Design of High-Order Multirate General Additive Runge Kutta Schemes

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Outline

Multirate systems involve mixed dynamics.

$$y' = \sum_{\sigma=1}^{N} f^{\{\sigma\}}(y), \quad y(t_0) = y_0, \quad y(t) \in \mathbb{R}^d.$$

$$y' = f(y) = f^{\{\mathfrak{s}\}}(y) + f^{\{\mathfrak{f}\}}(y), \quad y(t_0) = y_0, \quad y(t) \in \mathbb{R}^d,$$

$$M = H/h.$$

- Systems driven by hybrid dynamics that incur different time-scales.
- Fast dynamics (shock waves, diffusion, electro/magneto waves) interact with slow ones (long range transport, reaction processes, nuclear decay).
- Multiple discretization lead to varying stiffness and evaluation costs of the right hand side partitions.

Desired features of a multirate time-stepping method

- Flexible methods that work at different rates (M dependent coefficients).
- Treat different partitions of the system according to their stiffness (couple implicit and explicit methods).
- Avoid unnecessary computation cost (decouple stage computations across different partitions).
- Control both the error and the rates of integration in different partitions ($H - M$ adaptivity).

We design of multirate methods using the GARK framework.

- Multirating body of work is rich: Rice[1], Andrus[2], Gear and Wells, Kværnø and Rentrop[3] Bartel[4], ...
- GARK framework developed by Sandu and Günther[5] describes a general methodology and order condition theory for partitioned Runge-Kutta schemes
- Multirate GARK framework[6] lays out the order condition theory for MR GARK methods.
- We will consider methods discrete in all partitions

[1] Rice, "Split Runge-Kutta methods for simultaneous equations".

[2] Andrus, "Numerical Solution for Ordinary Differential Equations Separated into Subsystems"; Andrus, "Stability of a multirate method for numerical integration of ODEs".

[3] Kværnø, "Stability of multirate Runge-Kutta schemes"; Kværnø and Rentrop, *Low order multirate Runge-Kutta methods in electric circuit simulation*.

[4] Bartel and Günther, "A multirate W-method for electrical networks in state-space formulation".

[5] Sandu and Günther, "A generalized-structure approach to additive Runge-Kutta methods".

[6] Günther and Sandu, "Multirate generalized additive Runge-Kutta methods".

One step of a MR GARK scheme:

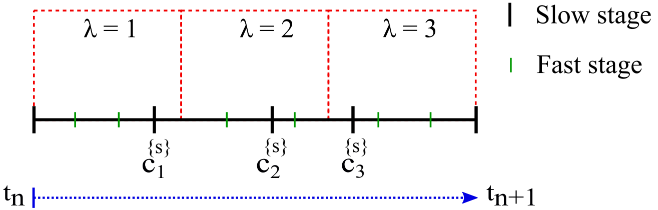
$$Y_i^{\{\mathfrak{s}\}} = y_n + H \sum_{j=1}^{s^{\{\mathfrak{s}\}}} a_{i,j}^{\{\mathfrak{s},\mathfrak{s}\}} f^{\{\mathfrak{s}\}}\left(Y_j^{\{\mathfrak{s}\}}\right) + h \sum_{\lambda=1}^{M} \sum_{j=1}^{s^{\{\mathfrak{f}\}}} a_{i,j}^{\{\mathfrak{s},\mathfrak{f},\lambda\}} f^{\{\mathfrak{f}\}}\left(Y_j^{\{\mathfrak{f},\lambda\}}\right), \quad i = 1, \dots, s^{\{\mathfrak{s}\}},$$

