Implicit Multirate GARK Methods

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Compute the Future!

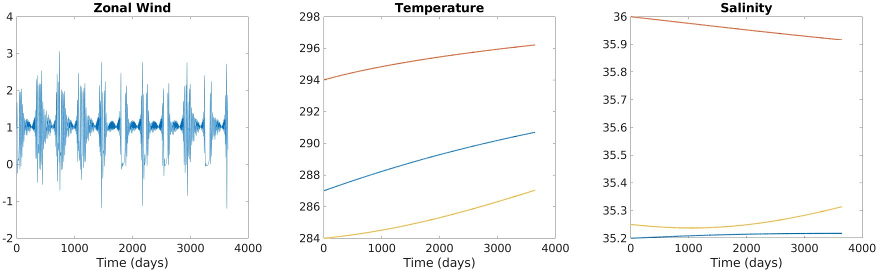
VIRGINIA TECH

Why use multirate methods?

- Many dynamical systems exhibit multiple characteristic timescales.

$$y' = f(y) = f^{\{\mathfrak{f}\}}(y) + f^{\{\mathfrak{s}\}}(y), \qquad y(t_0) = y_0$$

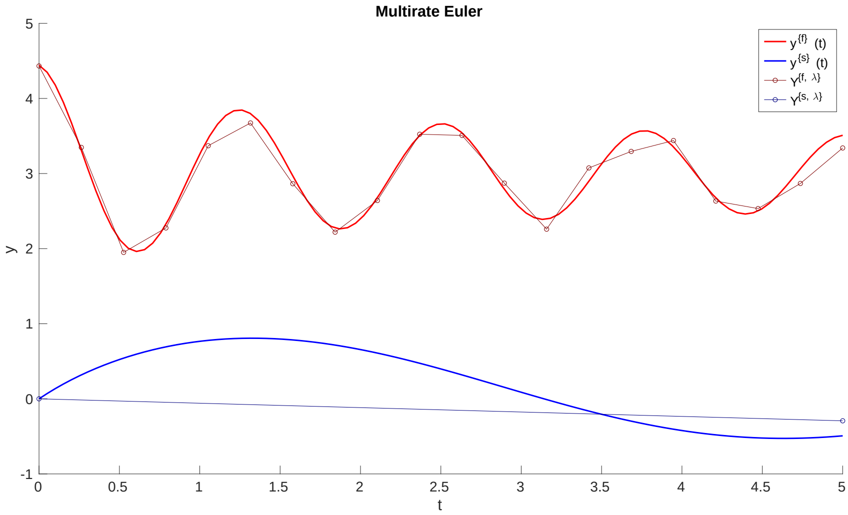
- Example: Wind, temperature, and salinity in a simplified climate model



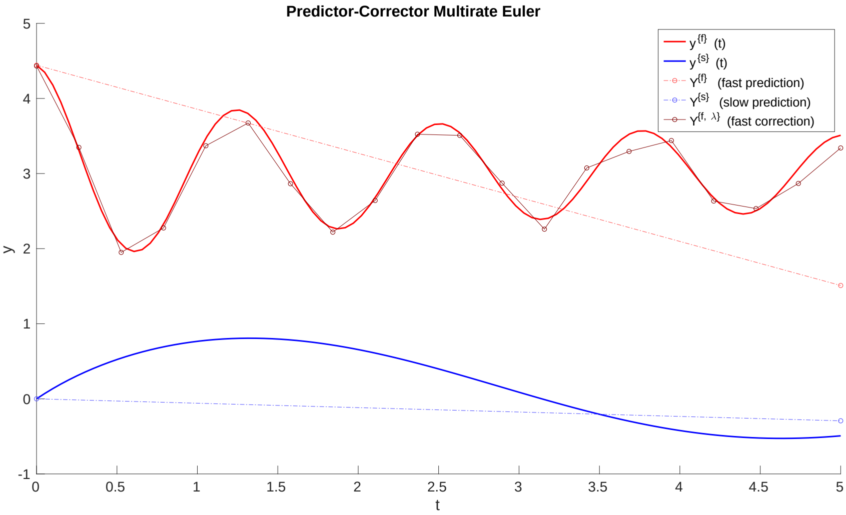
What are multirate methods?

