Partially Implicit Time Integration Methods for the Compressible Euler Equations

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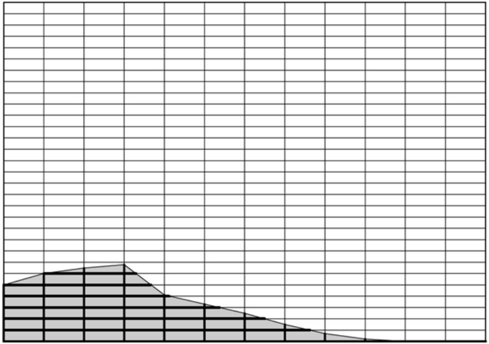
LEIBNIZ-INSTITUT FÜR TROPOSPHÄRENFORSCHUNG

ASAM
All Scale Atmospheric Model

- Cut cell approach with small grid cells



- In compressible models occur:
  - Energetically relevant slow waves (e.g. advection, Rossby waves)
  - Energetically irrelevant fast waves (e.g. sound waves)
- In explicit models the fast waves restrict the maximal time step size
- One ansatz to overcome this is operator splitting
  - Advantages: Every step is cheap, easy to implement, parallelization
  - Disadvantages: Still explicit (i.e. only small time steps allowed especially when used together with cut-cells), complicated derivation of order conditions and stability results
- Another ansatz is the use of implicit methods
  - Advantages: Allows very big time steps, order conditions and stability issues are obvious
  - Disadvantages: Requires solution of huge (non-)linear systems of equations, needs efficient (parallel) preconditioners

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- Consider PDE discretized in space

$$y' = f(y)$$

- Rosenbrock Method

$$\begin{aligned} y_{n+1} &= y_n + \sum_{i=1}^{s} b_i k_i, \\ k_i &= \tau f\left(y_n + \sum_{j=1}^{i-1} a_{ij} k_j\right) + \Delta t W \sum_{j=1}^{i} \gamma_{ij} k_j, \quad i = 1, ..., s. \end{aligned}$$

where $W \approx J_n = f('y_n)$.

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- Order conditions

Order p	Conditions
1	$\sum_{i=1}^{s} b_i = 1$
2	$\sum_{i=2}^{s} b_i a_i = 1/2$
	$\sum_{i=2}^{s} b_i d_i = 0$
3	$\sum_{i=2}^{s} b_i a_i^2 = 1/3$
	$\sum_{i=3}^{s} \sum_{j=2}^{i-1} b_i a_{ij} a_j = 1/6$
	$\sum_{i=3}^{s} \sum_{j=2}^{i-1} b_i a_{ij} d_j = 0$
	$\sum_{i=3}^{s} \sum_{j=2}^{i-1} b_i \gamma_{ij} a_j = 0$
	$\sum_{i=2}^{s} b_i d_i^2 = 0$

- Rosenbrock-W method based on RK3

$$
\begin{array}{c|ccc}
0 & & & \\
1/3 & 1/3 & & \\
1/2 & 0 & 1/2 & \\
\hline
 & 0 & 0 & 1
\end{array}
\qquad
\begin{array}{c|ccc}
\gamma & \gamma & & \\
\frac{1-9\gamma+24\gamma^2}{-9+36\gamma} & \frac{1-12\gamma^2}{-9+36\gamma} & \gamma & \\
0 & -1/4+2\gamma & 1/4-3\gamma & \gamma \\
\hline
 & 0 & 0 & 0
\end{array}
$$

$\mathcal{A}$-Matrix	Γ-Matrix

- Type of approximate Jacobian
  - Approximate matrix factorization

$$f = f_1 + f_2, \quad J = J_1 + J_2, \quad I - \gamma\tau W = (I - \gamma\Delta t J_1)(I - \gamma\Delta t J_2)$$

