Status report of

WG 2 – Numerical aspects

COSMO General meeting, online
13-17 Sept. 2021

Michael Baldauf, Florian Prill (DWD), Michal Ziemianski (IMGW)

Outline

- Status COSMO-EULAG
- Recent developments with the DG scheme
- Further WG2 stuff

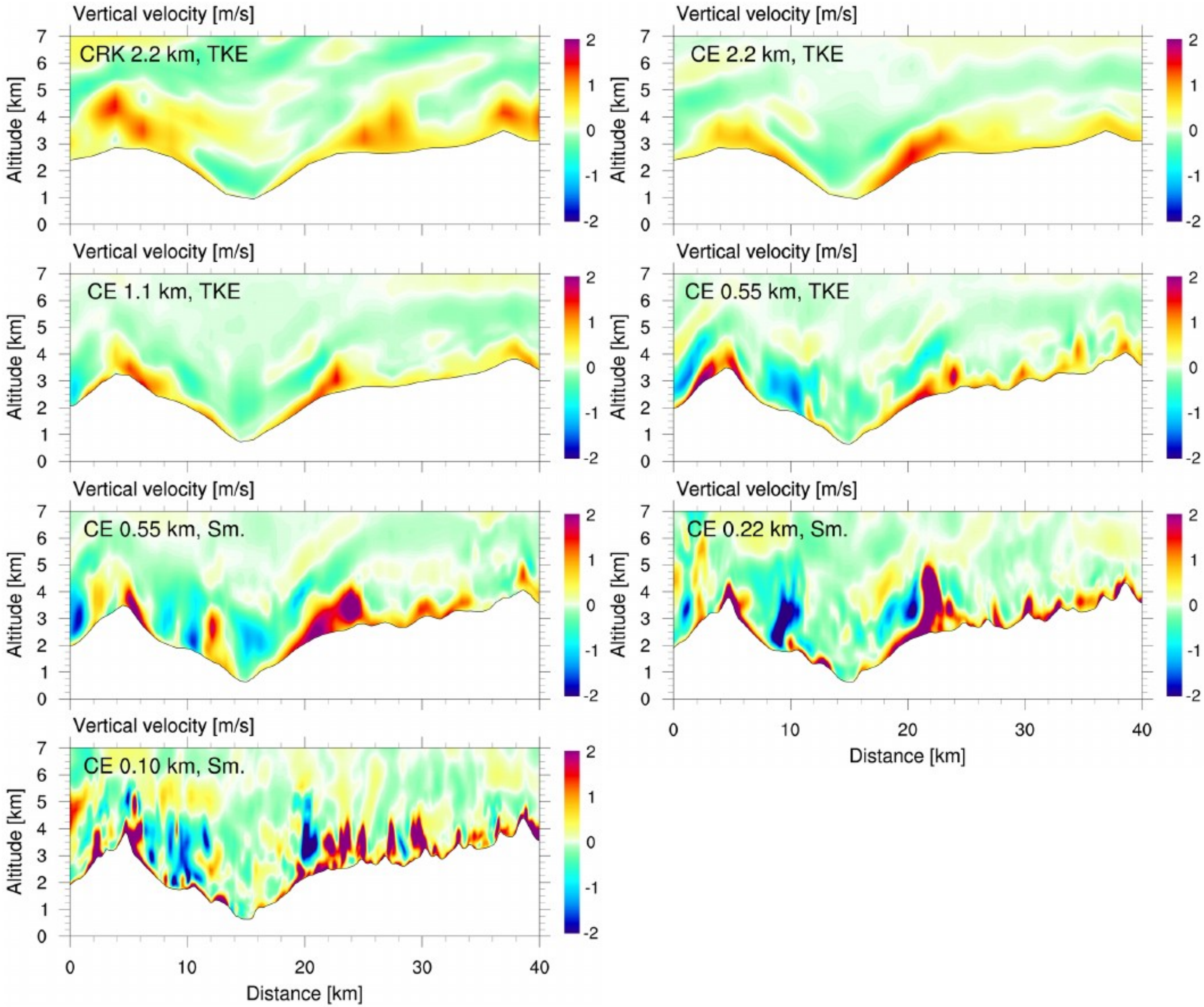
COSMO publication

M. Ziemiański

An article „Compressible EULAG dynamical core in COSMO: convective-scale Alpine weather forecasts" by M. Ziemiański, D. Wójcik, B. Rosa, and Z. Piotrowski was accepted for publication in Monthly Weather Review (August 2021)

- it contains :
  - description of the semi-implicit compressible EULAG dynamical core
  - discussion of the coupling of EULAG dynamical core with the COSMO computational and physical framework (version 5.05 was used)
  - comparison of standard verification statistics for 2.2 km COSMO-Runge-Kutta (CRK) and COSMO-EULAG (CE) for warm and colder season over Alpine domain
  - verification case-study for representation of summer convective clouds with CRK at 2.2 km grid and CE at 2.2, 1.1, and 0.55km grid
  - demonstration of the CE forecast of Alpine convection at 0.22 and 0.1 km grid
- it demonstrates the competitive CE verification scores and realism and robustness of its Alpine forecasts at O(100 m) horizontal grid with slopes reaching 85 deg.

CRK and CE vertical velocity over the Alps



Vertical velocity (m/s) over the Rhone valley (Bietschhorn on the left, Weiss-horn on the right) at 1230 UTC of 19 July 2013 for horizontal grids between 2.2 and 0.1 km and different turbu-lence schemes

(TKE or Smago-rinsky)

Recent developments in the Discontinuous Galerkin scheme

Michael Baldauf, Florian Prill (DWD)

Discontinuous Galerkin (DG) methods in a nutshell (I)

$$\frac{\partial q^{(k)}}{\partial t} + \nabla \cdot \mathbf{f}^{(k)}(q) = S^{(k)}(q), \qquad k = 1, ..., K$$

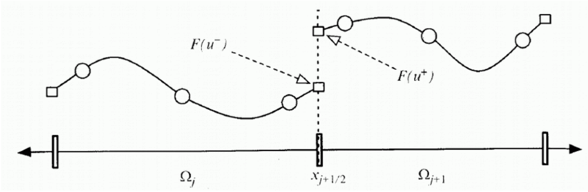
e.g.
Cockburn, Shu (1989) Math. Comput.
Cockburn et al. (1989) JCP
Hesthaven, Warburton (2008)

1.) weak formulation $\int_{\Omega_j} dx \, v(\mathbf{x}) \cdot \ldots$

$$\rightarrow \quad \frac{d}{dt} \int_{\Omega_j} q^{(k)} \, v \, dV + \int_{\partial \Omega_j} f^{(k)num,\perp} \, v \, da - \int_{\Omega_j} \mathbf{f}^{(k)} \cdot \nabla v \, dV = \int_{\Omega_j} S^{(k)} \, v \, dV$$

