Time integration methods and dynamic-physics coupling

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Contents

Dynamics versus Physics

- Dynamical core – inviscid dry Euler equation, which includes
  - Advection of momentum and passive traces
  - Pressure gradient
  - Gravitational term
  - Coriolis term
- Physical parameterizations
  - "Turbulent" diffusion
  - Surface fluxes, temperature and moisture in the soil
  - Phase transfer (microphysics)
  - Falling hydrometeors
  - Radiation depending on phase state of the atmosphere
  - Convection, large scale vertical redistribution

  All together we should have a well-defined "mathematical" model and look for suitable numerics

Numerical schemes for DyCore

How good are methods for a dry numerical core for a "full" model formulation

- Full Eulerian (finite differences/volumes/elements)
- Spatial low order methods, most of the codes
- High order discontinuous Galerkin methods and special methods for source terms
- Semi-Lagrangian methods and their large time steps are corroborated by fast physics

Parameterization should be suitable for "smooth" time integration

- Right hand sides differentiable with respect to state variables
- IF THEN ELSE constructs, MAX, MIN are problematic for numerical differentation
- No adhoc change of state variables
- Non-prognostic parameterization are hidden constraints like incompressibility
- New trend prognostic convection schemes
- No hidden time constants (Relaxation) and time steps and time derivatives (e.g. vertical acceleration)

Replace saturation adjustment by a "smooth" process
Burmeister-Fischer function

$$\varphi(a,b) = a + b - \sqrt{a^2 + b^2}\,.$$

with the property

$$\varphi(a,b) = 0 \quad \Leftrightarrow \quad a \geq 0, \quad b \geq 0, \quad ab = 0\,.$$

In our case we take

$$a \equiv \varrho_v^*(T) - \varrho_v$$

und

$$b \equiv \varrho_c\,,$$

The phase transition term is now

$$\frac{1}{t_{relax}} Q_{ph}(\varrho_v, \varrho_l, T) = \frac{1}{t_{relax}} \left(\varrho_v^*(T) - \varrho_v + \varrho_c - \sqrt{(\varrho_v^*(T) - \varrho_v)^2 + \varrho_c^2} \right)$$

Two case
$\varrho_v > \varrho_v^*(T)$ than $Q_{ph}<0$ and condensation
$\varrho_v < \varrho_v^*(T)$ and $\varrho_c > 0$ than evaporation

- Positive supersaturation possible, depends from relaxation time (cf. Reisner)
- Negative ϱ_c is "coming" back

- Move to prognostic mass flux schemes
- Boundary layer diffusion schemes and drag parametrizations are a naturally part of the numerics of the the dynamical core
- Transport in the upper soil layers and water levels can also be included
- In other areas we are solving advection-diffusion-reaction equations
- In the vertical diffusive fluxes are larger than resolved vertical movement

Method of lines

- Method of lines approach, spatial approximation leads to the time integration
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$$\dot{y} = F(t, y)$$

or with splitting in sub-problems

$$\dot{y} = \sum_i F_i(t, y)$$

$$k_i = \Delta t F(y_n + \sum_{j=1}^{s} a_{ij} k_j), \quad i = 1, \ldots, s$$

$$y_{n+1} = y_n + \sum_{i=1}^{s} b_i k_i$$

or

$$Y_i = y_n + \Delta t \sum_{j=1}^{s} a_{ij} F(Y_i), \quad i = 1, \ldots, s$$

$$y_{n+1} = y_n + \Delta t \sum_{i=1}^{s} b_i F(Y_i)$$

- Explicit methods for $a_{ij} = 0$ for $j > i$
- Error control and adaptive time step selection possible
- A lot of modifications

$$k_i = \Delta t F_1(y_n + \sum_{j=1}^{s} a_{ij} k_j + \sum_{j=1}^{s} \hat{a}_{ij} l_j), \quad i = 1, \ldots, s$$

$$l_i = \Delta t F_2(y_n + \sum_{j=1}^{s} a_{ij} k_j + \sum_{j=1}^{s} \hat{a}_{ij} l_j), \quad i = 1, \ldots, s$$

$$y_{n+1} = y_n + \sum_{i=1}^{s} b_i k_i + \sum_{i=1}^{s} \hat{b}_i l_i$$

or

$$Y_i = y_n + \Delta t \sum_{j=1}^{s} a_{ij} F_1(Y_i) + \Delta t \sum_{j=1}^{s} \hat{a}_{ij} F_2(Y_i), \quad i = 1, \ldots, s$$

$$y_{n+1} = y_n + \Delta t \sum_{i=1}^{s} b_i F_1(Y_i) + + \Delta t \sum_{i=1}^{s} \hat{b}_i F_2(Y_i)$$