  - Jacobian from a low order discretization

$$f_L \approx f, \quad W = J_L$$

  - Partial Jacobian, split with respect to space or processes

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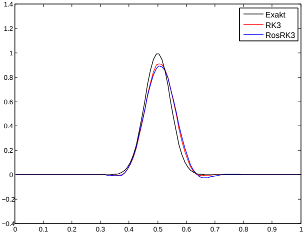
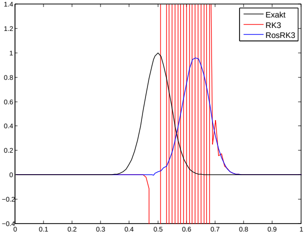
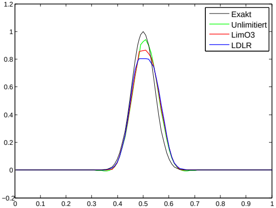
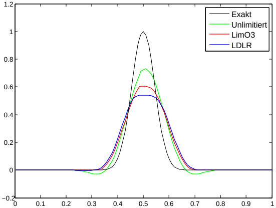
- Unit interval, 100 grid cells, comparison of a uniformly spaced grid and a uniformly grid cell with one small grid cell $h_{\text{small}} = 1/10000$.





- Uniformly grid cell with one small grid cell $h_{\text{small}} = 1/10000$, one and tenth revolution of the profile, two different limiters





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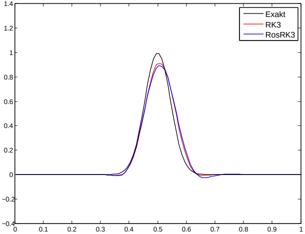

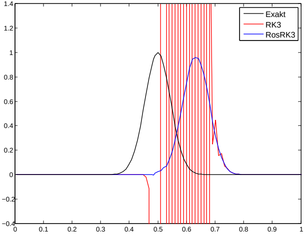

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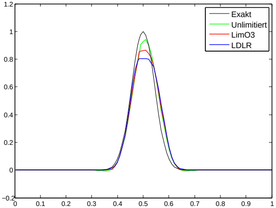

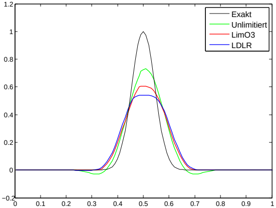

- Peer Method
- Write numerical solutions as:

$$Y_m := \begin{pmatrix} Y_{m1} \\ \vdots \\ Y_{ms} \end{pmatrix} \approx \begin{pmatrix} y(t_m + c_1 \Delta t) \\ \vdots \\ y(t_m + c_s \Delta t) \end{pmatrix} \in \mathbb{R}^{s \times n}, \qquad F_m := f(Y_m) \in \mathbb{R}^{s \times n}$$

- Runge-Kutta methods (for autonomous systems) read:

$$Y_m = Y_{m-1,s} + \Delta t A F_m$$

- Explicit peer methods are defined by:

$$Y_{mi} = B_i Y_{m-1} + \Delta t A_i F_{m-1} + \Delta t R_i F_m$$

- Performing one Newton step results in the considered class of linearly implicit peer methods:

$$Y_m (I - h\gamma J)^T = B Y_{m-1} + \Delta t A F_{m-1} + \Delta t R F_m + \Delta t G Y_{m-1} J^T + \Delta t H Y_m J^T$$

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- Order conditions $AB(k)=0$, $\widehat{AB}(k)=0$, $k\le s$, can be written in compact matrix form

$$\begin{aligned} B\mathbb{1} &= \mathbb{1},\\ A &= CV_0D^{-1}V_1^{-1} - B(C-I)V_1D^{-1}V_1^{-1} - RV_0V_1^{-1},\\ G &= -\Gamma V_0V_1^{-1} - HV_0V_1^{-1} \end{aligned}$$

with $\mathbb{1}=(1,\dots,1)^T$, $C=\mathrm{diag}(c_1,\dots,c_s)$, $\Gamma=\gamma I$, $D=\mathrm{diag}(1,2,\dots,s)$,

$$V_0=\begin{pmatrix}1 & c_1 & \cdots & c_1^{s-1}\\ \vdots & \vdots & \ddots & \vdots\\ 1 & c_s & \cdots & c_s^{s-1}\end{pmatrix} \quad\text{and}\quad V_1=\begin{pmatrix}1 & c_1-1 & \cdots & (c_1-1)^{s-1}\\ \vdots & \vdots & \ddots & \vdots\\ 1 & c_s-1 & \cdots & (c_s-1)^{s-1}\end{pmatrix}.$$