2.) Finite-element ingredient

$$q^{(k)}(x,t) = \sum_{l=0}^{p} q_{j,l}^{(k)}(t) \, p_l(x - x_j)$$



From *Nair et al. (2011)* in *‚Numerical techniques for global atm. models'*

Galerkin-idea: identify $v \equiv p_l$

Modal base: orthogonal functions e.g. Legendre-Polynomials
Nodal base: interpolation (Lagrange) polynomials

Discontinuous Galerkin (DG) methods in a nutshell (II)

Weak formulation

$$\frac{d}{dt}\int_{\Omega_j} q^{(k)}\, v\, dV + \int_{\partial\Omega_j} f^{(k)num,\perp}\, v\, da - \int_{\Omega_j} \mathbf{f}^{(k)} \cdot \nabla v\, dV = \int_{\Omega_j} S^{(k)}\, v\, dV$$

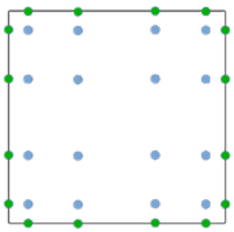
3.) Finite-volume ingredient:

Replace physical flux by a numerical flux in the surface integral
→ couple two neighbouring cells

Often used: simple Lax-Friedrichs flux

$$\mathbf{f}(q) \to f^{num,\perp}(q^+, q^-) = \frac{1}{2}\left(\mathbf{f}(q^+) + \mathbf{f}(q^-)\right) \cdot \mathbf{n} - \frac{\alpha}{2}(q^+ - q^-)$$

4.) Gaussian quadrature for the volume and surface integrals



→ ODE-system for $q^{(k)}{}_{jl}(t)$

5.) Use a time-integration scheme (Runge-Kutta, …)

DG – Pros …

- **local conservation** of every prognostic variable
- any **order of approximation (convergence)** possible
- flexible application on **unstructured grids** (also dynamic adaptation is possible, h-/p-adaptivity)
- very good **scalability** on massively-parallel computers (compact data transfer and no extensive halos)
- **separation** between (analytical) equations and numerical implementation
- **boundary conditions** are easily prescribed (fluxes or values in weak form) → coupling with other subcomponents (ocean model, …) should be easy
- higher accuracy helps to **avoid several awkward approaches** of standard 2nd order schemes: staggered grids (on triangles/hexagons, vertically heavily stretched), numerical hydrostatic balancing, grid imprints by pentagon points or along cubed sphere lines, …
- **unified numerical treatment** of all flux terms and source terms
- **explicit** schemes are relatively easy to build and are quite well understood

DG – … and Cons

- **high computational costs** due to
  - (apparently) **small Courant numbers** → small time steps
  - higher number of **degrees of freedom**
    - variables ‚live' both on interior *and* on edge quadrature points
    - this holds additionally for **parabolic problems (diffusion)**
  - HEVI approach leads to **block tridiagonal matrices** with larger blocks

→ All these expenses must be outperformed by:
higher convergence order, better computational intensity, and better parallelization!

- **well-balancing** (hydrostatic, perhaps also geostrophic?) in Euler equations is an issue → can be solved!
- basically ‚only' an **A-grid-method** →however, the ‚spurious pressure mode' is very selectively damped!

Step 1:

bring DG on the sphere …

How to construct a higher order numerical scheme on the sphere

annoying: the sphere doesn‘t allow a single coordinate system without singularities ☹

Straightforward approach to avoid this (for any 2D manifold!)

1.generate a triangulation for an arbitrary set of *points* on the manifold and by connecting them

a)by *geodetic lines* (=great circle arcs on the sphere) → curved triangles

b)and by *straight lines* in the embedding Euclidean space → flat triangles → unit triangle

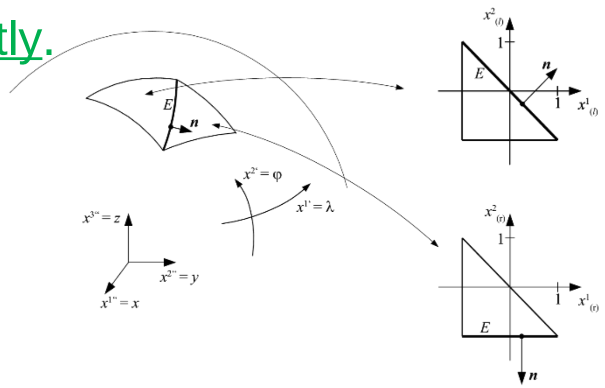
2.map every unit triangle (with *local coordinates* x^1, x^2) to the related curved triangle;
this can be done *exactly* (and without any ‚holes‘ or overlappings) for the

•sphere: by *gnomonial projection* (e.g. *Läuter, Giraldo, … (2008) JCP*)

•ellipsoid: by *gnomonial + affine projection*

→ all geometric properties (g_{ij}, Γ^i_{jk}, ...) are treated exactly.

→ higher order discretizations are straightforward.



In a FV scheme, one only has to *transform the fluxes* between neighboring unit triangles by

$$f^i_{(r \to l)} = \frac{\partial x^i_{(l)}}{\partial x^j_{(r)}} f^j_{(r)}, \qquad f^i_{(l \to r)} = \frac{\partial x^i_{(r)}}{\partial x^j_{(l)}} f^j_{(l)}$$

This is simplified by using the *covariant form* of the equations ...

Shallow-water equations in covariant form, i.e. only tensors occur
→ equations are valid *on any 2D manifold* (at least from a mathematical viewpoint)

$$\frac{\partial H}{\partial t} + \nabla_j M^j = 0,$$

$$\frac{\partial M^i}{\partial t} + \nabla_j T^{ij} = S^i, \quad i, j = 1, 2,$$

momentum flux tensor:

$$T^{ij} = \frac{M^i M^j}{H} + \frac{1}{2} g_{grav} H^2 g^{ij},$$

source vector of momentum:

$$S^i = -g_{grav} H g^{ij} \nabla_j h_B + f_c g^{ij} E_{jl} M^l,$$

E_{jl} : 2nd rank Levi-Civita pseudo tensor,
f_c : Coriolis parameter (a pseudo scalar field)

express covariant derviative ∇_j
by partial derivative and Christoffel symbols
→ accessible to a numerical implementation:

$$\frac{\partial \sqrt{g} H}{\partial t} + \frac{\partial}{\partial x^j} \sqrt{g} M^j = 0,$$

$$\frac{\partial \sqrt{g} M^i}{\partial t} + \frac{\partial}{\partial x^j} \sqrt{g}\, T^{ij} + \sqrt{g}\, \Gamma^i_{jk} T^{kj} = \sqrt{g} S^i.$$

