Recent numerics developments in the COSMO and ICON model

42nd EWGLAM/ 27th SRNWP meeting, online
28 Sept. - 02 Oct. 2020

Michael Baldauf, Sebastian Borchert, Florian Prill,
Günther Zängl, Daniel Reinert (DWD),
Zbigniew Piotrowski (IMGW)

Outline

- **COSMO-Runge-Kutta** (operational): no further developments
- **COSMO-EULAG**
- **ICON**
  - Current work:
    - Improved vertical discretization didn‘t show advantages (*D. Reinert*)
    - Continuity eq. for dry mass (*D. Reinert*, *KIT*)
    - c_p/c_v-Bugfix (*G. Zängl*, *V. Maurer*, …)
    - **Deep atmosphere modifications** (*S. Borchert)*
  - **Discontinuous Galerkin-discretisation** for ICON
    - Further work on the 2D toy model (*M. Baldauf*)
    - First steps in the infrastructure of a 3D ICON-prototype done (*F. Prill*)

Z. Piotrowski , … (IMGW)

COSMO-EULAG

EULAG dynamical core: combine the *MPDATA* advection scheme via the *non-oscillatory forward in time*-method with an implicit elliptic solver (*preconditioned generalized conjugate residual* (GCR) solver)

- in official code since COSMO 5.7 (2020)
- runs operationally at IMGW (Poland) since 2020

recent publ.: *Ziemianski et al. (2020) subm. to MWR*

Lowest level of advection substepping - split MPDATA scheme.

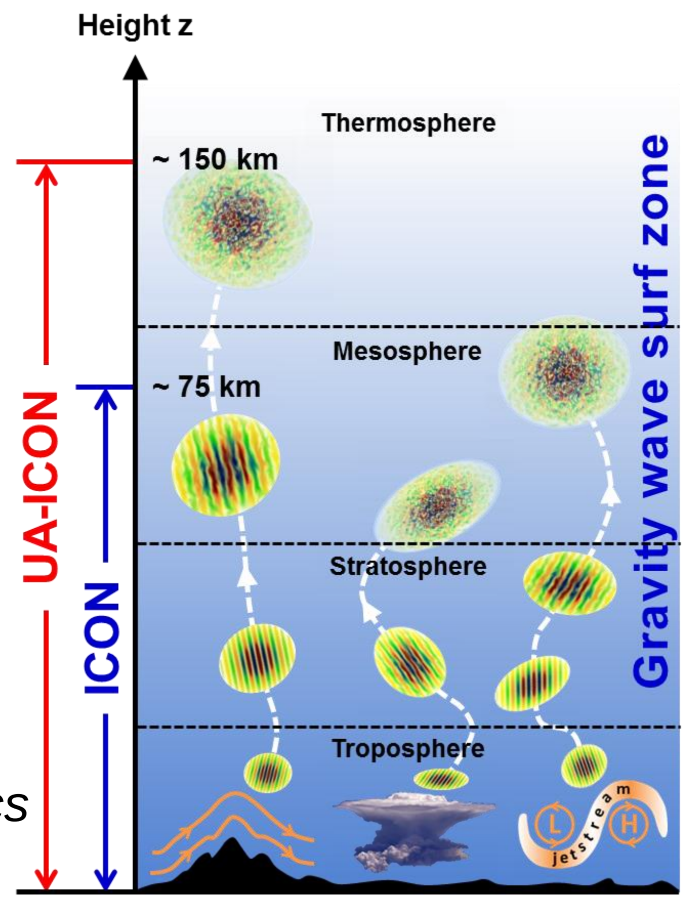
The vertical Courant number, in the context of regional NWP, typically exceeds the horizontal Courant number up to several times. This justifies the splitting approach typically employed in NWP, but has numerical consequences. The strategy is as follows: (Strang-Splitting)

- First perform vertical advection of density with half timestep, followed by horizontal advection with full timestep, then again vertical advection of rho with half timestep; intermediate results stored.
- Evaluate advection of a prognostic variable with the same three steps, using respective densities.
- Allows for twice larger Courant number in the vertical (horizontal variant possible as well, e.g. twice larger Courant in x direction as well if needed)
- Somewhat more diffusive than regular MPDATA due to effectively larger stencil as a result of full sequence (even though particular operators remain the same)

Modification of ICON* for the deep atmosphere: Motivation

S. Borchert (DWD)

- Work is part of DFG research group: **Multiscale Dynamics of Gravity Waves** (MS-GWaves**)
- Collaboration with colleagues from Max Planck Institute for Meteorology (Hamburg)
- Goal: simulation of large part of gravity wave life cycle, from sources in Troposphere to wave breaking in upper Mesosphere lower Thermosphere
- Implementation of upper-atmosphere physics package (by MPI-M)
- Implementation of *deep-atmosphere dynamics* (by DWD)

