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Implicit-Explicit Time Stepping Methods for Multiphysics Problems

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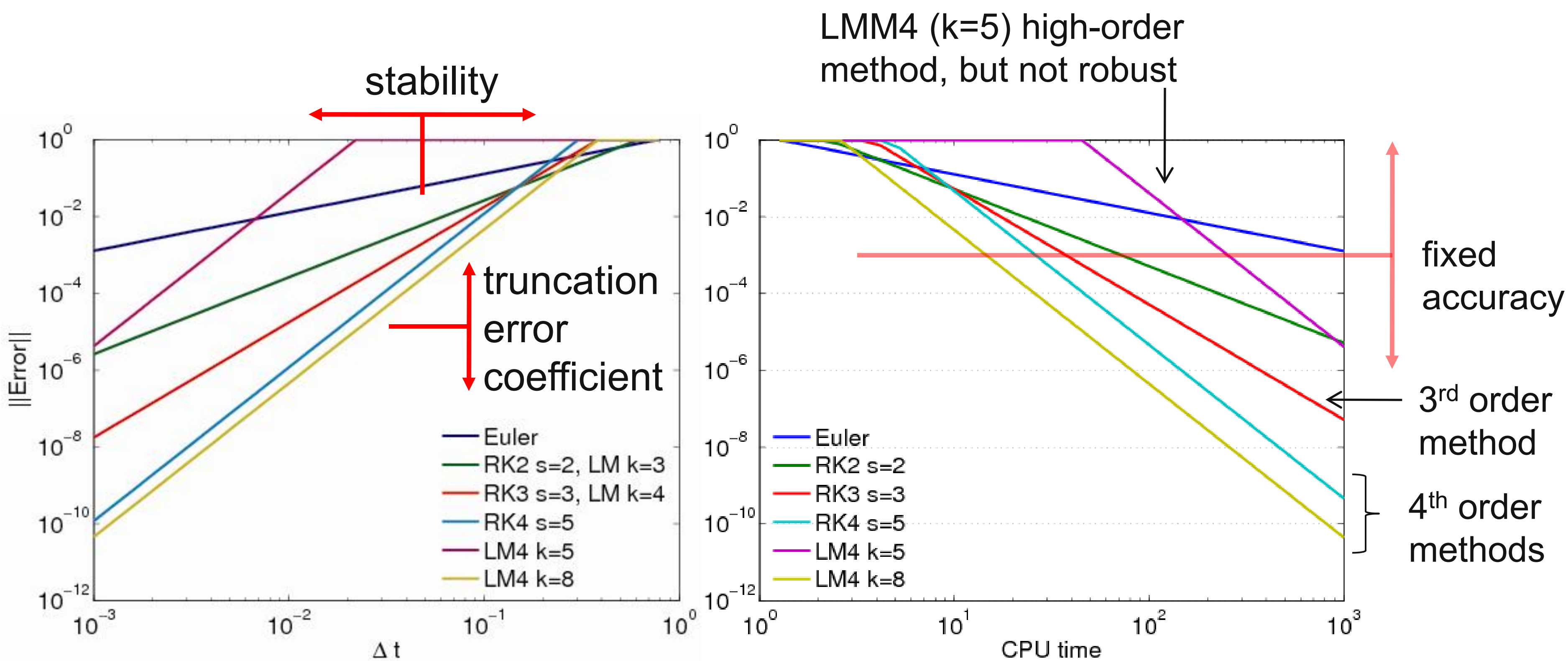
Outline: Implicit-Explicit Time Stepping Methods for Multiphysics Problems

- The need for high-order methods
- IMplicit-EXplicit (IMEX) time stepping for multiphysics problems
- Extend classical extrapolation methods to extrapolated IMEX
- Introduce three new very high-order IMEX methods for ODEs, DAEs, and PDEs
- Analyze linear stability and consistency
- Implementation considerations for multicore architectures

The need for high-order time stepping

- The order of convergence & stability play an important role in efficiency
- The focus is placed on high-order methods with large stability regions
- Representation of normalized asymptotic convergence rates:



Problems with processes that can be informally categorized according to their dynamics into fast (stiff) and slow (nonstiff)

- Problem: $y'(t) = F(t,y)\,,\ F(t,y) = f(t,y) + g(t,y)\,,\ t \geq t_0\,,\ y(t_0) = y_0$

- Additive partition: $y'(t) = f(t, y(t)) + g(t, y(t))\,,\ t > 0\,,\ y(t_0) = y_0$

$$\frac{\partial y}{\partial t} = \boxed{-u\nabla y} + \boxed{\frac{1}{\rho}\nabla(\rho K \nabla y) + \frac{1}{\rho}C(\rho y)}$$

(advection-diffusion-reaction)

nonstiff (slow) component

stiff (fast) component

time step larger than characteristic time

- Explicit methods are effective for slow processes b/c of low cost
- Implicit schemes are more efficient for fast processes b/c of stability considerations
- IMEX are more efficient for problems with both stiff and nonstiff components

IMEX methods for differential equations with stiff and nonstiff components

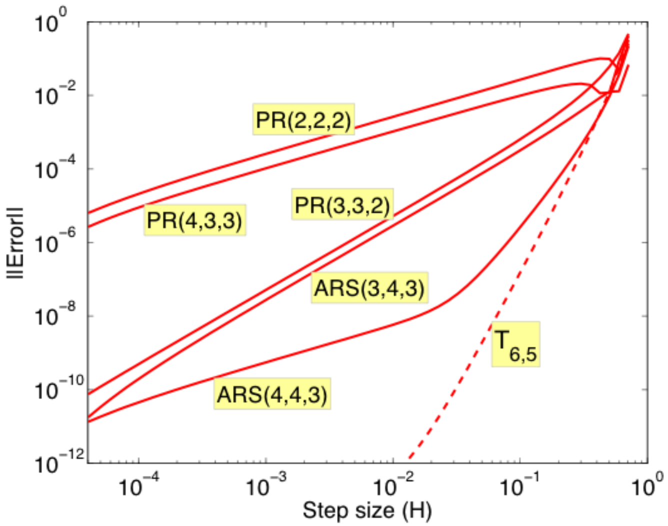
$$y'(t) = f(t, y(t)) + g(t, y(t)) \,,\ t > 0 \,,\ y(t_0) = y_0$$

