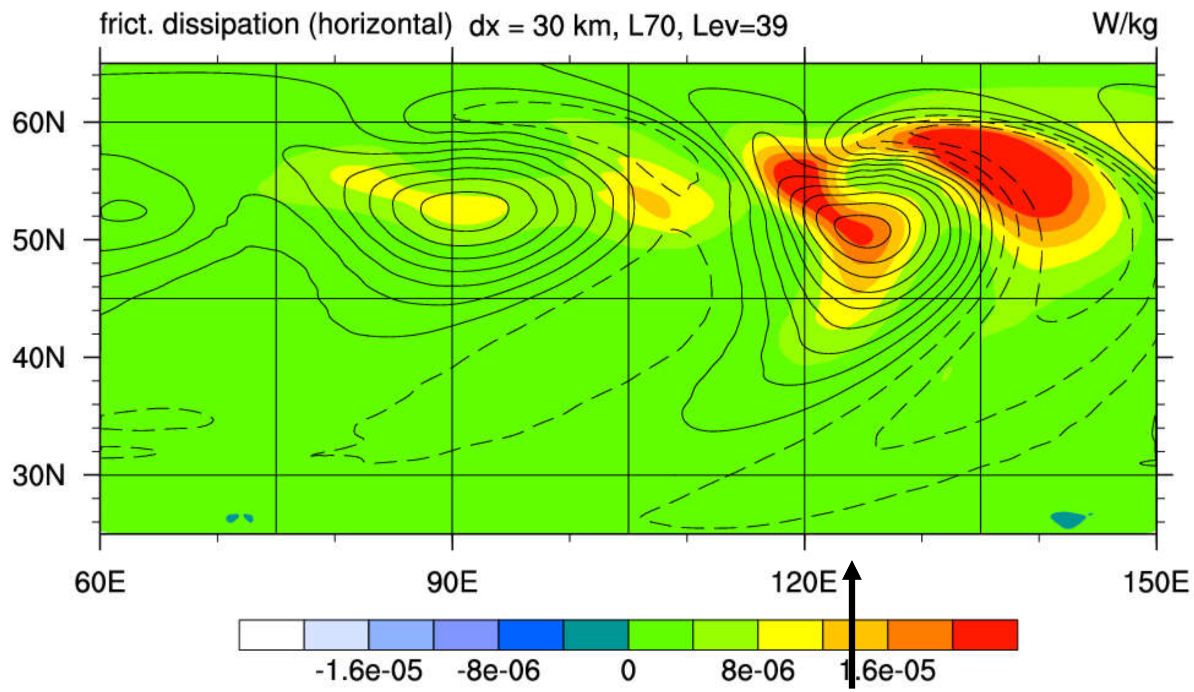
$$\nabla \cdot (\boldsymbol{f}\psi) = \psi \nabla \cdot (\boldsymbol{f}) + \boldsymbol{f} \cdot \nabla \psi$$

This plays also a role when deriving the entropy budget equation and disentangling entropy flux divergences from internal entropy production terms

$$\varrho d_t s = \underbrace{-\nabla \cdot \left(\frac{\mathbf{J}_s}{T} + \sum_i s_i \mathbf{J}_i \right)}_{\varrho d_{t,e} s} + \underbrace{\frac{\varepsilon_{fric} - \mathbf{J}_s/T \cdot \nabla T - \sum_i \mathbf{J}_i \cdot \nabla \mu_i|_T - \sum_i I_i \mu_i}{T}}_{\varrho d_{t,i} s \text{ internal entropy production } \geq 0}$$

