A New Multirate Time-Stepping Strategy for ODE Systems Equipped with a Surrogate Model

SIAM CSE

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Compute the Future!

VIRGINIA TECH

Solving large-scale systems of ODEs

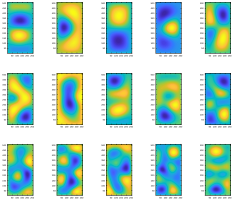
- Consider the system of ordinary differential equations (ODEs)

$$y' = f(y), \qquad y(t_0) = y_0, \qquad y \in \mathbb{C}^N.$$

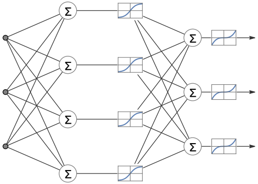
- We will limit our focus to nonstiff systems.
- In many scientific applications, f can be prohibitively expensive and the dimension N intractably large.
- This is common in method of lines discretized PDEs that require a fine spatial mesh.

What about surrogate models?

- In many cases, we can find a cheap but inaccurate surrogate model that approximates the full model f.
- Examples:



(a) Model Order Reduction



(b) Neural Network

(c) Coarser Meshes

- Integrating the surrogate model alone may lead to stability, accuracy, and convergence issues.

The best of both worlds: combining full and surrogate models

- How can we incorporate a surrogate model into the integration of f to reduce expensive full model evaluations?
- In the context of optimization, surrogate models have proved successful in reducing evaluations of expensive objective functions.
- There are some related ideas that can be used in the time-stepping context:
  - Rosenbrock-W methods admit approximate Jacobians
  - Coupling of model order reduction and multirate methods[1]
  - Projective integration
  - High-order/low-order (HOLO) algorithms[2]

[1] Hachtel, Kerler-Back, Bartel, Günther, and Stykel, "Multirate DAE/ODE-Simulation and Model Order Reduction for Coupled Field-Circuit Systems"; Bannenberg, Ciccazzo, and Günther, "Coupling of model order reduction and multirate techniques for coupled dynamical systems".

[2] Chacón et al., "Multiscale high-order/low-order (HOLO) algorithms and applications".

Surrogate model definition

- Suppose we have a surrogate model

$$y'_{\mathrm{sur}} = f_{\mathrm{sur}}(y_{\mathrm{sur}}), \qquad y_{\mathrm{sur}} \in \mathbb{C}^{S}.$$

- Recall that the full model was

$$y' = f(y), \qquad y \in \mathbb{C}^{N}.$$

- The surrogate model could evolve in lower-dimensional subspace: $S < N$.
- To move between the full and surrogate model spaces, we use $\mathrm{V}, \mathrm{W} \in \mathbb{C}^{N \times S}$:

$$y_{\mathrm{sur}} = \mathrm{W}^* y, \qquad y \approx \mathrm{V} y_{\mathrm{sur}}, \qquad \mathrm{W}^* \mathrm{V} = \mathrm{I}_{S \times S}.$$

Using multirating to combine full and surrogate models[3]

- Let's rewrite the original ODE as

$$y' = \underbrace{V f_{\mathrm{sur}}(W^* y)}_{f^{\{\mathfrak{f}\}}(y)} + \underbrace{f(y) - V f_{\mathrm{sur}}(W^* y)}_{f^{\{\mathfrak{s}\}}(y)} \in \mathbb{C}^N.$$

- Idea: Apply a multirate method to this ODE.
  - The fast partition is the surrogate model and is treated with a small timestep.
  - The slow partition is the surrogate model error and is treated with a large timestep.
- The surrogate model guides the solution while the occasional full model evaluation corrects for surrogate model error and ensures convergence.

[3] Roberts, Popov, Sarshar, and Sandu, "A fast time-stepping strategy for ODE systems equipped with a surrogate model".

Multirate methods

- Any multirate method suitable for additively partitioned ODEs could be used.
- Multirate infinitesimal step[4] (MIS) and the multirate infinitesimal GARK[5] (MRI-GARK) extensions make an excellent choice.
- Consider, for example, MIS/MRI Euler applied to $y' = f^{\{\mathfrak{f}\}}(y) + f^{\{\mathfrak{s}\}}(y)$:

$$
\begin{aligned}
v(0) &= y_n, \\
v'(\theta) &= f^{\{\mathfrak{f}\}}(v(\theta)) + f^{\{\mathfrak{s}\}}(y_n), \qquad \text{for } \theta \in [0, H], \\
y_{n+1} &= v(H).
\end{aligned}
$$

- Infinitesimal schemes blur the line between continuous and discrete methods and offer wonderful flexibility in the treatment of $f^{\{\mathfrak{f}\}}$.

[4] Knoth and Wolke, "Implicit-explicit Runge–Kutta methods for computing atmospheric reactive flows"; Wensch, Knoth, and Galant, "Multirate infinitesimal step methods for atmospheric flow simulation".

[5] Sandu, "A Class of Multirate Infinitesimal GARK Methods"; Roberts, Sarshar, and Sandu, "Coupled Multirate Infinitesimal GARK Schemes for Stiff Systems with Multiple Time Scales".