- Multistage (Runge-Kutta) IMEX: difficult to construct

$$Y_i = y_{n-1} + \Delta t \sum_{j=1}^{i-1} a_{ij} f(Y_j) + \Delta t \sum_{j=1}^{s} \widehat{a}_{ij} g(Y_j)$$

$$y_n = y_{n-1} + \Delta t \sum_{j=1}^{s} b_j f(Y_j) + \Delta t \sum_{j=1}^{s} \widehat{b}_j g(Y_j)$$

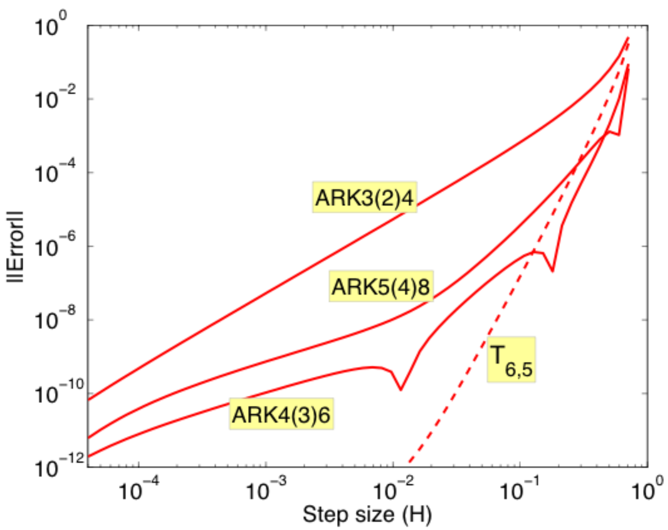
  - Ascher-Ruuth-Spiteri (ARS) [1997]
  - Pareschi-Russo (PR) [2000]
  - Kennedy-Carpenter (ARK) [2003]



- Linear multistep IMEX: stability restrictions

$$y_n = \sum_{j=1}^{k} a_j y_{n-j} + \Delta t \sum_{j=1}^{k} b_j f(y_{n-j}) + \Delta t \sum_{j=0}^{k} \widehat{b}_j g(y_{n-j})$$

  - Ascher-Ruuth-Spiteri [1995]
  - Hundsdorfer-Ruuth (IMEX-BFD) [2007]



High-order IMEX Runge-Kutta methods are very difficult to construct

- Fifth order IMEX Runge-Kutta method with embedded fourth order

explicit part

implicit part

[Kennedy and Carpenter 2003]

ARK5(4)8L[2]SA - ERK

0	0	0	0	0	0	0	0	0
$\frac{41}{100}$	$\frac{41}{100}$	0	0	0	0	0	0	0
$\frac{2935347310677}{11292855782101}$	$\frac{367902744464}{2072280473677}$	$\frac{677623207551}{8224143866563}$	0	0	0	0	0	0
$\frac{1426016391358}{7196633302097}$	$\frac{1268023523408}{10340822734521}$	0	$\frac{1029933939417}{13636558850479}$	0	0	0	0	0
$\frac{92}{100}$	$\frac{14463281900351}{6315353703477}$	0	$\frac{66114435211212}{5879490589093}$	$\frac{-54053170152839}{4284798021562}$	0	0	0	0
$\frac{24}{100}$	$\frac{14090043504691}{34967701212078}$	0	$\frac{15191511035443}{11219624916014}$	$\frac{-18461159152457}{12425892160975}$	$\frac{-281667163811}{9011619295870}$	0	0	0
$\frac{3}{5}$	$\frac{19230459214898}{13134317526959}$	0	$\frac{21275331358303}{2942455364971}$	$\frac{-38145345988419}{4862620318723}$	$\frac{-1}{8}$	$\frac{-1}{8}$	0	0
1	$\frac{-19977161125411}{11928030595625}$	0	$\frac{-40795976796054}{6384907823539}$	$\frac{177454434618887}{12078138498510}$	$\frac{782672205425}{8267701900261}$	$\frac{-69563011059811}{9646580694205}$	$\frac{7356628210526}{4942186776405}$	0
b_i	$\frac{-872700587467}{9133579230613}$	0	0	$\frac{22348218063261}{9555858737531}$	$\frac{-1143369518992}{8141816002931}$	$\frac{-39379526789629}{19018526304540}$	$\frac{32727382324388}{42900044865799}$	$\frac{41}{200}$
$\hat{b}_i$	$\frac{-975461918565}{9796059967033}$	0	0	$\frac{78070527104295}{32432590147079}$	$\frac{-548382580838}{3424219808633}$	$\frac{-33438840321285}{15594753105479}$	$\frac{3629800801594}{4656183773603}$	$\frac{4035322873751}{18575991585200}$

ARK5(4)8L[2]SA - ESDIRK

0	0	0	0	0	0	0	0	0
$\frac{41}{100}$	$\frac{41}{200}$	$\frac{41}{200}$	0	0	0	0	0	0
$\frac{2935347310677}{11292855782101}$	$\frac{41}{400}$	$\frac{-567603406766}{11931857230679}$	$\frac{41}{200}$	0	0	0	0	0
$\frac{1426016391358}{7196633302097}$	$\frac{683785636431}{9252920307686}$	0	$\frac{-110385047103}{1367015193373}$	$\frac{41}{200}$	0	0	0	0
$\frac{92}{100}$	$\frac{3016520224154}{10081342136671}$	0	$\frac{30586259806659}{12414158314087}$	$\frac{-22760509404356}{11113319521817}$	$\frac{41}{200}$	0	0	0
$\frac{24}{100}$	$\frac{218866479029}{1489978393911}$	0	$\frac{638256894668}{5436446318841}$	$\frac{-1179710474555}{5321154724896}$	$\frac{-60928119172}{8023461067671}$	$\frac{41}{200}$	0	0
$\frac{3}{5}$	$\frac{1020004230633}{5715676835656}$	0	$\frac{25762820946817}{25263940353407}$	$\frac{-2161375909145}{9755907335909}$	$\frac{-211217309593}{5846859502534}$	$\frac{-4269925059573}{7827059040749}$	$\frac{41}{200}$	0
1	$\frac{-872700587467}{9133579230613}$	0	0	$\frac{22348218063261}{9555858737531}$	$\frac{-1143369518992}{8141816002931}$	$\frac{-39379526789629}{19018526304540}$	$\frac{32727382324388}{42900044865799}$	$\frac{41}{200}$
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Extrapolated IMEX methods can be used to efficiently integrate multiphysics problems

- Problem: $y'(t) = f(t, y(t)) + g(t, y(t))\,,\ t > 0\,,\ y(t_0) = y_0$

$$y(t) - y_{\Delta t}(t) = e_{p+1}(t)\,\Delta t^{p+1} + \cdots + e_N(t)\,\Delta t^N + E_{\Delta t}(t)\,\Delta t^{N+1}$$