- 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

- A generalized-structure additively partitioned Runge–Kutta (GARK)[1] method with two partitions reads

$$
\begin{aligned}
Y_i^{\{\mathfrak{f}\}} &= y_n + H \sum_{j=1}^{s^{\{\mathfrak{f}\}}} a_{i,j}^{\{\mathfrak{f},\mathfrak{f}\}} f^{\{\mathfrak{f}\}}\left(Y_j^{\{\mathfrak{f}\}}\right) + H \sum_{j=1}^{s^{\{\mathfrak{s}\}}} a_{i,j}^{\{\mathfrak{f},\mathfrak{s}\}} f^{\{\mathfrak{s}\}}\left(Y_j^{\{\mathfrak{s}\}}\right), \qquad i = 1, \dots s^{\{\mathfrak{f}\}}, \\
Y_i^{\{\mathfrak{s}\}} &= y_n + H \sum_{j=1}^{s^{\{\mathfrak{f}\}}} a_{i,j}^{\{\mathfrak{s},\mathfrak{f}\}} f^{\{\mathfrak{f}\}}\left(Y_j^{\{\mathfrak{f}\}}\right) + H \sum_{j=1}^{s^{\{\mathfrak{s}\}}} a_{i,j}^{\{\mathfrak{s},\mathfrak{s}\}} f^{\{\mathfrak{s}\}}\left(Y_j^{\{\mathfrak{f}\}}\right), \qquad i = 1, \dots s^{\{\mathfrak{s}\}}, \\
y_{n+1} &= y_n + H \sum_{j=1}^{s^{\{\mathfrak{f}\}}} b_j^{\{\mathfrak{f}\}} f^{\{\mathfrak{f}\}}\left(Y_j^{\{\mathfrak{f}\}}\right) + H \sum_{j=1}^{s^{\{\mathfrak{s}\}}} b_j^{\{\mathfrak{s}\}} f^{\{\mathfrak{s}\}}\left(Y_j^{\{\mathfrak{s}\}}\right).
\end{aligned}
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$$

- 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}
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\end{array}.
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- 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 $c^{\{\mathfrak{s}\}} \equiv A^{\{\mathfrak{s},\mathfrak{f}\}} \mathbb{1}_{s^{\{\mathfrak{f}\}}} = A^{\{\mathfrak{s},\mathfrak{s}\}} \mathbb{1}_{s^{\{\mathfrak{s}\}}}$

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

Multirate Runge–Kutta methods are GARK methods

Standard MrGARK[2]:

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

Predictor-corrector MrGARK:

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

[2] Günther & Sandu, "Multirate generalized additive Runge Kutta methods".

Challenges in developing implicit multirate methods

- Order conditions grow quickly in quantity and complexity.
- How can we balance the cost of solving nonlinear equations with stability?
- Linear stability is surprisingly complex and there are many open research questions.
- Many results on stability are limited to particular methods.

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"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"

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"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"

MrGARK Order Conditions

- The MrGARK order conditions follow from substituting tableau structure into GARK order conditions.
- Assuming internal consistency, the cummulative number of order conditions is

Method	Order 1	Order 2	Order 3	Order 4
Standard MrGARK[3]	2	4	10	36
Predictor-corrector MrGARK	2	4	9	29

- Predictor-corrector order conditions more precise than usual technique of finding dense output of sufficient accuracy. The third order coupling condition, for example, is

$$\frac{M}{6} = \sum_{\lambda=1}^{M} b^T A^{\{\mathfrak{f},\mathfrak{s},\lambda\}} c.$$

[3] Sarshar *et al.*, "Design of High-Order Decoupled Multirate GARK Schemes".

