System of ODEs
\[ u'(t) = F(u(t)) + G(u(t)) \]
with \( F \) non-stiff or mildly stiff, and \( G \) a stiff term.

IMEX linear multistep methods: \( u_n \approx u(t_n) \), \( t_n = n\Delta t \),

\[
    u_n = \sum_{j=1}^{k} a_j u_{n-j} + \sum_{j=1}^{k} \hat{b}_j \Delta t F(u_{n-j}) + \sum_{j=0}^{k} b_j \Delta t G(u_{n-j}).
\]

Applications:

\[ u_t + \nabla \cdot f(u) = \frac{1}{\epsilon} g(u) \]\n\( \ldots \) conservation laws with stiff relaxation,

\[ u_t + \nabla \cdot f(u) = \nabla \cdot (K(u) \nabla u) \]\n\( \ldots \) convection-diffusion.
Requirements on IMEX LM

- **Accuracy**: e.g. order $p = k$
- **Implicit method**: stable for stiff systems, and good damping properties
- **Explicit method**: non-oscillatory/monotone, e.g. under assumption $\|v + \tau_0 F(v)\|_{TV} \leq \|v\|_{TV}$ with total variation semi-norm,
  - **TVD methods (Shu)**: $\|u_n\|_{TV} \leq \max_{0 \leq j \leq k-1} \|u_j\|_{TV}$, for $0 < \Delta t \leq C \tau_0$. This leads to $p < k$.
  - **TVB methods (Ruuth & H.)**: $\|u_n\|_{TV} \leq M \cdot \|u_0\|_{TV}$, for $0 < \Delta t \leq C \tau_0$, with $M \geq 1$ determined by the starting procedure.

Design of IMEX LM

- Start with an implicit method (BDF) and combine this with a corresponding $k$th order expl. method.
- Start with an explicit method (Adams or optimal TVB) and find corresponding $k$th order impl. method with good stability/damping properties (for example, $A(\alpha)$-stability and optimal damping at $\infty$).
Examples

- **IMEX BDF2**

\[ u_n = \frac{4}{3} u_{n-1} - \frac{1}{3} u_{n-2} + \frac{4}{3} \Delta t F_{n-1} - \frac{2}{3} \Delta t F_{n-2} + \frac{2}{3} \Delta t G_n. \]

- **IMEX BDF3**

\[ u_n = \frac{18}{11} u_{n-1} - \frac{9}{11} u_{n-2} + \frac{2}{11} u_{n-3} \]
\[ + \frac{18}{11} \Delta t F_{n-1} - \frac{18}{11} \Delta t F_{n-2} + \frac{6}{11} \Delta t F_{n-3} + \frac{6}{11} \Delta t G_n. \]

- **IMEX TVB3**

\[ u_n = \frac{3909}{2048} u_{n-1} - \frac{1367}{1024} u_{n-2} + \frac{873}{2048} u_{n-3} \]
\[ + \frac{18463}{12288} \Delta t F_{n-1} - \frac{1271}{768} \Delta t F_{n-2} + \frac{8233}{12288} \Delta t F_{n-3} \]
\[ + \frac{1089}{2048} \Delta t G_n - \frac{1139}{12288} \Delta t G_{n-1} - \frac{367}{6144} \Delta t G_{n-2} + \frac{1699}{12288} \Delta t G_{n-3}. \]
Stability for linear test equations (advection explicit)

(1) Advection diffusion \( \ldots \quad u_t + au_x = du_{xx} \) with \( d \geq 0 \).

(2) Advection reaction \( \ldots \quad u_t + au_x = -cu \) with \( c \geq 0 \).

Example for (2) : spatial discretization 2nd-order central. Boundaries of stability regions \( \mathcal{D}_{AR} \) are plotted with ‘growth factor’ \(-c\Delta t\) horizontal and Courant number \( \nu = |a|\Delta t/\Delta x \) vertical.

\[\begin{array}{cccc}
\text{Courant} & 2 & 1.5 & 1 & 0.5 & 0.0 \\
\text{growth factor} & -10 & -8 & -6 & -4 & -2 & 0
\end{array}\]

\( \text{Fig:} \) Boundaries of \( \mathcal{D}_{AR} \) for third-order methods BDF3 and TVB3 and Adams3. (Below boundary: stable. Above boundary: unstable.)
**Fig:** Boundaries of $\mathcal{D}_{AR}$ for fourth-order methods $BDF4$, $TVB4$ and $Adams4$.