- Extrapolation methods (easy construction) [Gragg, 1964]:

$$T_{i,1} := y_{\Delta t_i}(t_0 + \Delta T)\,, \Longrightarrow T_{j,k+1} = T_{j,k} + \frac{T_{j,k} - T_{j-1,k}}{\left(n_j/n_{j-1}\right) - 1}$$

order p order p+1   order p+2

$$\begin{array}{cccc} T_{11} & & & \\ T_{21} & \to T_{22} & & \\ T_{31} & \to T_{32} & \to T_{33} & \\ \cdots & \cdots & \cdots & \cdots \end{array}$$

$$\Delta t_i = \Delta T / n_j$$
$$n_j = 1, 2, 3, 4, \ldots$$

- "Base" methods:
- Extrapolation:

$$[\textit{Explicit}]\ y^{n+1} = y^n + \Delta t\, f(y^n) + \Delta t\, g(y^n)\,,$$

$$[\textit{L-Implicit}]\ y^{n+1} = y^n + [I - \Delta t\,(f+g)'(y^n)]^{-1}\ (\Delta t\, f(y^n) + \Delta t\, g(y^n))\,,$$

$$[\textit{W-Method}]\ y^{n+1} = y^n + [I - \Delta t\, g'(y^n)]^{-1}\ (\Delta t\, f(y^n) + \Delta t\, g(y^n))\,,$$

- Extrapolated IMEX

$$[\textit{IMEX}]\ y^{n+1} = y^n + \Delta t\, f(y^n) + [I - \Delta t\, g'(y^n)]^{-1}\ (\Delta t\, g(y^n))\,,$$

$$[\textit{Split-IMEX}]\ y^{n+1} = y^* + [I - \Delta t\, g'(y^n)]^{-1}\ (\Delta t\, g(y^*))\ ;\ \ y^* = y^n + \Delta t\, f(y^n)$$

Implementation of the proposed extrapolated IMEX schemes

- Problem: $y'(t) = f(t, y(t)) + g(t, y(t))\,,\ t > 0\,,\ y(t_0) = y_0$

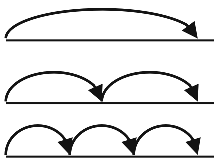
order p

order $p+1$

order $p+2$

$$\begin{array}{cccc} T_{11} & & & \\ T_{21} & T_{22} & & \\ T_{31} & T_{32} & T_{33} & \\ \cdots & \cdots & \cdots & \cdots \end{array}$$

$$T_{i,1} := y_{\Delta t_i}(t_0 + \Delta T)\,,$$



$$\begin{array}{ccc} T_{11} & & \\ T_{21} & T_{22} & \\ T_{31} & T_{32} & T_{33} \end{array} \longrightarrow T_{j,k+1} = T_{j,k} + \frac{T_{j,k} - T_{j-1,k}}{\left(n_j/n_{j-1}\right) - 1}$$

$$\Delta t_i = \Delta T / n_j$$
$$n_j = 1, 2, 3, 4, \ldots$$

$$y^{n+1} = y^n + \left[I - \Delta t\, g'(y^n)\right]^{-1} \left(\Delta t\, f(y^n) + \Delta t\, g(y^n)\right)\,,$$
$$y^{n+1} = y^n + \Delta t\, f(y^n) + \left[I - \Delta t\, g'(y^n)\right]^{-1} \left(\Delta t\, g(y^n)\right)\,,$$
$$y^{n+1} = y^* + \left[I - \Delta t\, g'(y^n)\right]^{-1} \left(\Delta t\, g(y^*)\right)\,;\ \ y^* = y^n + \Delta t\, f(y^n)$$

- Note: the Jacobians are evaluated once

Linear stability analysis for IMEX methods

- Classical linear stability: $y'(t) = \lambda y(t); \qquad y^{n+1} = R(\lambda \Delta t)\, y^n; \qquad |R(\lambda \Delta t)| \leq 1$

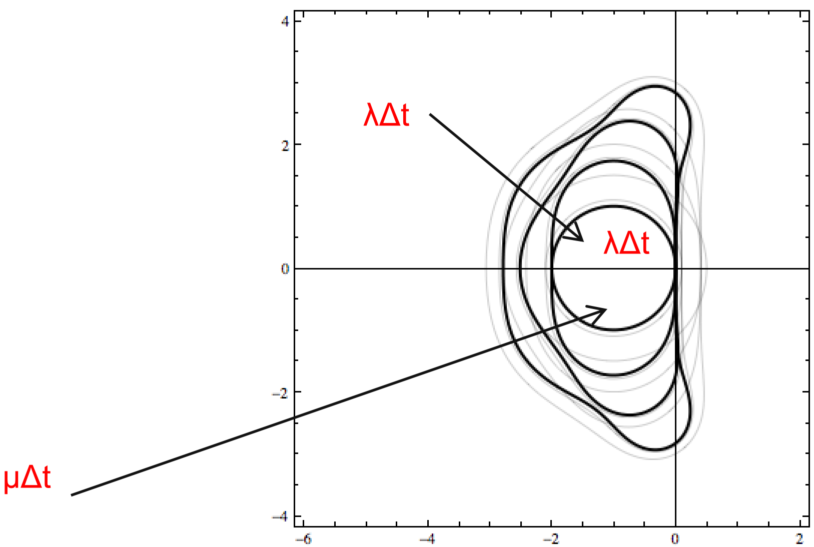
- IMEX linear stability:

  [nonstiff] [stiff]