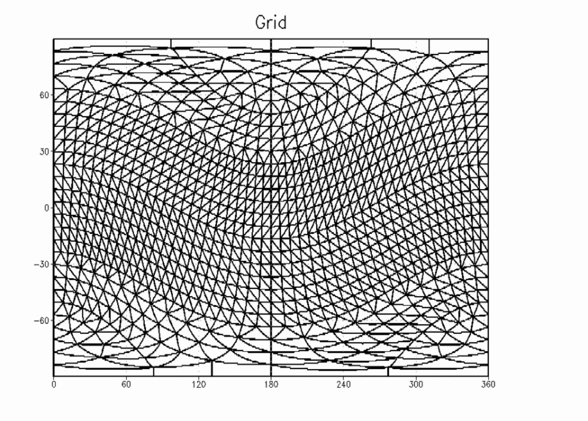
Baldauf, M. (2020): *Discontinuous Galerkin solver for the shallow-water equations in covariant form on the sphere and the ellipsoid,* J. Comp. Phys. 410

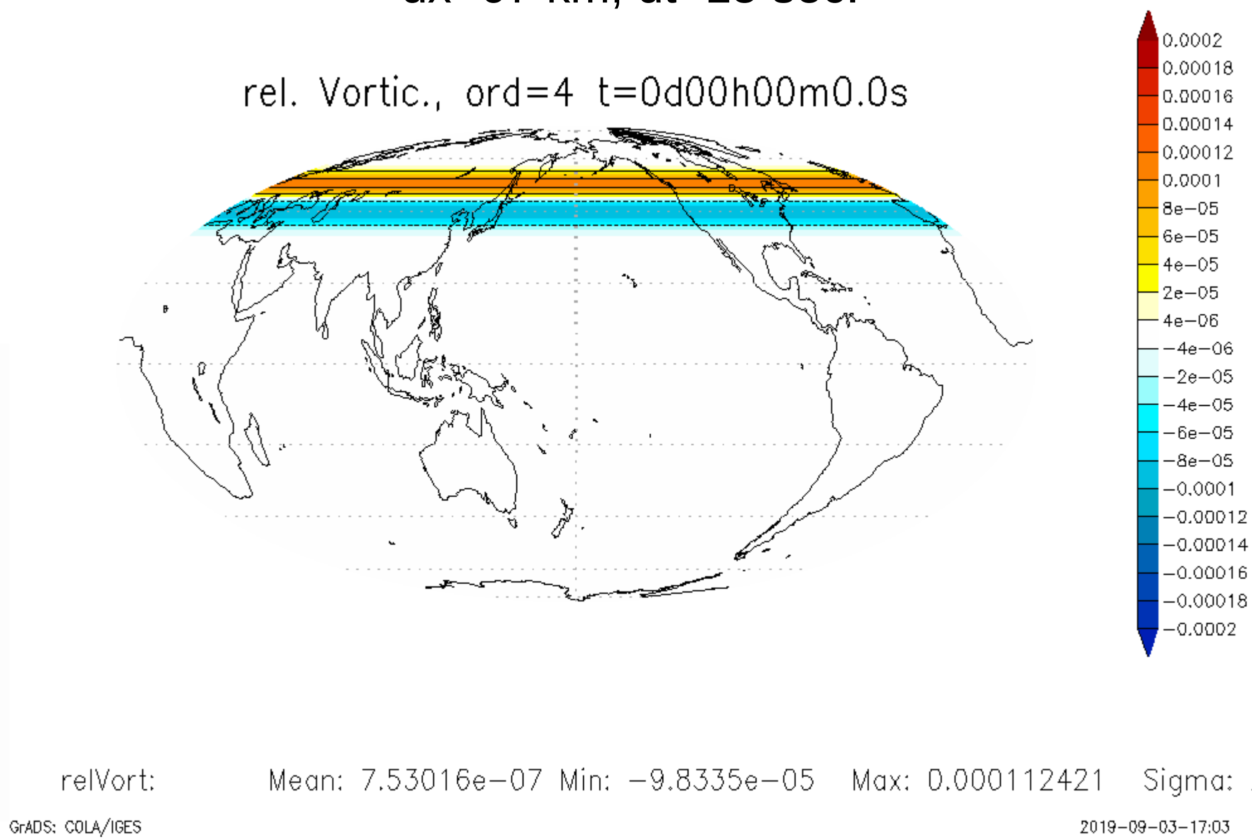
Barotropic instability test
Galewsky et al. (2004)

4th order DG scheme

without additional diffusion
dx~67 km, dt=15 sec.

simple triangle grid
on the sphere
dx ~ 500km:

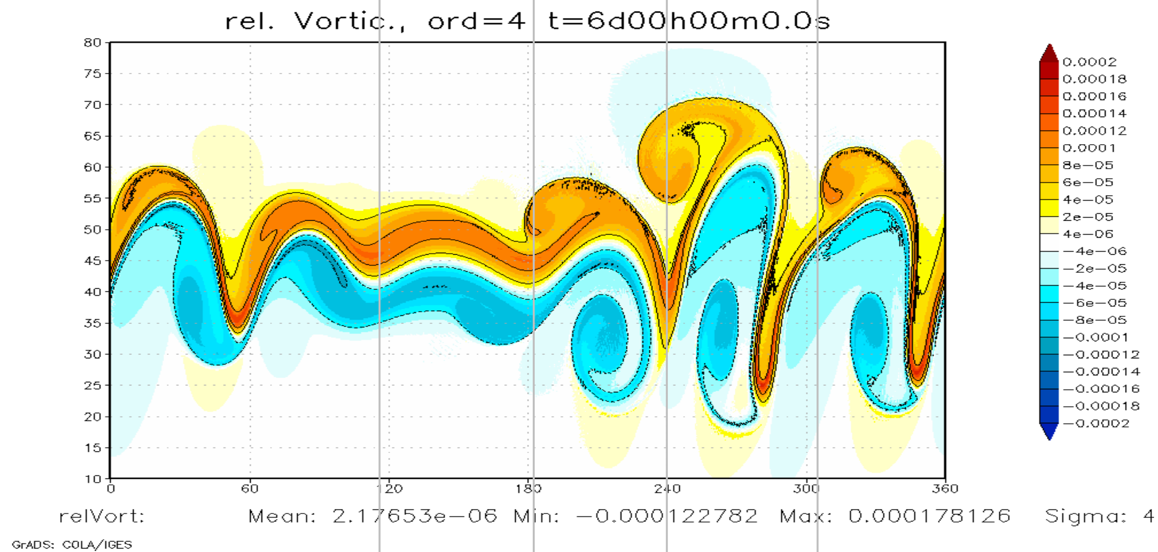




Barotropic instability test

Galewsky et al. (2004)

