



Further developments in the Discontinuous Galerkin based dynamical core for ICON (BRIDGE)

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The BRIDGE project (Basic Research for ICON with DG Extension)

BRIDGE is an *informal* project *at DWD*, started ~ mid 2020

currently: F. Prill, M. Baldauf, D. Reinert

Goals:

- develop a prototype for a Discontinuous Galerkin (DG) discretization of the 3D Euler equations (,DG-HEVI on the sphere')
- together with a minimal set of physical parameterizations
- using ICON infrastructure (parallelisation via YAXT, I/O, ...)
- more object-orientation and use of standard software (e.g. YAC coupler, ...)
- → BRIDGE is an intermediate step to a full–fledged ICON implementation. Later on (starting ~2024), the BRIDGE code will serve as a code base for the final ICON-DG model.







Discontinuous Galerkin (DG) methods in a nutshell

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

1.) weak formulation

e.g.

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

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

2.) Finite-element ingredient

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

3.) Finite-volume ingredient: numerical flux



From Nair et al. (2011) in ,Numerical techniques for global atm.

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

4.) Gaussian quadrature for the volume and surface integrals

 \rightarrow ODE-system for $q^{(k)}_{il}(t)$

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









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1.) weak formulation

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

2.) Finite-element ingredient $q^{(k)}(x,t) = \sum_{l=1}^{p} q_{j,l}^{(k)}(t) \ p_l(x-x_j)$

3.) Finite-volume ingredient: numerical flux

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

e.g.

works on unstructured grids \checkmark

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

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

4.) Gaussian quadrature for the volume and surface integrals

$$\rightarrow$$
 ODE-system for $q^{(k)}_{il}(t)$

allows massive parallelisation \checkmark

5.) Use a time-integration scheme (Runge-Kutta, high computational intensity v







Improvements in the efficiency of the HEVI solver





Efficiency of the HEVI (vertically implicit) solver

The HEVI approach applied to DG leads to (large) *block-tridiagonal linear system of equations* (*Baldauf (2021) JCP*).

Problem: the complexity of a direct solver for a linear system of *N* equations for LU-decomposition is $O(N^3)$, for matrix vector mult. is $O(N^2)$ with N = # of variables (5) * # of base functions in each cell (10*4) (for 4th order)

Efficiency improvement by **Collocation** (i.e. interpolation points = quadrature points) This decouples the equations horizontally (also in the BCs!) \rightarrow N = # of variables (5) * # of vertical base functions in each cell (4)

→ HEVI solver ~ 10 times faster than before!

 \rightarrow we are in the game again \odot





3D Euler equations: quasi-linear expansion of gravity and sound waves in a spherical shell

Baldauf, Reinert, Zängl (2014) QJRMS derive a linearized analytic solution for

- test scenario (A): f = 0
- test scenario (B): $f = 10 * f_{geo}(45^{\circ}) \rightarrow f/N \sim 0.05$

DG 4th order scheme with explicit time integration (4th order Runge-Kutta)







Deutscher Wetterdienst Wetter und Klima aus einer Hand

A very first (!), almost (!) fair comparison between ICON and BRIDGE

- test case Baldauf, Reinert, Zängl (2014) QJRMS: expansion of sound- and gravity waves in a spherical shell (uses shallow atmosph. approx., U₀=0, f=0).
 Analytic solution available!
- R= r_{earth} / 100 → almost isotropic grid cells
 → HEVI- (ICON) and purely expl. time integration (BRIDGE) are comparable!
- all simul. on our RCL (ICON: 32, 64, 384 proc. (thanks to D. Reinert!), BRIDGE: 16 proc.)