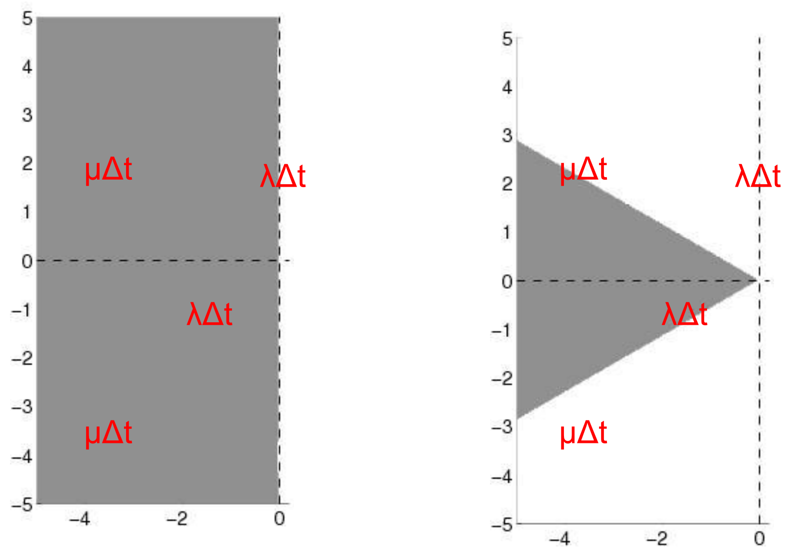
  $$y'(t) = \lambda y(t) + \mu y(t)\,,\ t > 0\,,\ y(t_0) = y_0\,,\ |Re(\mu)| \gg |Re(\lambda)|$$

  $$y^{n+1} = R(\lambda \Delta t, \mu \Delta t) y^n \quad \mathcal{S} = \{z \in \mathbb{C},\ w \in \mathbb{C} : |R(z,w)| \leq 1\}$$

Explicit stability region

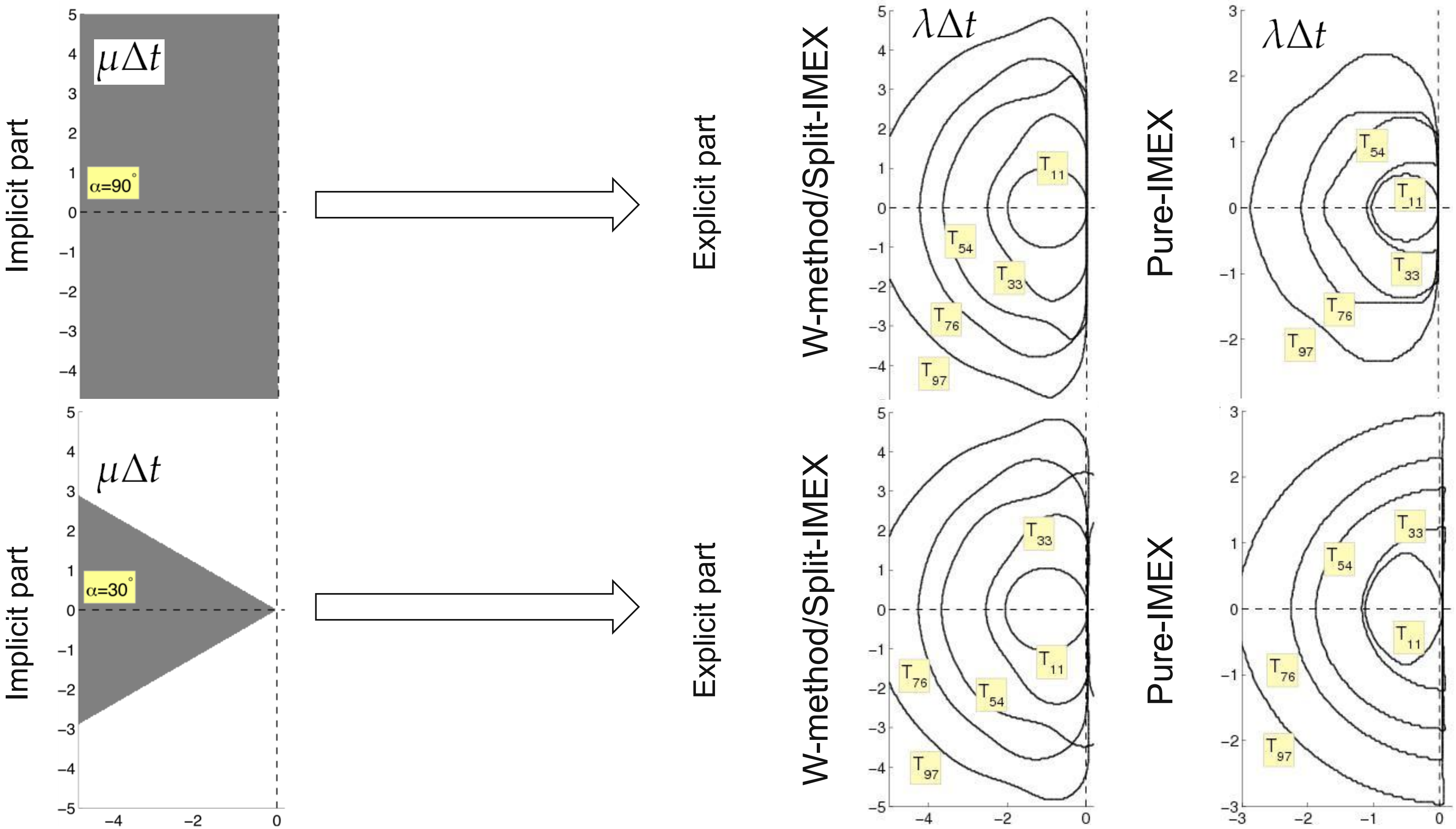


Implicit stability region



Linear stability analysis for the proposed extrapolated IMEX methods

$$y'(t) = \lambda y(t) + \mu y(t)\,,\ t > 0\,,\ y(t_0) = y_0\,,\ |Re(\mu)| \gg |Re(\lambda)|$$



Consistency analysis of extrapolated IMEX methods for stiff problems

- Perform a change of variables: $u' = f(x,u) + g(x,u) \quad \text{with } u = y + \varepsilon z$

$$\begin{cases} y' = \widehat{f}(y,z) = f(y + \varepsilon z) \\ \varepsilon z' = \widehat{g}(y,z) = g(y + \varepsilon z) \end{cases} \quad \text{with} \begin{cases} y^0 + \varepsilon z^0 = u^0 \\ y + \varepsilon z = u \\ (y + \varepsilon z)' = u' \end{cases}$$

- IMEX (SPP) ODE: $\begin{pmatrix} y \\ \varepsilon z \end{pmatrix}' = \begin{pmatrix} f(y,z) \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ g(y,z) \end{pmatrix}$

$\Delta t \gg \varepsilon$

- DAE (index-1): $\begin{pmatrix} y \\ 0 \end{pmatrix}' = \begin{pmatrix} f(y,z) \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ g(y,z) \end{pmatrix}$

$\varepsilon \to 0$

g_z is invertible

- The consistency analysis is done through the expansion of the global error

Asymptotic expansion of the global error for the extrapolated IMEX methods applied to DAEs