$$Y_i^{\{\mathfrak{f},\lambda\}} = \widetilde{y}_{n+(\lambda-1)/M} + H \sum_{j=1}^{s^{\{\mathfrak{s}\}}} a_{i,j}^{\{\mathfrak{f},\mathfrak{s},\lambda\}} f^{\{\mathfrak{s}\}}\left(Y_j^{\{\mathfrak{s}\}}\right) + h \sum_{j=1}^{s^{\{\mathfrak{f}\}}} a_{i,j}^{\{\mathfrak{f},\mathfrak{f}\}} f^{\{\mathfrak{f}\}}\left(Y_j^{\{\mathfrak{f},\lambda\}}\right), \quad i = 1, \dots, s^{\{\mathfrak{f}\}},$$

$$\widetilde{y}_{n+\lambda/M} = \widetilde{y}_{n+(\lambda-1)/M} + h \sum_{i=1}^{s^{\{\mathfrak{f}\}}} b_i^{\{\mathfrak{f}\}} f^{\{\mathfrak{f}\}}\left(Y_i^{\{\mathfrak{f},\lambda\}}\right), \quad \lambda = 1, \dots, M,$$

$$y_{n+1} = \widetilde{y}_{n+M/M} + H \sum_{i=1}^{s^{\{\mathfrak{s}\}}} b_i^{\{\mathfrak{s}\}} f^{\{\mathfrak{s}\}}\left(Y_i^{\{\mathfrak{s}\}}\right).$$

M = 3



Butcher tableau for a MR GARK method:

$$
\begin{array}{c|c}
\mathbf{A}^{\{\mathfrak{f},\mathfrak{f}\}} & \mathbf{A}^{\{\mathfrak{f},\mathfrak{s}\}} \\ \hline
\mathbf{A}^{\{\mathfrak{s},\mathfrak{f}\}} & \mathbf{A}^{\{\mathfrak{s},\mathfrak{s}\}} \\ \hline
\mathbf{b}^{\{\mathfrak{f}\}\,T} & \mathbf{b}^{\{\mathfrak{s}\}\,T}
\end{array}
:=
\begin{array}{ccc|c}
\frac{1}{M}\,A^{\{\mathfrak{f},\mathfrak{f}\}} & \cdots & 0 & A^{\{\mathfrak{f},\mathfrak{s},1\}} \\
\vdots & \ddots & \vdots & \vdots \\
\frac{1}{M}\,\mathbb{1}\,b^{\{\mathfrak{f}\}\,T} & \cdots & \frac{1}{M}\,A^{\{\mathfrak{f},\mathfrak{f}\}} & A^{\{\mathfrak{f},\mathfrak{s},M\}} \\ \hline
\frac{1}{M}\,A^{\{\mathfrak{s},\mathfrak{f},1\}} & \cdots & \frac{1}{M}\,A^{\{\mathfrak{s},\mathfrak{f},M\}} & A^{\{\mathfrak{s},\mathfrak{s}\}} \\ \hline
\frac{1}{M}\,b^{\{\mathfrak{f}\}\,T} & \cdots & \frac{1}{M}\,b^{\{\mathfrak{f}\}\,T} & b^{\{\mathfrak{s}\}\,T}
\end{array}
.
$$

Order 3 coupling conditions for Internally consistent MR GARK

$$\frac{M}{6} = \sum_{\lambda=1}^{M} b^{\{\mathfrak{f}\}\,T} A^{\{\mathfrak{f},\mathfrak{s},\lambda\}} c^{\{\mathfrak{s}\}}, \qquad \text{(order 3)}$$

$$\frac{M^2}{6} = \sum_{\lambda=1}^{M} b^{\{\mathfrak{s}\}\,T} A^{\{\mathfrak{s},\mathfrak{f},\lambda\}} \left((\lambda-1)\mathbb{1} + c^{\{\mathfrak{f}\}}\right), \qquad \text{(order 3)}$$