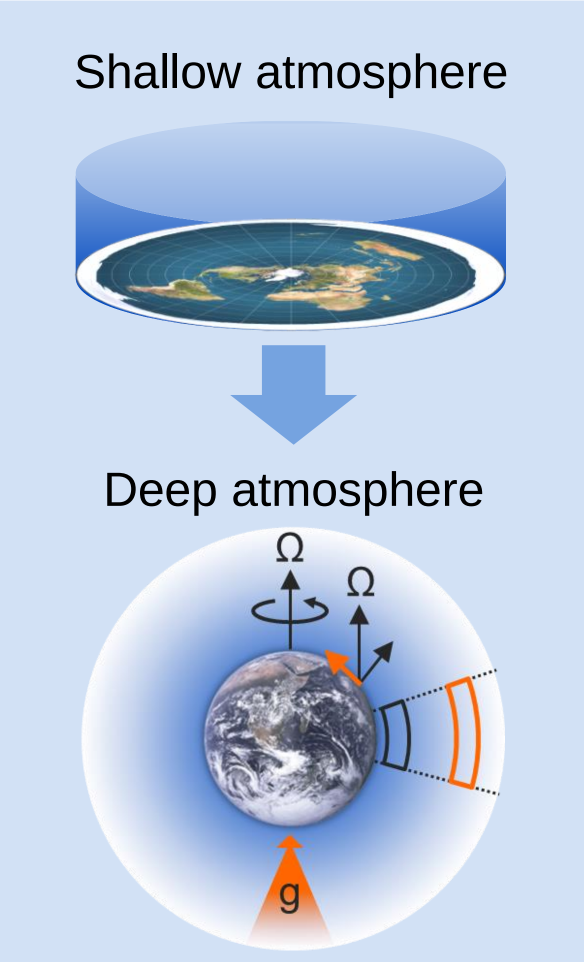


* Zängl et al (2015) Q. J. R. Met. Soc. **https://ms-gwaves.iau.uni-frankfurt.de/

Modification of ICON for the deep atmosphere: Overview

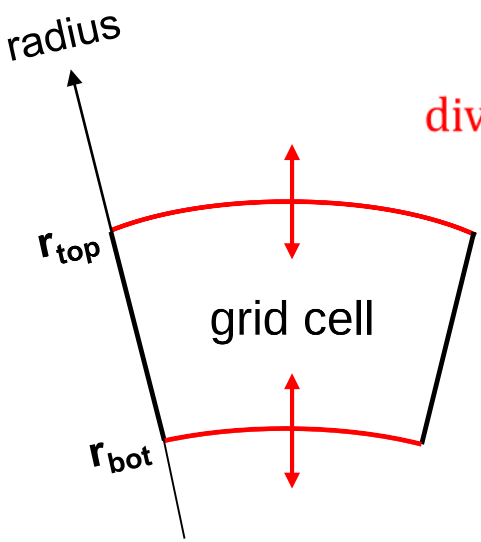
- **Shallow atmosphere***
  - Standard configuration in ICON
  - In particular, replace prefactors $1/r \rightarrow 1/a$

- **Deep-atmosphere modifications**
  - Abandon *shallow-atmosphere approximation*
    - Increase of grid cell extension with height
    - Gravitational field strength $|\boldsymbol{g}|$ decreases with height
  - Abandon *traditional approximation*
    - Coriolis acceleration due to $\boldsymbol{\Omega}_\mathrm{h}$
    - take all metric terms in advection



* See *Thuburn & White (2013) Q. J. R. Met. Soc.*

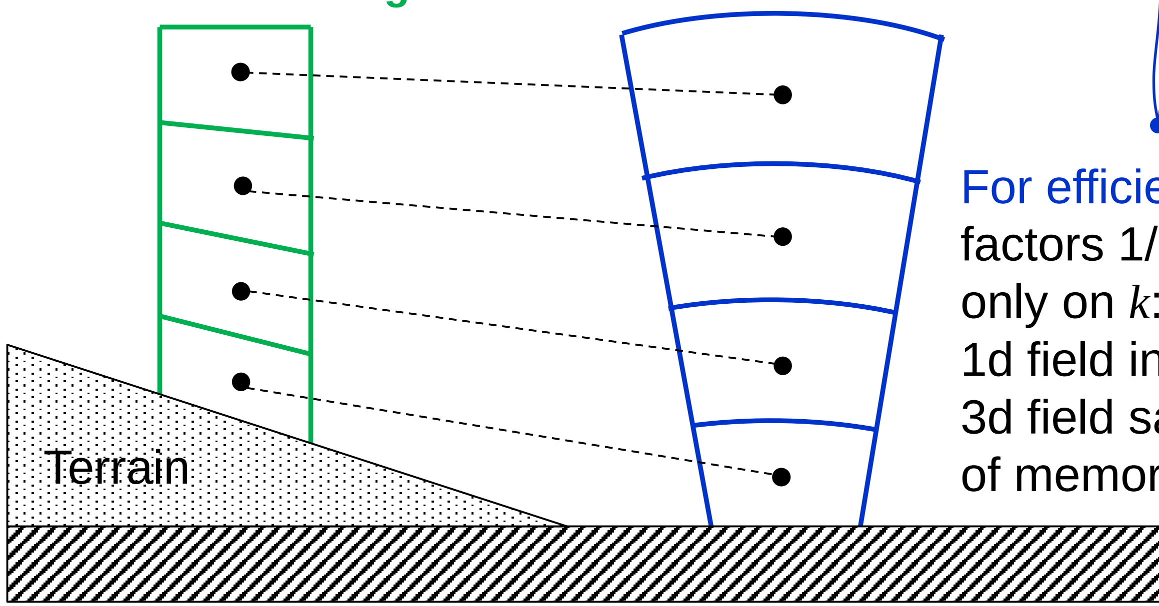
Example: vertical divergence of some flux ξ