- In the remainder we will concentrate on second-order methods with $s=2$ stages. Furthermore we choose $c_s=1$ so that $Y_{ms}\approx y(t_{m+1})$.
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- One-dimensional compressible Euler equations in conservative form:

$$
\begin{aligned}
\dot{\rho} &= -\frac{\partial \rho u}{\partial x} \\
\dot{\rho u} &= -\frac{\partial \rho u u}{\partial x} - \frac{\partial p}{\partial x} \\
\dot{\rho\theta} &= -\frac{\partial \rho u \theta}{\partial x} \\
p &= \left(\frac{R\rho\theta}{p_0^\kappa}\right)^{\frac{1}{1-\kappa}}
\end{aligned}
$$

- Elimination of pressure:

$$
\begin{aligned}
\frac{\partial p}{\partial x} &= \frac{\partial p}{\partial \rho\theta}\frac{\partial \rho\theta}{\partial x} \\
\frac{\partial p}{\partial \rho\theta} &= \frac{R}{p_0^\kappa(1-\kappa)}\left(\frac{R\rho\theta}{p_0^\kappa}\right)^{\frac{\kappa}{1-\kappa}} = \frac{1}{\rho\theta(1-\kappa)}\left(\frac{R\rho\theta}{p_0^\kappa}\right)^{\frac{1}{1-\kappa}} = \frac{c_s^2}{\theta}
\end{aligned}
$$

with c_s the speed of sound

$$
c_s := \sqrt{\frac{1}{\rho(1-\kappa)}\left(\frac{R\rho\theta}{p_0^\kappa}\right)^{\frac{1}{1-\kappa}}}
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- Elimination of pressure:

$$\frac{\partial p}{\partial x} = \frac{\partial p}{\partial \rho\theta}\frac{\partial \rho\theta}{\partial x}$$
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$$c_s := \sqrt{\frac{1}{\rho(1-\kappa)}\left(\frac{R\rho\theta}{p_0^\kappa}\right)^{\frac{1}{1-\kappa}}}$$

- Use of product rule for

$$\frac{\partial \rho u u}{\partial x} = -u^2 \frac{\partial \rho}{\partial x} + 2u \frac{\partial \rho u}{\partial x}$$
$$\frac{\partial \rho u \theta}{\partial x} = -u\theta \frac{\partial \rho}{\partial x} + \theta \frac{\partial \rho u}{\partial x} + u \frac{\partial \rho \theta}{\partial x}$$

- results in the nonlinear Euler equations in compact form:

$$\begin{pmatrix} \dot{\rho} \\ \dot{\rho u} \\ \dot{\rho\theta} \end{pmatrix} = -\begin{pmatrix} 0 & 1 & 0 \\ -u^2 & 2u & \frac{c_s^2}{\theta} \\ -u\theta & \theta & u \end{pmatrix} \begin{pmatrix} \rho_x \\ (\rho u)_x \\ (\rho\theta)_x \end{pmatrix}$$

- Linearization by considering the disturbed quantities (e.g. $\rho' := \rho - \overline{\rho}$) and dropping all nonlinear terms:

$$\begin{pmatrix} \dot{\rho}' \\ (\dot{\rho u})' \\ \frac{1}{\overline{\theta}}(\dot{\rho\theta})' \end{pmatrix} = -\underbrace{\begin{pmatrix} 0 & 1 & 0 \\ -\overline{u}^2 & 2\overline{u} & c_s^2 \\ -\overline{u} & 1 & \overline{u} \end{pmatrix}}_{M} \begin{pmatrix} \rho'_x \\ (\rho u)'_x \\ \frac{1}{\overline{\theta}}(\rho\theta)'_x \end{pmatrix}$$

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- To save storage and gain computational efficiency we make two simplifications for the Jacobian J:
    - Use Jacobian of the advection form of the Euler equations
    - Use first-order upwind scheme for spatial discretization
- Use $\overline{\rho}u' \approx (\rho u)' - \overline{u}\rho$ instead of $(\rho u)'$, i.e. use:

$$\widetilde{M} := -\begin{pmatrix} 1 & 0 & 0 \\ -\overline{u} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ -\overline{u}^2 & 2\overline{u} & c_s^2 \\ -\overline{u} & 1 & \overline{u} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ \overline{u} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = -\begin{pmatrix} \overline{u} & 1 & 0 \\ 0 & \overline{u} & c_s^2 \\ 0 & 1 & \overline{u} \end{pmatrix}$$

