IMEX Linear Multistep Methods for Stiff Hyperbolic Relaxation Systems

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(Talk based on joint work with Steve Ruuth, SFU)

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IMEX multistep methods

Applications :

$$u_t + \nabla \cdot f(u) = \frac{1}{\epsilon} g(u) \qquad \ldots \quad \text{conservation laws with stiff relaxation,}$$

$$u_t + \nabla \cdot f(u) = \nabla \cdot (K(u)\nabla u) \qquad \ldots \quad \text{convection-diffusion.}$$

PDE and spatial discretization $\rightsquigarrow$ 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: $u_n \approx u(t_n)$, $t_n = n\Delta t$,

$$u_n = \sum_{j=1}^{k} a_j u_{n-j} + \sum_{j=1}^{k} \widehat{b}_j \Delta t F(u_{n-j}) + \sum_{j=0}^{k} b_j \Delta t G(u_{n-j}),$$

with starting values: $u_0, u_1, \ldots, u_{k-1}$.

Direct combination of explicit and implicit methods *without splitting errors.*

Why IMEX ?

- **Why not only EX ? (fully explicit)**

Stability will require *very small* stepsizes for stiff sources, relaxation or diffusion terms.

- **Why not only IM ? (fully implicit)**

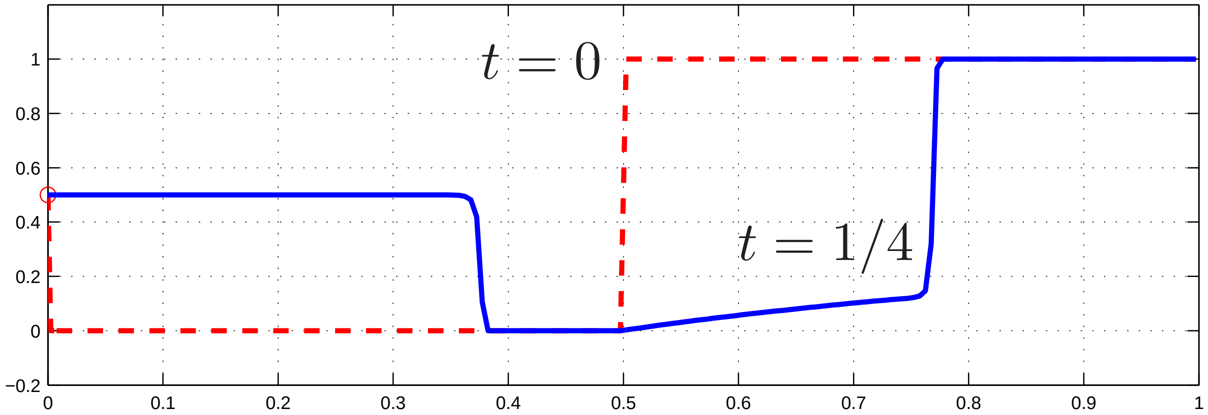
For problems with shocks or steep gradients, implicit methods are not much better than explicit ones. For advection discretizations with limiting or WENO in space, the implicit relations are hard (expensive) to solve.

Example: Implicit and extrapolated BDF2 for convection problem.
Buckley-Leverett equation:

$$u_t + f(u)_x = 0\,, \qquad f(u) = \frac{u^2}{u^2 + \frac{1}{3}(1-u)^2}\,,$$

with $u(0,t) = \frac{1}{2}$ and initial block-function (zero on $(0, \frac{1}{2}]$, one on $(\frac{1}{2}, 1]$).

Flux-limited spatial discretization (van Leer); fixed grid with $\Delta x = 5 \cdot 10^{-3}$.



- Implicit BDF2 scheme :

$$u_n = \frac{4}{3}u_{n-1} - \frac{1}{3}u_{n-2} + \frac{2}{3}\Delta t F(u_n)\,.$$

