Implicit Multirate Generalized Additive Runge-Kutta Methods

An analysis of stability

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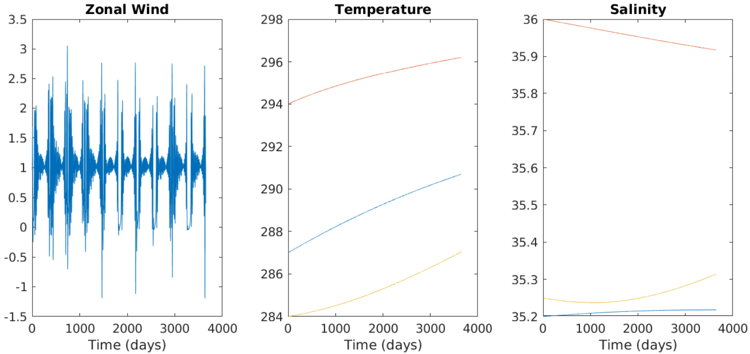
Why use multirate methods?

Many dynamical systems exhibit multiple characteristic timescales.

$$y' = f(y) = f^{\{\mathfrak{f}\}}(y) + f^{\{\mathfrak{s}\}}(y)$$

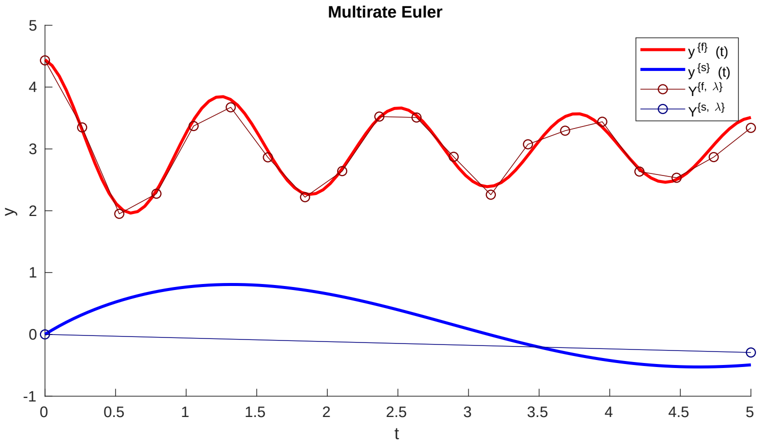
Example: Wind, temperature, and salinity in a simplified climate model.



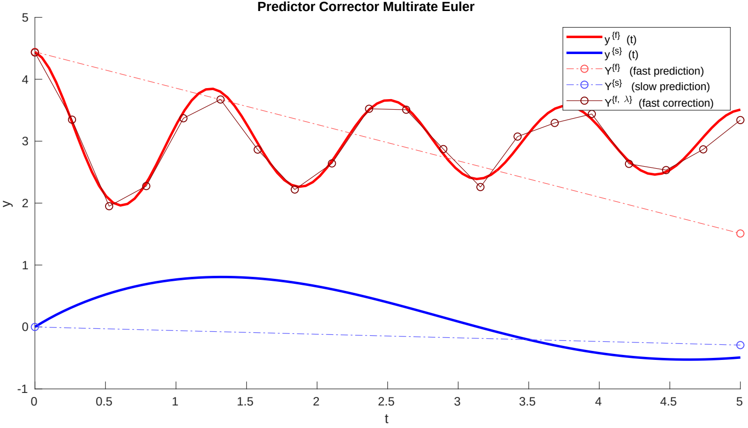
What are multirate methods?