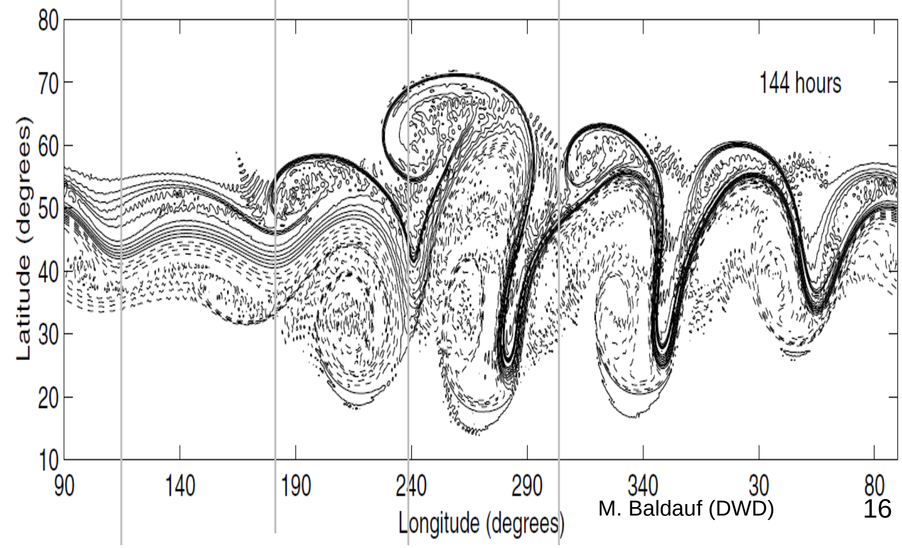
relative vorticity



4th order DG scheme
without additional diffusion
dx~67 km, dt=15 sec.

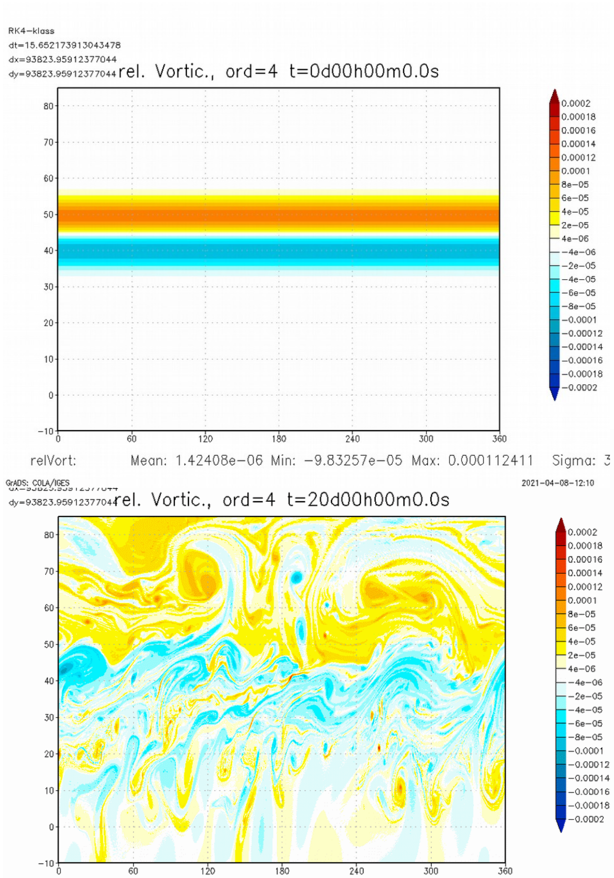
FMS-SWM (Geophys. Fl. Dyn. Lab.)
without additional diffusion
dx~60 km (T341), dt=30 sec.

Fig. 4 from *Galewsky et al. (2004)*



Barotropic instability test

Galewsky et al. (2004)



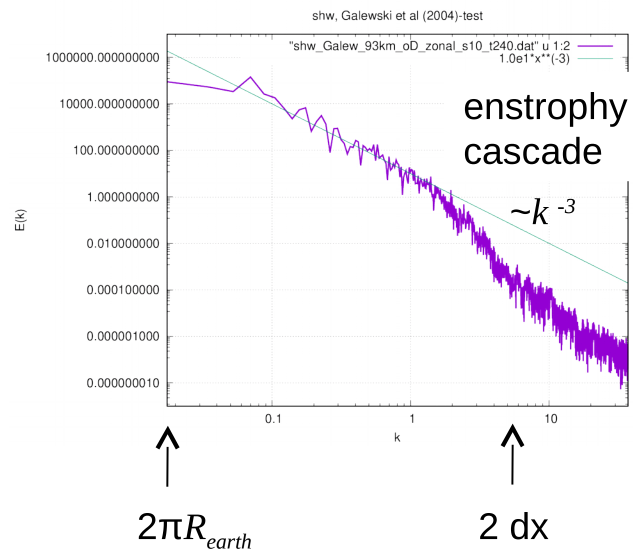
Generation of 2D turbulence

4th order DG scheme

without additional diffusion

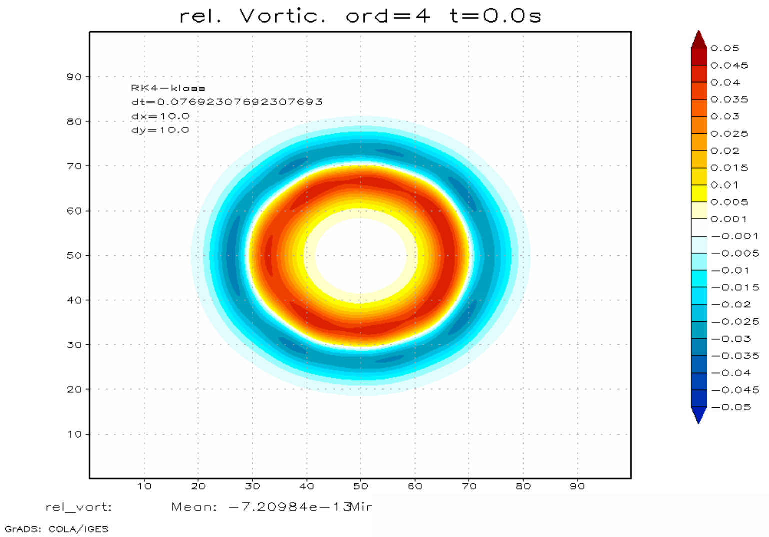
dx~67 km, dt=15 sec.