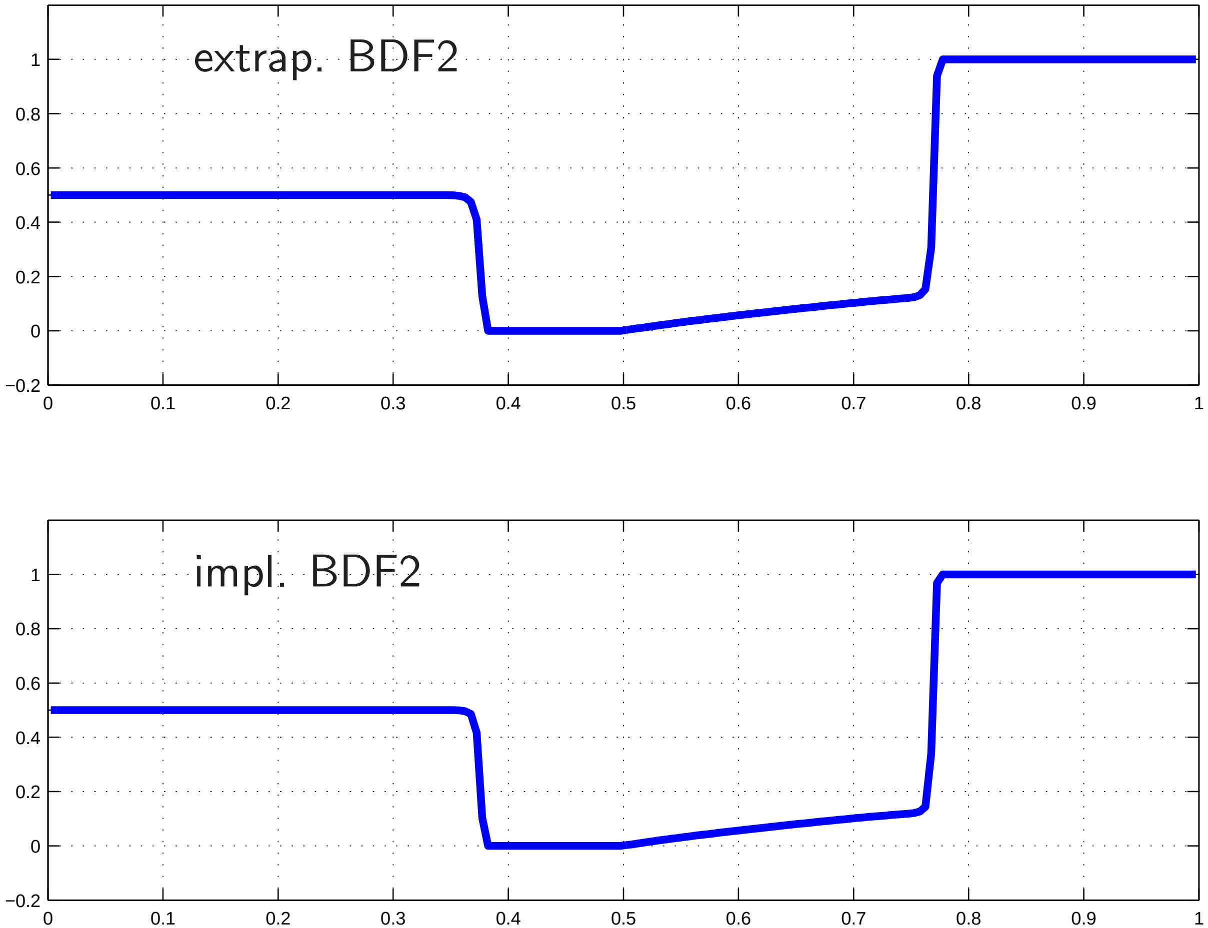
Order 2; unconditionally stable.

- Extrapolated BDF2 scheme :

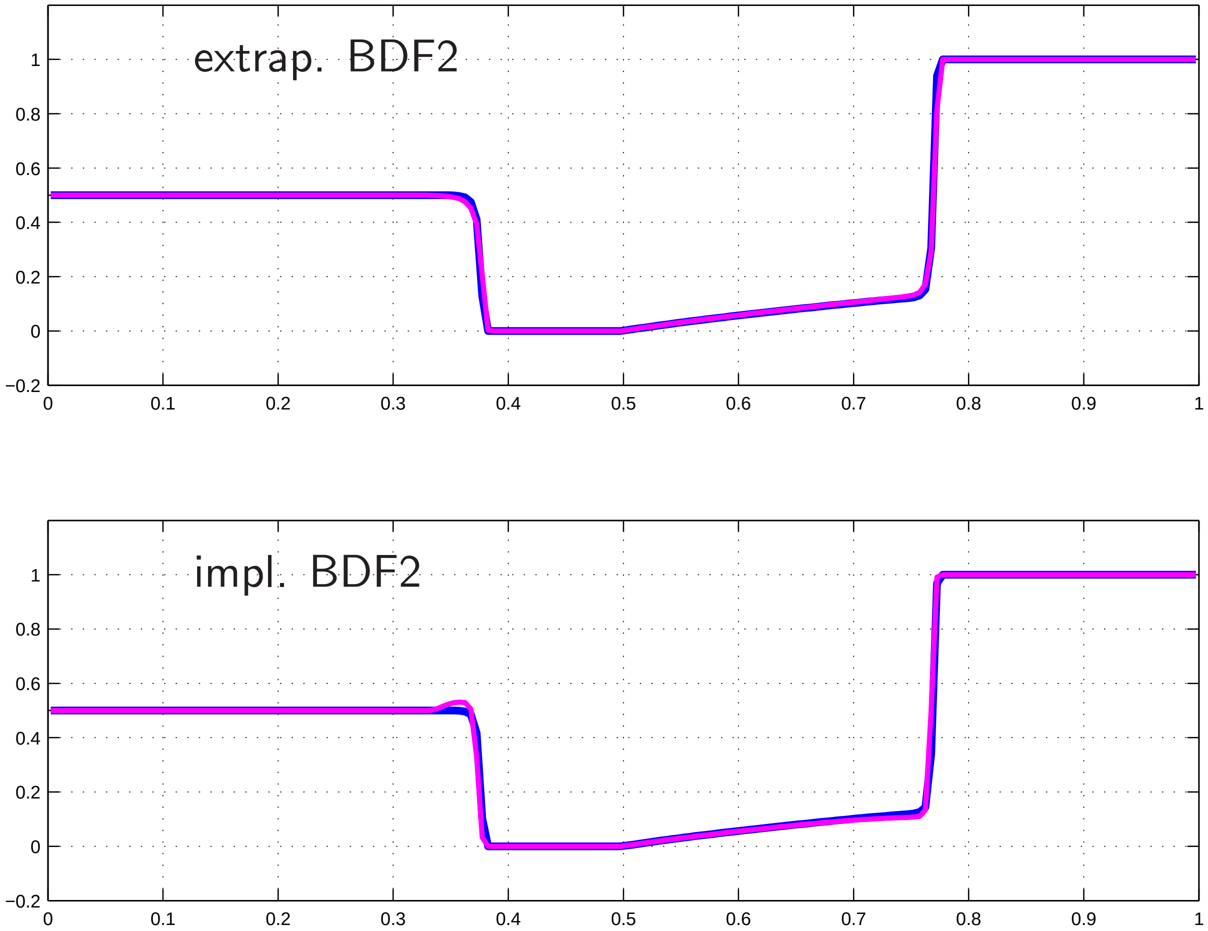
$$u_n = \frac{4}{3}u_{n-1} - \frac{1}{3}u_{n-2} + \frac{4}{3}\Delta t F(u_{n-1}) - \frac{2}{3}\Delta t F(u_{n-2})\,.$$