Order 4 coupling conditions for Internally consistent MR GARK

$$\frac{M^2}{8} = \sum_{\lambda=1}^{M} (\lambda - 1)\, b^{\{\mathfrak{f}\}\,T} A^{\{\mathfrak{f},\mathfrak{s},\lambda\}}\, c^{\{\mathfrak{s}\}} + \sum_{\lambda=1}^{M} b^{\{\mathfrak{f}\}\,T} \left(c^{\{\mathfrak{f}\}} \times A^{\{\mathfrak{f},\mathfrak{s},\lambda\}}\, c^{\{\mathfrak{s}\}} \right), \qquad \text{(order 4)}$$

$$\frac{M^2}{8} = b^{\{\mathfrak{s}\}\,T} \sum_{\lambda=1}^{M} \left(c^{\{\mathfrak{s}\}} \times \left(A^{\{\mathfrak{s},\mathfrak{f}\,\lambda\}} \left((\lambda - 1)\, \mathbb{1} + c^{\{\mathfrak{f}\}} \right) \right) \right), \qquad \text{(order 4)}$$

$$\frac{M}{12} = \sum_{\lambda=1}^{M} b^{\{\mathfrak{f}\}\,T} A^{\{\mathfrak{f},\mathfrak{s},\lambda\}} c^{\{\mathfrak{s}\}\times 2}, \qquad \text{(order 4)}$$

$$\frac{M^3}{12} = \sum_{\lambda=1}^{M} b^{\{\mathfrak{s}\}\,T} A^{\{\mathfrak{s},\mathfrak{f},\lambda\}}\, c^{\{\mathfrak{f}\}\times 2} + \sum_{\lambda=1}^{M} (\lambda - 1)^2 b^{\{\mathfrak{s}\}\,T} A^{\{\mathfrak{s},\mathfrak{f},\lambda\}}\, \mathbb{1} + 2 \sum_{\lambda=1}^{M} (\lambda - 1) b^{\{\mathfrak{s}\}\,T} A^{\{\mathfrak{s},\mathfrak{f},\lambda\}}\, c^{\{\mathfrak{f}\}}, \qquad \text{(order 4)}$$

$$\frac{M^2}{24} = \sum_{\lambda=1}^{M} b^{\{\mathfrak{s}\}\,T} A^{\{\mathfrak{s},\mathfrak{s}\}}\, A^{\{\mathfrak{s},\mathfrak{f},\lambda\}} \left((\lambda - 1)\mathbb{1} + c^{\{\mathfrak{f}\}} \right), \qquad \text{(order 4)}$$

More order 4 coupling conditions for Internally consistent MR GARK

$$\frac{M}{24} = \sum_{\lambda=1}^{M} b^{\{\mathfrak{s}\}\,T} A^{\{\mathfrak{s},\mathfrak{f},\lambda\}} A^{\{\mathfrak{f},\mathfrak{s},\lambda\}} c^{\{\mathfrak{s}\}}, \qquad \text{(order 4)}$$

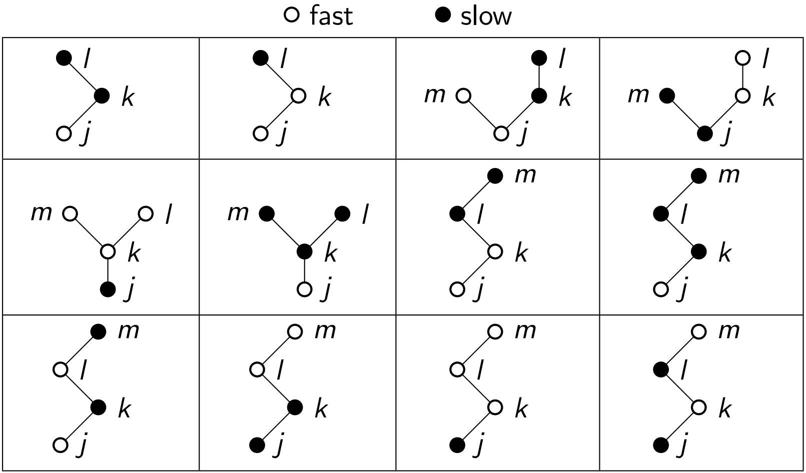
$$\frac{M^3}{24} = \sum_{\lambda=1}^{M} \frac{(\lambda-1)^2}{2} b^{\{\mathfrak{s}\}\,T} A^{\{\mathfrak{s},\mathfrak{f},\lambda\}} \mathbb{1} + \sum_{\lambda=1}^{M} (\lambda-1) b^{\{\mathfrak{s}\}\,T} A^{\{\mathfrak{s},\mathfrak{f},\lambda\}} c^{\{\mathfrak{f}\}} + \sum_{\lambda=1}^{M} b^{\{\mathfrak{s}\}\,T} A^{\{\mathfrak{s},\mathfrak{f},\lambda\}} A^{\{\mathfrak{f},\mathfrak{f}\}} c^{\{\mathfrak{f}\}}, \qquad \text{(order 4)}$$

