Multirate Infinitesimal Step methods for compressible atmospheric flow

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OVERVIEW

Atmospheric transport code ASAM at IfT, Leipzig

- Nonhydrostatic Euler equations + chemical reaction-advection-diffusion
- staggered $\lambda - \phi$ grid, finite volumes, 3rd order upwind (advection), central differences (sound)
- semi-implicit time integration with Approximate Matrix Factorization (AMF) for advection/sound terms
- Heterogenous grids in space and (in the future) time

Starting point: Split-explicit RK3 scheme [Wicker/Skamarock]

- Governing equations
- Infinitesimal step approach to time integration MIS-RK methods, Peer methods, Exponential integrators
- Order and Stability
- Nonlinear test examples

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EULER EQUATIONS (2D)

- Conservation form with entropy as thermodynamic quantity

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} = Q$$

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho w \\ \rho\theta \end{bmatrix}, \quad F(U) = \begin{bmatrix} u\rho \\ \rho u^2 + p \\ u\rho w \\ u\rho\theta \end{bmatrix}, \quad G(U) = \begin{bmatrix} w\rho \\ w\rho u \\ \rho w^2 + p \\ w\rho\theta \end{bmatrix}.$$

- Q denotes the gravity source terms.
- diagnostic equation: Pressure $p = p(\rho\theta) = p_0 \left(\frac{R\rho\theta}{p_0}\right)^\gamma$
- Red terms are ”sound” terms, spatial discretization $\Rightarrow$

$$y' = B(y, y) = C(y)y + f(y) + g(y)$$

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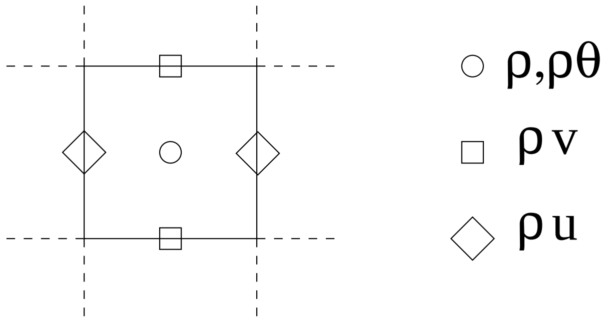
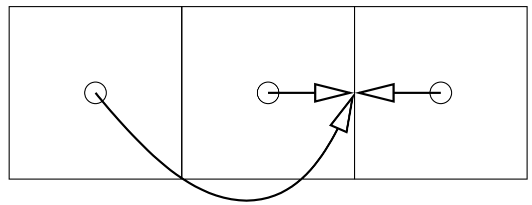
SPATIAL DISCRETIZATION: FINITE VOLUMES

- Staggered grid (Arakawa C-grid)





From Cell to Face: upwind, 3rd order

- shift $\rho u, \rho v \longrightarrow \rho u_{L/R}, \rho v_{U/D}$
- For $\phi \in \{1, \theta, u_{L/R}, v_{U/D}\}$ we interpolate from center to face

$$\frac{\partial}{\partial t}(\rho\phi)_{ij} = -\frac{1}{\Delta x}\left[(\rho u)_{i+1/2,j}\phi_{i+1/2,j} - (\rho u)_{i-1/2,j}\phi_{i-1/2,j}\right] - \frac{1}{\Delta z}\left[(\rho v)_{i,j+1/2}\phi_{i,j+1/2} - (\rho v)_{i,j-1/2}\phi_{i,j-1/2}\right]$$

  - ρu: average advection update of $\rho u_{L/R}$ (no fast terms!), pressure gradient: $(p(\rho\theta_{i+1/2,j}) - p(\rho\theta_{i-1/2,j}))/\Delta x$, same for v, gravitational force $-g\rho$ as fast term

TIME INTEGRATION: RUNGE-KUTTA

- Runge-Kutta method for integration of $y' = f(y)$ uses internal stages

$$
\begin{aligned}
Y_{ni} =& y_n + h \sum_j a_{ij} f(Y_{nj}) \\
y_{n+1} =& Y_{n,s+1} \qquad \text{(final update=additional stage)}
\end{aligned}
$$

- Stage is interpreted as the exact solution of $y' = c := \sum_j a_{ij} f(Y_{nj})$

$$
\begin{aligned}
Z_{ni}(0) =& y_n \\
Z'_{ni}(\tau) =& \sum_j a_{ij} f(Y_{nj}) \\
Y_{ni} =& Z_{ni}(h).
\end{aligned}
$$