$$\mathrm{div}_z(\xi) = \frac{\xi_{top}\left\{3\left[1+\frac{r_{bot}}{r_{top}}+\left(\frac{r_{bot}}{r_{top}}\right)^2\right]^{-1}\right\} - \xi_{bot}\left\{3\left[1+\frac{r_{top}}{r_{bot}}+\left(\frac{r_{top}}{r_{bot}}\right)^2\right]^{-1}\right\}}{z_{top}-z_{bot}}$$

Shallow-atmosphere formulation:
terrain-following

Deep-atmosphere modification:
as if there is no terrain!

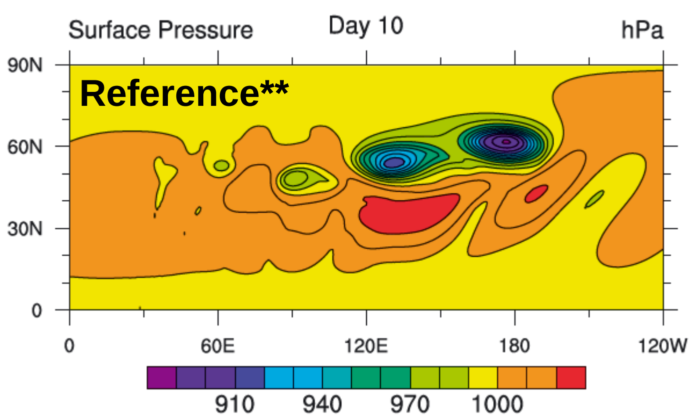


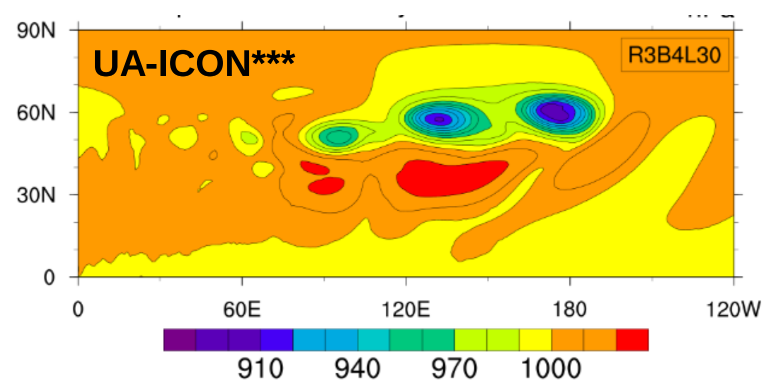
For efficiency:
factors $1/r$ depend only on k:
1d field instead of 3d field saves a lot of memory access

$r = a + z$
$a = \text{Earth radius}$

Modification of ICON for the deep atmosphere: Test II

- Jablonowski-Williamson baroclinic instability test case*
  in its extension for deep-atmosphere dynamical cores**
- Focus on hydrostatic balance and baroclinic waves as important atmospheric synoptic-scale features
- No analytic solution available: model intercomparison





→ If you are interested in the upper-atmosphere extension of ICON:
*** Borchert, Zhou, Baldauf, Schmidt, Zängl, Reinert (2019) *The upper-atmosphere extension of the ICON general circulation model (version ua-icon-1.0),* GMD

* Jablonowski & Williamson (2006) Q. J. R. Met. Soc. ** Ullrich et al (2014) Q. J. R. Met. Soc.

CONSORTIUM FOR SMALL SCALE MODELING

COSMO

Deutscher Wetterdienst

Wetter und Klima aus einer Hand

A Discontinuous Galerkin solver as a possible alternative dynamical core for ICON

- Further development of the 2D toy model

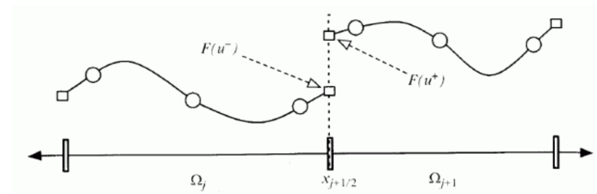
Michael Baldauf (DWD)

MetStröm

ESCAPE

Discontinuous Galerkin (DG) methods in a nutshell

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



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

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

Finite-element ingredient

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

e.g. Legendre-Polynomials

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

Finite-volume ingredient

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

Gaussian quadrature for the integrals of the weak formulation

→ ODE-system for $q^{(k)}{}_{jl}(t)$

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 **band diagonal matrices** with many bands
- **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!