Order 2; stable for Courant numbers $\lesssim \frac{1}{2}$.

Plots of numerical solutions at time $t = \frac{1}{4}$ with $\Delta t/\Delta x = 1/8$.

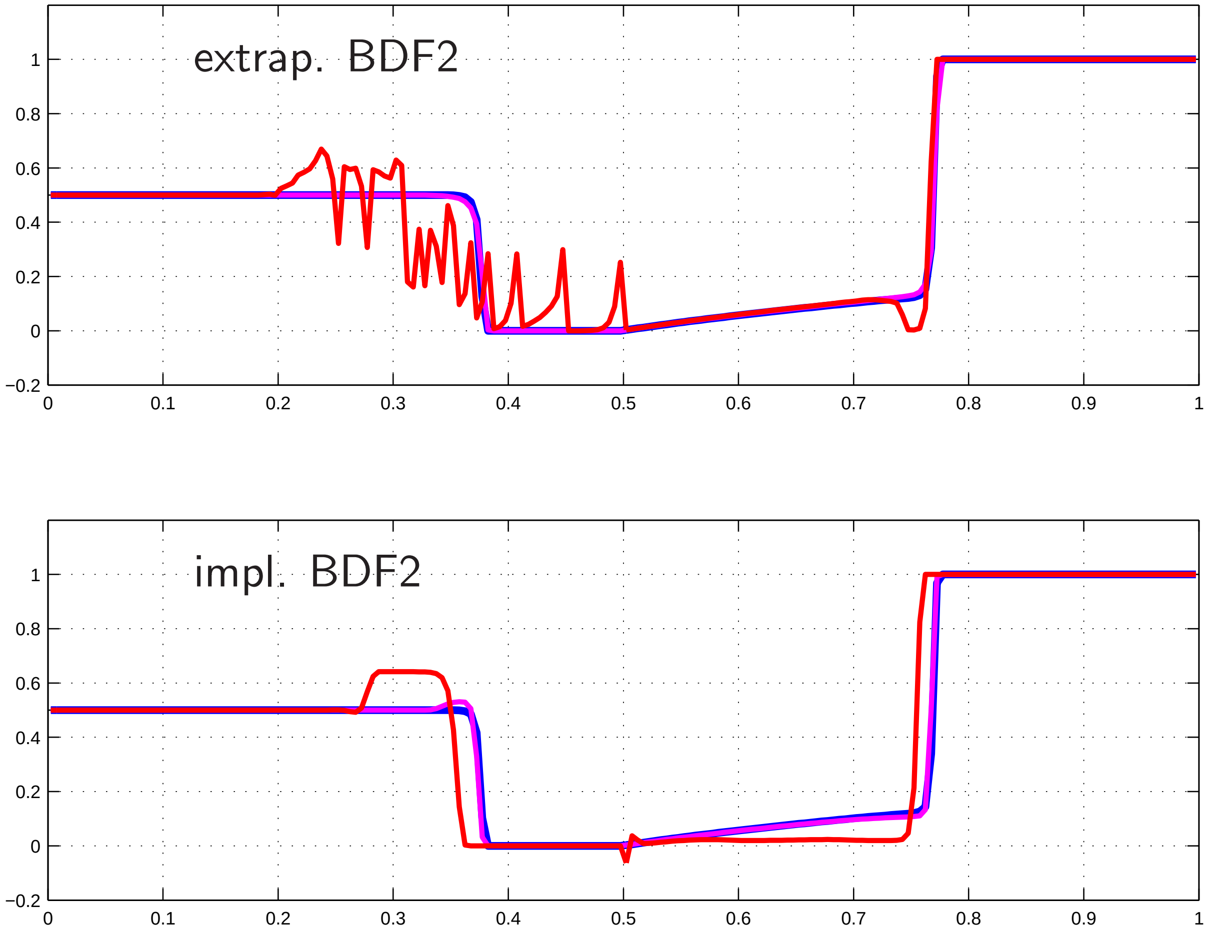


Plots of numerical solutions at time $t = \frac{1}{4}$ with
$\Delta t/\Delta x = 1/8$, $\Delta t/\Delta x = 1/4$.