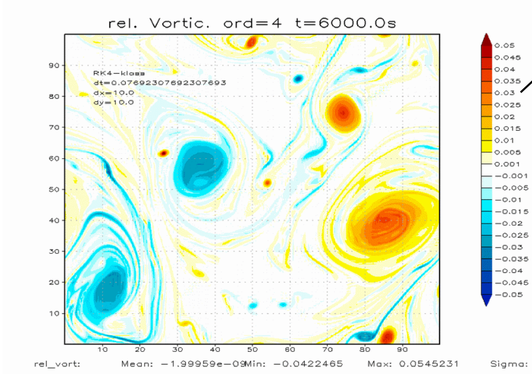
Power spectrum of KE along 45°:



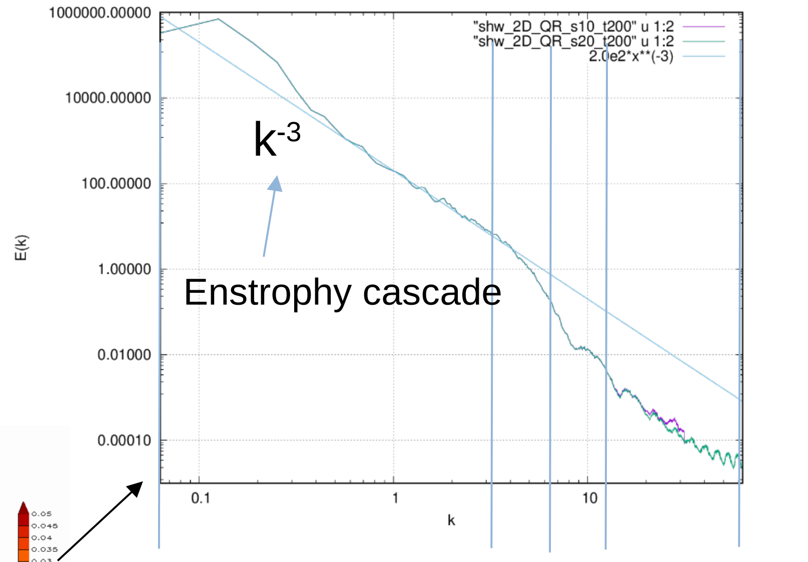
DG toy model, 4th order, shallow water equations on a plane, without Coriolis force

L*L=1*1 km², Δx=Δy=10m





1D-power spectrum of the kinetic energy after t=6000sec.

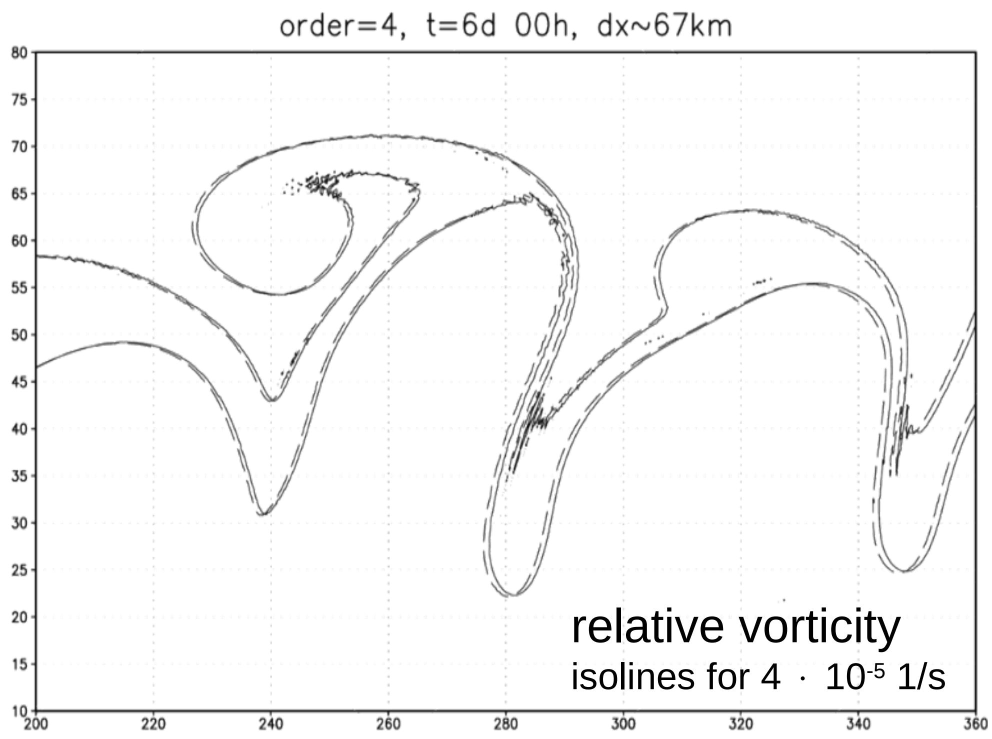


Each grid cell is sampled by 20*20 points (only at the output)

Barotropic instability test
Galewsky et al. (2004)

Comparison between the sphere and the ellipsoid

4th order DG scheme
without additional diffusion
dx~67 km, dt=15 sec.



solid line: sphere
R = 6371.22 km

dashed line: ellipsoid
a = 6378.137 km
c = 6356.752 km
→ numer. excentr. = 0.082

relative vorticity
isolines for 4 · 10^{-5} 1/s

→ ellipsoidal solution shows westward phase shift of ~1° after 6 days
→ is in qualitative agreement with *Bénard (2015) QJRMS*

Step 2:

extension for the Euler equations in terrain-following coordinates and a HEVI time integration

Extension to the 3D Euler equations on the sphere together with terrain-following coordinates

Additional metric terms of terrain-following coordinates can destroy numerical local conservation → use *strong conservation form* of the equations, i.e. use both base vectors for a smooth (e.g. spherical) coordinate system K‘ and for the terrain-following system K.

example: strong cons. form of the momentum equation:

$$\frac{\partial}{\partial t}\sqrt{g}\,M^{i'} + \frac{\partial}{\partial x^k}\sqrt{g}\,T^{i'k} = \sqrt{g}\,(S^{i'}_{(M)} - \Gamma^{i'}_{k'l'}T^{l'k'})$$

↑ now: additional metric terms only from the smooth system K‘

momentum flux for Euler eqns.

$$T^{ik} = \frac{1}{\rho}M^i M^k + \tilde{p}g^{ik}$$

for diffusion (D^{ik} = deformation tensor), add

$$T^{ik}_{diff} = -\rho K_a 2D^{ik} - \rho K_b g^{ik}\nabla_l v^l$$

Additionally: Continuity eq. (for ρ) and energy equation (for $\rho\theta$)

Horizontally explicit - vertically implicit (HEVI)-scheme with DG

Motivation: get rid of the **strong time step restriction** by vertical sound wave expansion in **flat grid cells** (in particular near the ground)

$$\frac{\partial q^{(s)}}{\partial t} + \underbrace{\nabla \cdot \mathbf{f}^{(s)}_{slow}}_{\text{explicit}} + \underbrace{\nabla \cdot \mathbf{f}^{(s)}_{fast}}_{\text{implicit}} = \underbrace{S^{(s)}_{slow}}_{\text{explicit}} + \underbrace{S^{(s)}_{fast}}_{\text{implicit}}$$

$$\mathbf{f}^{(s)}_{fast} = f^{(s)}_{z,fast}\mathbf{e}_z$$

$$f^{(s)}_{z,fast} = \sum_{s'} H^{ss'} q^{(s')}$$

- Use of **IMEX-Runge-Kutta** (SDIRK) schemes: SSP3(3,3,2), SSP3(4,3,3) (*Pareschi, Russo (2005) JSC*)
- The implicit part leads to several band diagonal matrices
  → here a direct solver is used (expensive!)