**Fig:** Boundaries of $\mathcal{D}_{AR}$ for fifth-order methods $BDF5$, $TVB5$. 
IMEX Runge-Kutta methods

\[ u_{n,i} = u_{n-1} + \sum_{j=1}^{i-1} \hat{a}_{ij} \Delta t \, F(u_{n,j}) + \sum_{j=1}^{i} a_{ij} \Delta t \, G(u_{n,j}), \quad i = 1, \ldots, s, \]

\[ u_n = u_{n-1} + \sum_{j=1}^{s} \hat{b}_{j} \Delta t \, F(u_{n,j}) + \sum_{j=1}^{s} b_{j} \Delta t \, G(u_{n,j}). \]

Examples:  
ARS3 [Ascher, Ruuth & Spiteri]: \( p = 3, \ s = 4, \)
PR3  [Pareschi & Russo]: \( p = 3, \ s = 4, \)
KC4  [Kennedy & Carpenter]: \( p = 4, \ s = 6, \)
KC5  [Kennedy & Carpenter]: \( p = 5, \ s = 8. \)

Let \( \hat{c}_i = \sum_j \hat{a}_{ij}, \ c_i = \sum_j a_{ij}. \) For most methods \( \hat{c}_i = c_i, \ i = 1, \ldots, s. \)

Exception: Pareschi-Russo methods; first stage backward Euler for \( G \) only, to make the method "asymptotic preserving".
**Fig:** Boundaries of $\mathcal{D}_{AR}$ for the IMEX Runge-Kutta methods ARS3, PR3, KC4 and KC5.

Stability plots (also with 1st-order and 3rd-order upwind advection) are slightly better for the IMEX LM methods BDF$k$ and in particular for TVB$k$. Same for advection-diffusion test equation.
Temporal discretization errors

For LM: if the explicit method and the implicit method are of order $p$, then the IMEX scheme is of order $p$ independent of the stiffness.

For RK: for the IMEX scheme to have order $p$ for non-stiff problems, we need order $p$ for the explicit and the implicit method, together with compatibility conditions.

For stiff problems there can be order reduction with the RK methods:

- If all $\hat{c}_i = c_i$, then order of accuracy may reduce to 2.

- If $\hat{c}_i \neq c_i$ for some $i$, then the order may reduce to 1. This can happen already for stationary problems.
Numerical example: order reduction

Linear advection-reaction problem (advection explicit)

\[ u_t + u_x = -k_1 u + k_2 v, \]
\[ v_t = k_1 u - k_2 v + 1. \]

for \( 0 < x < 1, \ 0 < t < 1, \) with \( k_1 = 10^6, \ k_2 = 2 \cdot 10^6. \) Initial and boundary values:

\[ u(x, 0) = 1 + x, \quad v(x, 0) = \frac{k_1}{k_2} u(x, 0) + \frac{1}{k_2}, \quad u(0, t) = 1. \]

This gives simple stationary solution. Results not good for the PR schemes.

<table>
<thead>
<tr>
<th>( \Delta t )</th>
<th>1.00 ( \cdot 10^{-2} )</th>
<th>5.00 ( \cdot 10^{-3} )</th>
<th>2.50 ( \cdot 10^{-3} )</th>
<th>1.25 ( \cdot 10^{-3} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>PR2</td>
<td>2.36 ( \cdot 10^{-3} )</td>
<td>1.18 ( \cdot 10^{-3} )</td>
<td>5.89 ( \cdot 10^{-4} )</td>
<td>2.93 ( \cdot 10^{-4} )</td>
</tr>
<tr>
<td>PR3</td>
<td>9.47 ( \cdot 10^{-4} )</td>
<td>4.74 ( \cdot 10^{-4} )</td>
<td>2.37 ( \cdot 10^{-4} )</td>
<td>1.18 ( \cdot 10^{-4} )</td>
</tr>
<tr>
<td>BDF2</td>
<td>1.74 ( \cdot 10^{-11} )</td>
<td>9.40 ( \cdot 10^{-12} )</td>
<td>1.49 ( \cdot 10^{-11} )</td>
<td>1.35 ( \cdot 10^{-11} )</td>
</tr>
</tbody>
</table>

**Table:** \( L_1 \)-errors versus step size for fixed spatial grid \( \Delta x = 1/100. \)
Numerical example: accuracy test

Simplified adsorption-desorption problem with a dissolved concentration $u$ and adsorbed concentration $v$,

$$u_t + au_x = \kappa(v - \phi(u)),$$
$$v_t = -\kappa(v - \phi(u)),$$

for $0 < x < 1$ and $0 < t \leq \frac{5}{4}$, with $\phi(u) = k_1 u / (1 + k_2 u)$. Parameters $\kappa = 10^6$, $k_1 = 50$, $k_2 = 100$. Initial values $u = v = 0$, boundary values

$$\begin{cases} 
    u(0, t) = 1 - \cos^2(6\pi t) & \text{if } a > 0, \\
    u(1, t) = 0 & \text{if } a < 0.
\end{cases}$$

Velocity given as

$$a = -\frac{3}{\pi} \arctan(100(t - 1)) \approx \begin{cases} 
    1.5 & \text{for } t < 1 \text{ (adsorption phase)}, \\
    -1.5 & \text{for } t > 1 \text{ (desorption phase)}.
\end{cases}$$
accuracy test (cont.)