- The W-method, Pure-IMEX, and Split-IMEX schemes have global error expansions:

$$
\begin{aligned}
y_i - y(t_i) &= \sum_{j=1}^{M} \Delta t^j \left(a_j(t_i) + \alpha_i^{(j)} \right) + \mathcal{O}\left(\Delta t^{M+1}\right) \\
z_i - z(t_i) &= \sum_{j=1}^{M} \Delta t^j \left(b_j(t_i) + \beta_i^{j} \right) + \mathcal{O}\left(\Delta t^{M+1}\right)
\end{aligned}
$$

numerical approx.
after *i* steps

exact solution

smooth
functions

perturbations

- The extrapolation method cancels the smooth coeff. *a*, *b*; but not the perturbations

  - W-method:

$$
\begin{aligned}
\alpha_i^{(1)} = 0\,,\ \alpha_i^{(2)} = 0\,,\ \beta_i^{(1)} = 0\,,\ \forall i \geq 0\,, \\
\alpha_i^{(3)} = 0\,,\ \alpha_i^{(4)} = 0\,,\ \beta_i^{(2)} = 0\,,\ \forall i \geq 1\,, \\
\alpha_i^{(j)} = 0\,,\ \forall i \geq j-3\,,\ j \geq 5\,, \\
\beta_i^{(j)} = 0\,,\ \forall i \geq j-2\,,\ j \geq 3\,.
\end{aligned}
$$

  - Pure-IMEX scheme:

$$
\begin{aligned}
\alpha_i^{(2)} = 0\,,\ \beta_i^{(1)} = 0\,,\ \forall i \geq 1\,, \\
\alpha_i^{(1)} = 0\,,\ \forall i \geq 0\,, \\
\alpha_i^{(3)} = 0\,,\ \beta_i^{(2)} = 0\,,\ \forall i \geq 2\,, \\
\alpha_i^{(j)} = 0\,,\ \forall i \geq j-1\,,\ j \geq 4\,, \\
\beta_i^{(j)} = 0\,,\ \forall i \geq j\,,\ j \geq 3\,.
\end{aligned}
$$

  - Split-IMEX scheme

$$
\begin{aligned}
\alpha_i^{(1)} = 0\,, \alpha_i^{(2)} = 0\,,\ \beta_i^{(1)} = 0\,,\ \forall i \geq 0\,, \\
\alpha_i^{(3)} = 0\,,\ \beta_i^{(2)} = 0\,,\ \forall i \geq 1\,, \\
\alpha_i^{(j)} = 0\,,\ \forall i \geq j-2\,,\ j \geq 4\,, \\
\beta_i^{(j)} = 0\,,\ \forall i \geq j-1\,,\ j \geq 3\,.
\end{aligned}
$$

Asymptotic expansion of the global error for the extrapolated Split-IMEX scheme applied to DAEs

$$y_i - y(t_i) \;=\; \sum_{j=1}^{M} \Delta t^j \left(a_j(t_i) + \alpha_i^{(j)}\right) + \mathcal{O}\left(\Delta t^{M+1}\right) \qquad z_i - z(t_i) \;=\; \sum_{j=1}^{M} \Delta t^j \left(b_j(t_i) + \beta_i^{j}\right) + \mathcal{O}\left(\Delta t^{M+1}\right)$$

- Extrapolated Split-IMEX: $y^{n+1} = y^* + [I - \Delta t\, g'(y^n)]^{-1}\ (\Delta t\, g(y^*))\ ;\ \ y^* = y^n + \Delta t\, f(y^n)$

$$\begin{pmatrix} I & 0 \\ -\Delta t g_y(0) & -\Delta t g_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1} - y_i \\ z_{i+1} - z_i \end{pmatrix} = \Delta t \begin{pmatrix} f(y_i, z_i) \\ g(y_i + \Delta t f(y_i, z_i), z_i) - \Delta t g_y(0) f(y_i, z_i) \end{pmatrix}$$

- Accuracy Split-IMEX

entry *jk* in the extrapolation tableau

$$Y_{jk} - y(t_0 + \Delta t) = \mathcal{O}\left(\Delta T^{r_{jk}}\right), \qquad Z_{jk} - z(t_0 + \Delta t) = \mathcal{O}\left(\Delta T^{s_{jk}}\right)$$

1	2									
2	2	3								
3	2	3	3							
4	2	3	3	4						
5	2	3	3	4	4					
6	2	3	3	4	5	4				
7	2	3	3	4	5	5	4			
8	2	3	3	4	5	6	5	4		
9	2	3	3	4	5	6	6	5	4	
10	2	3	3	4	5	6	7	6	5	4
	1	2	3	4	5	6	7	8	9	10

2									
2	2								
2	2	3							
2	2	3	3						
2	2	3	4	3					
2	2	3	4	4	3				
2	2	3	4	5	4	3			
2	2	3	4	5	5	4	3		
2	2	3	4	5	6	5	4	3	
2	2	3	4	5	6	6	5	4	3
1	2	3	4	5	6	7	8	9	10

$$\alpha_i^{(1)} = 0\,, \alpha_i^{(2)} = 0\,,\ \beta_i^{(1)} = 0\,,\ \forall i \geq 0\,,$$
$$\alpha_i^{(3)} = 0\,,\ \beta_i^{(2)} = 0\,,\ \forall i \geq 1\,,$$
$$\alpha_i^{(j)} = 0\,,\ \forall i \geq j-2\,,\ j \geq 4\,,$$
$$\beta_i^{(j)} = 0\,,\ \forall i \geq j-1\,,\ j \geq 3\,.$$

Theoretical local extrapolation orders for linearly implicit, W-IMEX, Pure-IMEX, and Split-IMEX methods for index-1 DAEs

Orders (r_{jk}) for component y_{jk} for Linearly implicit| W-IMEX|Pure-IMEX|Split-IMEX