- Integrate the slow partition with Runge–Kutta method $\left(A^{\{\mathfrak{s},\mathfrak{s}\}}, b^{\{\mathfrak{s}\}}\right)$ using a stepsize H
- Integrate the fast partition with Runge–Kutta method $\left(A^{\{\mathfrak{f},\mathfrak{f}\}}, b^{\{\mathfrak{f}\}}\right)$ using a stepsize $h = H/M$
- M is called the multirate ratio
- Coupling information needs to be shared between slow and fast integrations
- Why use implicit method for both fast and slow dynamics?
  - Adapting timesteps to accuracy requirements can improve efficiency
  - Decoupled methods simplify Newton iterations
  - Certain parts of system may slow down Newton iterations

Multirate Runge–Kutta



Predictor Corrector Multirate Runge–Kutta



GARK provides a theoretical foundation I

A generalized-structure additively partitioned Runge–Kutta (GARK) method with two partitions reads

$$Y_i^{\{\mathfrak{f}\}} = y_n + H \sum_{j=1}^{s^{\{\mathfrak{f}\}}} a_{i,j}^{\{\mathfrak{f},\mathfrak{f}\}} f^{\{\mathfrak{f}\}}\left(Y_j^{\{\mathfrak{f}\}}\right) + H \sum_{j=1}^{s^{\{\mathfrak{s}\}}} a_{i,j}^{\{\mathfrak{f},\mathfrak{s}\}} f^{\{\mathfrak{s}\}}\left(Y_j^{\{\mathfrak{s}\}}\right), \qquad i = 1, \ldots s^{\{\mathfrak{f}\}},$$

$$Y_i^{\{\mathfrak{s}\}} = y_n + H \sum_{j=1}^{s^{\{\mathfrak{f}\}}} a_{i,j}^{\{\mathfrak{s},\mathfrak{f}\}} f^{\{\mathfrak{f}\}}\left(Y_j^{\{\mathfrak{f}\}}\right) + H \sum_{j=1}^{s^{\{\mathfrak{s}\}}} a_{i,j}^{\{\mathfrak{s},\mathfrak{s}\}} f^{\{\mathfrak{s}\}}\left(Y_j^{\{\mathfrak{f}\}}\right), \qquad i = 1, \ldots s^{\{\mathfrak{s}\}},$$

$$y_{n+1} = y_n + H \sum_{j=1}^{s^{\{\mathfrak{f}\}}} b_j^{\{\mathfrak{f}\}} f^{\{\mathfrak{f}\}}\left(Y_j^{\{\mathfrak{f}\}}\right) + H \sum_{j=1}^{s^{\{\mathfrak{s}\}}} b_j^{\{\mathfrak{s}\}} f^{\{\mathfrak{s}\}}\left(Y_j^{\{\mathfrak{s}\}}\right).$$

The corresponding tableau is

$$\begin{array}{c|c} \mathbf{A}^{\{\mathfrak{f},\mathfrak{f}\}} & \mathbf{A}^{\{\mathfrak{f},\mathfrak{s}\}} \\ \hline \mathbf{A}^{\{\mathfrak{s},\mathfrak{f}\}} & \mathbf{A}^{\{\mathfrak{s},\mathfrak{s}\}} \\ \hline \mathbf{b}^{\{\mathfrak{f}\}\,T} & \mathbf{b}^{\{\mathfrak{s}\}\,T} \end{array}.$$

Often assume internal consistency: $c^{\{\mathfrak{f}\}} \equiv A^{\{\mathfrak{f},\mathfrak{f}\}} \mathbb{1}_{s^{\{\mathfrak{f}\}}} = A^{\{\mathfrak{f},\mathfrak{s}\}} \mathbb{1}_{s^{\{\mathfrak{s}\}}}$ and $c^{\{\mathfrak{s}\}} \equiv A^{\{\mathfrak{s},\mathfrak{f}\}} \mathbb{1}_{s^{\{\mathfrak{f}\}}} = A^{\{\mathfrak{s},\mathfrak{s}\}} \mathbb{1}_{s^{\{\mathfrak{s}\}}}$.

GARK provides a theoretical foundation II

MrGARK:

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

Predictor corrector MrGARK:

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

Substitute these structures into GARK order conditions and stability.

Even linear stability analysis is challenging

"...little theoretical study has been made on the accuracy and stability of such methods." Gear, *Multirate methods for ordinary differential equations*

"Stability properties of various multirate schemes have been disussed .... However, most of these discussions are not very detailed, nor very conclusive." Kværnø, "Stability of multirate Runge–Kutta schemes"

"Even though the multirate scheme considered in this paper is quite simple, the stability analysis will turn out to be complicated." Hundsdorfer & Savcenco, "Analysis of a Multirate Theta-method for Stiff ODEs"

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How can linear stability be assessed?