PARTITIONED RK-METHODS

- Extend to a partitioned equation $y' = f(y) + g(y)$.
- In each stage compute $Z_{ni}(\tau)$ as solution of $Z'(\tau) = F + g(Z(\tau))$, where $F = \mathrm{const}$ are the fixed slow tendencies $\Rightarrow$ Multirate Infinitesimal Step approach (MIS)

$$
\begin{aligned}
Z_{ni}(0) &= y_n \\
Z'_{ni}(\tau) &= \sum_j a_{ij} f(Y_{nj}) + c_i g(Z_{ni}(\tau)) \\
Y_{ni} &= Z_{ni}(h).
\end{aligned}
$$

- Split-explicit RK3-method uses finite number of steps of forward-backward Euler:

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \text{ nodes } c = (0, 1/2, 1/3, 1)^T$$

GENERALISED PARTITIONED METHODS

- We generalise the exact integration procedure in two directions:
  - arbitrary starting points based on preceeding stages

$$Z_{ni}(0) = y_n + \sum_j \alpha_{ij}(Y_{nj} - y_n)$$

  - increments in the constant term F based on preceeding stages

$$Z'_{ni}(\tau) = \frac{1}{h}\sum_j \gamma_{ij}(Y_{nj} - y_n) + \sum_j \beta_{ij} f(Y_{nj}) + d_i g(Z_{ni}(\tau))$$

- Extends to general case via $y' = B(y, y)$, where $d_i := \sum_j \beta_{ij}$ (balanced)

$$Z'_{ni}(\tau) = \frac{1}{h}\sum_j \gamma_{ij}(Y_{nj} - y_n) + \sum_j \beta_{ij} B(Y_{nj}, Z_{ni}(\tau))$$

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MIS-RK METHODS

- The complete method is given by

$$
\begin{aligned}
Z_{ni}(0) &= y_n + \sum_j \alpha_{ij}(Y_{nj} - y_n) \\
\frac{\partial}{\partial \tau} Z_{ni}(\tau) &= \frac{1}{h} \sum_j \gamma_{ij}(Y_{nj} - y_n) + \sum_j \beta_{ij} f(Y_{nj}) + d_i g(Z_{ni}(\tau)) \\
Y_{ni} &= Z_{ni}(h) \\
y_{n+1} &= Y_{n,s+1}.
\end{aligned}
$$

- $g = 0 \Rightarrow$ underlying RK method

$$
\begin{aligned}
Y &= \mathbb{1} \otimes y_n + ((\boldsymbol{\alpha} + \boldsymbol{\gamma}) \otimes I)(Y - \mathbb{1} \otimes y_n) + h(\boldsymbol{\beta} \otimes I) f(Y) \\
Y &= \mathbb{1} \otimes y_n + h((I - \boldsymbol{\alpha} - \boldsymbol{\gamma})^{-1} \boldsymbol{\beta} \otimes I) f(Y) \\
\Rightarrow A &= (I - \boldsymbol{\alpha} - \boldsymbol{\gamma})^{-1} \boldsymbol{\beta} =: R\beta
\end{aligned}
$$

DERIVATION OF ORDER CONDITIONS

Expand numerical solution in a Taylor series.
Note: Z_{ni} is a function of τ and h. Define
$G(Y_{ni})^{(k)} := \frac{\partial^k}{\partial h^k}\Big|_{h=0} G(Y_{ni})$, $G(Z_{ni})^{(k,l)} := \frac{\partial^{k+l}}{\partial \tau^k \partial h^k}\Big|_{\tau=h=0} G(Z_{ni})$

- Recursion for derivatives of Y_{ni}:

$$Y_{ni} = Z_{ni}(h,h) \quad \Rightarrow \quad Y_{ni}^{(k)} = \sum_{l=0}^{k} \binom{k}{l} Z_{ni}^{(l,k-l)}.$$

- 3 different recursions for derivatives of Z_{ni}:

$$\begin{aligned} Z_{ni}^{(0,l)} &= \sum_j \alpha_{ij} Y_{nj}^{(l)} \\ Z_{ni}^{(1,l)} &= \frac{1}{l+1} \sum_j \gamma_{ij} Y_{nj}^{(l+1)} + \sum_j \beta_{ij} f(Y_{nj})^{(l)} + d_i g(Z_{ni})^{(0,l)} \\ \Rightarrow \quad Z_{ni}^{(k,l)} &= d_i g(Z_{ni})^{(k-1,l)}, \quad k \geq 2. \end{aligned}$$