Status of the toy model at the last SRNWP/EWGLAM-meeting 2019

<u>Euler-equations in a 2D x-z-slice model</u>

- Fully explicit solver in *terrain-following* coordinates
- *HEVI* solver on *cartesian* coordinates (but t-f coord. didn‘t work yet)
- Additionally (physical) ‚3D‘-*diffusion* on *cartesian* coordinates

<u>Shallow-water equations on the sphere</u>

- Explicit solver on an arbitrary triangle grid

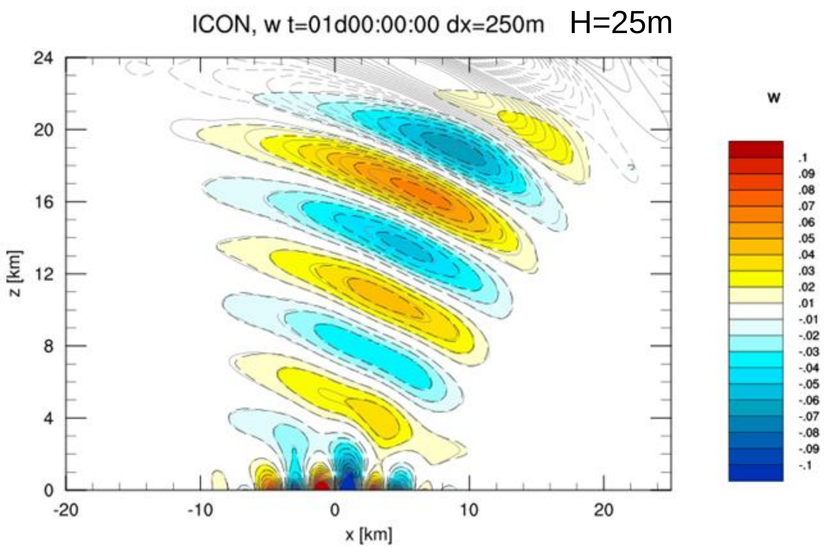
… what‘s new in 2020

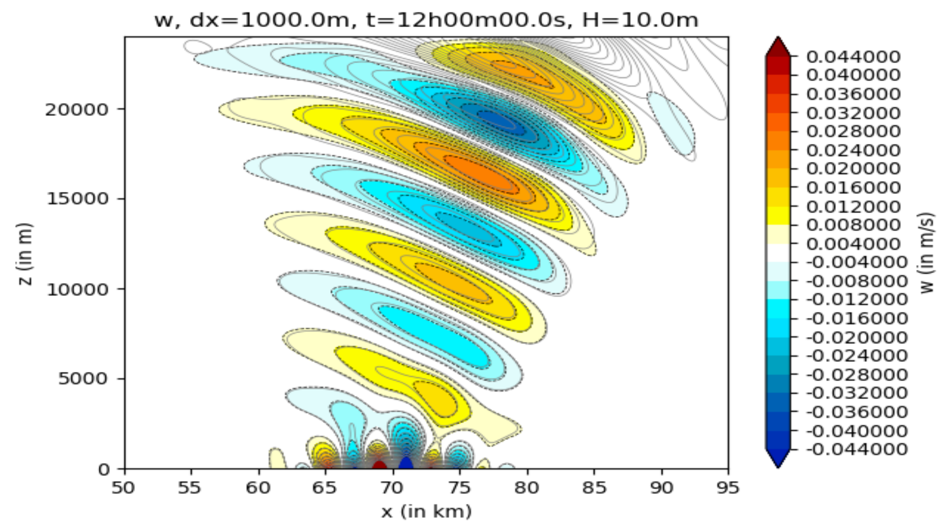
- *HEVI*-solver works on *terrain-following* coordinates
- Filtering of the source terms in HEVI-solver (and for a nodal base)
- (physical) *diffusion* in *terrain-following* coordinates, fully explicit or *vertically implicit*
- Optimization of the implicit solver

Flow over mountain with the HEVI-solver

ICON Δx=250m Δz=150m

HEVI-DG 4th order Δx=1000m Δz= 600m





colors and black dotted lines: model

grey lines: analytic solution *(Baldauf, 2008, COSMO-Newsl.)*

Computing time on 160 processors
(Cray XC40 Broadwell)
for t_{total}=24h, 26min
→on 1 processor: 69h

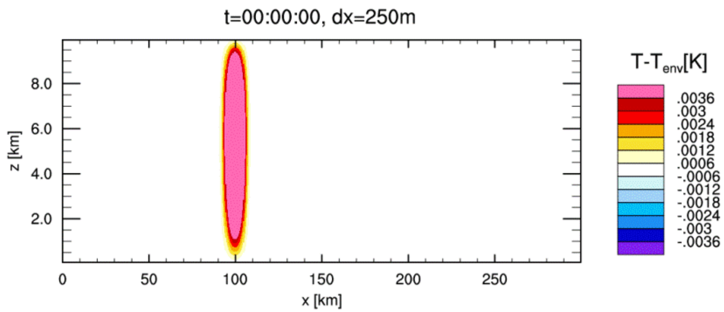
Computing time on 1 processor:
(Intel(R) Core(TM) i7-4790 CPU @ 3.60GHz)
for t_{total}=24h, 4th order DG: 160h