Newton iterations

- The most computationally expensive part of implicit multirate methods
- Decoupled methods
  - Implicitness only comes from base methods
  - Only requires decompositions of $I - h\gamma J^{\{\mathfrak{f}\}}$ and $I - H\gamma J^{\{\mathfrak{s}\}}$
  - Efficient for component partitioned problems
- Coupled methods
  - Fast and slow stages solved together
  - Potentially very expensive
  - Practical methods require linear solves no more expensive than those of their singlerate counterparts.
  - Potential for better stability

Scalar stability function

- We can generalize the Dahlquist test problem by

$$y' = f^{\{\mathfrak{f}\}}(y) + f^{\{\mathfrak{s}\}}(y) \xRightarrow{\text{linearize}} y' = J^{\{\mathfrak{f}\}}\, y + J^{\{\mathfrak{s}\}}\, y \xRightarrow{\text{change basis*}} y' = \lambda^{\{\mathfrak{f}\}}\, y + \lambda^{\{\mathfrak{s}\}}\, y$$

[4] Gear, *Multirate methods for ordinary differential equations.*

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- *Only if $J^{\{\mathfrak{f}\}}(y)$ and $J^{\{\mathfrak{s}\}}(y)$ are simultaneously triangularizable
- *Multirate methods are not invariant under change of basis[4].

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- *Only if $J^{\{\mathfrak{f}\}}(y)$ and $J^{\{\mathfrak{s}\}}(y)$ are simultaneously triangularizable
- *Multirate methods are not invariant under change of basis[4].
- Applying the scalar test problem yields a stability function $R_1(z^{\{\mathfrak{f}\}}, z^{\{\mathfrak{s}\}})$ with $z^{\{\mathfrak{f}\}} = H\lambda^{\{\mathfrak{f}\}}$ and $z^{\{\mathfrak{s}\}} = H\lambda^{\{\mathfrak{s}\}}$.
- Stability criteria
  - 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 $R_1(\infty, z^{\{\mathfrak{s}\}}) = R_1(z^{\{\mathfrak{f}\}}, \infty) = 0$
  - A(α)- and L(α)-stability: A 4D wedge fits in stability region

[4] Gear, *Multirate methods for ordinary differential equations.*

2D stability function

- At least two variables are needed for a component partitioned test problem:

$$\begin{bmatrix} y^{\{\mathfrak{f}\}} \\ y^{\{\mathfrak{s}\}} \end{bmatrix}' = \underbrace{\begin{bmatrix} \lambda^{\{\mathfrak{f}\}} & \eta^{\{\mathfrak{s}\}} \\ \eta^{\{\mathfrak{f}\}} & \lambda^{\{\mathfrak{s}\}} \end{bmatrix}}_{\Lambda} \begin{bmatrix} y^{\{\mathfrak{f}\}} \\ y^{\{\mathfrak{s}\}} \end{bmatrix}.$$

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- Applying the scalar test problem yields a stability function $R_2(Z) \in \mathbb{C}^{2 \times 2}$ with $Z = H\Lambda$.
- Stability criteria
  - A-Stability: $R_2(Z)$ power bounded for all Z exponentially bounded with $z^{\{\mathfrak{f}\}}, z^{\{\mathfrak{s}\}} \in \mathbb{C}^-$
  - Many have restricted the problem to real entries to simplify analysis.

Even more ways to assess stability

- Others have looked at block test problems:

$$\begin{bmatrix} y^{\{\mathfrak{f}\}} \\ y^{\{\mathfrak{s}\}} \end{bmatrix}' = \begin{bmatrix} \Lambda^{\{\mathfrak{f}\}} & E^{\{\mathfrak{s}\}} \\ E^{\{\mathfrak{f}\}} & \Lambda^{\{\mathfrak{s}\}} \end{bmatrix} \begin{bmatrix} y^{\{\mathfrak{f}\}} \\ y^{\{\mathfrak{s}\}} \end{bmatrix}.$$

- Algebraic stability: If $f^{\{\mathfrak{f}\}}$ and $f^{\{\mathfrak{s}\}}$ are dissipative, then $\|y_{n+1} - \widetilde{y}_{n+1}\| \leq \|y_n - \widetilde{y}_n\|$.
- **Which stability cirteria should we use?**

Our findings on stability analysis

- E-Polynomial can be generalized for scalar test problem

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

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

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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.