Plots of numerical solutions at time $t = \frac{1}{4}$ with

$\Delta t/\Delta x = 1/8$, $\Delta t/\Delta x = 1/4$, $\Delta t/\Delta x = 1/2$.



Requirements on IMEX LM

- Accuracy : order $p = k$, moderate error constants
- Implicit method : stable for stiff systems, and good damping properties
- Explicit method : non-oscillatory/monotone. Theory: under assumption $\|v + \tau_0 F(v)\|_{TV} \leq \|v\|_{TV}$ with total variation semi-norm,
  - TVD methods (Shu) :
  $$\|u_n\|_{TV} \leq \max_{0 \leq j \leq k-1} \|u_j\|_{TV} \quad \text{for } 0 < \Delta t \leq C\tau_0,$$
  with constant C determined by the method (not the problem).
  Having $C > 0$ leads to $p < k$.
  - TVB methods (H. & Ruuth) :
  $$\|u_n\|_{TV} \leq M \cdot \|u_0\|_{TV} \quad \text{for } 0 < \Delta t \leq C\tau_0,$$
  with $M \geq 1$ determined by the starting procedure.
    - This allows much larger class of interesting methods, $p = k$ (e.g. Adams and BDF type).
    - Example: for impl. BDF2 : $C = \frac{1}{2}$; for extrap. BDF2 : $C = \frac{5}{8}$.
    - In practice, $M \approx 1 + \epsilon$ for any "decent" starting procedure.

Design of IMEX LM : possibility I

Start with an implicit method (BDF) and combine this with a corresponding kth order expl. method.

Examples based on implicit BDF [Crouzeix, Varah, 1980]:

- IMEX BDF2

$$u_n = \frac{4}{3}u_{n-1} - \frac{1}{3}u_{n-2} + \frac{4}{3}\Delta t\, F_{n-1} - \frac{2}{3}\Delta t\, F_{n-2} + \frac{2}{3}\Delta t\, G_n$$

  Most popular IMEX method of order two.

- IMEX BDF3

$$\begin{aligned} u_n = {} & \frac{18}{11}u_{n-1} - \frac{9}{11}u_{n-2} + \frac{2}{11}u_{n-3} \\ & + \frac{18}{11}\Delta t\, F_{n-1} - \frac{18}{11}\Delta t\, F_{n-2} + \frac{6}{11}\Delta t\, F_{n-3} + \frac{6}{11}\Delta t\, G_n \end{aligned}$$

Design of IMEX LM : possibility II

Start with an explicit method (Adams or optimal TVB) and find correspondig kth order impl. method with good stability/damping properties (for example, $A(\alpha)$-stability and optimal damping at ∞).

Examples:

- IMEX Adams2

$$u_n = u_{n-1} + \frac{3}{2}\Delta t\, F_{n-1} - \frac{1}{2}\Delta t\, F_{n-2} + \frac{9}{16}\Delta t\, G_n + \frac{3}{8}\Delta t\, G_{n-1} + \frac{1}{16}\Delta t\, G_{n-2}$$

- IMEX TVB3

$$\begin{aligned} u_n = &\frac{3909}{2048}u_{n-1} - \frac{1367}{1024}u_{n-2} + \frac{873}{2048}u_{n-3} \\ &+ \frac{18463}{12288}\Delta t\, F_{n-1} - \frac{1271}{768}\Delta t\, F_{n-2} + \frac{8233}{12288}\Delta t\, F_{n-3} \\ &+ \frac{1089}{2048}\Delta t\, G_n - \frac{1139}{12288}\Delta t\, G_{n-1} - \frac{367}{6144}\Delta t\, G_{n-2} + \frac{1699}{12288}\Delta t\, G_{n-3} \end{aligned}$$

IMEX Runge-Kutta methods

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

$$u_n = u_{n-1} + \sum_{j=1}^{s} \widehat{b}_j \Delta t\, F(u_{n,j}) + \sum_{j=1}^{s} b_j \Delta t\, G(u_{n,j})\,.$$

Examples:

- PR2 [Pareschi & Russo, 2005] : $p = 2,\ s = 2,$
- PR3 [Pareschi & Russo, 2005] : $p = 3,\ s = 4,$
- ARS3 [Ascher, Ruuth, Spiteri, 1995] : $p = 3,\ s = 4,$
- KC4 [Kennedy & Carpenter, 2003] : $p = 4,\ s = 6,$
- KC5 [Kennedy & Carpenter, 2003] : $p = 5,\ s = 8.$

The PR2, PR3 schemes are based on expl. TVD methods; the others are not.