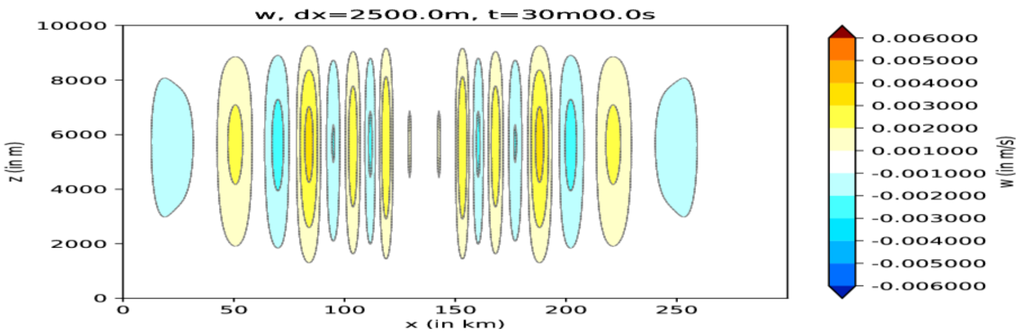
But don‘t take the computing times too serious!

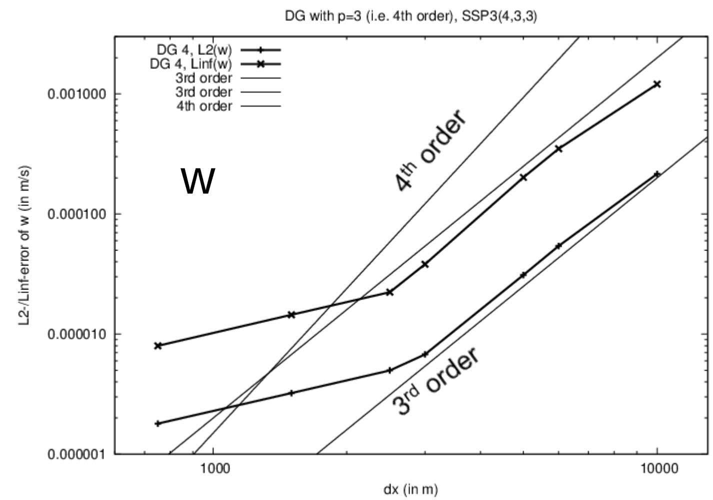
Linear gravity/sound wave expansion in a channel

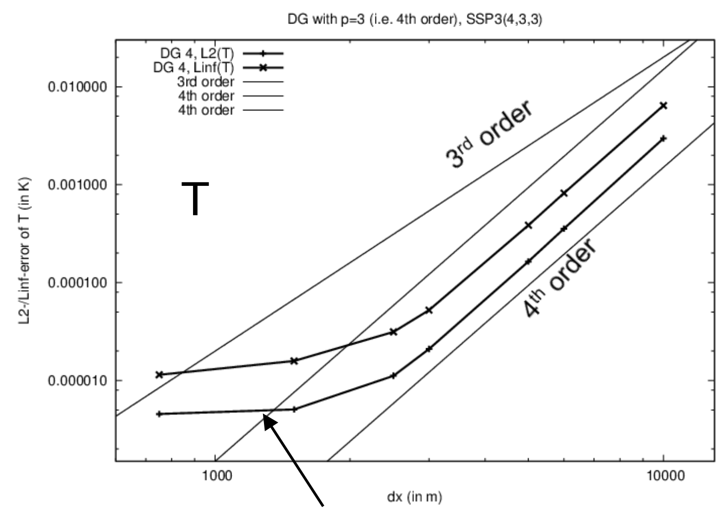
setup similar to *Skamarock, Klemp (1994) MWR*

Deutscher Wetterdienst
Wetter und Klima aus einer Hand









colors : simulation with p=3/SSP3(4,3,3)
dx=2500m, dz=1250m

black lines: analytic solution for compressible, non-hydrostatic Euler eqns.
(*Baldauf, Brdar (2013) QJRMS*)

Nonlinear effect?

General treatment of diffusion in DG

Simple replacement of a flux $f(q)$ by $f(q, \partial q/\partial x)$, where $\partial q/\partial x$ is directly calculated from q, does not work.
Instead (*Bassi, Rebay, 1997*, and similar for ‚local DG'):

- define a new variable $d = \partial q/\partial x$
- treat q as a flux and apply the DG formalism to this equation, too.
- Replace $f(q) \rightarrow f(q) + f_{\text{diffus}}(q,d)$
  Remark: the numerical flux for f_{diffus} does not need additional numerical diffusion.

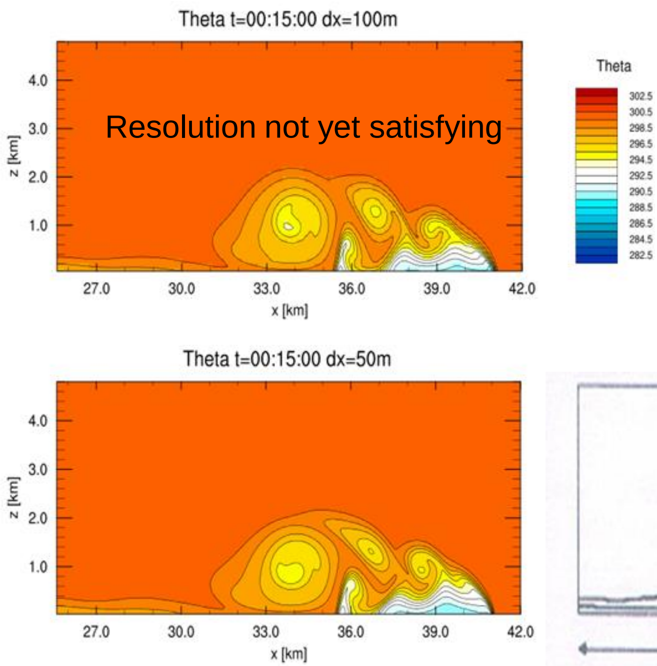
3D-diffusion in terrain-following coordinates