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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 real 2D test problem.

GARK stability hierarchy

$$
\begin{tikzcd}
\text{2D A-stability} \arrow[r, Rightarrow] \arrow[dr, Rightarrow] & \text{Real 2D A-stability} & \\
\text{Algebraic stability} \arrow[r, Rightarrow] & \text{Scalar A-stability} \arrow[r, Rightarrow] & \text{Scalar A}(\alpha)\text{-stability} \\
\text{Scalar L-stability} \arrow[r, Rightarrow] \arrow[ur, Rightarrow] & \text{Scalar L}(\alpha)\text{-stability} \arrow[ur, Rightarrow] &
\end{tikzcd}
$$

- In general, no implication arrows are reversible.

New general stability function for predictor-corrector MrGARK

- Using the particular structure of predictor-corrector coupling, we found the scalar stability function is

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

  with $z = z^{\{\mathfrak{f}\}} + z^{\{\mathfrak{s}\}}$.
- If $R(\infty) = 0$ for the base method, then the condition

$$A^{\{\mathfrak{f},\mathfrak{s},\lambda\}} A^{-1} \mathbb{1}_s = \mathbb{1}_s$$

  ensures $R_1(\infty, z^{\{\mathfrak{s}\}}) = 0$.

First order multirate methods

- Many coupling structures have been explored.
- Surprising stability limitation:

Theorem

An internally consistent MrGARK method of order exactly one has conditional scalar stability for all but a finite number of multirate ratios.

Higher order multirate methods

- We found a decoupled multirate midpoint method that preserves the algebraic stability, symmetry, and symplecticity of the midpoint method.
- New predictor-corrector up to order four that are close to scalar A-stable:

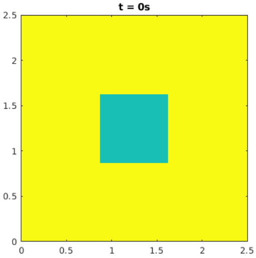
Method	$M = 2$	$M = 3$	$M = 4$	$M = 8$	$M = 16$	$M = 32$
SDIRK 2	84.6°	83.5°	83.2°	83.0°	83.0°	83.0°
SDIRK 3	88.6°	87.8°	87.3°	86.9°	86.8°	86.8°
SDIRK 4	81.7°	81.2°	81.2°	81.2°	81.2°	81.2°

Table: Scalar $L(\alpha)$-stability for new predictor-corrector MrGARK methods.

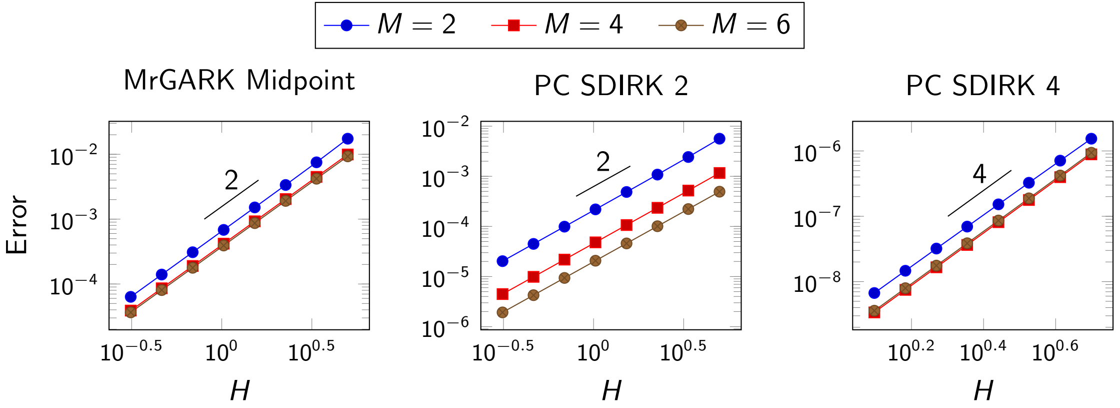
- Internal consistency seems to inhibit stability.

