Implicit Multirate GARK Methods for Stiff, Multiscale ODEs

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Abstract

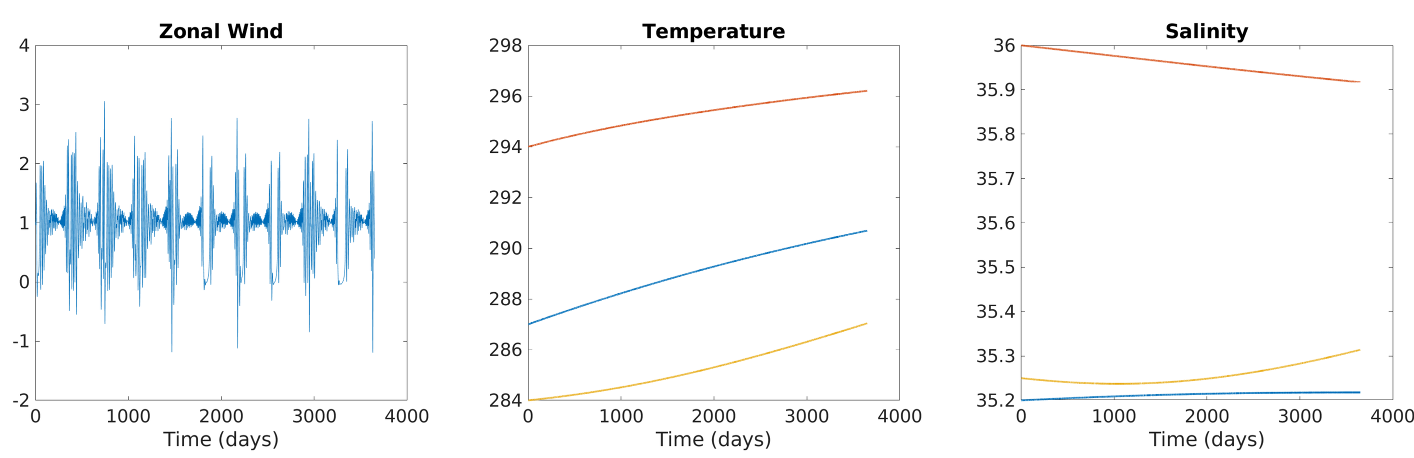
This work considers Multirate General-structure Additive Runge–Kutta (MrGARK) methods [1] for solving stiff systems of ordinary differential equations (ODEs) with multiple time scales. These methods treat different partitions of the system with different timesteps for a more targeted and efficient solution compared to singlerate approaches. With implicit methods used across all partitions, methods must find a balance between stability and the cost of solving nonlinear equations. New implicit multirate methods up to fourth order are derived, and their accuracy and efficiency properties are validated with numerical tests.

Objective

We seek to develop numerical methods to efficiently integrate stiff systems of ODEs:

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

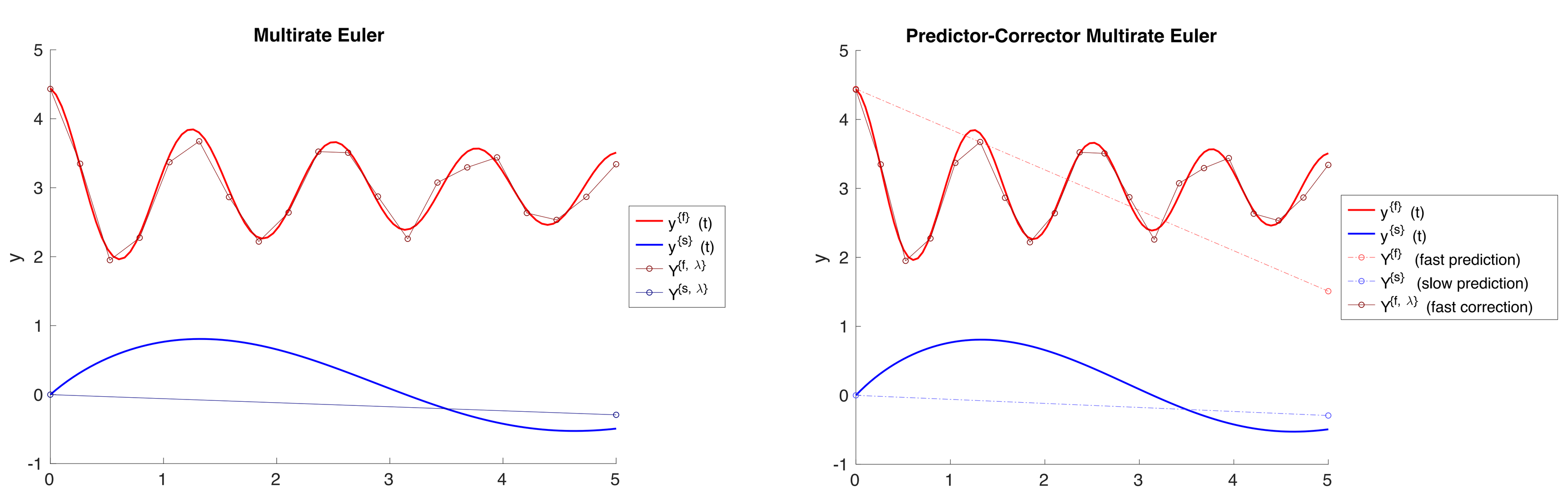
Our focus in on problems where certain parts of the system evolve at very different rates than others. Here the fast dynamics are described by $f^{\{f\}}$, and the slow dynamics are described by $f^{\{s\}}$. Examples include chemical reactions, fluid flow, electric circuits, and many other physical phenomena. The figure below shows the multiscale behavior of a simple climate model.



Multirate GARK Methods

Singlerate	Multirate
• Traditional time integration methods can be inefficient for multiscale problems • A single, global timestep must accommodate the fastest or stiffest dynamics	• Multirate methods use different timesteps for different partitions of an ODE • Stability analysis not well understood • Few high order methods

We use the General-structure Additive Runge–Kutta (GARK) framework [2] to create and analyze new implicit multirate Runge–Kutta methods. The methods integrate $f^{\{s\}}$ with a macro-step H and $f^{\{f\}}$ with a micro-step $h = H/M$. We consider two main types of coupling structures: standard and predictor-corrector.



Example Method: Multirate Midpoint

$$y_{n+\lambda/M} = y_{n+(\lambda-1)/M} + h\, f^{\{f\}}\left(\frac{y_{n+\lambda/M} + y_{n+(\lambda-1)/M}}{2}\right), \qquad \lambda = 1, \dots, \frac{M}{2},$$

$$\tilde{y}_{n+1/2} = y_{n+1/2} + H\, f^{\{s\}}\left(\frac{\tilde{y}_{n+1/2} + y_{n+1/2}}{2}\right),$$

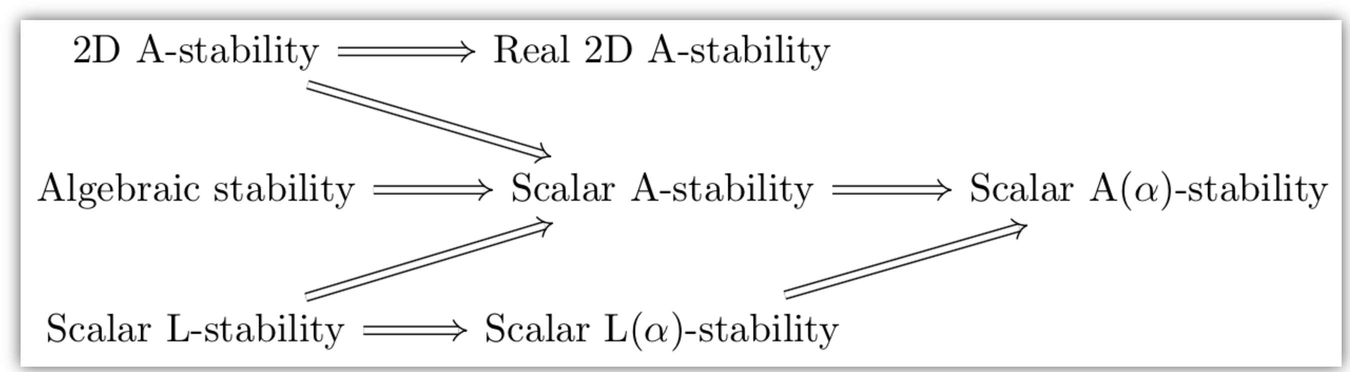
$$\tilde{y}_{n+\lambda/M} = \tilde{y}_{n+(\lambda-1)/M} + h\, f^{\{f\}}\left(\frac{\tilde{y}_{n+\lambda/M} + \tilde{y}_{n+(\lambda-1)/M}}{2}\right), \qquad \lambda = \frac{M}{2} + 1, \dots, M$$