New developments:

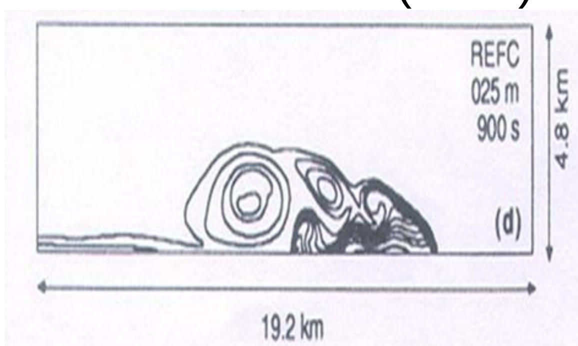
- In terrain-following coord. there are several choices for d possible.
  here: covariant derivatives of the prognostic variables
- If diffusion is treated vertically implicit (i.e. HEVI), too
  → extension of the band diagonal matrix necessary
- Currently: ‚HEVI-diffusion' is done in every sound time-step
  → expensive! Appropriate time-integration necessary.

Falling bubble test case

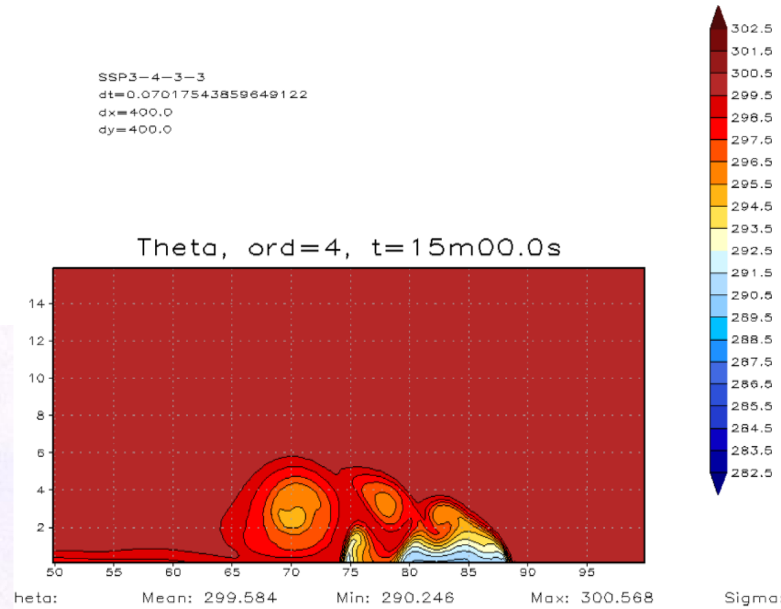
ICON



Reference solution for θ
Straka et al. (1993):



DG-HEVI



Computing time on 40 processors
(Cray XC40 Broadwell)
dx=dz=50m: 5min
→ on 1 processor: 3h30min

Computing time on 1 processor
(Intel(R) Core(TM) i7-4790 CPU @ 3.60GHz)
dx=dz=400m, 4th order DG
Euler HEVI, diffusion explicit: 1h40min
Euler + diffusion in HEVI: 3h50min

But don‘t take the computing times too serious!

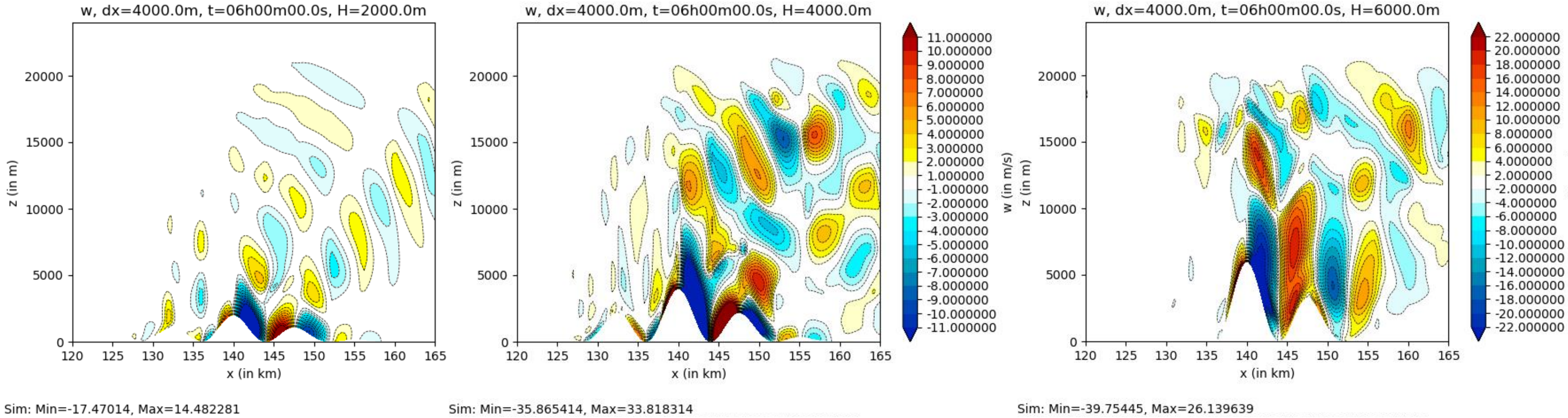
Flow over mountain with steep slopes and vertical grid stretching