$$\frac{M^2}{24} = \sum_{\lambda=1}^{M} \sum_{k=1}^{\lambda-1} b^{\{\mathfrak{f}\}\,T} A^{\{\mathfrak{f},\mathfrak{s},k\}} c^{\{\mathfrak{s}\}} + \sum_{\lambda=1}^{M} b^{\{\mathfrak{f}\}\,T} A^{\{\mathfrak{f},\mathfrak{f}\}} A^{\{\mathfrak{f},\mathfrak{s},\lambda\}} c^{\{\mathfrak{s}\}}, \qquad \text{(order 4)}$$

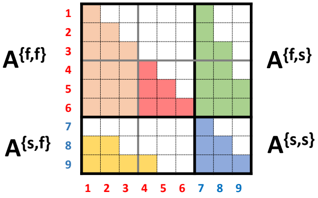
$$\frac{M}{24} = \sum_{\lambda=1}^{M} b^{\{\mathfrak{f}\}\,T} A^{\{\mathfrak{f},\mathfrak{s},\lambda\}} A^{\{\mathfrak{s},\mathfrak{s}\}} c^{\{\mathfrak{s}\}}, \qquad \text{(order 4)}$$

$$\frac{M^3}{24} = \sum_{\lambda=1}^{M} \sum_{k=1}^{M} b^{\{\mathfrak{f}\}\,T} A^{\{\mathfrak{f},\mathfrak{s},\lambda\}} A^{\{\mathfrak{s},\mathfrak{f},k\}} \left((k-1)\mathbb{1} + c^{\{\mathfrak{f}\}}\right). \qquad \text{(order 4)}$$

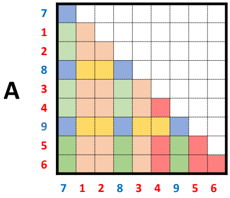
Coupling order conditions in 2-color tree representation.



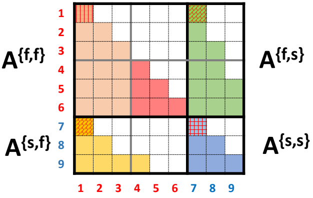
Examining the coupling structure reveals a pattern.



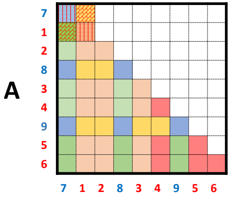
(a) decoupled



(b) permuted decoupled



(c) coupled MrGARK



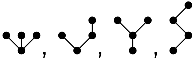
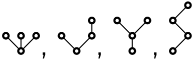
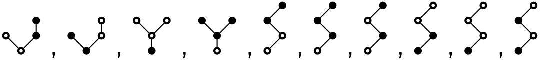
(d) permuted coupled

Decoupled methods are computationally more efficient.