- It holds:

$$\begin{pmatrix} \dot{\rho}' \\ \overline{\rho}\dot{u}' \\ \frac{1}{\overline{\theta}}(\rho\dot{\theta})' \end{pmatrix} = -\begin{pmatrix} \overline{u} & 1 & 0 \\ 0 & \overline{u} & c_s^2 \\ 0 & 1 & \overline{u} \end{pmatrix} \begin{pmatrix} \rho_x' \\ (\overline{\rho}u')_x \\ \frac{1}{\overline{\theta}}(\rho\theta)_x' \end{pmatrix}$$

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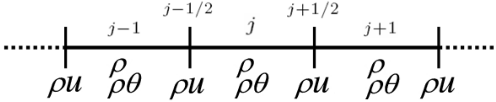
- Variables are defined on a staggered grid



- For investigation of spatial discretizations perform von Neumann stability analysis, e.g. it holds:

$$\rho u(t, x_{j+1/2}) = \rho u(t) e^{ikx_{j+1/2}}$$

$$\Rightarrow \quad \left.\frac{\partial \rho u}{\partial x}\right|_{(t,x_j)} = \rho u(t) \frac{e^{ikx_j}}{\Delta x}\left(e^{\frac{ik\Delta x}{2}} - e^{-\frac{ik\Delta x}{2}}\right)$$

- Three spatial discretizations appear:

$$\mathcal{D}_1 = \frac{1}{\Delta x}\left(1 - e^{-ik\Delta x}\right)$$

$$\mathcal{D}_2 = \frac{1}{\Delta x}\left(e^{\frac{ik\Delta x}{2}} - e^{-\frac{ik\Delta x}{2}}\right)$$

$$\mathcal{D}_3 = \frac{1}{6\Delta x}\left(2e^{ik\Delta x} + 3 - 6e^{-ik\Delta x} + e^{-2ik\Delta x}\right)$$

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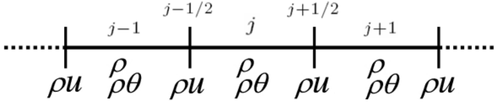

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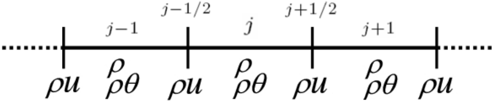

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- Using these operators results in the ODE:

$$\begin{pmatrix} \dot{\rho}' \\ (\dot{\rho u})' \\ \frac{1}{\overline{\theta}}(\rho\dot{\theta})' \end{pmatrix} = -\begin{pmatrix} 0 & \mathcal{D}_2 & 0 \\ -\overline{u}^2\mathcal{D}_3 & 2\overline{u}\mathcal{D}_3 & c_s^2\mathcal{D}_2 \\ -\overline{u}\mathcal{D}_3 & \mathcal{D}_2 & \overline{u}\mathcal{D}_3 \end{pmatrix} \begin{pmatrix} \rho' \\ (\rho u)' \\ \frac{1}{\overline{\theta}}(\rho\theta)' \end{pmatrix}$$

- For the Jacobian we instead use the matrix which belongs to:

$$\begin{pmatrix} \dot{\rho}' \\ \overline{\rho}\dot{u}' \\ \frac{1}{\overline{\theta}}(\rho\dot{\theta})' \end{pmatrix} = -\begin{pmatrix} \overline{u}\mathcal{D}_1 & \mathcal{D}_2 & 0 \\ 0 & \overline{u}\mathcal{D}_1 & c_s^2\mathcal{D}_2 \\ 0 & \mathcal{D}_2 & \overline{u}\mathcal{D}_1 \end{pmatrix} \begin{pmatrix} \rho' \\ \overline{\rho}u' \\ \frac{1}{\overline{\theta}}(\rho\theta)' \end{pmatrix}$$