- IMEX methods for $a_{ij} = 0$ for $j > i$
- Again a lot of modifications

- Classical split-explicit methods for the dynamical core can be written as partitioned Runge-Kutta methods with splitting the right hand side with three parts
- HEVI methods are a further generalization with five or even more Runge-Kutta tableaux
- Sandu and Günther and others developed the so called Multirate General Additive Runge-Kutta methods (MGARK)
- Can have final implicit stages

$$k_i = \Delta t F(y_n + \sum_{j=1}^{i-1} a_{ij} k_j) + \Delta t W \sum_{j=1}^{i} \gamma_{ij} k_j, \quad i = 1, \ldots, s$$

$$y_{n+1} = y_n + \sum_{i=1}^{s} b_i k_i$$

or in a matrix free form

$$(I - \gamma_{ii} \Delta t_n W) v_i = \Delta t_n F(y_n + \sum_{j=1}^{i-1} \omega_{ij} k_j) + \sum_{j=1}^{i} d_{ij} k_j, \quad i = 1, \ldots, s$$

$$y_{n+1} = y_n + \sum_{i=1}^{s} m_i v_i$$

- Matrix $W \approx \partial F(y_n)/\partial y$
- Convergence order does not depend on W
- In practical applications $\gamma_{ii} = \gamma_0$
- Mainly for stability reasons
- If W is identical zero a explicit Runge-Kutta is obtained
- IMEX methods with linear implicit term and diagonal form are Rosenbrock-Methods
- With $F = \sum F_i$ the matrix $W \approx \sum_i \partial F_i(y_n)/\partial y$

Options for choice of the matrix W

- Order processes with respect to time scales and include fast scales
- Decompose between vertical and horizontal transport processes
- Decompose W on the linear algebra level, approximate matrix factorization (AMF)
- Solve linear system approximately or with a fixed number of time steps

- To reduce further computational cost the following approximation to the Jacobian are applied
- The Jacobian with respect to advection is computed for a first order approximation in space
- For a generic variable χ and advection in x-direction

$$\frac{\partial(\rho u)\frac{\rho\chi}{\rho}}{\partial x}$$

  the differentiation with respect to ρ is ignored
- $(I - \gamma_0 \Delta t W)$ is replaced by $(I - \gamma_0 \Delta t W_T)(I - \gamma_0 \Delta t W_S)$ with $W = W_T + W_S$
- W_T is an approximation to the transport part, W_S is an approximation to the sound part
- Further simplifications are possible for special applications

- Sound part means differentiation of the pressure in the momentum equations with respect to the thermodynamic variables, differentiation of the right hand side of the thermodynamic variables with respect to momentum
- $$W_S = \begin{pmatrix} D_u & D_{u1}\mathrm{Grad}D_1 & \dots & D_{us}\mathrm{Grad}D_s \\ \mathrm{Div}T_{1u} & T_1 & \dots & 0 \\ \mathrm{Div}T_{su} & 0 & 0 & T_s \end{pmatrix}$$

  where D and T are diagonal matrices
- In the anelastic cases $T_i = 0$
- Choice of the diagonal matrices for the different formulations

	D_{u1}	D_1	T_{1u}
C	1	$\partial p/\partial\rho\theta$	θ
A	ρ_0	1	1
P	$\rho_0\theta_0$	1	$(\rho_0\theta_0)/\rho$

Transport/source system

$$(I - \gamma \Delta t W_{AD} - \gamma \Delta t W_S)\Delta w = R$$

Two types of preconditioning I. With the block-lower-upper triangular decomposition

$$I - \gamma \Delta t W_{AD} - \gamma \Delta t W_S = L + D + U$$

the linear system is preconditioned (Block-Gauss-Seidel) by

$$P = (U + D)^{-1} D (L + D)^{-1}$$

II. Preconditioning from the right and the left with

$$P_r = (I - \gamma \Delta t W_{AD})^{-1}$$

$$P_l = (I - \gamma \Delta t W_S)^{-1}.$$

- J_{AD} stands for advection/diffusion, elements are coupled between grid cells
- J_S assembles the source terms, coupling is between different components in each grid cell

$$P_l(I - \gamma \Delta t W_{AD} - \gamma \Delta t W_S) P_r$$

can be written in the form

$$(I - \gamma \Delta t P_l W_{AD}) P_r = (I + P_l((I - \gamma \Delta t W_{AD}) + I)) P_r.$$

- Need to store only the LU-decomposition of the matrix $(I - \gamma \Delta t W_S)$
- $(I - \gamma \Delta t W_{AD})$ is inverted by a fixed number of Gauss-Seidel iterations
- In the parallel case we use one cell overlap

- Split-explicit and Rosenbrock-W-methods in one code
- Processes are called in an additive fashion
- Each process comes with a function and a Jacobian
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