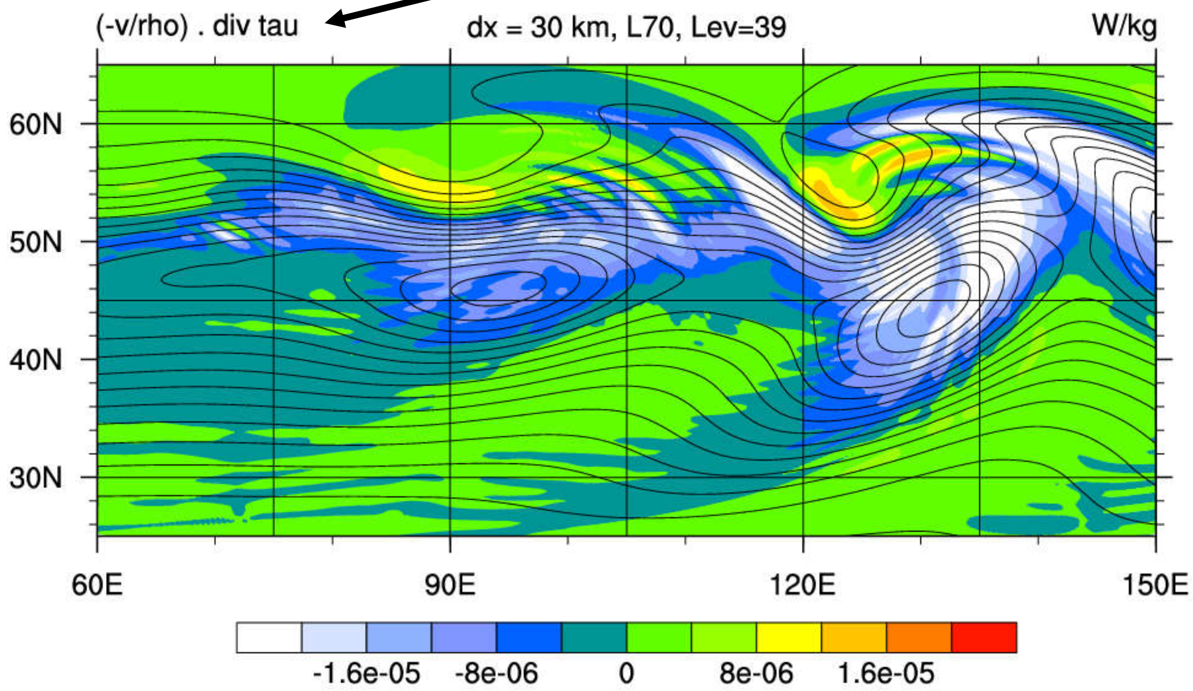
dissipation: ε = T*internal entropy production

The subgridscale fluxes must be proportional to the above gradients.
The numerical operators for the divergences and gradients in the parameterizations must be the same as in the dynamical core.



Frictional dissipation (colors) and vorticity (contours by 10 e^{-6}/s)
Run used only hori diffusion with a conventional Smagorinsky scheme.
Note that this is positive definit, hence a slight heating – in fact it is the produced TKE by shear.

$$-\nabla\cdot(\overleftrightarrow{\boldsymbol{\tau}}\cdot\boldsymbol{v}) = -\boldsymbol{v}\cdot\nabla\cdot\overleftrightarrow{\boldsymbol{\tau}} - \overleftrightarrow{\boldsymbol{\tau}}\cdot\cdot\nabla\boldsymbol{v}$$



Tendency to the kinetic energy due to friction (colors) and kinetic energie (contours). Kinetic energy is eroded, but not everywhere.