- Opting in for better computational efficiency at the cost of losing *some* stability.
- Decoupled methods have complementary structure in the slow-to-fast and fast-to-slow coupling:

$$\mathbf{A}^{\{\mathfrak{s},\mathfrak{f}\}} \times \mathbf{A}^{\{\mathfrak{f},\mathfrak{s}\}\ T} = \mathbf{0}_{s^{\{\mathfrak{s}\}} \times M s^{\{\mathfrak{f}\}}}.$$

Isolating the slow, fast and coupling error is a challenging task.

- 4 order 4 slow trees: 
- 4 order 4 fast trees: 
- 10 order 4 coupling trees:


Controlling the step sizes by balancing the projected errors:

- Choose macro step size according to traditional error control theory.
- Choose step size ratio M to balance the projected slow and fast errors.

$$
\begin{aligned}
H_{\text{new}} &= \text{fac} \cdot H \cdot \left(\widehat{\varepsilon}_{n+1}\right)^{-\frac{1}{p}}\,, \\
\widehat{\varepsilon}_{n+2}^{\{\mathfrak{s}\}} &= \widehat{\varepsilon}_{n+2}^{\{\mathfrak{f}\}}, \\
M_{\text{new}} &\approx M \cdot \left(\frac{\widehat{\varepsilon}_{n+1}^{\{\mathfrak{f}\}}}{\widehat{\varepsilon}_{n+1}^{\{\mathfrak{s}\}}}\right)^{\frac{1}{q}}\,.
\end{aligned}
$$

Controlling the step sizes by balancing the projected errors vs computational cost:

- Monitor the computational cost of evaluating right-hand-side pieces
- Solve an online univariate optimization to minimize function evaluation cost along with error

$$\min_{H_{\text{new}}, M_{\text{new}}} \frac{t^{\{\mathfrak{s}\}} + M_{\text{new}}\, t^{\{\mathfrak{f}\}}}{H_{\text{new}}} \quad \text{subject to} \quad \widehat{\varepsilon}_{n+2} = 1,$$

$$\min_{M_{\text{new}}} \frac{t^{\{\mathfrak{s}\}} + M_{\text{new}}\, t^{\{\mathfrak{f}\}}}{H} \left(\widehat{\varepsilon}^{\{\mathfrak{s}\}}_{n+1} + \widehat{\varepsilon}^{\{\mathfrak{f}\}}_{n+1} \cdot \frac{M^q}{M_{\text{new}}^q} \right)^{\frac{1}{q+1}} .$$

Overview of type-A Multirate GARK methods developed:

Order	Fast Method	Slow Method	Stiff Accuracy	FSAL FSAL	$H - M$ Adaptive	High-Order Coupling
2	Ralston's ERK2(1)2 {Ralston, 1962}	Ralston's ERK2(1)2 {Ralston, 1962}			✓	✓
2	SDIRK2(1)2 {Alexander, 1977}	Ralston's ERK2(1)2 {Ralston, 1962}	✓		✓	
2	Ralston's ERK2(1)2 {Ralston, 1962}	SDIRK2(1)2 {Alexander, 1977}	✓		✓	
3	Ralston's ERK3(2)3 {Ralston, 1962}	Ralston's ERK3(2)3 {Ralston, 1962}			✓	
3	SDIRK3(2)3 {Alexander, 1977}	Ralston's ERK3(2)3 {Ralston, 1962}	✓		✓	
3	Ralston's ERK3(2)3 {Ralston, 1962}	SDIRK3(2)3 {Alexander, 1977}	✓		✓	
3	Custom ERK3(2)3	Custom ERK3(2)3			✓	✓
4	ERK4(3)5 {Sofroniou and Spaletta, 2004}	ERK4(3)5 {Sofroniou and Spaletta, 2004}		✓	✓	
4	Fehlberg's ERK4(5)6 {Fehlberg, 1969}	SDIRK4(3)5 {Kennedy and Carpenter, 2016}	✓		✓	
4	ERK4(3)4 {Sofroniou and Spaletta, 2004}	Custom SDIRK4(3)6	✓		✓	