The Gray–Scott model

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

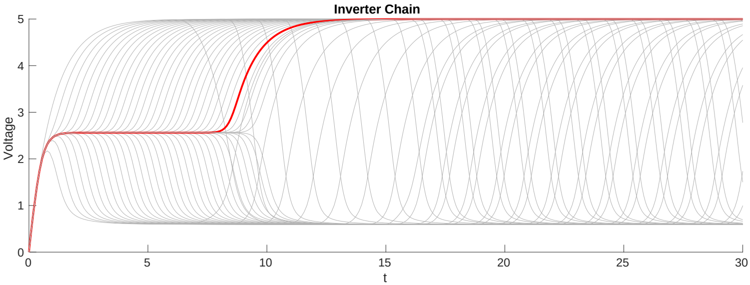


Gray–Scott convergence test



Inverter chain: a classic multirate test problem

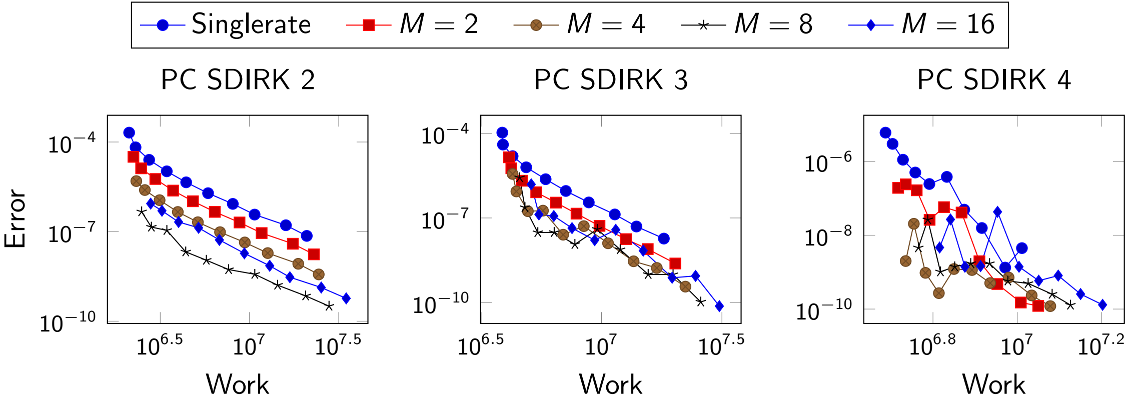
$$
\begin{aligned}
U_1' &= U_{op} - U_1 - g(U_{in}, U_1, U_0), \\
U_i' &= U_{op} - U_i - g(U_{i-1}, U_i, U_0), \qquad i = 2, \dots m, \\
g(U_g, U_D, U_S) &= (\max(U_G - U_S - U_T, 0))^2 - (\max(U_G - U_D - U_T, 0))^2
\end{aligned}
$$



Setup for inverter chain performace results

- Dynamic partitioning is used to select fast parts of circuit
- Performance depends heavily on implementation details
  - Linear solver
  - Stage value predictor
  - Newton tolerances
  - Programming language
- Work is measured by accumulating the dimension of each linear solve performed across integration.

Inverter chain performance results



Conclusions

- Linear stability is surprisingly challenging for multirate methods.
- GARK provides overarching framework to analyze multirate 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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Questions?

- Slides available at `https://steven-roberts.github.io/`