- **Remark:** While M and $\widetilde{M}$ are similar the matrices

$$A := \begin{pmatrix} 0 & \mathcal{D}_2 & 0 \\ -\overline{u}^2\mathcal{D}_3 & 2\overline{u}\mathcal{D}_3 & c_s^2\mathcal{D}_2 \\ -\overline{u}\mathcal{D}_3 & \mathcal{D}_2 & \overline{u}\mathcal{D}_3 \end{pmatrix} \quad \text{and} \quad \widetilde{A} := \begin{pmatrix} \overline{u}\mathcal{D}_1 & \mathcal{D}_2 & 0 \\ 0 & \overline{u}\mathcal{D}_1 & c_s^2\mathcal{D}_2 \\ 0 & \mathcal{D}_2 & \overline{u}\mathcal{D}_1 \end{pmatrix}$$

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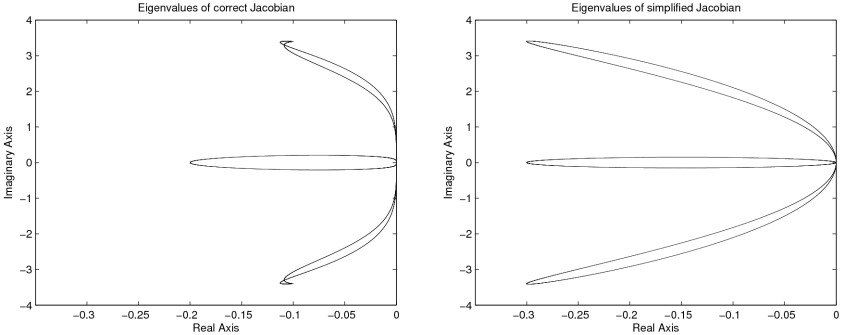
Eigenvalues of correct and simplified Jacobian



- Application of the peer method to the Dahlquist test equation

$$\dot{y} = \lambda y$$

leads to:

$$(1 - \Delta t \gamma J) Y_m = B Y_{m-1} + \Delta t A \lambda Y_{m-1} + \Delta t R \lambda Y_m + \Delta t G J Y_{m-1} + \Delta t H J Y_m$$

- With notations $z := \Delta t \lambda$ and $\widetilde{z} := \Delta t J$ it holds:

$$Y_m = (I - zR - \widetilde{z}(\gamma I + H))^{-1}(B + zA + \widetilde{z}G) Y_{m-1}$$

- Side conditions for optimization are
  - A-stability in common sense, i.e. for $\widetilde{z} = z$
  - A-stability for simplified Jacobian, i.e. for $\mathrm{Re}\widetilde{z} = 2.5\mathrm{Re}z$, $\mathrm{Im}\widetilde{z} = \mathrm{Im}z$

- Application of the peer method to the Dahlquist test equation

$$\dot{y} = \lambda y$$

leads to:

$$(1-\Delta t\gamma J)Y_m = BY_{m-1}+\Delta t A\lambda Y_{m-1}+\Delta t R\lambda Y_m+\Delta t GJY_{m-1}+\Delta t HJY_m$$

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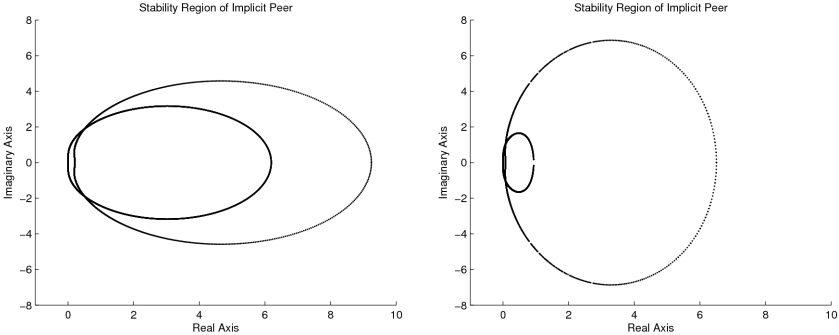
Stability regions for exact and simplified Jacobian