Overview of type-S Multirate GARK methods developed:

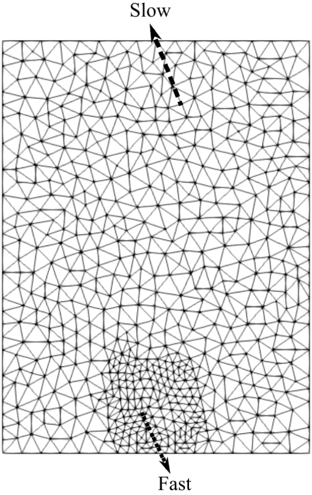
Order	Fast Method	Slow Method	$H - M$ Adaptivity
2	Ralston's ERK2(1)2 {Ralston, 1962}	Ralston's ERK2(1)2 {Ralston, 1962}	✓
3	Ralston's ERK3(2)3	Ralston's ERK3(2)3	✓
3	SDIRK3(2)3	Ralston's ERK3(2)3 {Ralston, 1962}	✓
3	Ralston's ERK3(2)3 {Ralston, 1962}	SDIRK3(2)3	✓

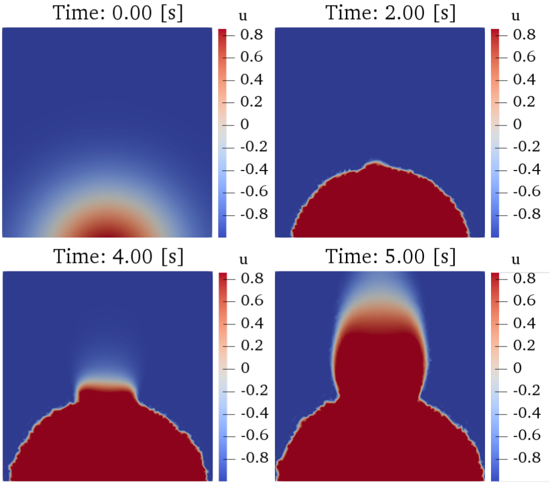
Component partitioning test

We use the reaction-diffusion equation:

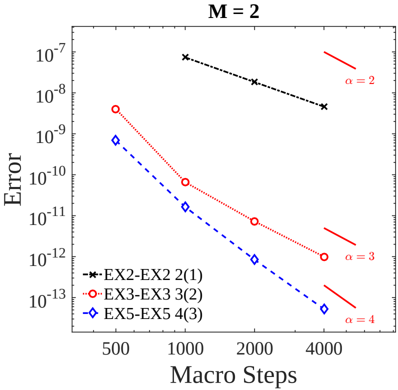
$$u_t = \nabla \cdot \left(D(x,y)\nabla u\right) + 10\left(1-u^2\right)(u+0.6), \quad x,y \in \Omega,$$
$$u(x,y,0) = 2\exp\left(-10(x-0.5)^2 - 10(y+0.1)^2\right),$$
$$D(x,y) = 0.1\sum_{i=1}^{3} e^{-100(x-0.5)^2+(y-y_i)^2},$$
$$D(x,y)\nabla u \cdot \vec{n} = 0, \qquad x,y \in \partial\Omega,\ t \in [0,t_F].$$

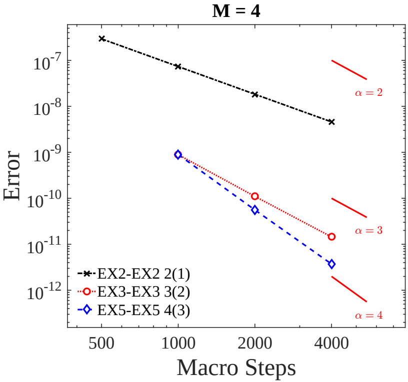
Slow and fast partitions are defined on mesh points.