References:
Giraldo et al. (2010) SIAM JSC: propose a HEVI semi-implicit scheme
Bao, Klöfkorn, Nair (2015) MWR: use of an iterative solver for HEVI-DG
Blaise et al. (2016) IJNMF: use of IMEX-RK schemes in HEVI-DG
Abdi et al. (2019) IJHighPerfCompAppl: use of multi-step or multi-stage IMEX for HEVI-DG

IMEX-Runge-Kutta

- general stability function for the Dahlquist problem is known
- general order conditions are known
- described by double Butcher tableaus

e.g. SSP3(3,3,2) by *Pareschi, Russo (2005) JSC:*

$$\begin{array}{c|ccc} 0 & 0 & & \\ 1 & 1 & 0 & \\ 1/2 & 1/4 & 1/4 & 0 \\ \hline & 1/6 & 1/6 & 2/3 \end{array} \qquad \begin{array}{c|ccc} a & a & & \\ 1\text{-}a & 1\text{-}2a & a & \\ 1/2 & 1/2\text{-}a & 0 & a \\ \hline & 1/6 & 1/6 & 2/3 \end{array}$$

$$a = 1 - 1/\sqrt{2}$$

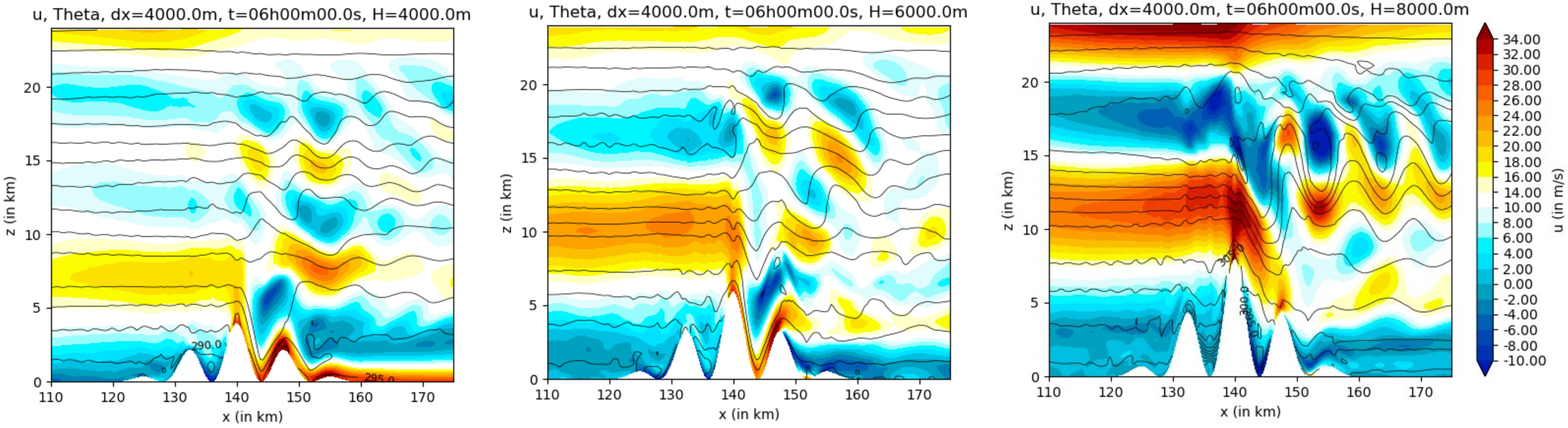
- practically SDIRK schemes are preferred

Lock, Wood, Weller (2014) QJRMS
Pareschi, Russo (2005) JSC: SSP3(3,3,2), SSP3(4,3,3)
Giraldo et al. (2012) Siam JSC: ARK2(2,3,2)
Kang, Giraldo, Bui-Thanh (2020) JCP: IMEX-RK in hybridiz. DG

Flow over mountains with steep slopes and vertical grid stretching

Schaer et al. (2002) MWR, test case 5b: U_0=10m/s, N=0.01 1/s, but a=10km

H_{oro}= 4000m, α_{max} = 58° | H_{oro}= 6000m, α_{max} = 67° | H_{oro}= 8000m, α_{max} = 72°



Δx=4 km; vertical grid stretching: Δz_{min}~46m, Δz_{max}~736m, $z_{lowest\ QP}$~10.3m

HEVI-DG simulation (4th order) remains stable even for steeper slopes!

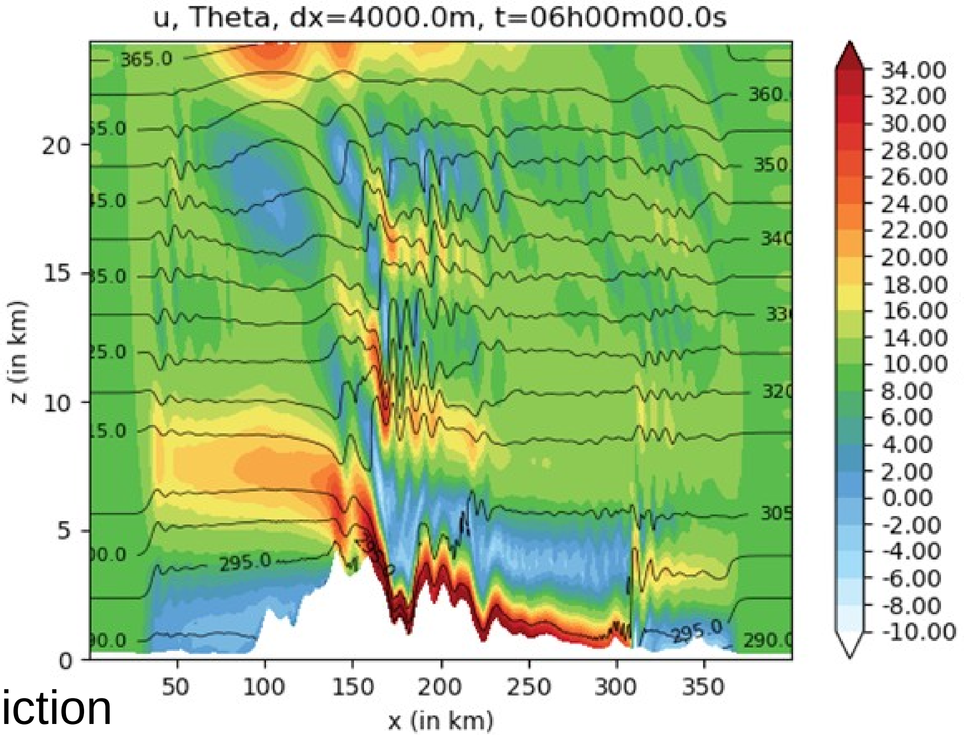
to avoid instability by strong gravity wave breaking, vertically implicit ‚3D‘ Smagorinsky diffusion was used