ORDER CONDITIONS

- The recursion leads to following order conditions for 3rd order
  - four classical order conditions

$$b^T \mathbb{1} = 1, b^T c = 1/2, b^T c^2 = 1/3, b^T A c = 1/6$$

  - and five additional order conditions

$$\begin{aligned} \tilde{b}(c + \tilde{c}) &= 1 \\ \tilde{b}(I + \boldsymbol{\alpha})Ac &= 1/3 \\ 3\tilde{b}(\boldsymbol{\alpha} + \boldsymbol{\gamma}/2)RD(c + \tilde{c}) + \tilde{b}^T D(c + 2\tilde{c}) &= 1 \\ b^T RD(c + \tilde{c}) &= 1/3 \\ \tilde{b}^T (c^2 + \tilde{c}^2 + c \cdot \tilde{c}) &= 1 \end{aligned}$$

where we use $\tilde{c} := \boldsymbol{\alpha} c$ and $\tilde{b} = e_{s+1}^T RD$.

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PEER METHODS

- General linear method ⇒ multivalue + multistage
- For an ODE $y' = f(y)$ the method is given by

$$Y_{ni} = \sum_{j=1}^{s} b_{ij} Y_{n-1,j} + \sum_{j=1}^{i-1} s_{ij} Y_{nj} + h \sum_{j=1}^{s} a_{ij} f_{n-1,j} + h \sum_{j=1}^{i-1} r_{ij} f_{nj}$$

Note: We compute approximations $Y_{ni} \approx y(t_n + c_i h)$!
Equivalent to cyclic multistep method on grid $\{t_m\} = \{t_n + c_i h\}$.

- Apply MIS-approach

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

$$Z'(\tau) = \left(\sum_{j=1}^{s} a_{ij} f_{n-1,j} + \sum_{j=1}^{i-1} r_{ij} f_{nj} \right) + d_i g(Z(\tau))$$

$Y_{ni} = Z(h)$ No update!

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EXPONENTIAL INTEGRATORS

Assume an ODE $y' = B[y](y)$ where we can solve $y' = B[p](y)$ and even

$$y' = \sum_k \alpha_k B[p_k](y).$$

Abstract solution operator $\exp$

$$y(t) := \exp(t \sum_k \alpha_k B[p_k]) y(0).$$

Time integration procedure

$$Y_{ni} = \exp(h \sum_{j<i} a_{ij}^{(l)} B[Y_{nj}]) \ldots \exp(h \sum_{j<i} a_{ij}^{(1)} B[Y_{nj}]) y_n$$

Example: $y' = A(y)y + c(y) \Rightarrow y' = A(p)y + c(p)$, exact solution

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$$y(t) = \mathrm{Exp}(tA)y(0) + t\phi(tA)c, \quad \text{where } \phi(z) := (e^z - 1)/z$$

CONSTRUCTION OF METHODS

- MIS-RK:
  - 3 stage 3rd order $\Rightarrow$ 12 parameters for 9 eqns
  - No 3rd order method for $\boldsymbol{\alpha} = \boldsymbol{\gamma} = 0$ (classic splitting like RK3)
  - $\boldsymbol{\alpha}, \boldsymbol{\gamma} \neq 0$: Eliminate 8 order conditions
    4 free parameters and 1 complex nonlinear condition remain
  - Here: MIS3B [W.,K.,G., BIT 2009]
- Peer methods: 3 stages, order 2 [K.,J., MWR 2008]
- Exponential integrators: Lie group theory [Owren 06],
  method CF3 based on $c = (0, 1/3, 2/3)$ and 3rd order Radau-weights,
  $\boldsymbol{\alpha} \neq 0$, $\alpha_{ij} \in \{0, 1\}$, $\boldsymbol{\gamma} = 0$
- Peer/MIS-RK construction: Exhaustive search of parameter space for methods with good stability properties
- NOTE: MIS-approach is used to derive methods and investigate stability, in practical computations we use forward-backward Euler!

