Multirate Infinitesimal Step methods for compressible atmospheric flow

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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
EULER EQUATIONS (2D)

- Conservation form with entropy as thermodynamic quantity

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

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

- \(Q\) 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 \(\Rightarrow\)

\[
y' = B(y, y) = C(y)y + f(y) + g(y)
\]
SPATIAL DISCRETIZATION: FINITE VOLUMES

- Staggered grid (Arakawa C-grid)

- **Shift** $\rho u, \rho v \rightarrow \rho u_{L/R}, \rho v_{U/D}$

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

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

- $\rho u$: 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

\[ Y_{ni} = y_n + h \sum_j a_{ij} f(Y_{nj}) \]

\[ y_{n+1} = Y_{n,s+1} \] (final update=additional stage)

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

\[ Z_{ni}(0) = y_n \]
\[ Z'_{ni}(\tau) = \sum_j a_{ij} f(Y_{nj}) \]
\[ Y_{ni} = Z_{ni}(h). \]
PARTITIONED RK-METHODS

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

\[
Z_{ni}(0) = y_n \\
Z'_{ni}(\tau) = \sum_{j} a_{ij} f(Y_{nj}) + c_{i} g(Z_{ni}(\tau)) \\
Y_{ni} = Z_{ni}(h).
\]

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

\[
A = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 \\
1/3 & 0 & 0 & 0 & 0 \\
0 & 1/2 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0
\end{pmatrix}, \quad \text{nodes} \ c = (0, 1/2, 1/3, 1)^T
\]
GENERALISED PARTITIONED METHODS

We generalise the exact integration procedure in two directions:

- arbitrary starting points based on preceding stages

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

- increments in the constant term \( F \) based on preceding 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)

\[ Z'_{ni}(\tau) = \frac{1}{h} \sum_j \gamma_{ij} (Y_{nj} - y_n) + \sum_j \beta_{ij} B(Y_{nj}, Z_{ni}(\tau)) \]
The complete method is given by

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

\[
\frac{\partial}{\partial \tau} Z_{ni}(\tau) = \frac{1}{h} \sum_j \gamma_{ij} (Y_{nj} - y_n) + \sum_j \beta_{ij} f(Y_{nj}) + d_i g(Z_{ni}(\tau))
\]

\[
Y_{ni} = Z_{ni}(h)
\]

\[
y_{n+1} = Y_{n,s+1}.
\]

\(g = 0 \Rightarrow\) underlying RK method

\[
Y = 1 \otimes y_n + ((\alpha + \gamma) \otimes I)(Y - 1 \otimes y_n) + h(\beta \otimes I)f(Y)
\]

\[
Y = 1 \otimes y_n + h((I - \alpha - \gamma)^{-1} \beta \otimes I)f(Y)
\]

\(\Rightarrow A = (I - \alpha - \gamma)^{-1} \beta =: R\beta\)
DERIVATION OF ORDER CONDITIONS

Expand numerical solution in a Taylor series. 
Note: $Z_{ni}$ is a function of $\tau$ and $h$. Define 

$$G(Y_{ni})^{(k)} := \frac{\partial^k}{\partial h^k} G(Y_{ni}), \ G(Z_{ni})^{(k,l)} := \frac{\partial^k}{\partial \tau^k} \frac{\partial^l}{\partial h^l} |_{\tau=h=0} G(Z_{ni})$$

- **Recursion for derivatives of $Y_{ni}$:**

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

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

$$Z_{ni}^{(0,l)} = \sum_j \alpha_{ij} Y_{nj}^{(l)}$$

$$Z_{ni}^{(1,l)} = \frac{1}{l+1} \sum_j \gamma_{ij} Y_{nj}^{(l+1)} + \sum_j \beta_{ij} f(Y_{nj})^{(l)} + d_i g(Z_{ni})^{(0,l)}$$

$$\Rightarrow \ Z_{ni}^{(k,l)} = d_i g(Z_{ni})^{(k-1,l)}, \quad k \geq 2.$$
ORDER CONDITIONS

The recursion leads to following order conditions for 3rd order

four classical order conditions

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

and five additional order conditions

\[ \tilde{b}(c + \tilde{c}) = 1 \]
\[ \tilde{b}(I + \alpha) A c = 1/3 \]
\[ 3\tilde{b}(\alpha + \gamma/2) R D(c + \tilde{c}) + \tilde{b}^T D(c + 2\tilde{c}) = 1 \]
\[ b^T R D(c + \tilde{c}) = 1/3 \]
\[ \tilde{b}^T(c^2 + \tilde{c}^2 + c \cdot \tilde{c}) = 1 \]

where we use \( \tilde{c} := \alpha c \) and \( \tilde{b} = e_{s+1}^T R D \).
PEER METHODS

- General linear method $\Rightarrow$ 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

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

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

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

\[
Y_{ni} = \exp(h \sum_{j<i} a^{(l)}_{ij} B[Y_{nj}]) \cdots \exp(h \sum_{j<i} a^{(1)}_{ij} B[Y_{nj}])y_n
\]

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

\[
y(t) = \text{Exp}(tA)y(0) + t\phi(tA)c, \quad \text{where } \phi(z) := (e^z - 1)/z
\]
CONSTRUCTION OF METHODS

- MIS-RK:
  - 3 stage 3rd order $\Rightarrow$ 12 parameters for 9 eqns
  - No 3rd order method for $\alpha = \gamma = 0$ (classic splitting like RK3)
  - $\alpha, \gamma \neq 0$: 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,
  $\alpha \neq 0, \alpha_{ij} \in \{0, 1\}, \gamma \neq 0$

- 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 → upwind-differences, sound terms → symmetric differences.

- Stability: Maximum amplification for all waves for fixed Courant numbers
  \[ C_A = U \Delta t / \Delta x, \quad C_S = c_s \Delta t / \Delta x \]

- 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

\( n_s = [3, 6, 6] \).
Euler equations, rising bubble with advection
- Domain $20\text{km} \times 10\text{km}$, Grid $\text{dx} = \text{dy} = 125\text{ m}$;
- Final time = 17 minutes
- Initial state: $u = 20\text{m/s}$, $v = 0$, hydrostatic balance, $\theta = 300K$.
- Thermal bubble with $\Delta \theta = +2K$, radius $2\text{km}$
- Boundary conditions: periodic/no-flux

<table>
<thead>
<tr>
<th>Method</th>
<th>RK3</th>
<th>CF3</th>
<th>WKG3Bb</th>
<th>PEER</th>
</tr>
</thead>
<tbody>
<tr>
<td>Macro Time Step in s</td>
<td>0.9</td>
<td>0.5</td>
<td>1.8</td>
<td>5.0</td>
</tr>
</tbody>
</table>
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 (→ 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

\[
\begin{array}{c|ccc}
0 & & \\
1/3 & 1/3 & \\
2/3 & 0 & 2/3 \\
1 & 1/3 & \\
\hline
\end{array}
\]

In our notation we have

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