Modeling and Approximation of Moist Atmospheric Flows with Consideration of Topographical Effects

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Introduction

In computational fluid dynamics significance is being ascribed to conserving properties.

If moist processes are present discontinuities appear at phase transformations. Therefore a weak formulation of mass, momentum and energy conservation is the correct description from a mathematical point of view. In meteorological modeling there are many other formulations which allow simpler discretizations and incorporate discontinuities in different ways.

In this project we compare mass and momentum conserving methods which distinguish from each other by the description of thermodynamics. We consider two different classes of finite volume methods: Wave propagation algorithms (where the flux calculation is based on the solution of local Riemann problems) and methods which are widely used in numerical weather prediction (where the flux calculation is done componentwise by interpolation).

In order to consider meteorological relevant problems one should be able to represent orography, small Mach and Froude numbers and stiff phase transformation processes with the numerical method.

We consider discretizations on Cartesian grids with cut cells for the orography.

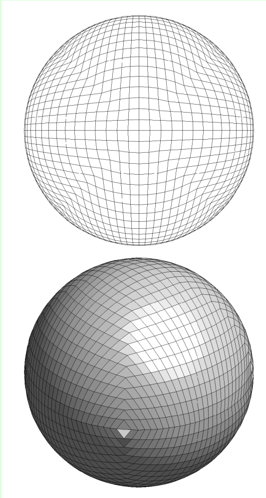
Finite volume methods in circular and spherical domains

D.A. Calhoun, C. Helzel and R.J. Leveque suggested mappings for circular and spherical domains (e.g. the sphere and spherical shell). These mappings lead to quadrilateral or hexahedral grids with nearly uniform cell sizes, thus avoiding the pole singularity.

Calhoun et al. (2008) showed how to solve hyperbolic equations on these circular and sphere grids and demonstrated that they can obtain accurate results for Euler equations on a disk, the shallow water wave equations on the sphere, and acoustic equations on a mesh with embedded cylinders.

Calhoun and Helzel (2008) developed a finite volume discretization of the surface Laplacian that complements the hyperbolic solvers from Calhoun et al. (2008) and is suitable for solving parabolic problems on surface grids. Their method does not require analytic metric terms, shows second order accuracy on the disk and sphere grids, can be easily coupled to existing finite volume solvers for logically Cartesian meshes and handles general mixed boundary conditions.

Currently M. Berger, D.A. Calhoun, C. Helzel and R.J. Leveque are working on discretizations of the spherical nappes, i.e. 3D, for hyperbolic problems with the use of adaptive mesh refinement techniques.



On the top is a grid for the disk which redistributes points near the boundary and which is used to construct the sphere grid shown below.

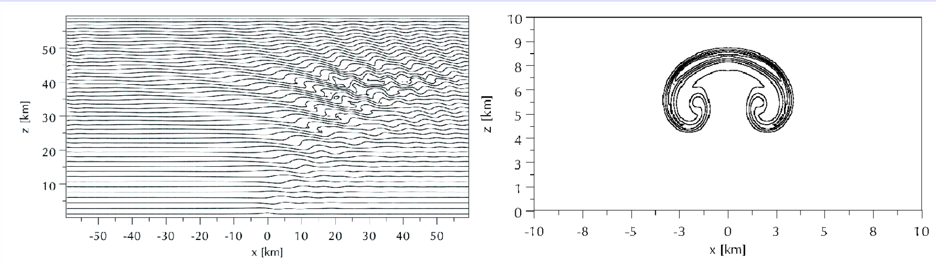
Godunov-type projection method for sound-proof models

(following Schneider et al., JCP (1999), for incompressible flows)

Anelastic	**Pseudo-incompressible**
$\times \quad \nabla\cdot(\overline{\rho}\boldsymbol{v}) = 0$	$\rho_t + \nabla\cdot(\rho\boldsymbol{v}) = 0$
$(\overline{\rho}\boldsymbol{v})_t + \nabla\cdot(\overline{\rho}\boldsymbol{v}\circ\boldsymbol{v}) + \overline{\rho}\nabla\pi = \frac{\theta'}{\overline{\theta}}\overline{\rho}g\boldsymbol{k}$	$(\rho\boldsymbol{v})_t + \nabla\cdot(\rho\boldsymbol{v}\circ\boldsymbol{v}) + \overline{P}\nabla\pi = \frac{\theta'}{\overline{\theta}}\rho g\boldsymbol{k}$
$P_t + \nabla\cdot(P\boldsymbol{v}) = 0$	$\times \quad \nabla\cdot(\overline{P}\boldsymbol{v}) = 0$
$\overline{\rho}(z)\theta = P, \quad \theta = \overline{\theta}(z) + \theta'$	$\rho(z)\theta = \overline{P}, \quad \theta = \overline{\theta}(z) + \theta'$

Klein (2008):

- Asymptotic analysis reveals three distinct time scales
- Sound-proof models are not accessible via classical scale analysis
- Numerics uses structural similarity with compressible flow equations, not their limiting asymptotic behavior



Breaking of internal waves (left) and rising warm, dry bubble (right).