STABILITY: LINEAR ACOUSTICS

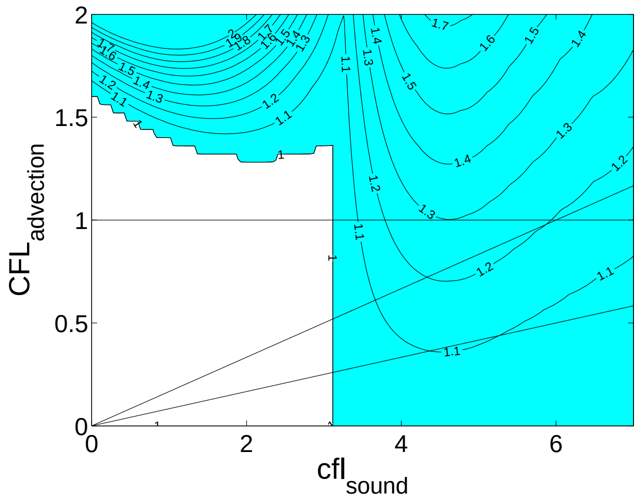
- Linear acoustics equation

$$u_t + U u_x = -c_s \pi_x$$
$$\pi_t + U \pi_x = -c_s u_x$$

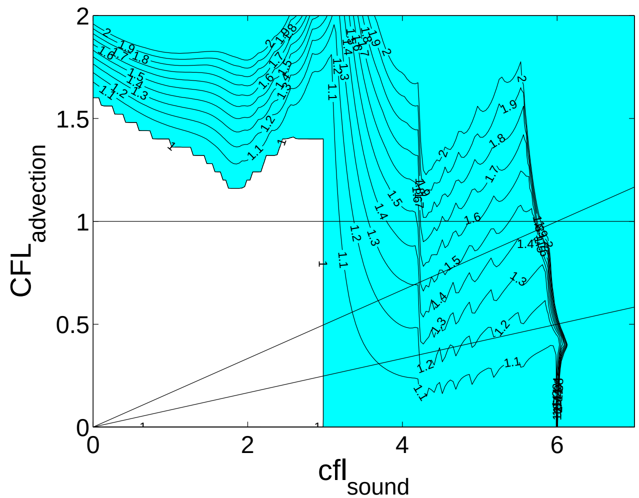
- Spatial discretisation on staggered grid, advection $\longrightarrow$ upwind-differences, sound terms $\longrightarrow$ symmetric differences.
- Stability: Maximum amplification for all waves for fixed Courant numbers $C_A = U\Delta t/\Delta x$, $C_S = c_s \Delta t/\Delta x$
- NOTE: Even if we execute a finite number of small forward-backward Euler steps, C_S is computed with respect to the large time step!

STABILITY REGIONS

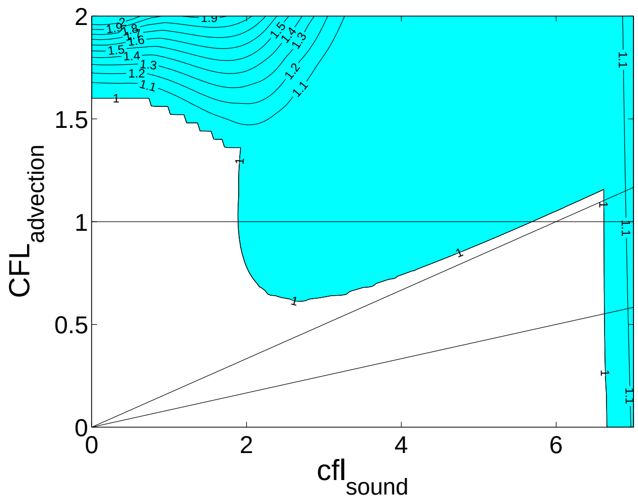
RK3, exact integration.



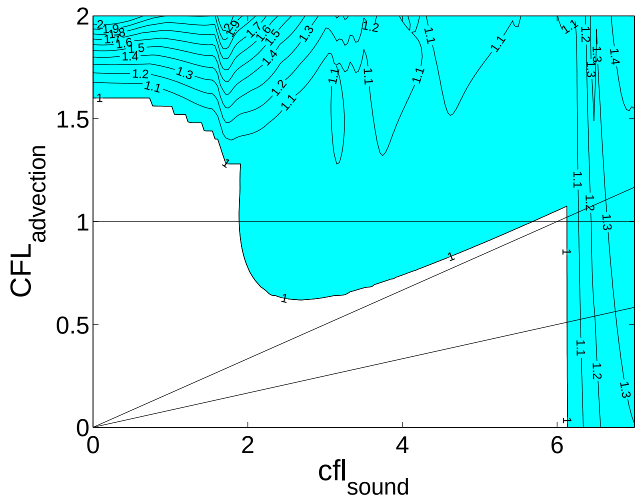
RK3, forward-backward Euler ($n_s = [2, 3, 6]$).