For a simple test problem, find conditions that ensure errors are not amplified from step to step. There are many choices of test problems:

- Scalar test problem:
$$y' = \lambda^{\{\mathfrak{f}\}} y + \lambda^{\{\mathfrak{s}\}} y.$$
- 2D test problem:
$$\begin{bmatrix} y^{\{\mathfrak{f}\}} \\ y^{\{\mathfrak{s}\}} \end{bmatrix}' = \underbrace{\begin{bmatrix} \lambda^{\{\mathfrak{f}\}} & \eta^{\{\mathfrak{s}\}} \\ \eta^{\{\mathfrak{f}\}} & \lambda^{\{\mathfrak{s}\}} \end{bmatrix}}_{\Lambda} \begin{bmatrix} y^{\{\mathfrak{f}\}} \\ y^{\{\mathfrak{s}\}} \end{bmatrix}.$$
- 2x2 block test problem:
$$\begin{bmatrix} y^{\{\mathfrak{f}\}} \\ y^{\{\mathfrak{s}\}} \end{bmatrix}' = \begin{bmatrix} \Lambda^{\{\mathfrak{f}\}} & E^{\{\mathfrak{s}\}} \\ E^{\{\mathfrak{f}\}} & \Lambda^{\{\mathfrak{s}\}} \end{bmatrix} \begin{bmatrix} y^{\{\mathfrak{f}\}} \\ y^{\{\mathfrak{s}\}} \end{bmatrix}.$$
- And others...

Comparison of stability

Scalar test problem

- Let $z^{\{\mathfrak{f}\}} = H\lambda^{\{\mathfrak{f}\}}$ and $z^{\{\mathfrak{s}\}} = H\lambda^{\{\mathfrak{s}\}}$.
- A-Stability: $\left|R_1(z^{\{\mathfrak{f}\}}, z^{\{\mathfrak{s}\}})\right| \leq 1$ for all $z^{\{\mathfrak{f}\}}, z^{\{\mathfrak{s}\}} \in \mathbb{C}^-$
- L-Stability: A-stability and $R_1 \to 0$ as $z^{\{\mathfrak{f}\}} \to -\infty$ and $z^{\{\mathfrak{s}\}} \to -\infty$

2D test problem

- Let $Z = H\Lambda$.
- A-Stability: $R_2(Z)$ power bounded for all Z exponentially bounded with $z^{\{\mathfrak{f}\}}, z^{\{\mathfrak{s}\}} \in \mathbb{C}^-$
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Algebraic stability

- If $f^{\{\mathfrak{f}\}}$ and $f^{\{\mathfrak{s}\}}$ are dissipative, then $\|y_{n+1} - \widetilde{y}_{n+1}\| \leq \|y_n - \widetilde{y}_n\|$.

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Our findings on stability analysis

- E-Polynomial can be generalized for scalar test problem
- The scalar and 2D stability functions are related:

$$R_1\left(z^{\{\mathfrak{f}\}}, z^{\{\mathfrak{s}\}}\right) = \begin{bmatrix} 1 & 1 \end{bmatrix} R_2(Z) \begin{bmatrix} \alpha \\ 1-\alpha \end{bmatrix}.$$

- There are algebraically stable methods that are conditionally stable for the 2D problem.

Theorem

If a GARK method is A-stable with respect to the 2D test problem, then it is A-stable with respect to the scalar test problem.

Theorem

A decoupled GARK method is conditionally stable for the 2D test problem.