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

H_{oro}= 2000m, α_{max} = 38°

H_{oro}= 4000m, α_{max} = 58°

H_{oro}= 6000m, α_{max} = 67°



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‘ diffusion with K=100m²/s was used

"BRIDGE" - Basic 3D Test Code

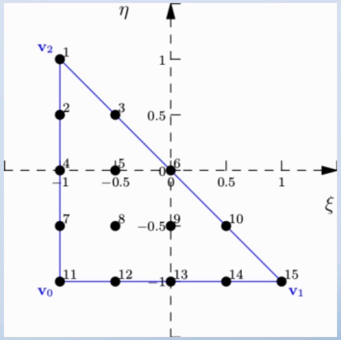
Florian Prill (DWD)

- 3D test code with as little infrastructure overhead as possible
- Discontinuous Galerkin discretizations
- Test platform for DSLs and new infrastructure libraries
- Benchmark "dwarfs”
- Fortran 2003
- MPI parallelization
- Modules and interfaces closely resemble ICON
- ICON triangular grid
- Storage layout: MPI parallel domain decomposition, arrays of 2D triangulations are **`nproma`**-blocked

2.5D: Restrict to quadrature points and node sets which are built from 2Dx1D tensor products.

Consequently, restriction to expansions

$$q(r(x^1,x^2),s(x^3),t) = \sum_{l=1}^{M}\sum_{m=1}^{N} Q_{l,m}(t)\phi_l(x^1,x^2)\psi_m(x^3) \ .$$



Modularization, Encapsulation

Deutscher Wetterdienst
Wetter und Klima aus einer Hand

Libraries

... as little infrastructure overhead as possible:

- Use of supporting libraries like **YAXT**
  The communication library YAXT (DKRZ, Hamburg) abstracts the communication on MPI level from the application.
- better separation between scientific code and infrastructure:
  two auxiliary libraries have been created: **`libftnbasic`** and **`libcbasic`**.

F2003 object-oriented features

The code uses F2003 objects to a far greater extent than ICON:

- to avoid global variables
- to make the data flow in the model more transparent
  which variable is touched by whom, and when ...

Vectors (FE coefficients, evaluated shape fct., ...) remain **`REAL(wp)`** vectors
= no derived type abstraction.
The user takes care of the index ordering
or the fact if they are global or local, synched or not.

DG and Parameterisations

General principle: spatial transport (advection, sedimentation, diffusion, …) must be treated in the DG-scheme!
Otherwise we loose conservation.

Box-models (e.g. **cloud physics**, **chemistry/aerosol-packages**):
are evaluated and deliver tendencies in every quadrature point
→ at the first place no adaptations necessary!
Nevertheless, the ‚classical' physics/dynamics-coupling questions remain:
overall time integration scheme? how to achieve positive definiteness?

Turbulence:
Remark: diffusion needs special treatment in DG (local DG, compact DG, …)
Advantage of local DG: derivatives of fields are directly available for turbulence modeling!

…

Summary

- **2D toy model** for
  - explicit DG-RK (unstructured grids, triangle or quadrilateral grid cells) and
  - **HEVI DG-IMEX-RK**

  now works for *Euler equations* with *terrain-following coordinates* and optionally with *3D diffusion* (explicit or HEVI): several tests show correct convergence behaviour, well-balancing problems solved, …
- Efficiency problems with band diagonal matrix solver strongly improved: the whole implicit part (build coeff. matrix, *LU decomposition*, matrix-vector-mult.) takes ~60% of total run time.
- **DG on the sphere** on a triangle grid possible by the use of local (rotated gnomonial) coordinates and the covariant formulation of the equations. (*Baldauf (2020) JCP*)

→ 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!

Outlook

- Current tasks in the **2D toy model**
  - Consolidation of what has been achieved so far:
    further testing; what are the true limits of the method?

Further **milestones** (for the next years!)