MIS3B, exact integration.

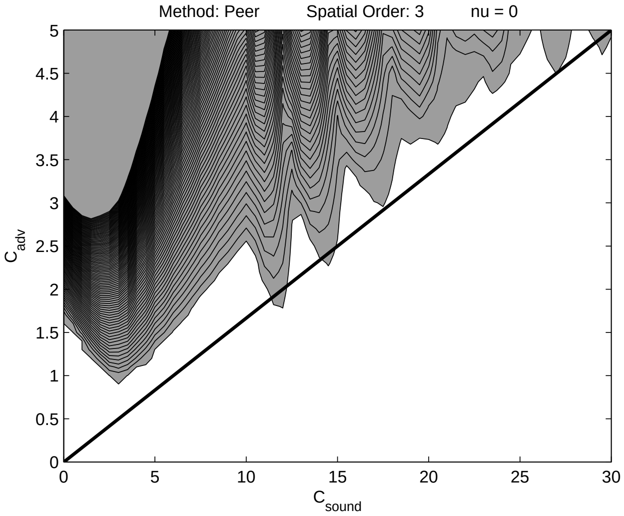


MIS3Ba, forward-backward Euler ($n_s = [2, 3, 4]$).

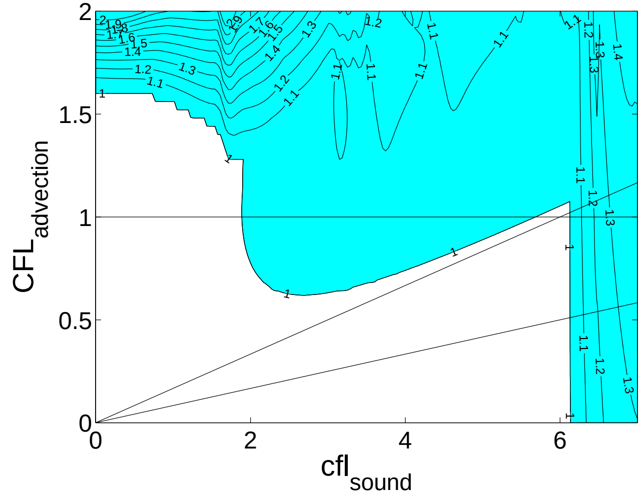


STABILITY REGIONS

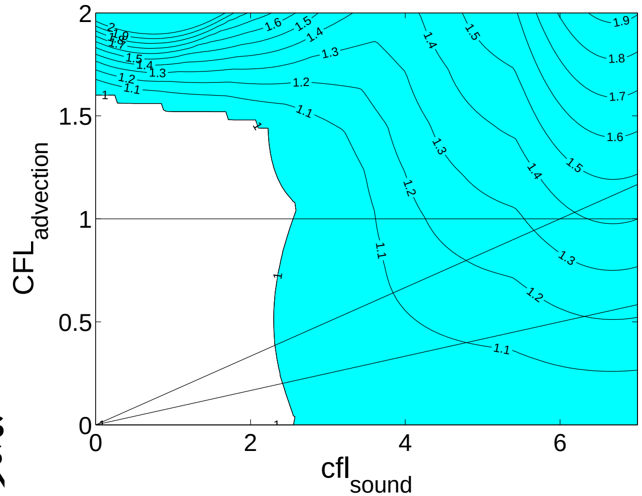
Peer method, FB-Euler (different scale!)



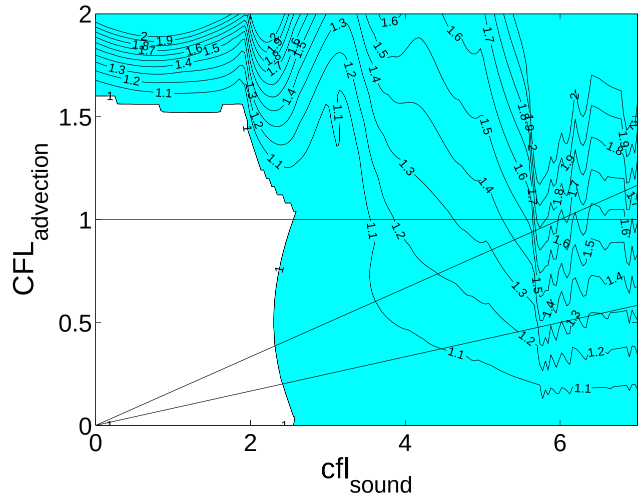
MIS3Bb, forward-backward Euler ($n_s = [4, 6, 8]$).