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GARK stability hierarchy

$$
\begin{tikzcd}
\text{2D L-Stability} \arrow[r, Rightarrow] \arrow[dr, Rightarrow, "?"] & \text{2D A-Stability} \arrow[dr, Rightarrow] & \\
& \text{Scalar L-Stability} \arrow[r, Rightarrow] & \text{Scalar A-Stability} \\
& \text{Algebraic Stability} \arrow[ur, Rightarrow] &
\end{tikzcd}
$$

New general stability function for predictor corrector MrGARK

Starting with the GARK scalar stability function

$$R_1\left(z^{\{\mathfrak{f}\}}, z^{\{\mathfrak{s}\}}\right) = 1 + \mathbf{b}^T \mathbf{Z}(I - \mathbf{A}\mathbf{Z})^{-1}\mathbb{1}, \qquad \mathbf{Z} = \begin{bmatrix} z^{\{\mathfrak{f}\}} I & 0 \\ 0 & z^{\{\mathfrak{s}\}} I \end{bmatrix},$$

we can derive the stability function for a predictor corrector MrGARK method

$$\begin{aligned} R_1\left(z^{\{\mathfrak{f}\}}, z^{\{\mathfrak{s}\}}\right) &= R\left(\frac{z^{\{\mathfrak{f}\}}}{M}\right)^M \\ &\quad + z^{\{\mathfrak{s}\}} \left(b^T + \frac{z^{\{\mathfrak{f}\}}}{M} b^T \left(I_{s\times s} - \frac{z^{\{\mathfrak{f}\}}}{M} A \right)^{-1} \sum_{\lambda=1}^{M} R\left(\frac{z^{\{\mathfrak{f}\}}}{M}\right)^{M-\lambda} A^{\{\mathfrak{f},\mathfrak{s},\lambda\}} \right) R_{\text{int}}(z), \end{aligned}$$

with $z = z^{\{\mathfrak{f}\}} + z^{\{\mathfrak{s}\}}$.

Stability guides method derivation

- Scalar stability most practical, but 2D more insightful
- Interesting result at first order:

Theorem

An internally consistent MrGARK method of order exactly one is conditionally stable for all but a finite number of multirate ratios.

- Methods derived up to order four
  - Both coupling strategies
  - Based on SDIRK methods

Stability of new fourth order method

$$\mathcal{S}^{1\mathrm{D}}_{\alpha,\rho} = \left\{ z^{\{\mathfrak{s}\}} \in \mathbb{C} \,\middle|\, \left| R_1\left(z^{\{\mathfrak{f}\}}, z^{\{\mathfrak{s}\}}\right) \right| \leq 1, \forall z^{\{\mathfrak{f}\}} \in \mathbb{C}^- : \left| z^{\{\mathfrak{f}\}} \right| \leq \rho, \left| \arg\left(-z^{\{\mathfrak{f}\}}\right) \right| \leq \alpha \right\}$$

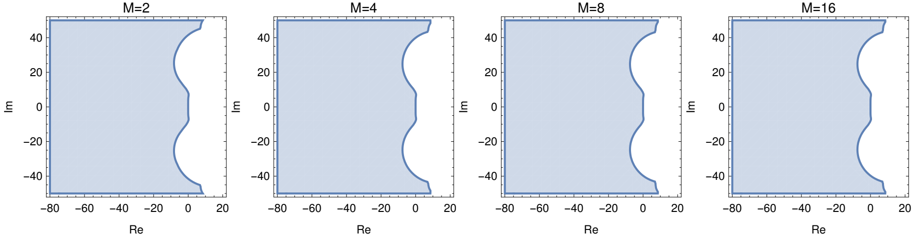
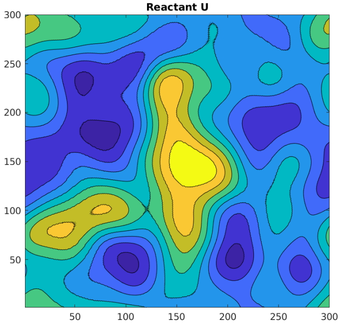
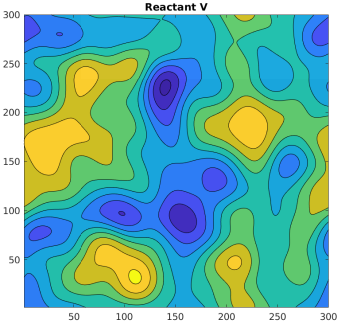


Figure: Stability region $\mathcal{S}^{1\mathrm{D}}_{80^\circ,\infty}$ for different M