- Development of a **3D prototype: (**DG-HEVI on the sphere)
  BRIDGE (**B**asic **R**esearch for **I**CON with **DG E**xtension) (start ~mid 2020)
  - **Further design decisions**: nodal vs. modal,
    local DG vs. interior penalty vs. …,
    allow non-conformal grids?,
    efficient data layout, …
  - Coupling of **tracer advection** (mass-consistency)?
  - Develop coupling ideas for parameterizations
    time-integration, preserve pos. def., …
- Implementation into **ICON** (start ~2024)
  - choose optimal convergence order p and grid spacing
    estimated: $p_{horiz} \sim 4 \ldots 6$, $p_{vert} \sim 3 \ldots 4$ ($p_{time} \sim 3 \ldots 4$)
    currently I favor: $p_{horiz} = 4$, $p_{vert} = 4$, $p_{time} = 3$

Announcement:

The next

„Partial differential equations on the sphere“ – workshop

will take place at
DWD, Offenbach, Germany
~~5-9 October 2020~~
postponed due to Covid-19 to (probably)
17-21 May 2021

2D Euler-equations (non-hydrostatic, compressible) with diffusion (=Navier-Stokes eqns.) with terrain-following coordinates (x, z‘) on a plane

$$
\begin{aligned}
\frac{\partial}{\partial t}\sqrt{G'}\rho' + \frac{\partial}{\partial x}\sqrt{G'}M^{*x} + \frac{\partial}{\partial z'}\sqrt{G'}\left(\frac{\partial z'}{\partial x}M^{*x} + \frac{\partial z'}{\partial z}M^{*z}\right) &= 0,\\
\frac{\partial}{\partial t}\sqrt{G'}M^{*x} + \frac{\partial}{\partial x}\sqrt{G'}T^{*x*x} + \frac{\partial}{\partial z'}\sqrt{G'}\left(\frac{\partial z'}{\partial x}T^{*x*x} + \frac{\partial z'}{\partial z}T^{*x*z}\right) &= 0,\\
\frac{\partial}{\partial t}\sqrt{G'}M^{*z} + \frac{\partial}{\partial x}\sqrt{G'}T^{*z*x} + \frac{\partial}{\partial z'}\sqrt{G'}\left(\frac{\partial z'}{\partial x}T^{*z*x} + \frac{\partial z'}{\partial z}T^{*z*z}\right) &= -\sqrt{G'}g\rho' - \sqrt{G'}\frac{M^{*z}}{\tau},\\
\frac{\partial}{\partial t}\sqrt{G'}\eta' + \frac{\partial}{\partial x}\sqrt{G'}H^{*x} + \frac{\partial}{\partial z'}\sqrt{G'}\left(\frac{\partial z'}{\partial x}H^{*x} + \frac{\partial z'}{\partial z}H^{*z}\right) &= 0,
\end{aligned}
$$

$$
p = p_{ref}\left(\frac{\eta R_d}{p_{ref}}\right)^{cp/cv},
$$

$$M^{*i} = \rho\, v^i$$

$$\eta = \rho\theta$$

Momentum fluxes:

$$
\begin{aligned}
T^{*x*x} &= \frac{M^{*x}M^{*x}}{\rho} + p' - 2K\rho\left(\frac{\partial v^{*x}}{\partial x} + \frac{\partial z'}{\partial x}\frac{\partial v^{*x}}{\partial z'}\right),\\
T^{*x*z} \equiv T^{*z*x} &= \frac{M^{*x}M^{*z}}{\rho} - K\rho\left(\frac{\partial z'}{\partial z}\frac{\partial v^{*x}}{\partial z'} + \frac{\partial v^{*z}}{\partial x} + \frac{\partial z'}{\partial x}\frac{\partial v^{*z}}{\partial z'}\right),\\
T^{*z*z} &= \frac{M^{*z}M^{*z}}{\rho} + p' - 2K\rho\frac{\partial z'}{\partial z}\frac{\partial v^{*z}}{\partial z'},
\end{aligned}
$$

Heat fluxes:

$$
\begin{aligned}
H^{*x} &= \frac{\eta M^{*x}}{\rho} - K\rho\left(\frac{\partial\Theta}{\partial x} + \frac{\partial z'}{\partial x}\frac{\partial\Theta}{\partial z'}\right),\\
H^{*z} &= \frac{\eta M^{*z}}{\rho} - K\rho\frac{\partial z'}{\partial z}\frac{\partial\Theta}{\partial z'}.
\end{aligned}
$$

strong conservation form with terrain following coordinates but cartesian base vectors (*Schuster et al. (2014) MetZ, appendix*, for the sphere*)*

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

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. (2017) arXiv: use of multi-step or multi-stage IMEX for HEVI-DG

Flow over mountain with the HEVI-solver

Setup : Schär et al. (2002)

Orography: $$h(x) = h_0 \cdot e^{-x^2/b^2} \cdot \cos^2 \pi \frac{x}{\lambda}$$

h_0=25m, b=5km, λ=4km → Fr_h =40, Fr_a =0.1 … 0.5
u_0=10m/s, N=0.01 1/s, $T(z=0)$=288K

compare with analytic linear solution: *Baldauf, 2008, COSMO-NL*
(uses only a few further approximations, e.g. it is a fully compressible solution)

DG and physics perturbations in ensembles

Some recommendations …
… to keep conservation properties of the DG scheme:

- in the **transport terms**, only (physical) fluxes should be perturbed.
- in the **source terms**: e.g. moisture var., perturb in a way that $\rho_{dry} + \rho_v + \rho_r + ... + \rho_g$ is unchanged (while keeping positive definitness)

DG and data assimilation

At least adaptations in the forward operators necessary:

- by the modified output grid; better say: to the position of the I/O-grid points (these are probably the quadrature points in the triangle grid)
- different prognostic variables (conserved var.)