Let $\widehat{c}_i = \sum_j \widehat{a}_{ij}$, $c_i = \sum_j a_{ij}$. For most methods $\widehat{c}_i = c_i$, $i = 1, \ldots, s$.
Exception: Pareschi-Russo methods; first stage backward Euler for G only, to make the method "asymptotic preserving".

Stability

Stabiltity analysis is quite complicated, even for scalar test equation

$$u'(t) = \lambda\, u(t) + \mu\, u(t)\,, \qquad \lambda, \mu \in \mathbb{C}\,.$$

Also relevant for systems $u'(t) = Au(t) + Bu(t)$ with normal, commuting matrices A, B (e.g. von Neumann analysis). In general:

$$\left.\begin{array}{l}\text{stability expl. method for } \Delta t\lambda \\ \text{stability impl. method for } \Delta t\mu\end{array}\right\} \not\Longrightarrow \quad \text{stabilty of the IMEX scheme}$$

Some sufficient conditions for stability of the IMEX scheme:

- Linear equations: [Ascher et. al (1995, 1997), Frank et. al (1997) Pareschi & Russo (2000), ...].
- Nonlinear equations: [Akrivis, Crouzeix, et. al (1998, 1999, 2003)].

Not much literature, and from these results it is not really possible to determine whether one scheme is better than another.

Stability for linear test equations (advection explicit)

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

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

Below: Examples for (2) with 2nd-order central spatial discretization; boundaries of stability regions $\mathcal{D}_{AR}$ are plotted with

- on horizontal axis the 'growth factor' $-c\Delta t$,
- on vertical axis the Courant number $\nu = |a|\Delta t/\Delta x$.

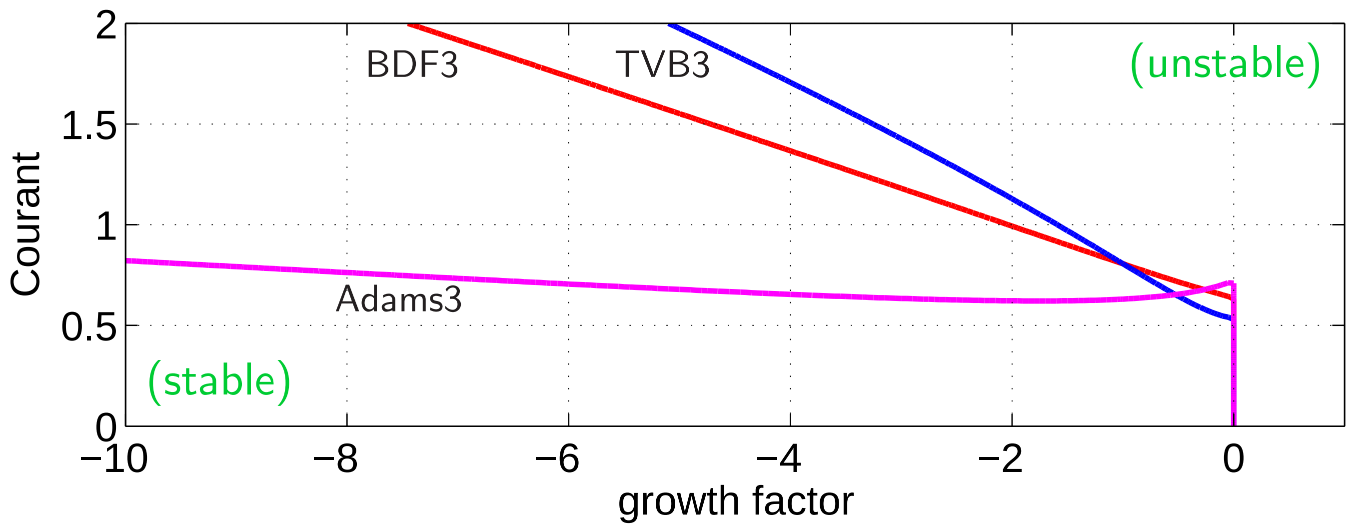


Fig: Boundaries of $\mathcal{D}_{AR}$ for third-order methods BDF3 and TVB3 and Adams3 (stable below boundary, unstable above boundary).