Choice of prognostic variables







Euler equations (in covariant form)

$$\begin{array}{ll} \text{Continuity eq.:} & \frac{\partial \rho}{\partial t} + \nabla_k M^k = 0 & M^k = \rho v^k \\\\ \text{Momentum eq.:} & \frac{\partial M^i}{\partial t} + \nabla_k T^{ik} = S^i_{(M)} \\\\ & T^{ik} = \frac{1}{\rho} M^i M^k + p g^{ik} & S^i_{(M)} = -g \rho e^i - 2g^{il} \epsilon_{ljk} \Omega^j M^k \end{array}$$

Energy budget eq.:

Variant 1: use density weighted potential temperature $\theta = \rho \Theta$ $\frac{\partial \theta}{\partial t} + \nabla_k v^k \theta = 0 \qquad p = p(\theta)$ Variant 2: use total energy density $E = E_{kin} + E_{pot} + E_{int}$

$$\frac{\partial E}{\partial t} + \nabla_k v^k (E+p) = 0 \qquad p = p(E_{int})$$





Falling cold bubble in a viscous medium







Baroclinic instability test on the sphere

Jablonowski, Williamson (2006) QJRMS

With $\rho\theta$, source term filtering



ord.5 HEVI jstep=5400 t=01d06:00:00.000 i=50 -> lon=-122.468354430379

latitude (in °)



Becomes quickly unstable!

Observation: slowly increasing disturbances in the vertical.

0.0455 🗐 -0.1364 R2B2L10, 4th order, after t=30h



Clear advantage by the use of E





Baroclinic instability test on the sphere

Jablonowski, Williamson (2006) QJRMS

- With $\rho\Theta,$ the simulation breaks after only ~30h, obviously due to heavy well-balancing problems
- Using total energy *E* and without any further actions, the test runs about 7d and then breaks
- Tests with any kind of physical diffusion (Smagorinsky or K=const.) either damps the unstable wave too much or doesn't prevent instability
- Exponential filtering (e.g. Hesthaven, Warburton (2008)): in each time step reduce a bit the amplitude in dependence of the polynomial degree (but no change of degree 0! ← conservation) This is a relatively cheap proxy for hyperdiffusion; but acts separately on each grid cell
- With the filter settings for exponential filtering found until now, the test runs until 15d
- \rightarrow Obviously, further testing is necessary
- Far future: use kinetic energy conserving DG schemes (Gassner et al. (2021), ...)







Baroclinic instability test on the sphere

Jablonowski, Williamson (2006) QJRMS

BRIDGE DG 4th order R2B3 $\rightarrow \Delta x \sim 315$ km, Δt =40s

T in z=1.5km



Feld 1: Min=224.6468132269569, Max=301.052790588424

Stabilization by an exponential filter (formally of 8th order)



T in 850 hPa at *t*=9d (Fig. 7 from *JW06*)







The DG scheme applied to the TKE equation





Example: Turbulence closure by a one-equation TKE model

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Density of the turbulent kinetic energy (TKE density): $\bar{e} := \frac{1}{2} \bar{\rho} \, \overline{v'^i v'_i}$

TKE equation: $\frac{\partial \bar{e}}{\partial t} = -\nabla_k (\bar{v}^k \bar{e}) + \nabla_k (g^{kj} K_e \nabla_j \bar{e}) - \bar{\rho} \, \overline{v'^i v'^j} \, \nabla_j v^k g_{ik} + g \, \frac{\bar{\rho}}{\bar{\Theta}} \, \overline{v'^i \Theta'} g_i^3 - \epsilon$

Parameterizations:

Diffusion coefficients:

$$\overline{v'^{i}v'^{j}} = -K_{M}2D^{ij} + \frac{2}{3}g^{ij}\overline{e} \qquad K_{x} = c_{x}l_{m}\sqrt{\overline{e}}, \quad x = M, H, e
\overline{v'^{i}\Theta'} = -K_{H}g^{ij}\frac{\partial\overline{\Theta}}{\partial x^{j}} \qquad \text{Mixing lengths (here only neutral case):}
\epsilon = C_{\epsilon}\overline{\rho}\frac{1}{l}\left(\frac{\overline{e}}{\overline{\rho}}\right)^{3/2} \qquad l_{m} = \frac{\kappa z}{1 + \frac{\kappa z}{l_{B}}}$$

BCs from a simplified ,transfer scheme' (wall law) for neutral stratification:

u* from
$$u(z) = \frac{u_*}{\kappa} \log \frac{z}{z_0} \rightarrow \text{ in } z=0: \overline{u'w'} = u_*^2, v=0 \text{ and } \overline{e} = c\rho u_*^2$$

Note: it is not the purpose of this implementation to have a ,good' turbulence parameterization, but to have the main ingredients that must be considered for a DG treatment!