Stability Analysis Results

- Do small perturbations in initial conditions lead to small changes in trajectory?
- The stability of multirate schemes is significantly more complicated than singlerate schemes.
- It not only depends on method coefficients but also the linear test problem:

$$y' = \lambda^{\{f\}}\, y + \lambda^{\{s\}}\, y \qquad \text{or} \qquad \begin{bmatrix} y^{\{f\}} \\ y^{\{s\}} \end{bmatrix}' = \begin{bmatrix} \lambda^{\{f\}} & \eta^{\{s\}} \\ \eta^{\{f\}} & \lambda^{\{s\}} \end{bmatrix} \begin{bmatrix} y^{\{f\}} \\ y^{\{s\}} \end{bmatrix}.$$

- We proved decoupled GARK cannot be A-stable for the 2D test problem.
- Internal consistency simplifies order conditions but inhibits stability.

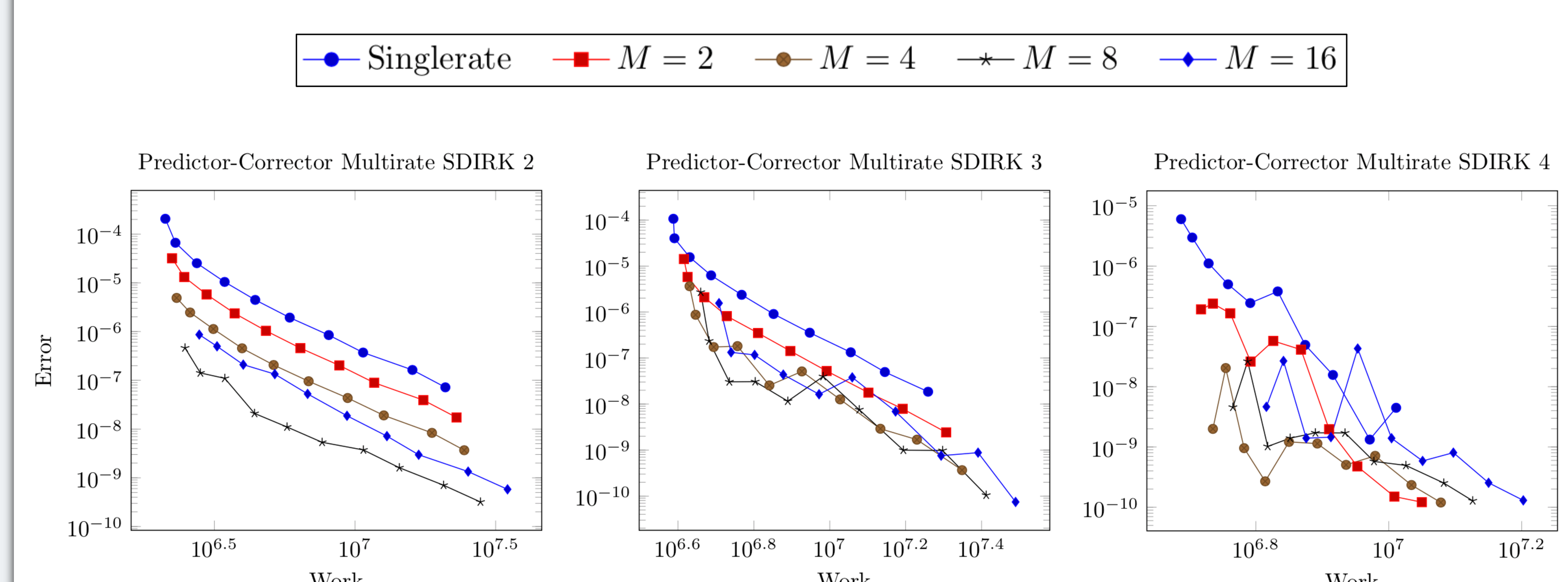


Performance Results

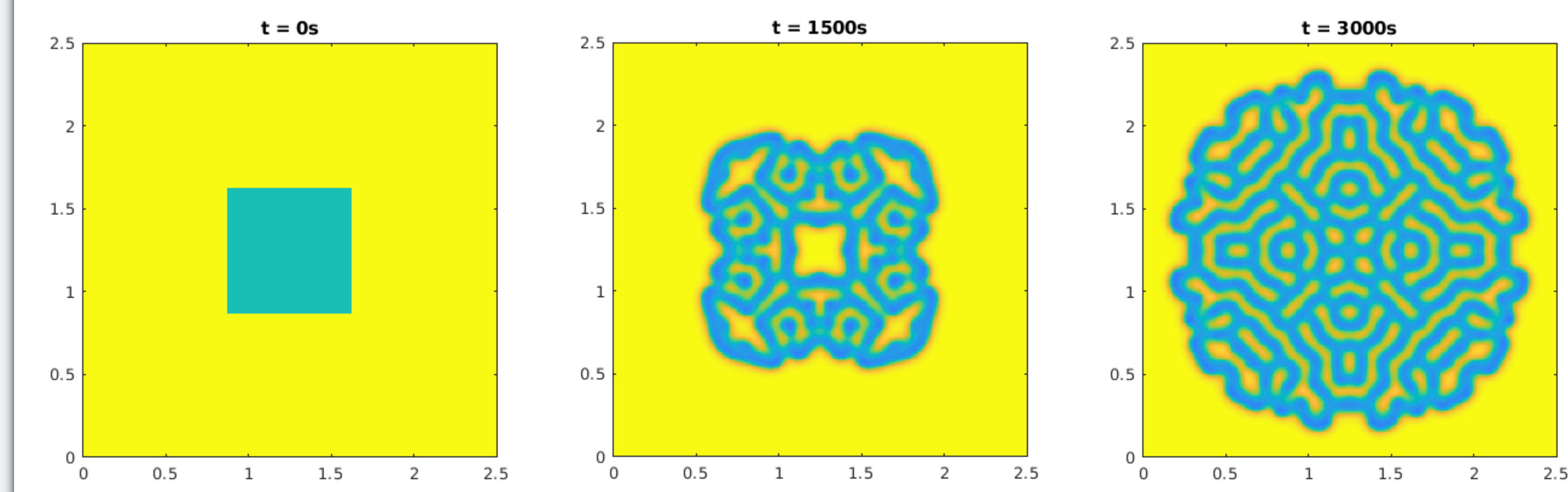
The inverter chain is a classic multirate test problem that simulates the propagation of a signal through a series of MOSFET inverters:

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

As an idealized measure of work, we accumulate the dimensions of all linear solves performed while solving the ODEs. Dynamic partitioning is used at each step to determine the fast and slow variables.