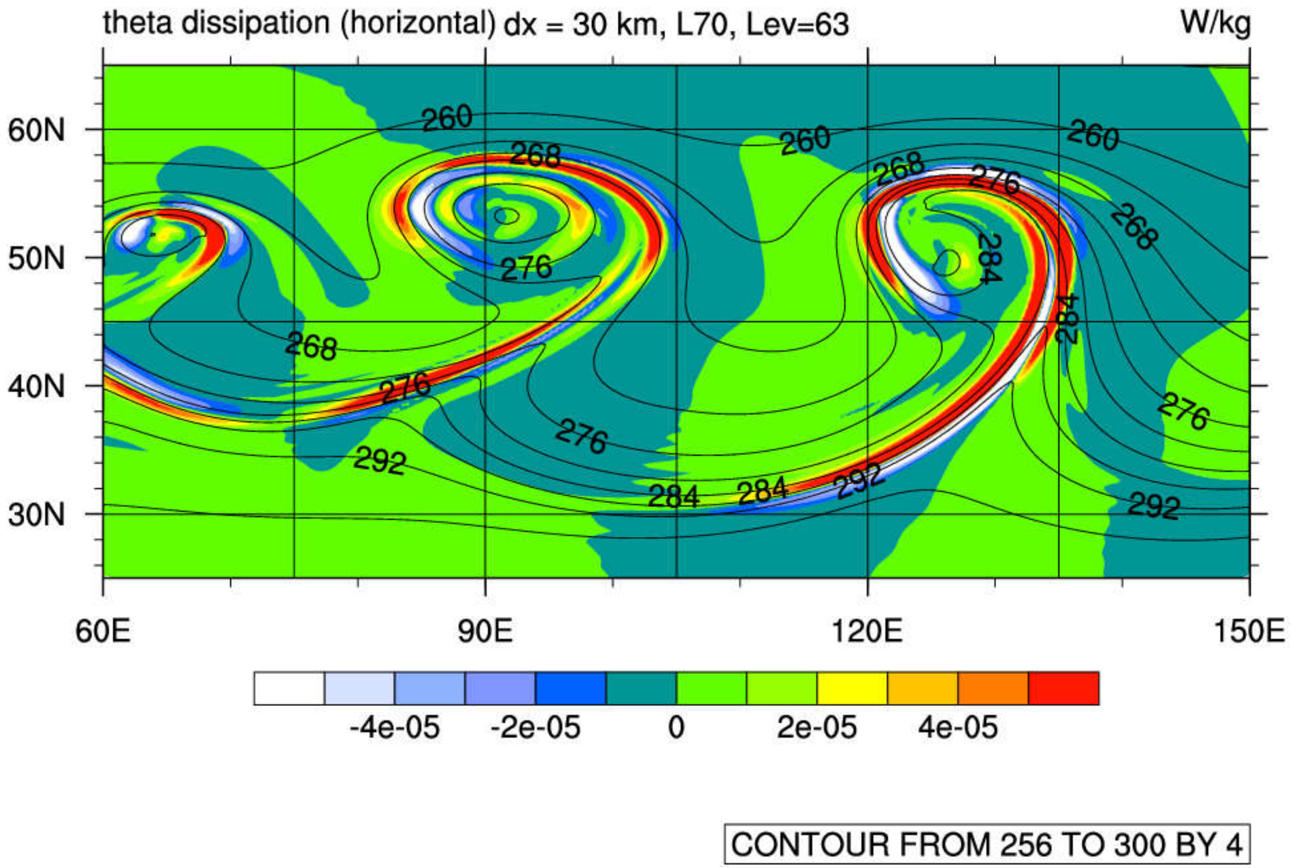
Note that the pattern of this field is less smooth than the field above.

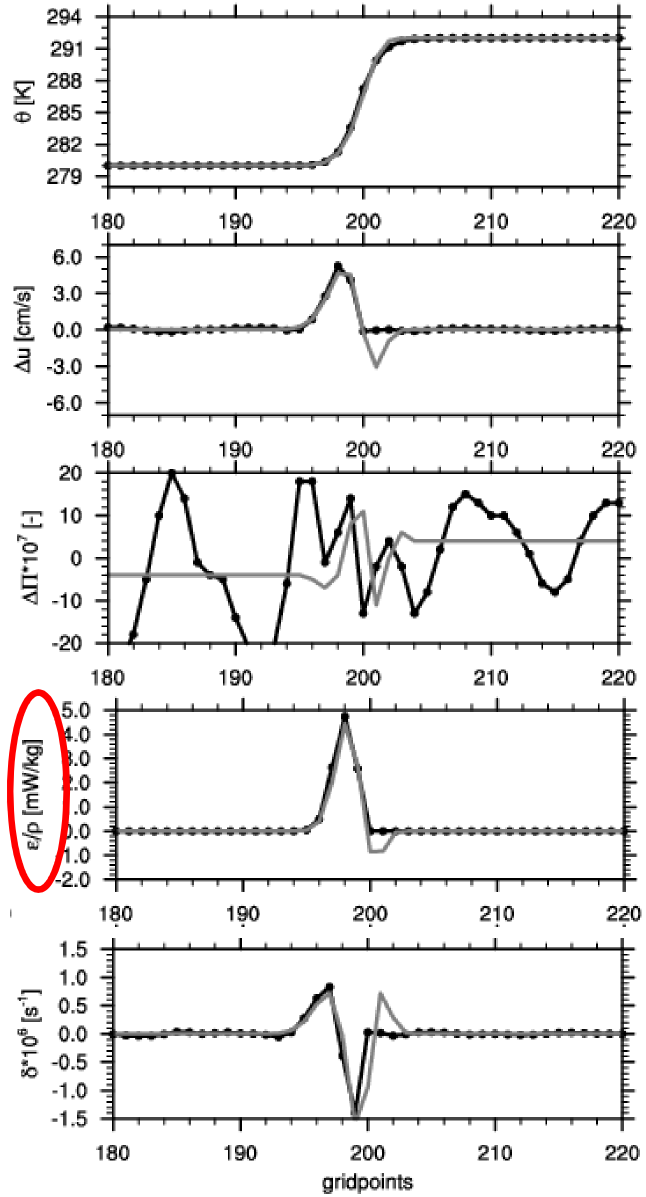
The 3rd order θ-advection is inherently (anti)diffusive → locally negative dissipation rates.