Euler equations + TKE-turbulence model

Simulation of the ,Leipzig wind profile' (from 1931!) u_g =17.5 m/s, z_0 =0.3m, l_B =40m (u, v obs. data from *Detering, Etling (1985)*)









Euler equations + TKE turbulence model:







 first version of a FE/DG framework available, MPI parallelized shallow water equations on the sphere, explicit time integration (RK) 3D Euler equations on the sphere, explicit time integration (RK) with 3D diffusion (+ a simple turbulence scheme) BR1/BR2 grid refinement works 	Q2/2021 ✓ Q3/2021 ✓ Q1/2022 ✓ Q2/2022 ✓/% Q2/2022 ✓
3. Euler equations, HEVI time integration (IMEX-RK)	Q3/2022 🗸
3.b optimization of the vertically implicit solver (Schur compl.,)	Q4/2022 ✓/
3.c with 3D diffusion (+ a simple turbulence scheme), HEVI	Q1/2023 🗸
4. cloud microphysics (Kessler) + tracer advection (positive definit)	
+ explicit sedimentation scheme	Q4/2022 🛠 !
4.b cloud microphysics (cloud ice, Graupel)	
 vertically implicit sedimentation scheme 	Q1/2023
4.c HEVI diffusion on physics time step; overall time integration	Q4/2023
5. limited area version available	Q1/2023
5.b vectorized version available	Q2/2023
5.c GPU version	Q1/2024
6. coupling of a full fledged turbulence + BL scheme	Q2/2023 🛠





Summary(I): BRIDGE, current status (Sept. 2023)

- DG-solver with explicit time integration (RK schemes) or implicit-explicit time integration (IMEX-RK schemes) for HEVI
- **Coordinate systems:** on the sphere, ellipsoid or flat plane (3D or x-z) and terrain-following in case of orography
- Nodal base
- **Tensor product** representation on prism grid cells
- **MPI** parallelisation, using YAXT library by



- Grid refinement on non-conformal grid
- Shallow-water or 3D Euler equations (compressible, non-hydrostatic, deep atmosph. or shallow atmosph. approx.)
- Simplified turbulence parameterizations (Prandtl, TKE eq., Smagorinsky)
- **Diffusion** via Bassi, Rebay 1 (expl. or HEVI) (BR2 under devel.)

Currently, bridge/src/ contains ~80000 lines of code







Summary (II)

- Large efficiency improvement in the HEVI solver by collocation • \rightarrow horizontal decoupling of FE amplitudes in one grid column! Further efficiency improvements by Schur complement technique?
- Equation system using **total energy** E has clear advantages with regard to ٠ a well-balancing problem in comparison to the use of $\rho \Theta$
 - Source term filtering is no longer needed (since no problems to cure ٠ with the buoyancy term)
 - No other detrimental effects visible by using E•
- The **baroclinic instability test case** (JW06) is quite demanding ٠ and needs totel energy E formulation. High order exponential filtering stabilizes this case.
- Successful treatment of a **one-equation TKE turbulence model** with the DG • approach could be demonstrated.
- Now, real **orography data** can be used, work has been started.... ٠







Summary (III)

- Coupling of a **turbulence model**
 - The wish for local conservation requires a **separation of the turbulence model** into a transport part (DG treatment) and a ,pure' parameterization part
 - Use of total energy as prognostic variable is quite probable \rightarrow instead of developing a new turbulence scheme, can we just express the new covariances by known ones (+ only a few additional covariances)?
 - Extend all considerations for **moisture** and by moist transport equations! •
 - Similar considerations are in principle necessary for ٠ convection param., gravity wave param., ...
- Many problems still must be solved in BRIDGE:
 - Collocation for use of different bases ٠
 - Positive definite and mass consistent tracer transport; microphysics coupl. ٠
 - Consistent higher (3rd) order time integration with multiple time steps ٠
 - **Overall efficiency**
- Nevertheless, we hope to start the marriage of BRIDGE with ICON in 2024 ...