- The analytical solution of the Dahlquist test equation satisfies

$$y(t_m) = e^z y(t_{m-1}) = e^{\mathrm{Re}z} e^{i\mathrm{Im}z} y(t_{m-1}),$$

i.e. the analytical solution has
  - the amplification factor $e^{\mathrm{Re}z}$
  - the relative phase speed 1
- Let λ be an eigenvalue of the amplification matrix $(I - zR - \widetilde{z}(\gamma I + H))^{-1}(B + zA + \widetilde{z}G)$ of a peer method applied to the Dahlquist test equation
  - The amplification factor is $|\lambda|$
  - The relative phase speed is $\frac{\arctan \frac{\mathrm{Im}\lambda}{\mathrm{Re}\lambda}}{\mathrm{Im}\lambda}$
- Optimization goal are good amplitude and phase errors for the case $z = (-0.05 + i)\mathrm{Im}z$ (i.e. eigenvalues of advection and acoustics) when using the simplified Jacobian (i.e. for $\mathrm{Re}\widetilde{z} = 2.5\mathrm{Re}z$, $\mathrm{Im}\widetilde{z} = \mathrm{Im}z$)

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  - the relative phase speed 1
- Let λ be an eigenvalue of the amplification matrix $(I - zR - \widetilde{z}(\gamma I + H))^{-1}(B + zA + \widetilde{z}G)$ of a peer method applied to the Dahlquist test equation
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- The analytical solution of the Dahlquist test equation satisfies

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i.e. the analytical solution has
  - the amplification factor $e^{\mathrm{Re} z}$
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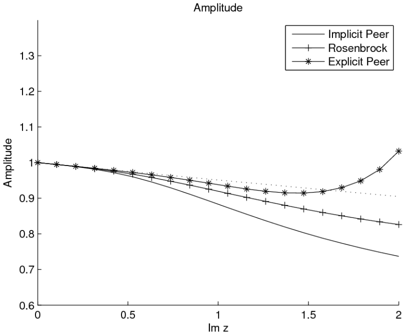
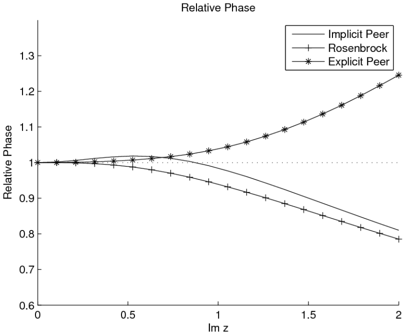
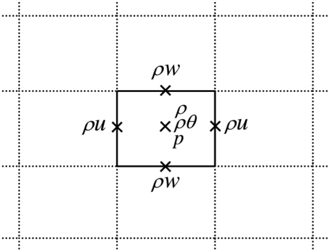
Amplitude and phase for the simplified Jacobian