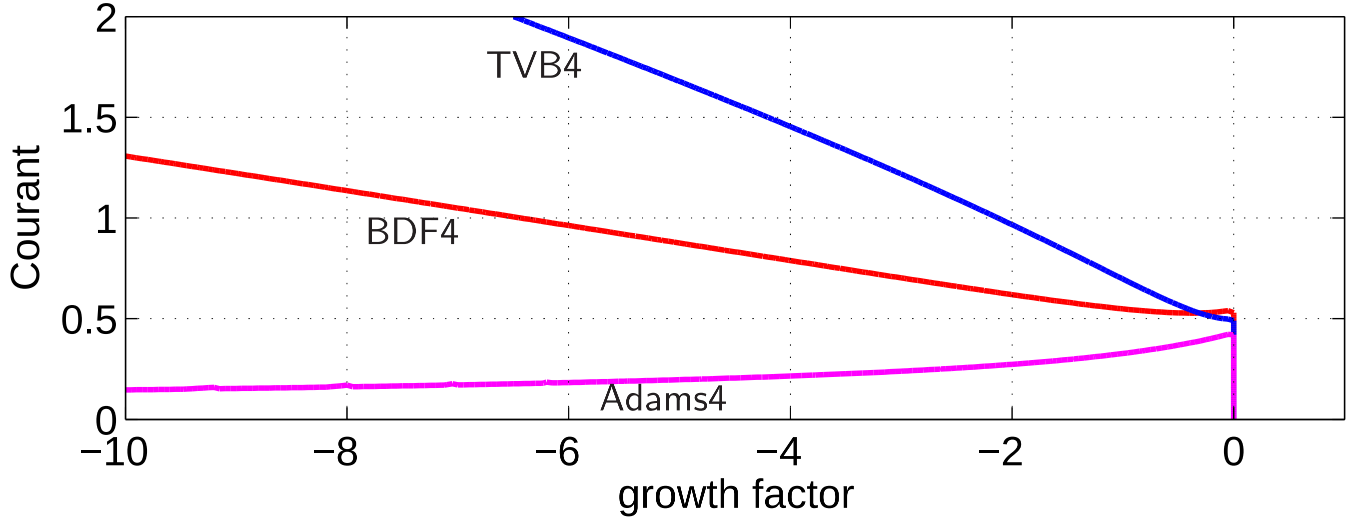


Fig: Boundaries of $\mathcal{D}_{AR}$ for fourth-order methods BDF4, TVB4 and Adams4.

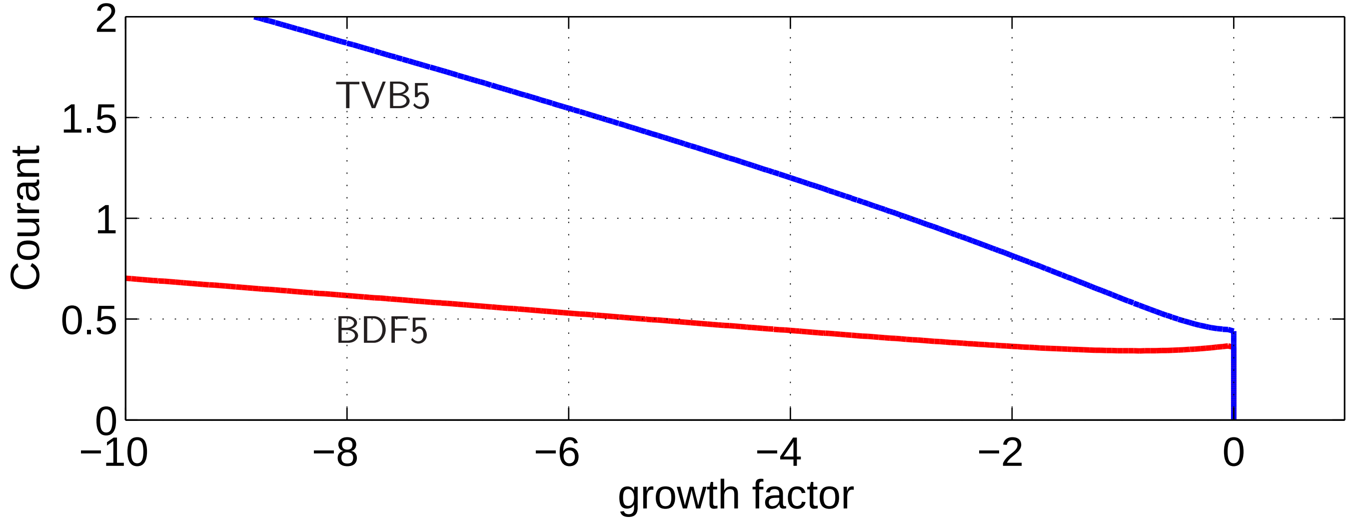


Fig: Boundaries of $\mathcal{D}_{AR}$ for fifth-order methods BDF5, TVB5.