DG 2D toy model: semi-realistic case study

Setup:
U_0= 10 m/s, N=0.01 1/s
Δx=4 km
vertical grid stretching as before

2D cross section over the Alps (Monte Rosa region) using orography data on a 0.05° mesh

DG HEVI scheme 4th order, Smagorinsky model, no surface friction



Additionally done

- Treatment of diffusion in a HEVI-DG scheme with terrain-following coordinates (by the Bassi, Rebay approach)
- Efficiency improvement of the implicit solver
(perform expensive LU-decomposition only after several dozen time steps)
- Formulation of boundary conditions for higher order schemes
- Method for consistent use of real orography

Baldauf, M. (2021): *A horizontally explicit, vertically implicit (HEVI) discontinuous Galerkin scheme for the 2-dim. Euler and Navier-Stokes equations using terrain-following coordinates*, J. Comp. Phys. 446

Difficulties in finding a Schur complement in the vertical implicit solver

In the ICON or COSMO dynamical core, an equation for *only one* variable w is vertically solved ←→ linear algebra analogon:

Schur complement: linear system of equations (LSE) $Mx=b$ with a matrix

$$M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

solve instead: one LSE with $S = D - CA^{-1}B$
and one LSE with A

→ efficiency gain, if A is large and can easily be inverted.

Difficulties in finding a Schur complement in the vertical implicit solver

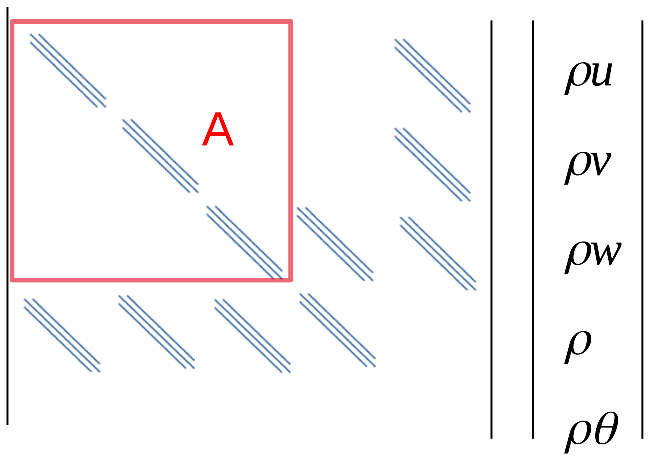
In the ICON or COSMO dynamical core, an equation for *only one* variable w is vertically solved ←→ linear algebra analogon:

Schur complement: linear system of equations (LSE) $Mx=b$ with a matrix

$M = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$ solve instead: one LSE with $S = D - CA^{-1}B$ and one LSE with A

→ efficiency gain, if A is large and can easily be inverted.

Structure of Euler equations:



= rhs.

In ICON / COSMO: A is diagonal!

In DG, the numerical diffusion in LF-flux

$$f^{num,\perp}(q^+, q^-) = \frac{1}{2}\left(\mathbf{f}(q^+) + \mathbf{f}(q^-)\right) \cdot \mathbf{n} - \frac{\alpha}{2}(q^+ - q^-)$$

couples vertical grid points →
→ A is block-tridiagonal
→ A^{-1} is a full matrix ☹
→ S is a full matrix → no efficiency gain

The **BRIDGE** project (**B**asic **R**esearch for **I**CON with **DG E**xtension)

started ~mid 2020
currently: F. Prill, M. Baldauf / joining later: D. Reinert, U. Schättler, S. Borchert, …

Goals:
- develop a prototype for a DG implementation of the 3D Euler equations (‚DG-HEVI on the sphere‘)
- together with a minimal set of physical parameterizations
- using ICON infrastructure (parallelisation, I/O, ...)
- more object-orientation and use of standard software (e.g. YAC coupler, ...)

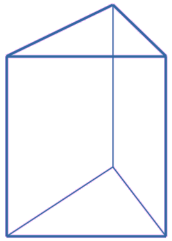
as an intermediate step to a full–fledged ICON implementation

Milestones:
- Shallow-water equations on the sphere ready in Q3/2021
- 3D explicit Euler solver ready in Q4/2021
- 3D HEVI Euler solver ready in Q1/2022 → decision about prolongation of the project
- Implementation into **ICON** (start ~2024)
- choose optimal approx. order (currently I favor: $p_{horiz}=4$, $p_{vert}=4$, $p_{time}=3$) and grid spacing
- Operationally useable version ready ~2028

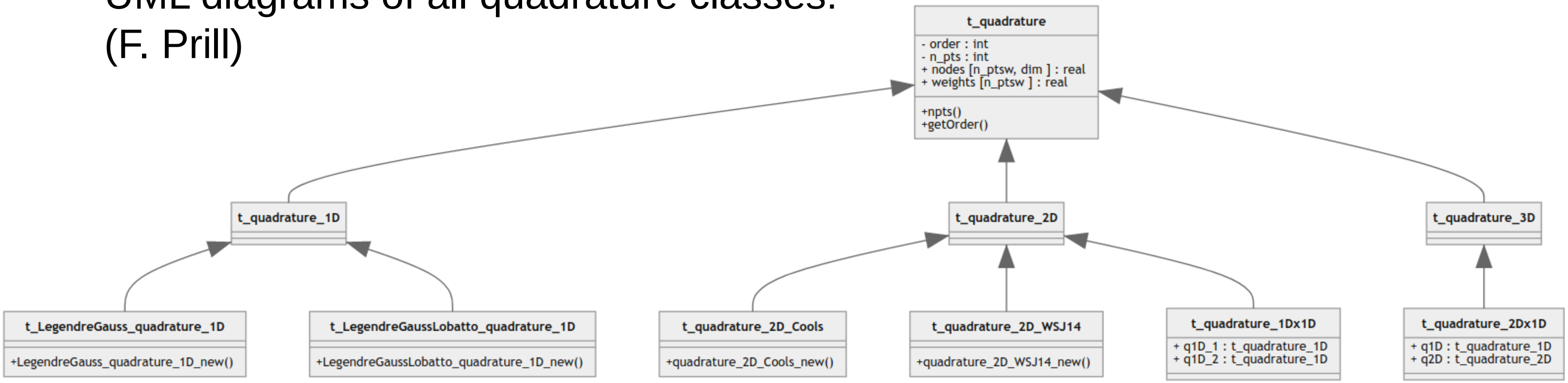
More object orientation with the BRIDGE code

Helps in keeping things as transparent as possible

Example: quadrature classes for the numerical integration over prism volumes or prism faces