$$\partial_t u|_{sub,2} = c_p \frac{K_\theta \partial_x \theta}{u} \partial_x \Pi$$

$$\partial_t (c_v \varrho T)|_{sub,2} = -c_p \Pi \partial_x (-\varrho K_\theta \partial_x \theta)$$

$$\partial_t (\varrho s)|_{sub,2} = \partial_x \left(\frac{c_p \varrho K_\theta \partial_x \theta}{\theta} \right) + \frac{c_p \varrho K_\theta (\partial_x \theta)^2}{\theta^2}$$





We see an impact onto the gravity wave formation near fronts.

Right: 1-dimensional impact of inherent θ-diffusion/antidiffusion on the dynamical fields.

Wind blows from left to right. Black: no antidiffusion allowed

Challenge: 2nd law forces downgradient T-diffusion – which is out of our experience, contemporary understanding and state of the art.
How to bring perspectives together?

Dry: Turbulence modelling requires TKE and TPE equations, both.

$$\varrho d_t E_k = -\varrho K_\theta N^2 - \partial_z(-\varrho K_{E_k}\partial_z E_k) + \varepsilon_{sh} - \varepsilon_{E_k}$$ turb. kinetic energy

$$\varrho d_t E_{tpe} = +\varrho K_\theta N^2 - \partial_z(-c_p \varrho K_\theta \Pi \partial_z \theta) - \varepsilon_{E_p} = -c_p \Pi \partial_z(-\varrho K \partial_z \theta) - \varepsilon_{E_p}$$ turb. potential energy

$$\varrho c_v d_t T|_{mv} = +\varepsilon_{E_k} + \varepsilon_{E_p}$$ energy on molecular and viscous scales

The resolved grid does not see the 'true' dissipation on mol. and viscous scales
It does only see the terms at the resolved scales, and so also only the resolved dissipation

$$\varrho d_t(E_k + E_p + c_v T|_{mv}) = \varepsilon_{sh} - \partial_z(-\varrho K_{E_k}\partial_z E_k - c_p \varrho K_\theta \Pi \partial_z \theta)$$

$$\varrho d_t(E_k + E_p + c_v T|_{mv}) = \varepsilon_{sh} + \varepsilon_{th} - T\partial_z\left(\frac{-\varrho K_{E_k}\partial_z E_k - c_p \varrho K_\theta \Pi \partial_z \theta}{T}\right)$$

Such kind of concept enforces the following inequality for the sensible heat flux

$$\varepsilon_{th} = \frac{\varrho K_{E_k}\partial_z E_k + c_p \varrho K_\theta \Pi \partial_z \theta}{T}\partial_z T \geq 0$$

Turbulence modelers should check whether their fluxes support this condition.
It means that a heat flux at stable stratification can only happen if it is supported by a TKE flux.
TKE is depositing energy into the stable layer.

Summary

1. C-grid staggering is advantageous for wave propagation

2. Poisson brackets for dynamics may be easily be discretized on C-grids. They formalize energy conversions and energy conservation.

3. One property of the brackets is the duality between gradient and divergence operator. This duality is also needed when deriving the 2^{nd} law of thermodynamics. At this place, challenges for research on turbulence schemes come to the fore.