Time-splitting methods

The numerical solution of the Euler equations requires the treatment of processes in different temporal scales. Sound waves propagate fast compared to advective processes. This makes the use of split-explicit scheme, which treat the different physical processes with different time step sizes, attractive: The advective terms are integrated by a Runge-Kutta method with a macro step size restricted by the CFL number. Sound wave terms are treated by small time steps respecting the CFL restriction dictated by the speed of sound. The splitting for the 2D Euler equations (with the red terms evaluated only at the macro time steps) becomes:

$$\begin{aligned}
\frac{\partial\rho}{\partial t} &= -\frac{\partial\rho u}{\partial x} - \frac{\partial\rho w}{\partial z}\\
\frac{\partial\rho u}{\partial t} &= -\frac{\partial\rho uu}{\partial x} - \frac{\partial\rho wu}{\partial z} - \frac{\partial p}{\partial x}\\
\frac{\partial\rho w}{\partial t} &= -\frac{\partial\rho uw}{\partial x} - \frac{\partial\rho ww}{\partial z} - \frac{\partial p}{\partial z} - \rho g\\
\frac{\partial\rho\theta}{\partial t} &= -\frac{\partial\rho u\theta}{\partial x} - \frac{\partial\rho w\theta}{\partial z}\\
p &= \left(\frac{R\rho\theta}{p_0^\kappa}\right)^{\frac{1}{1-k}}
\end{aligned}$$

Generalized split-explicit Runge-Kutta and peer methods

Wensch et al. (2008) generalized split-explicit Runge-Kutta methods by the inclusion of fixed tendencies of previous stages and by starting the integration of the fast part at some intermediate point instead of the beginning of the time intervals. For the solution of the split-differential equation $\dot{y} = f(y) + g(y)$, where f represents the advection and g the acoustics, their scheme reads:

$$Z_{ni}(0) = y_n + \sum_{j=1}^{i-1}\alpha_{ij}(Y_{nj} - y_n)$$

$$\frac{\partial}{\partial\tau}Z_{ni}(\tau) = \frac{1}{d_i}\left(\frac{1}{h}\sum_{j=1}^{i-1}\gamma_{ij}(Y_{nj} - y_n) + \sum_{j=1}^{i-1}\beta_{ij}f(Y_{nj})\right) + g(Z_{ni}(\tau))$$

$$Y_{ni} = Z_{ni}(d_i h), \qquad y_{n+1} = Y_{n,s+1}$$

In practice the integration of the fast differential equation is done with forward-backward Euler.

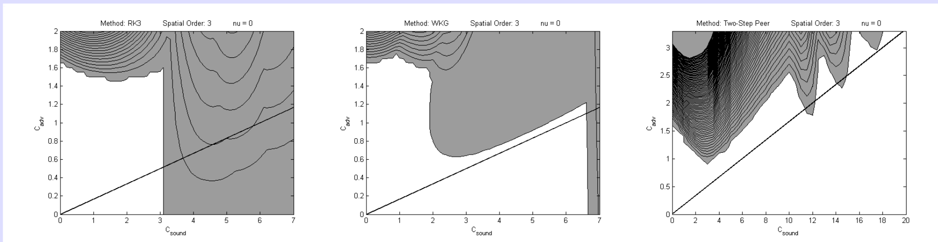
A further more generalization of time-splitting schemes is to use peer methods for the integration of the slow part. Peer methods are general linear methods with the same order in every stage. Jebens et al. (2008) used the representation

$$Z_{ni}(0) = \sum_{j=1}^{s} b_{ij}Y_{n-1,j} + \sum_{j=1}^{i-1} s_{ij}Y_{nj}$$

$$\frac{\partial}{\partial\tau}Z_{ni}(\tau) = \frac{1}{d_i}\left(\sum_{j=1}^{s} a_{ij}f(Y_{n-1,j}) + \sum_{j=1}^{i-1} r_{ij}f(Y_{nj})\right) + g(Z_{ni}(\tau))$$

$$Y_{ni} = Z_{ni}(d_i h).$$

Applying the Multirate Infinitesimal Step method (MIS) of Wensch et al. (2008) and the peer method of Jebens et al. (2008) to a linearized version of the Euler equations and comparing it with the common split-explicit Runge-Kutta method RK3 (which is implemented in the codes WRF of NCAR and COSMO of DWD amongst others) results in the following stability diagrams:



Stability regions of RK3 (left), MIS (middle) and Peer (right) for the linear test equation.

Both new time-splitting schemes were applied to the compressible Euler equations and tested with several examples. They produced good results even with time step sizes which nearly are the maximal stable step sizes from linear stability theory. For the compressible Euler equations (with wind speeds below of 30m/s) they run stable (and no clear differences between the solutions are visible) with time step sizes (and the third-order upwind-scheme for the spatial derivatives with a spatial resolution of 125m) given in the table below, $||d||_1$ is the sum of the fast integration intervals and therefore a measure for the effort of the integration of the fast part.