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



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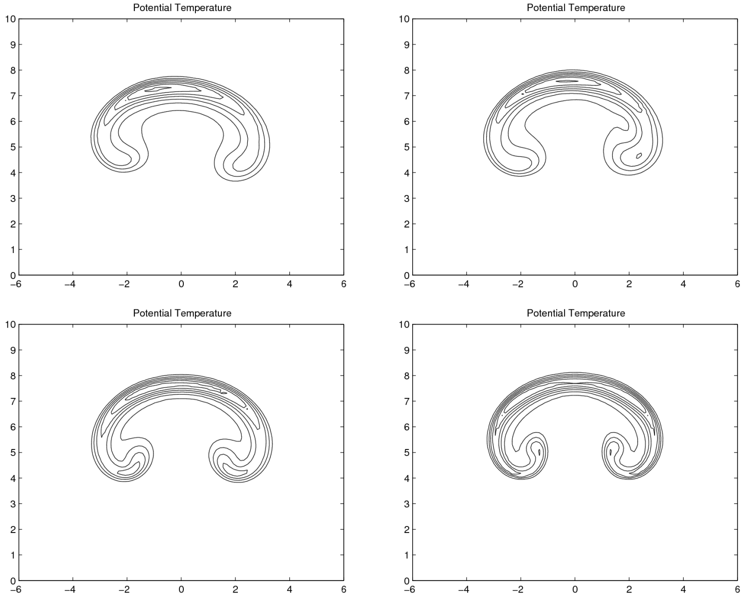
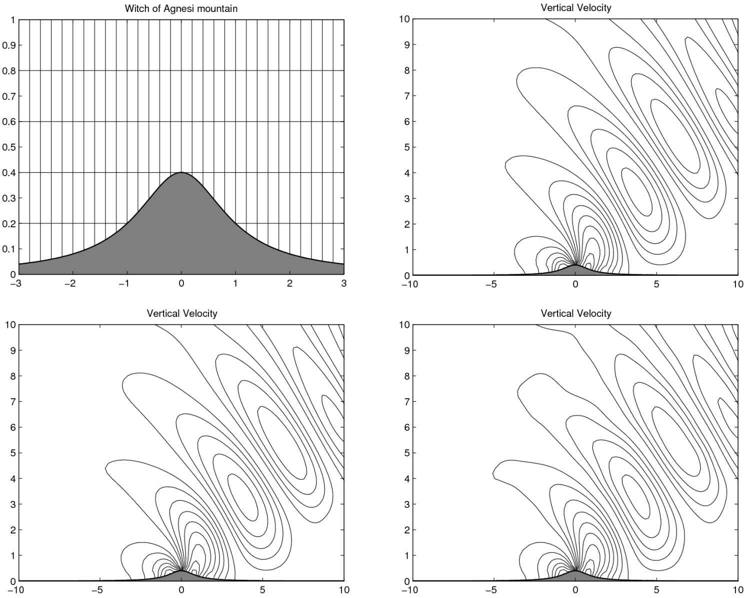
	correct Jacobian	simplified Jacobian	ratio
1D	$3\mathcal{D}_2 + 4\mathcal{D}_3 = 22$	$3\mathcal{D}_2 + 3\mathcal{D}_1 = 12$	55%
2D	$6\mathcal{D}_2 + 14\mathcal{D}_3 = 68$	$6\mathcal{D}_2 + 8\mathcal{D}_1 = 28$	41%
3D	$9\mathcal{D}_2 + 30\mathcal{D}_3 = 138$	$9\mathcal{D}_2 + 15\mathcal{D}_1 = 48$	35%

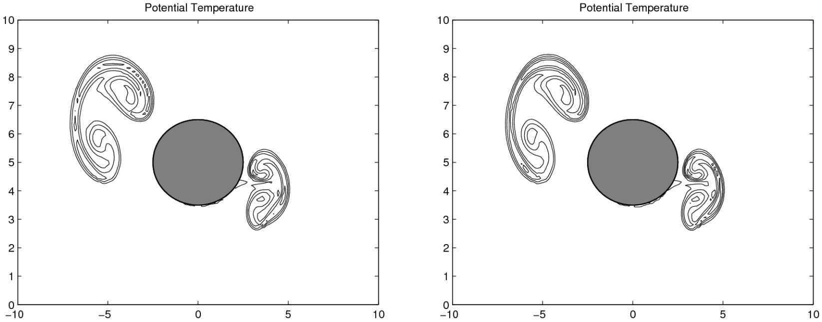
Rising bubble



Flow over mountain



Zeppelin test



Conclusions

- Development of a linearly implicit two-stage peer method which
  - is second-order independently of the Jacobian
  - is A-stable in the common sense and for the simplified Jacobian
  - has acceptable amplitude and phase errors
- Despite of the large CFL numbers the solutions of the linearly implicit peer method are as good as the solutions computed with the explicit method with tiny time steps
- Only exception is the transported rising bubble where the impact of damping and phase errors is visible, but
  - the explicit method is a three-stage method, there is no explicit two-stage method which is stable with the time steps used in the first test
  - the implicit peer method might not be the best one, perhaps there are better optimization criteria

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Outlook

- Determination of the practical speed-up when using the simplified Jacobian instead of the correct one
- Mixing of linearly implicit and explicit peer methods:
  - Use of full Jacobian in regions where orography results in cut-cells
  - In free regions without cut-cells only the parts of the Jacobian which come from acoustics have non-zeros entries
- Such a peer method should
  - compute with time step sizes restricted only by the CFL condition of the underlying explicit method in the free regions
  - produce as good results as the split-explicit peer method

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Danke für eure/Ihre Aufmerksamkeit!