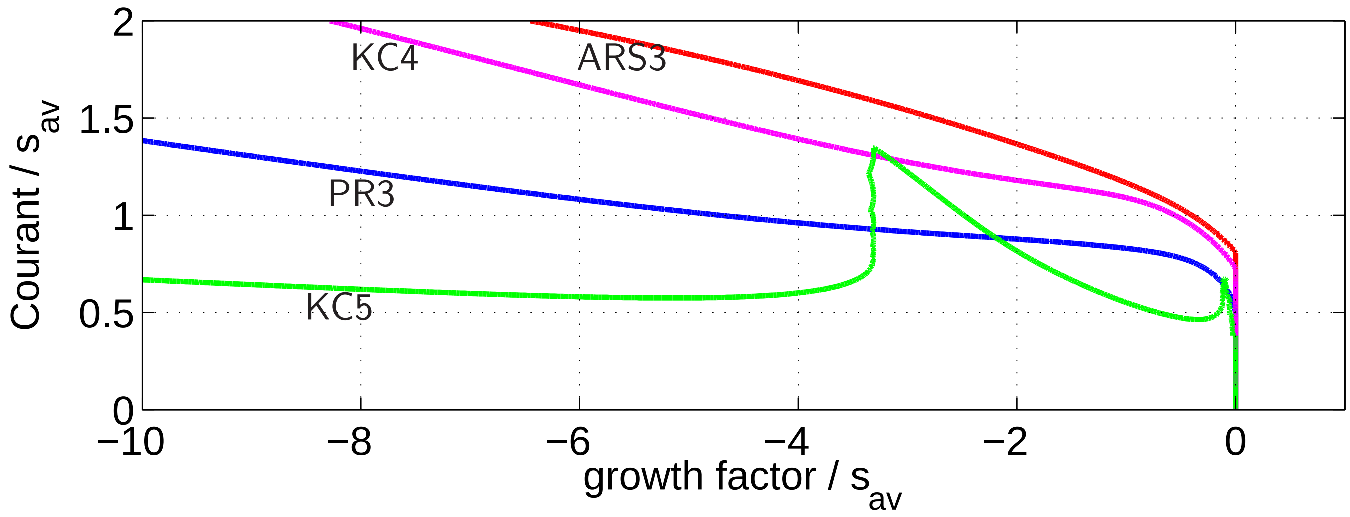


Fig: Boundaries of $\mathcal{D}_{AR}$ for the IMEX Runge-Kutta methods ARS3, PR3, KC4 and KC5.

Compared with these Runge-Kutta methods, the regions of stability are slightly better for the IMEX LM methods BDFk and in particular for TVBk.

- Also with 1st-order and 3rd-order upwind advection.
- Same for advection-diffusion test equation.

Temporal discretization errors

- **LM :** if the explicit method and the implicit method are of order p, then
  - the IMEX scheme is of order p
  - the local errors are *independent of the stiffness*

- **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.* Moreover
  - for stiff problems there can be *order reduction* with the RK methods:
    * if all $\widehat{c}_i = c_i$, then order of accuracy may reduce to 2;
    * if $\widehat{c}_i \neq c_i$ for some i, then the order may reduce to 1, and this can happen already for *stationary problems*.

  Such order reduction of RK schemes is due to the fact that in general $(\Delta t A)^j u^{(m)}(t) \neq \mathcal{O}(\Delta t^j)$ if A is a discretized differential operator (with negative powers of Δx), no matter how smooth the solution.

Numerical example: order reduction

Linear advection-reaction problem (advection explicit)

$$
\begin{aligned}
u_t + u_x &= -k_1 u + k_2 v \,, \\
v_t &= k_1 u - k_2 v + 1 \,.
\end{aligned}
$$

for $0 < x < 1$, $0 < t < 1$, with $k_1 = 10^6$, $k_2 = 2\;10^6$. Init.& bd. values:

$$
u(x,0) = 1 + x \,, \qquad v(x,0) = \frac{k_1}{k_2} u(x,0) + \frac{1}{k_2} \,, \qquad u(0,t) = 1 \,.
$$

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

Δt	$1.00 \cdot 10^{-2}$	$5.00 \cdot 10^{-3}$	$2.50 \cdot 10^{-3}$	$1.25 \cdot 10^{-3}$
PR2	$2.36 \cdot 10^{-3}$	$1.18 \cdot 10^{-3}$	$5.89 \cdot 10^{-4}$	$2.93 \cdot 10^{-4}$
PR3	$9.47 \cdot 10^{-4}$	$4.74 \cdot 10^{-4}$	$2.37 \cdot 10^{-4}$	$1.18 \cdot 10^{-4}$
BDF2	$1.74 \cdot 10^{-11}$	$9.40 \cdot 10^{-12}$	$1.49 \cdot 10^{-11}$	$1.35 \cdot 10^{-11}$

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,

$$
\begin{aligned}
u_t + a u_x &= \kappa(v - \phi(u)) \, , \\
v_t &= -\kappa(v - \phi(u)) \, ,
\end{aligned}
$$

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.)

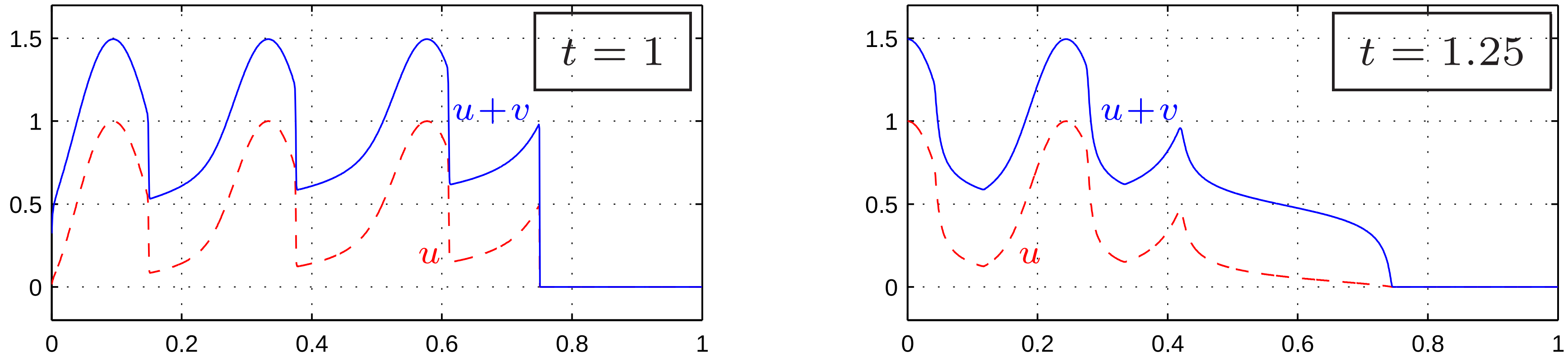


Fig: Dissolved concentration u and total concentration $u + v$ for the adsorption-desorption problem at times $t = 1, \frac{5}{4}$.