Convergence diagram for component partitioning test





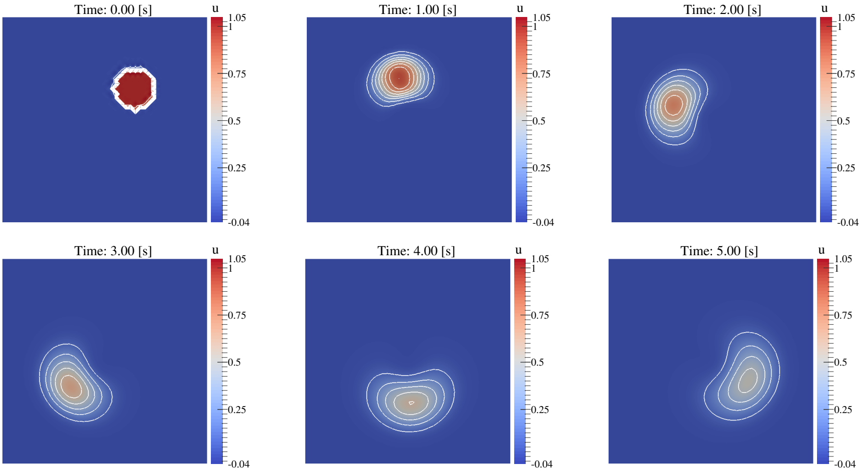
Additive partitioning test

We use the advection-diffusion equation:

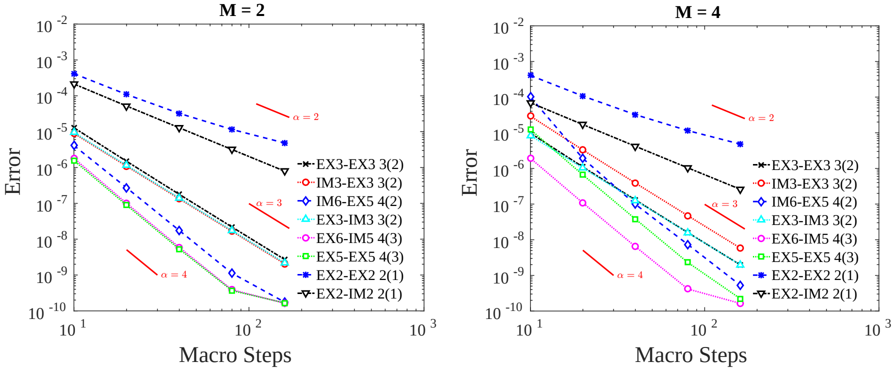
$$u_t - \varepsilon \nabla^2 u + w \cdot \nabla u = 0 \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega,$$
$$w = \begin{bmatrix} 2y(1-x^2) \\ -2x(1-y^2) \end{bmatrix}.$$

A Streamline Upwind Petrov-Galerkin (SUPG) spatial discretization is used, which leads to a semi-discrete system of linear ODEs:

$$\mathbf{M}^h u_t^h = \mathbf{A}\, u^h + (\vec{n} + \vec{n}^{stab})\, u^h,$$


Time: 0.00 [s]
Time: 1.00 [s]
Time: 2.00 [s]
Time: 3.00 [s]
Time: 4.00 [s]
Time: 5.00 [s]
u
1.05
1
0.75
0.5
0.25
-0.04

Convergence diagram for additive partitioning test



Conclusions

- MR GARK EX-EX, EX-IM and IM-EX methods of up to order 4
- Applied to component and operator splitting systems
- Developed adaptivity strategies

- What about stability considerations and Implicit-Implicit methods ?
  - Steven Robert's talk on Friday (MS390)

- What if you need full control over the fast system ?
  - Adrian Sandu's talk on Friday (MS358)
  - `arxiv.org/abs/1802.07188`
  - `arxiv.org/abs/1812.00808`

- Where can I find the coefficients ?
  - `arxiv.org/abs/1804.07716`
  - `wolfr.am/BsWkAHiM`
  - MatlODE package

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