**Fig:** Dissolved concentration $u$ and total concentration $u + v$ for the adsorption-desorption problem at times $t = 1, \frac{5}{4}$.

Spatial discretization by WENO5 scheme, mesh width $\Delta x = 1/800$.

IMEX schemes with advection explicit.
accuracy test (cont.)

Results for IMEX schemes of order 4 and 5:

Fig: Temporal $L_1$-errors vs. scaled step sizes $\in (4 \cdot 10^{-5}, 6 \cdot 10^{-4})$. Left: fourth-order IMEX methods BDF4, TVB4, Adams4 and KC4. Right: fifth-order IMEX methods BDF5, TVB5 and KC5. Spatial error $\approx 1.2 \cdot 10^{-3}$. 
Numerical example: positivity preservation

Biological population density model

\[ u_t = d u_{xx} + r_b(x) \frac{\epsilon u}{\epsilon + u} - r_d u + f(t, x), \]

for \( t > 0, \ x \in (0, 1) \) with spatial periodicity and \( u(x, 0) = 0 \). Implicit diffusion, standard 2nd order discr., \( \Delta x = 1/100 \). Parameters \( r_d = 1, \ \epsilon = 0.005, \)

\[ r_b(x) = \begin{cases} 
1 & \text{if } x \in [0, 1/2], \\
100 & \text{otherwise.} 
\end{cases} \]

The forcing term gives an impuls (random \( \in [0.8, 1.2] \)) at \( t = 0 \). Examples of steady state profiles:

![Graph showing steady state profiles for different diffusion coefficients](image)
For this model the *maximal time step* has been determined such that the numerical solution remains non-negative.

<table>
<thead>
<tr>
<th>IMEX meth.</th>
<th>$d = 0$</th>
<th>$d = 0.01$</th>
<th>$d = 0.04$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adams2</td>
<td>0.447</td>
<td>0.445</td>
<td>0.478</td>
</tr>
<tr>
<td>BDF2</td>
<td>0.628</td>
<td>0.636</td>
<td>0.686</td>
</tr>
<tr>
<td>Adams3</td>
<td>0.161</td>
<td>0.152</td>
<td>0.163</td>
</tr>
<tr>
<td>BDF3</td>
<td>0.391</td>
<td>0.390</td>
<td>0.414</td>
</tr>
<tr>
<td>TVB3</td>
<td>0.540</td>
<td>0.541</td>
<td>0.575</td>
</tr>
<tr>
<td>Adams4</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>BDF4</td>
<td>0.221</td>
<td>0.214</td>
<td>0.226</td>
</tr>
<tr>
<td>TVB4</td>
<td>0.461</td>
<td>0.460</td>
<td>0.487</td>
</tr>
<tr>
<td>BDF5</td>
<td>0.088</td>
<td>0.074</td>
<td>0.082</td>
</tr>
<tr>
<td>TVB5</td>
<td>0.379</td>
<td>0.376</td>
<td>0.397</td>
</tr>
<tr>
<td>PR2</td>
<td>1.004</td>
<td>0.745</td>
<td>0.745</td>
</tr>
<tr>
<td>PR3</td>
<td>1.004</td>
<td>0.498</td>
<td>0.572</td>
</tr>
</tbody>
</table>

For the other IMEX RK schemes (ARS, KC) the maximal step size was 0. The results for $d = 0$ agree closely with general theory. For the IMEX LM schemes results remain the same (approx.) for $d > 0$. 
Conclusions

- IMEX LM methods have some advantages over IMEX RK methods:
  - (slightly) better stability, much better monotonicity properties,
  - better accuracy behaviour for stiff problems.

- IMEX Adams methods not sufficiently stable/monotone for \( k \geq 4 \).

- Good results for the IMEX BDF and IMEX TVB schemes. The TVB class is more stable/monotone, the BDF class somewhat more accurate.

Note. The IMEX RK methods are self-starting. The IMEX LM methods need starting procedures. An automatic IMEX multistep code has not yet been developed!

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