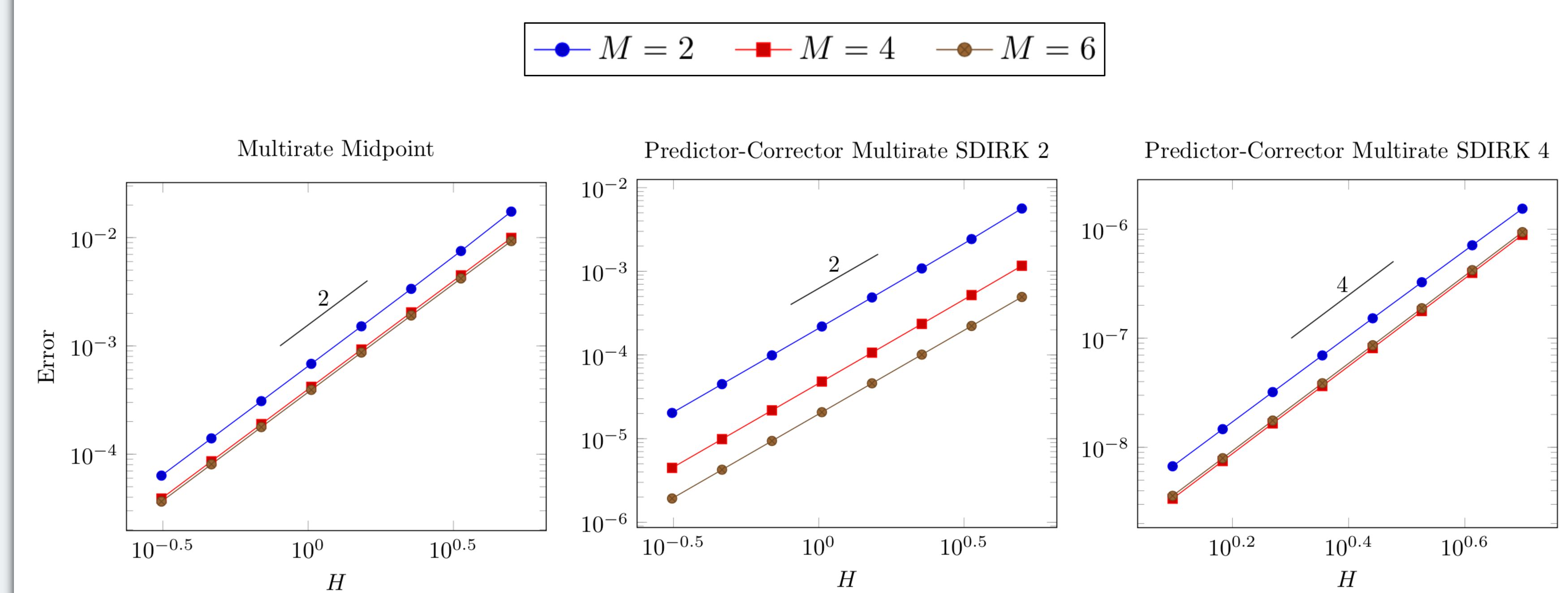
Convergence Results



The Gray–Scott model is a reaction-diffusion PDE given by

$$\begin{bmatrix} U \\ V \end{bmatrix}' = \begin{bmatrix} D_u\, \nabla U \\ D_v\, \nabla V \end{bmatrix} + \begin{bmatrix} -U\, V^2 + F(1-U) \\ U\, V^2 - (F+k)V \end{bmatrix}.$$

The reaction terms form the fast partition and the diffusion terms form the slow partition. The convergence plots below show the new methods achieve the theorical order for three different values of M.



Conclusions

- We derived new MrGARK methods up to order four designed to efficiently integrate stiff, multiscale ODEs.
- We discovered theoretical stability limitations for GARK and MrGARK methods.
- Many stability results were surprising and will be the subject of further investigation.
- Certain structures in coupled methods lead to simplifications in the Newton iterations.
- Numerical tests confirm the order of convergence and demonstrate the potential for speedup over singlerate counterparts.

References

1. Günther, M., & Sandu, A. (2016). Multirate generalized additive Runge–Kutta methods. *Numerische Mathematik*, *133*(3), 497-524.
2. Sandu, A., & Günther, M. (2015). A Generalized-Structure Approach to Additive Runge–Kutta Methods. *SIAM Journal on Numerical Analysis*, *53*(1), 17-42.

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