Method	RK3	MIS	Peer
Time step	0.9s	1.6s	5.0s
$\|\|d\|\|_1$	1.83	1.93	1.44

Euler's equations in Exterior Calculus

Overview

A formulation with Exterior Calculus (EC) gives us a deeper insight into the geometrical structure of Euler's equations. Our aim is to compare this formulation with the Energy-Vorticity-Theory (ETV) developed by Peter Névir. By using Discrete Exterior Calculus (DEC), we are going to investigate several methods on how to define the geometrical operators on the ICON-grid.

Shallow-water equations in Exterior Calculus

We computed a general and comprehensive derivation of Euler's equations in Exterior Calculus. In the following as an example, the shallow-water equations:

$$\frac{\partial(\vec{u}^\flat)}{\partial t} + \mathbf{i}_{\vec{u}}\circ\mathbf{d}\vec{u}^\flat + \frac{1}{2}\mathbf{d}(\vec{u}^\flat(\vec{u})) + \mathbf{d}\phi = 0, \qquad \frac{\partial(*\phi)}{\partial t} + \mathbf{d}*(\phi\vec{u})^\flat = 0$$

Discretization via Discrete Exterior Calculus

We are aiming to develop a systematical way of discretizing Euler's equations by using Discrete Exterior Calculus (DEC) by Anil Hirani. Therefore, we are developing an algorithm on how to discretize Euler's equations on the ICON-grid under the constraint of energy and enstrophy conservation. In addition, the properties of operators on continuous manifolds should also be fulfilled in the discretized case. Finally, we compare this approach with the Energy-Vorticity-Theory (ETV).

Grid refinement

Bossavit et al. developed prolongation and restriction operators for multigrid-methods used for interpolating information between different grid levels. These operators conserve the properties of differential operators on different grid levels. We will apply these tools on Euler's equations, formulated in EC, for grid refinement strategies on the ICON-grid.

Conservative formulation of the Euler equations

Our correct derivation of model equations for a moist and turbulent flow (Gassmann and Herzog, 2008, further on GH08) rests on the extended Energy-Vorticity-Theory originally developed by Névir (1998) for an ideal fluid.

The only way to come to a consistent entropy or potential temperature equation and a satisfying pressure gradient term is to define the potential temperature with a constant exponent in the Exner pressure. The related prognostic variable is the virtual potential temperature defined by

$$\theta_v = T_v/(p/p_{00})^{\frac{R_d}{c_{pd}}}, \qquad T_v = T\left(1 + \left(\frac{R_v}{R_d} - 1\right)q^{vapour} - q^{liquid} - q^{ice}\right).$$

Within the Hamiltonian viewpoint the internal energy reads then $\varrho c_{v,d}T_v$. This does not contradict with the overall energy conservation, if an additional apparent source term in the θ_v equation is taken into account. Now it is possible to write down a whole bunch of prognostic equations, given in GH08. By the use of the Poisson brackets, mass, energy and entropy conservation are automatically given, if the antisymmetry of the brackets is retained during disretisation. The integration by parts rule is applied to temporal discretisation, so that energy, entropy and mass conservation is exactly given for sound wave dynamics. The approximations to model physics were given in GH08 in such a way, that no conservation property is violated, especially the dissipation of energy is correctly represented. The problem of sedimenting particles was also tackled in GH08.

Thus, major parts of the project proposal are already fulfilled, at least the theoretical part.

Submitted and published Papers

D.A. Calhoun and C. Helzel, Finite volume methods for parabolic problems on curved surfaces, submitted to *SIAM Journal on Scientific Computing.*

D.A. Calhoun, C. Helzel and R.J. Leveque, Logically rectangular grids and finite volume methods for PDEs in circular and spherical domains, to appear in *SIAM Review.*

A. Gassmann and H.-J. Herzog, Towards a consistent numerical compressible non-hydrostatic model using generalized Hamiltonian tools, *Quarterly Journal of the Royal Meteorological Society* (2008), doi:10.1002/qj.297.

S. Jebens, O. Knoth and R. Weiner, Explicit Two-Step Peer Methods for the Compressible Euler Equations, submitted to *Monthly Weather Review.*

R. Klein, Asymptotics, structure, and integration of sound-proof atmospheric flow equations, submitted to *Theoretical and Computational Fluid Dynamics.*

M. Schlegel, O. Knoth, M. Arnold and R. Wolke, Multirate Runge–Kutta schemes for advection equations, *Journal of Computational and Applied Mathematics* (2008), doi:10.1016/j.cam.2008.08.009.

S. Vater and R. Klein, Stability of Cartesian grid projection methods for Zero Froude number shallow water flows, submitted to *Numerische Mathematik.*

J. Wensch, O. Knoth and A. Galant, Multirate infinitesimal step methods for atmospheric flow simulation, submitted to *BIT Numerical Mathematics.*

J. Wensch, O. Knoth and A. Galant, Multirate time integration for compressible atmospheric flow, *American Institute of Physics Conference Proceedings* (2008), Volume 1048, pp. 904-908.