CF3, exact integration.

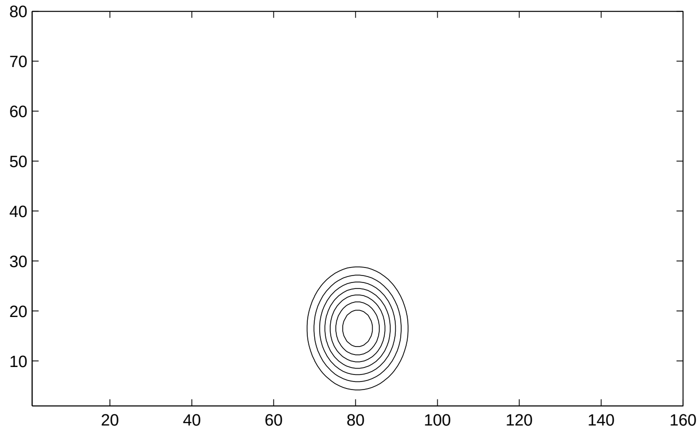


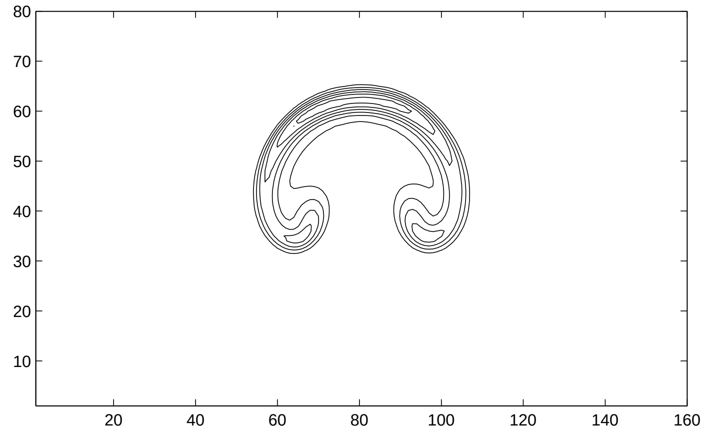
CF3, forward-backward Euler ($n_s = [3, 6, 6]$).



NONHYDROSTATIC EULER EQUATIONS

- Euler equations, rising bubble with advection
  - Domain $20km \times 10km$, Grid dx = dy = 125 m;
  - Final time = 17 minutes
  - Initial state: $u = 20m/s, v = 0$, hydrostatic balance, $\theta = 300K$.
  - Thermal bubble with $\Delta\theta = +2K$, radius $2km$
  - Boundary conditions: periodic/no-flux





- Maximum step sizes

Method	RK3	CF3	WKG3Bb	PEER
Macro Time Step in s	0.9	0.5	1.8	5.0

SUMMARY

- Even with MIS-approach all methods suffer from a sound-CFL-restriction. The reason for this coupling is unclear up to now.
- Sophisticated time integration techniques may help to construct methods with improved stability properties.
- Peer methods have extraordinary large stability area.
- Remark: Divergence damping may overcome the instability, too.
- Future directions:
  - Multistage semi-implicit methods ($\longrightarrow$ Rosenbrock methods/W methods) with full third order, efficient linear Algebra with AMF/dimension splitting/iterative solvers.
  - Real multirate in space and time for semiimplicit methods

THE METHOD CF3

Butcher tableau of CF3 (Celledoni et.al. 03, Owren 06), method has order 3

$$\begin{array}{c|ccc} 0 & & & \\ 1/3 & 1/3 & & \\ 2/3 & 0 & 2/3 & \\ \hline 1 & 1/3 & & \\ & -1/12 & 0 & 3/4 \end{array}$$

In our notation we have

$$\boldsymbol{\beta} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1/3 & 0 & 0 & 0 \\ 0 & 2/3 & 0 & 0 \\ -1/12 & 0 & 3/4 & 0 \end{pmatrix}, \boldsymbol{\alpha} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \boldsymbol{\gamma} = 0.$$