We consider IMEX schemes with advection explicit.

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

accuracy test (cont.)

Results for IMEX schemes of order 4 and 5:

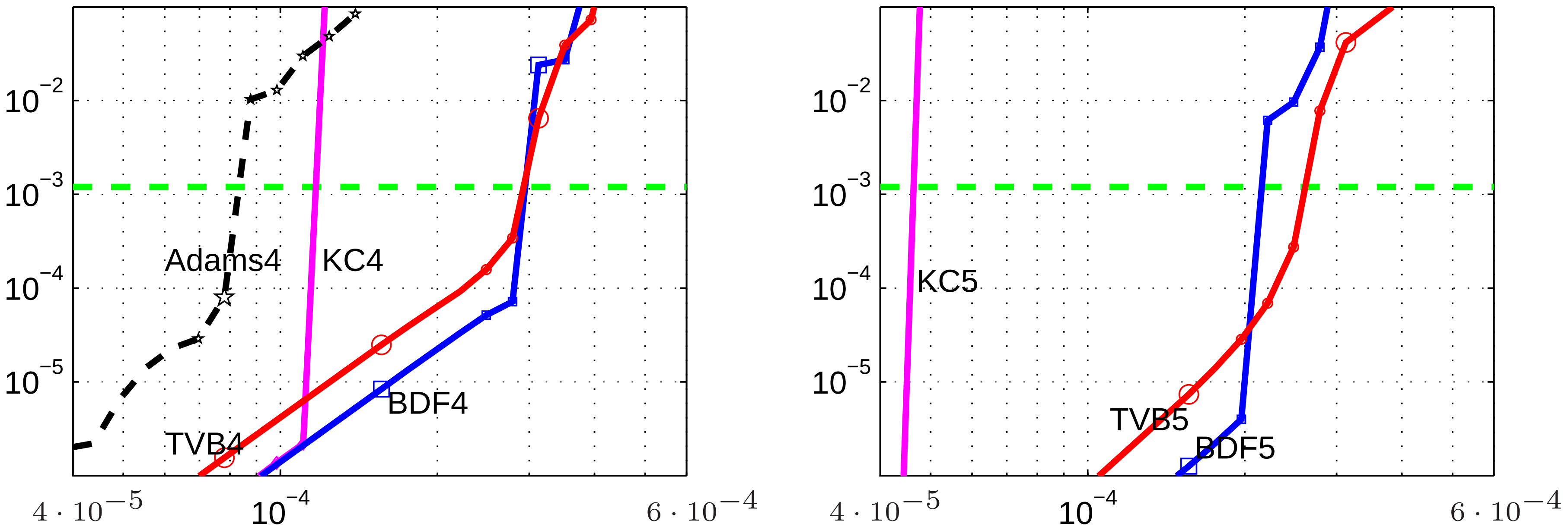


Fig: Temporal L_1-errors vs. scaled step sizes $\in (4 \cdot 10^{-5}, 6 \cdot 10^{-4})$.
Left: fourth-order IMEX methods BDF4, TVB4, Adams4 and KC4.
Right: fifth-order IMEX methods BDF5, TVB5 and KC5.
Spatial error $\approx 1.2 \cdot 10^{-3}$.

Numerical example: positivity preservation

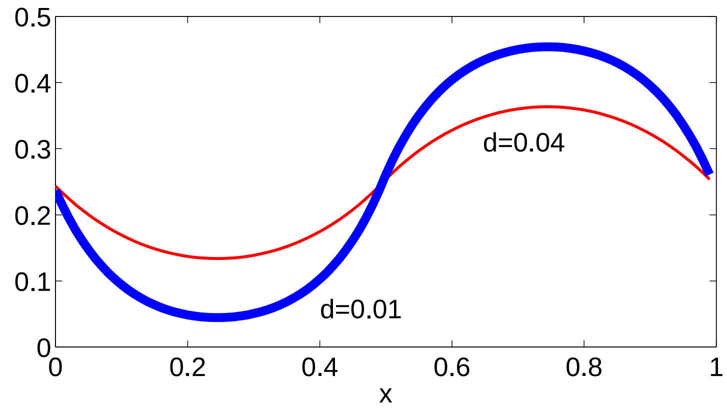
Biological population density model

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

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 :



For this model the *maximal time step* has been determined such that the numerical solution remains non-negative.

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

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.

  Of course, the IMEX RK methods are self-starting.

- 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.

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