UML diagrams of all quadrature classes:
(F. Prill)



Integration over plane triangles

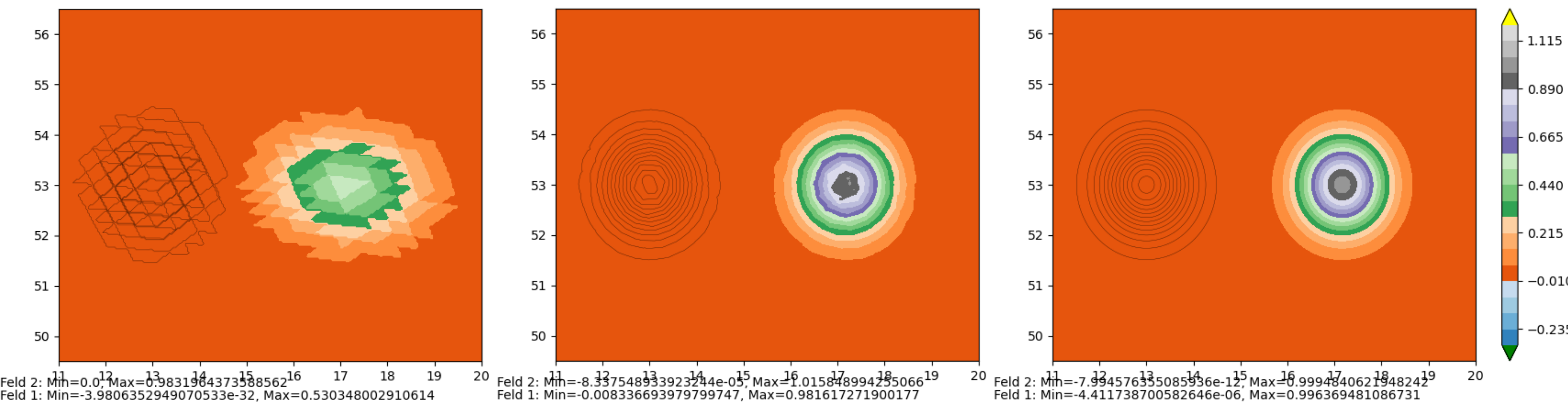
Integration over lateral faces

Integration over prism volume

A first very preliminary result of the BRIDGE code:

Advection by a solid body rotation wind field after 100 time steps (Δt=50 s)

1st order | 2nd order | 4th order



F. Prill (DWD)

BRIDGE is not just a 3D extension of the **2D toy model** but allows much **more flexibility** and **efficiency increase** by

- 2D×1D tensor product representations of quadratures and finite elements; and consequent use of matrix-vector operations
- Option to use different FE
for different progn. variables (e.g. for tracer var.) → use an indexing operator
and for different grid points → use of an ‚iterator over cells' concept
- Additional MPI-parallelization
- Optional use of non-conformal grids (i.e. hanging nodes are allowed)
- Consequent use of existing ICON infrastructure code:
triangular grid, nproma blocking, patch, mtime, …
- Consequent use of standard software tools:
YAC coupler (DKRZ/MPI-M), YAXT communication (DKRZ), …

However, BRIDGE is not yet ICON (no restart, no local parent grid, …)

Urgent ToDo‘s:

•Further optimizations of the vertical implicit solver
(e.g. can one find a Schur complement form?)

•Coupling of tracer advection (mass-consistency?)

•Sedimentation by an implicit, positive-definite tracer advection scheme

•Develop coupling ideas for parameterizations (time-integration, preserve pos. def., …)
including adaptations of first param. (turbulence, microphys.)

•Further design decisions: nodal v. modal, local DG vs. interior penalty vs. …,
allow non-conformal grids?, efficient data layout, …

•Real case applications probably need further stabilization mechanisms (filtering, entropy stable/conserving schemes, …)

For many of these questions there exist a large amount of literature; and we probably don‘t have to do this alone, since there is a great interest in academia in similar questions.

Summary for the DG development

- Basic questions are solved for (by the **2D toy model**)
  - **DG on the sphere** on a triangle grid possible by the use of local coordinates and the covariant formulation of the equations.
  - **HEVI-DG** for *Euler equations* with *terrain-following coordinates* and optionally with *3D diffusion*

Baldauf, M. (2020): *Discontinuous Galerkin solver for the shallow-water equations in covariant form on the sphere and the ellipsoid,* J. Comp. Phys. 410
Baldauf, M. (2021): *A horizontally explicit, vertically implicit (HEVI) Discontinuous Galerkin scheme for the 2-dim. Euler and Navier-Stokes equations using terrain-following coordinates*, J. Comp. Phys. 446

- With respect to the pure dynamical core (=solver for the Euler equations), no show–stopper occured until now. However, total efficiency is still an issue! In particular the vertically implicit solver is still too expensive.
- Further questions must be solved for coupling with parameterizations
- All this further work is done in the **BRIDGE** project, which is well on the way …

Status of PPs/PTs in WG2

PP CDIC
Final report is ready and will be available as COSMO Technical Report No. ??

PP CELO
Final report is ready and available as reviewed article:
Ziemiansky et al. (2021) MWR
An additional extended abstract will be prepared for the COSMO newsletter

PP EX-CELO
Final report is still due

PT CCE
An extended abstract will be prepared for the COSMO newsletter

PDEs
THE WORKSHOP ON PARTIAL DIFFERENTIAL EQUATIONS ON THE SPHERE

PDEs on the sphere, 17-21 May 2021

this year was organized by DWD

51 presentations,
about 90 participants

Topics:
- Time integration (exponential, IMEX, implicit)
- Grids/Interpolation, vertical coordinate
- spectral model + SISL
- FV, FE/SE, DG
- advective (tracer) transport
- Hamilton formulation
- Ocean
- test cases, machine learning
- Scaling, applications
- physics-dynamics-coupling

Organization team

Daniel Egerer, Michael Baldauf, Bernd Kress, Florian Prill

Scientific committee

Jörn Behrens (Univ. Hamburg)
Christiane Jablonowski (Univ. Michigan)
Peter Lauritzen (NCAR)
Thomas Dubos (Ecole Polytechnique)

WG2 - a few general remarks

•The CLM dynamics group has stopped ist activity and has joined WG2. Nevertheless, COSMO WG2 is quite small

•Everybody is welcome to take part;
please also have a look to the **WG2 Guidelines**
(available on the COSMO web page → WG2), if one of the short-to-mid term topics might be of interest for you.

Loose ideas beyond WG2…

COSMO fosters PPs/PTs about new developments (which is fine).
However, shouldn‘t we also encourage PPs/PTs about *model code investigation*? … that means ‚*is actually coded what has been documented*?‘
→ active search for bugs by code inspection
→ active search for missing documentation
→ overall quality assurance in our model
Applications are welcome …

Thank you very much for your attention!