<table>
<tr><td>1</td><td>2|2|2|2</td><td>$\cancel{a^{(2)}(\cdot)}$</td><td>$\cancel{a^{(3)}(\cdot)}$</td><td>$\cancel{a^{(4)}(\cdot)}$</td><td>$\cancel{a^{(5)}(\cdot)}$</td><td>$\cancel{a^{(6)}(\cdot)}$</td><td>$\cancel{a^{(7)}(\cdot)}$</td><td>$\cancel{a^{(8)}(\cdot)}$</td><td>$\cancel{a^{(9)}(\cdot)}$</td><td>$\cancel{a^{(10)}(\cdot)}$</td><td>$\cancel{a^{(11)}(\cdot)}$</td><td>$\cancel{a^{(12)}(\cdot)}$</td></tr>
<tr><td>2</td><td>2|2|2|2</td><td>3|3|2|3</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
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<tr><td>4</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|3|4</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
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<tr><td>6</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|4|4</td><td>5|5|4|5</td><td>6|5|3|4</td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>7</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|4|4</td><td>5|5|5|5</td><td>6|6|4|5</td><td>6|5|3|4</td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>8</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|4|4</td><td>5|5|5|5</td><td>6|6|5|6</td><td>7|6|4|5</td><td>6|5|3|4</td><td></td><td></td><td></td><td></td></tr>
<tr><td>9</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|4|4</td><td>5|5|5|5</td><td>6|6|6|6</td><td>7|7|5|6</td><td>7|6|4|4</td><td>6|5|3|4</td><td></td><td></td><td></td></tr>
<tr><td>10</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|4|4</td><td>5|5|5|5</td><td>6|6|6|6</td><td>7|7|6|7</td><td>8|7|5|6</td><td>7|6|4|5</td><td>6|5|3|4</td><td></td><td></td></tr>
<tr><td>11</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|4|4</td><td>5|5|5|5</td><td>6|6|6|6</td><td>7|7|7|7</td><td>8|8|6|7</td><td>8|7|5|6</td><td>7|6|4|5</td><td>6|5|3|4</td><td></td></tr>
<tr><td>12</td><td>2|2|2|2</td><td>3|3|2|3</td><td>4|3|3|3</td><td>5|4|4|4</td><td>5|5|5|5</td><td>6|6|6|6</td><td>7|7|7|7</td><td>8|8|7|8</td><td>9|8|6|7</td><td>8|7|5|6</td><td>7|6|4|5</td><td>6|5|3|4</td></tr>
<tr><td></td><td>1</td><td>2</td><td>3</td><td>4</td><td>5</td><td>6</td><td>7</td><td>8</td><td>9</td><td>10</td><td>11</td><td>12</td></tr>
</table>

Orders (s_{jk}) for component z_{jk} for Linearly implicit| W-IMEX|Pure-IMEX|Split-IMEX

<table>
<tr><td>1</td><td>2|2|1|2</td><td>$\cancel{b^{(2)}(\cdot)}$</td><td>$\cancel{b^{(3)}(\cdot)}$</td><td>$\cancel{b^{(4)}(\cdot)}$</td><td>$\cancel{b^{(5)}(\cdot)}$</td><td>$\cancel{b^{(6)}(\cdot)}$</td><td>$\cancel{b^{(7)}(\cdot)}$</td><td>$\cancel{b^{(8)}(\cdot)}$</td><td>$\cancel{b^{(9)}(\cdot)}$</td><td>$\cancel{b^{(10)}(\cdot)}$</td><td>$\cancel{b^{(11)}(\cdot)}$</td><td>$\cancel{b^{(12)}(\cdot)}$</td></tr>
<tr><td>2</td><td>2|2|1|2</td><td>2|2|2|2</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
<tr><td>3</td><td>2|2|1|2</td><td>2|2|2|2</td><td>3|3|2|3</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></tr>
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</table>

Example of nonlinear DAE index-1 solved with extrapolated Split-IMEX extrapolation method

- DAE example:

$$
\begin{aligned}
y' &= \frac{y^2}{z\sqrt{\frac{y^2}{z^2} - 1}} && = f(y,z) \\
0 &= z^2 - \frac{1}{1+y^2} - y^2\left(\frac{1}{z^2} - 1\right) && = g(y,z)
\end{aligned}
$$

- exact solution:

$$y(t) = \sinh(t),\ z(t) = \tanh(t)$$

Theoretical orders

1	2						2					
2	2	3					2	2				
3	2	3	3				2	2	3			
4	2	3	3	4			2	2	3	3		
5	2	3	3	4	4		2	2	3	4	3	
6	2	3	3	4	5	4	2	2	3	4	4	3

Numerical orders

$\boxed{y}$

1	2.0					
2	1.9	3.0				
3	1.9	3.0	3.0			
4	2.0	3.0	2.9	4.0		
5	2.0	3.0	3.0	4.0	4.0	
6	2.0	3.0	3.0	3.9	4.9	4.0

$\boxed{z}$

1	2.0					
2	2.0	2.0				
3	2.2	2.0	3.0			
4	1.8	2.0	2.9	3.0		
5	1.9	2.0	2.9	4.0	3.0	
6	1.9	2.0	2.9	3.9	4.0	3.1

Asymptotic expansion of the global error for the extrapolated IMEX methods applied to ODEs

- ODE solved with extrapolated W-method: $\begin{pmatrix} I & 0 \\ -\Delta t g_y(0) & \varepsilon I - \Delta t g_z(0) \end{pmatrix} \begin{pmatrix} y_{i+1} - y_i \\ z_{i+1} - z_i \end{pmatrix} = \Delta t \begin{pmatrix} f(y_i, z_i) \\ g(y_i, z_i) \end{pmatrix}$

$\varepsilon \leq \Delta t$

- Perturbed expansion:

$$y_i = y(x_i) + \Delta t a^{(1)}(x_i) + \Delta t^2 a^{(2)}(x_i) + \mathcal{O}(\Delta t^3) - \\ - \varepsilon f_z(0) g_z^{-1}(0) \left(I - \frac{\Delta t}{\varepsilon} g_z(0) \right)^{-i+1} \left(\Delta t b^{(1)}(0) + \Delta t^2 b^{(2)}(0) \right),$$

$$z_i = z(x_i) + \Delta t b^{(1)}(x_i) + \Delta t^2 b^{(2)}(x_i) + \mathcal{O}(\Delta t^3) - \\ - \left(I - \frac{\Delta t}{\varepsilon} g_z(0) \right)^{-i+1} \left(\Delta t b^{(1)}(0) + \Delta t^2 b^{(2)}(0) \right),$$