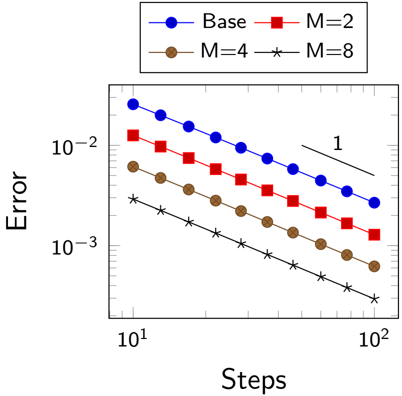
The Gray–Scott model

$$\underbrace{\begin{bmatrix} u \\ v \end{bmatrix}'}_{y'} = \underbrace{\begin{bmatrix} \nabla \cdot (\varepsilon_u \nabla u) \\ \nabla \cdot (\varepsilon_v \nabla v) \end{bmatrix}}_{f^{\{\mathfrak{s}\}}(y)} + \underbrace{\begin{bmatrix} -uv^2 + \mathfrak{f}(1-u) \\ uv^2 - (\mathfrak{f} + \mathfrak{k}) \end{bmatrix}}_{f^{\{\mathfrak{f}\}}(y)}$$

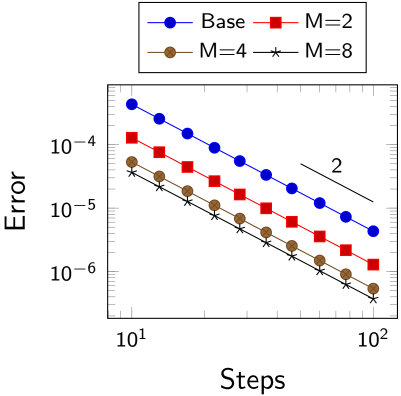




Gray–Scott convergence test I

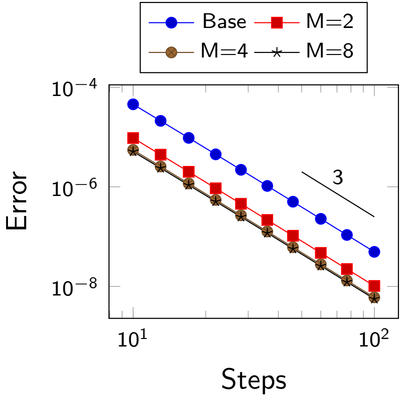


(a) First order MrGARK

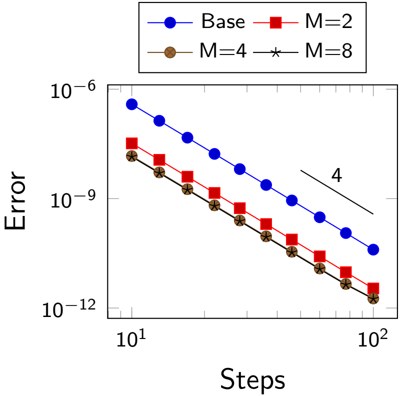


(b) Second order predictor corrector MrGARK

Gray–Scott convergence test II



(c) Third order predictor corrector MrGARK



(d) Fourth order predictor corrector MrGARK

Conclusions

- Linear stability is surprisingly challenging for multirate methods.
- GARK provides overarching framework to analyze multriate Runge–Kutta methods.
  - Order conditions
  - Stability
- We derive **general** stability results and fundamental stability limitations.
- New methods are derived up to order four.

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Roberts, S., Sarshar, A. & Sandu, A. Coupled Multirate Infinitesimal GARK Schemes for Stiff Systems with Multiple Time Scales. *arXiv preprint arXiv:1812.00808* (2018).

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Thank you

Website: `https://steven-roberts.github.io/`

Related work

- Explicit-explicit, implicit-explicit, and explicit-implicit MrGARK methods:
  Sarshar, A. *et al.* Design of High-Order Decoupled Multirate GARK Schemes. *arXiv preprint arXiv:1804.07716* (2018)
- MrGARK methods as $M \to \infty$ become infinitesimal methods:
  Roberts, S. *et al.* Coupled Multirate Infinitesimal GARK Schemes for Stiff Systems with Multiple Time Scales. *arXiv preprint arXiv:1812.00808* (2018)