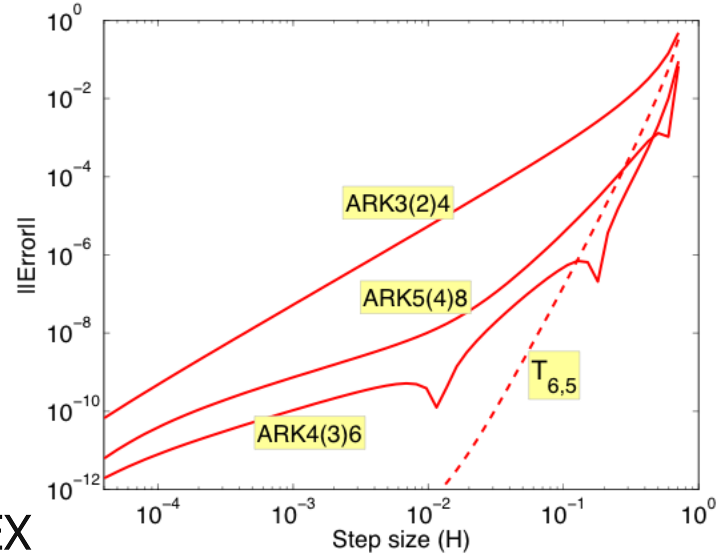
$$a^{(1)}(0) = \mathcal{O}(\varepsilon \Delta t),\ a^{(2)}(0) = \mathcal{O}(\Delta t),\ b^{(1)}(0) = \mathcal{O}(\varepsilon),\ b^{(2)}(0) = \mathcal{O}(1)$$

- Same orders as obtained for DAEs, but with an extra $\mathcal{O}(\varepsilon^2)$ term

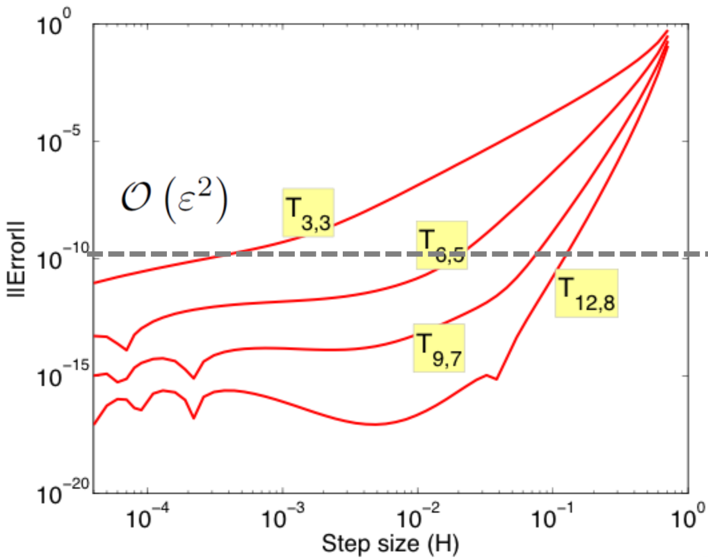
Asymptotic expansion of the global error for the extrapolated IMEX methods applied to ODEs

- ODE (van der Pol): $\varepsilon = 10^{-5}$

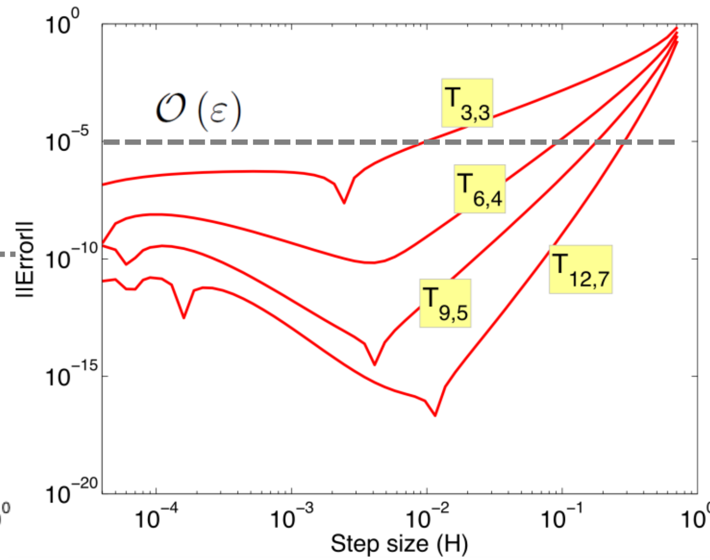
$$\begin{aligned} y' &= z \\ \varepsilon\, z' &= \left(1-y^2\right) z - y \end{aligned} = \begin{pmatrix} z \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \left(1-y^2\right) z - y \end{pmatrix}$$



- W- and Split-IMEX



- Pure-IMEX



- ARK

Efficient implementation considerations

- Extrapolation methods can accommodate:
  - very high accuracy
  - variable orders
  - lower order embedded approximations for error control
- Each approximation in the first column is independent:
  - parallelize easy

embedded method

variable order

1	2									
2	2	3								
3	2	3	3							
4	2	3	3	4						
5	2	3	3	4	4					
6	2	3	3	4	5	4				
7	2	3	3	4	5	5	4			
8	2	3	3	4	5	6	5	4		
9	2	3	3	4	5	6	6	5	4	
10	2	3	3	4	5	6	7	6	5	4
	1	2	3	4	5	6	7	8	9	10

first column is expensive

$$T_{i,1} := y_{\Delta t_i}(t_0 + \Delta T)$$

the rest are very cheap

$$T_{j,k+1} = T_{j,k} + \frac{T_{j,k} - T_{j-1,k}}{\left(n_j / n_{j-1}\right) - 1}$$

Very high accuracy experiments with an advection-reaction PDE problem

- Advection-reaction PDE example:

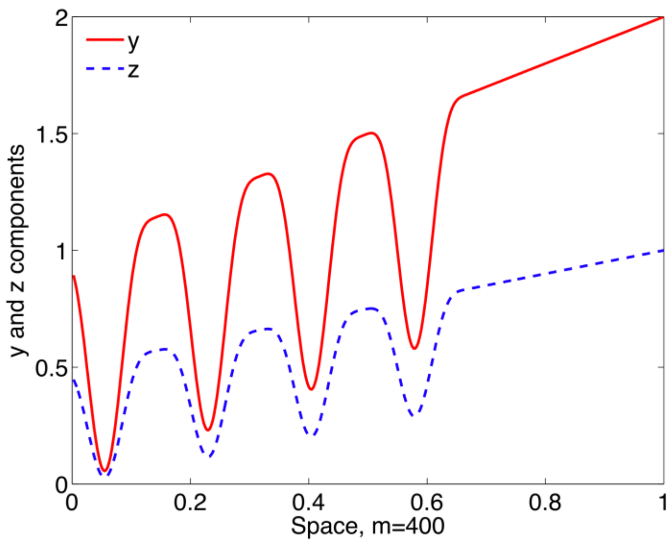
$$\begin{aligned} y_t + \alpha_1 y_x &= -k_1 y + k_2 z + s_1 \\ z_t + \alpha_2 z_x &= k_1 y - k_2 z + s_2 \end{aligned}, \quad \begin{aligned} 0 &< x < 1 \\ 0 &< t \le t_{\max} \end{aligned}, \quad \begin{aligned} \alpha_1 &= 1,\ k_1 = 10^6,\ s_1 = 0 \\ \alpha_2 &= 0,\ k_2 = 2k_1,\ s_2 = 1 \end{aligned},$$

$$y(x,0) = 1 + s_2 x,\ z(x,0) = \frac{k_1}{k_2} y(x,0) + \frac{1}{k_2} s_2,\ y(0,t) = 1 - \sin(12t)^4$$

$$x_i = i\Delta x,\ i = 1 \dots m \text{ with } \Delta x = 1/m,\ m = 400$$

- Global orders (W-|Pure-|Split-IMEX):

1.0|1.0|1.0				
1.0|1.0|1.0	2.0|1.0|2.0			
1.0|1.0|1.0	2.0|1.0|2.0	3.0|1.9|3.0		
1.2|1.0|1.2	2.0|1.0|2.0	3.0|2.0|3.0	4.0|2.0|4.0	
1.0|1.0|1.0	2.0|1.0|2.0	3.0|2.0|3.0	4.0|3.0|4.0	5.0|2.0|5.0

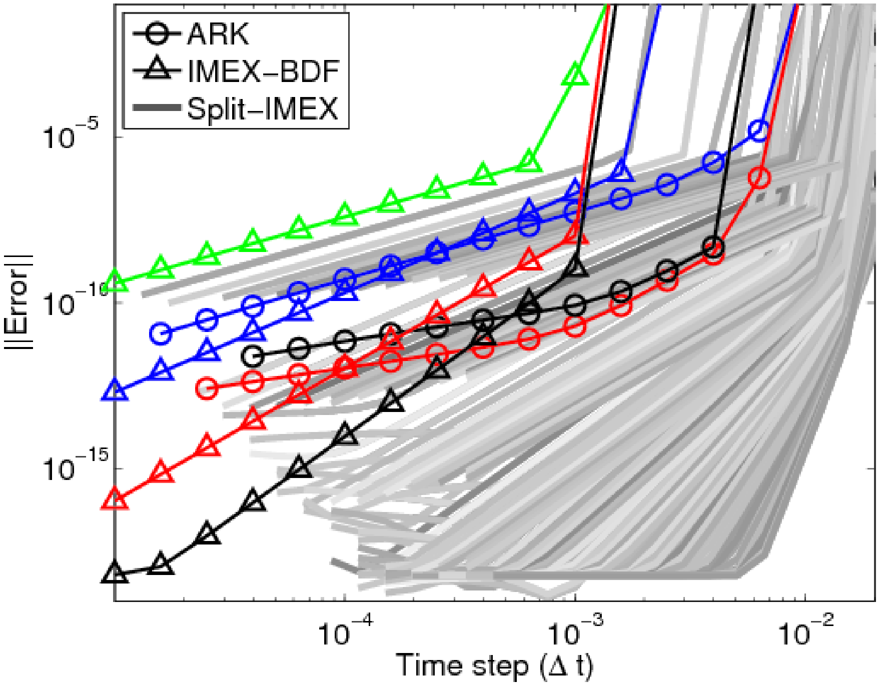


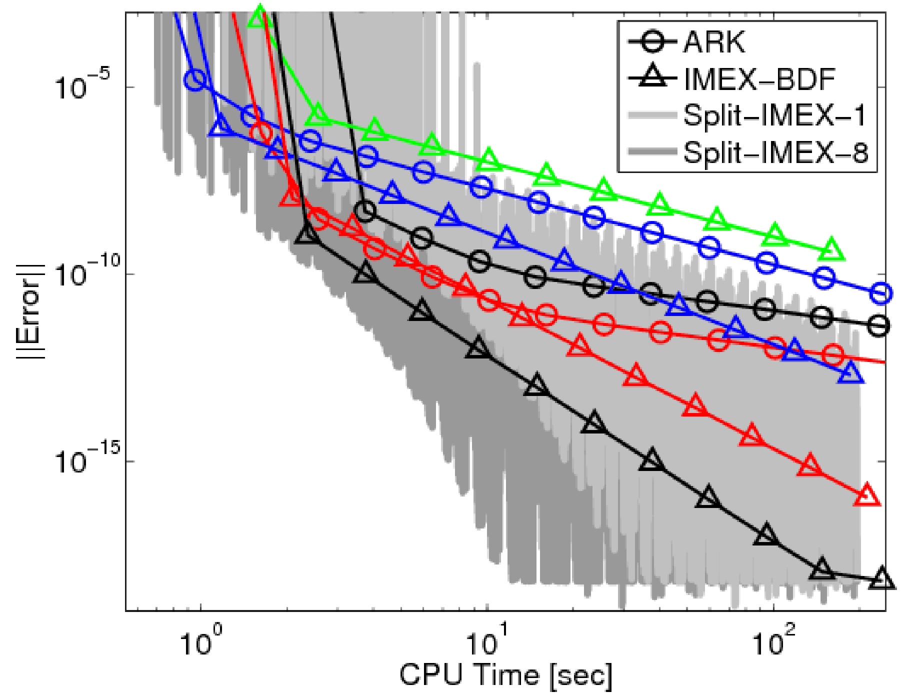
Very high accuracy experiments show the method robustness

- Advection-reaction PDE example:

$$\begin{aligned} y_t + \alpha_1\, y_x &= -k_1 y + k_2 z + s_1 \\ z_t + \alpha_2\, z_x &= k_1 y - k_2 z + s_2 \end{aligned}, \quad \begin{aligned} &0 < x < 1 \\ &0 < t \le t_{\max} \end{aligned}, \quad \begin{aligned} &\alpha_1 = 1,\ k_1 = 10^6,\ s_1 = 0 \\ &\alpha_2 = 0,\ k_2 = 2k_1,\ s_2 = 1 \end{aligned},$$

- Advection-reaction convergence: Comparison among IMEX-BDF, ARK, and extrapolated IMEX up to order 18 on (one and eight cores)





Conclusions

- Extrapolated W-, Split-, Pure-IMEX can be efficient integrators for multiphysics problems
- Computationally less expensive than fully implicit methods
- Easy to construct and implement w/ favorable accuracy properties
- Embedded lower order approximations/variable order are automatic
- Applicable to ODEs, DAEs index-1, PDEs via MOL
- Easy to parallelize and suitable for multicore architectures

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