Two types of multirate infinitesimal GARK methods

MRI-GARK:

$$Y_1 = y_n$$

$$\begin{cases} v_i(0) = Y_i, \\ v_i' = \Delta c_i^{\{\mathfrak{s}\}} \, f^{\{\mathfrak{f}\}}(v_i) + \sum_{j=1}^{i+1} \gamma_{i,j}\left(\frac{\theta}{H}\right) f^{\{\mathfrak{s}\}}(Y_j), \\ \qquad \text{for } \theta \in [0, H], \\ Y_{i+1} = v_i(H), \qquad i = 1, \dots, s^{\{\mathfrak{s}\}}, \end{cases}$$

$$y_{n+1} = Y_{s^{\{\mathfrak{s}\}}+1}.$$

Step predictor-corrector MRI-GARK (SPC-MRI-GARK):

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

$$\begin{cases} v(0) = y_n, \\ v' = f^{\{\mathfrak{f}\}}(v) + \sum_{j=1}^{s^{\{\mathfrak{s}\}}} \gamma_j\left(\frac{\theta}{H}\right) f^{\{\mathfrak{s}\}}(Y_j), \\ \qquad \text{for } \theta \in [0, H], \\ y_{n+1} = v(H). \end{cases}$$

Applying MRI-GARK to the ODE

- Now we apply an MRI-GARK method to

$$y' = V f_{\mathrm{sur}}(W^* y) + f(y) - V f_{\mathrm{sur}}(W^* y).$$

- This yields the surrogate model MRI-GARK (SM-MRI-GARK) method

$$
\begin{aligned}
&Y_1 = y_n, \\
&\begin{cases}
z_i(0) = W^* Y_i \in \mathbb{C}^S, \\
z_i'(\theta) = \Delta c_i^{\{\mathfrak{s}\}} f_{\mathrm{sur}}(z_i(\theta)) + \sum_{j=1}^{i+1} \gamma_{i,j}\left(\frac{\theta}{H}\right)\left(W^* f(Y_j) - f_{\mathrm{sur}}(W^* Y_j)\right), \quad \text{for } \theta \in [0, H], \\
Y_{i+1} = V z_i(H) + (I_{d\times d} - V W^*)\left(Y_i + H \sum_{j=1}^{i+1} \overline{\gamma}_{i,j} f(Y_j)\right), \\
\qquad i = 1, \dots, s^{\{\mathfrak{s}\}},
\end{cases} \\
&y_{n+1} = Y_{s^{\{\mathfrak{s}\}}+1}.
\end{aligned}
$$

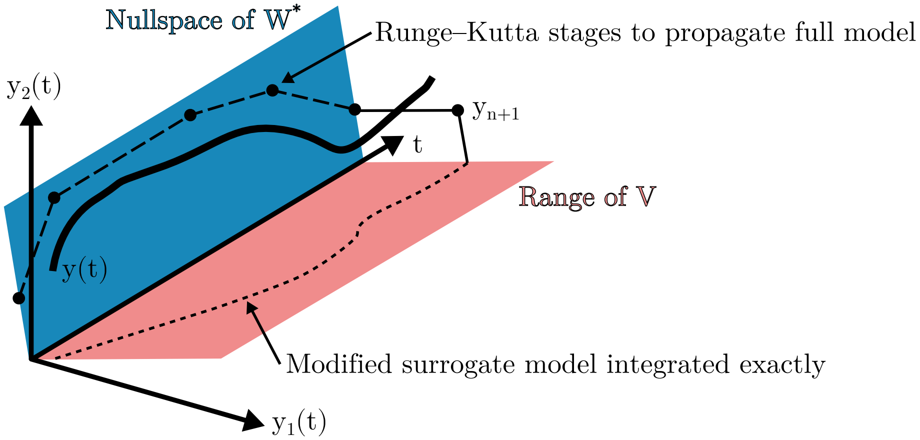
SM-MRI-GARK Euler

- When we use Euler's method as the base method and the coupling $\gamma_{1,1}(t) = 1$, we have the simple method

$$
\begin{aligned}
z(0) &= \mathrm{W}^* y_n \\
z'(\theta) &= f_{\mathrm{sur}}(z(\theta)) + \mathrm{W}^* f(y_n) - f_{\mathrm{sur}}(\mathrm{W}^* y_n), \qquad \text{for } \theta \in [0, H], \\
y_{n+1} &= \mathrm{V} z(H) + (\mathrm{I}_{d \times d} - \mathrm{V}\mathrm{W}^*)(y_n + H f(y_n)).
\end{aligned}
$$

- An ODE is solved in the range of V.
- An Euler step is taken in the nullspace of W^*.

Illustration of SM-MRI-GARK



SM-SPC-MRI-GARK

- We can also apply SPC-MRI-GARK to the ODE to get SM-SPC-MRI-GARK:

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

$$\begin{cases} z(0) = \mathrm{W}^* y_n \in \mathbb{C}^S, \\ z(\theta)' = f_{\mathrm{sur}}(z(\theta)) + \sum_{j=1}^{s^{\{\mathfrak{s}\}}} \gamma_j\left(\frac{\theta}{H}\right)(\mathrm{W}^* f(Y_j) - f_{\mathrm{sur}}(\mathrm{W}^* Y_j)), \\ \qquad \text{for } \theta \in [0, H], \\ y_{n+1} = \mathrm{V} z(H) + (\mathrm{I}_{d \times d} - \mathrm{V}\mathrm{W}^*)\left(y_n + H \sum_{j=1}^{s^{\{\mathfrak{s}\}}} b_j f(Y_j)\right). \end{cases}$$

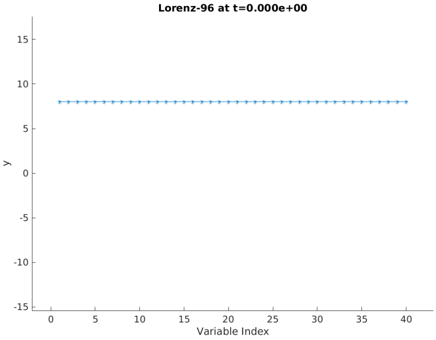
Numerical experiment: Lorenz '96 I

- The Lorenz '96 problem is given by

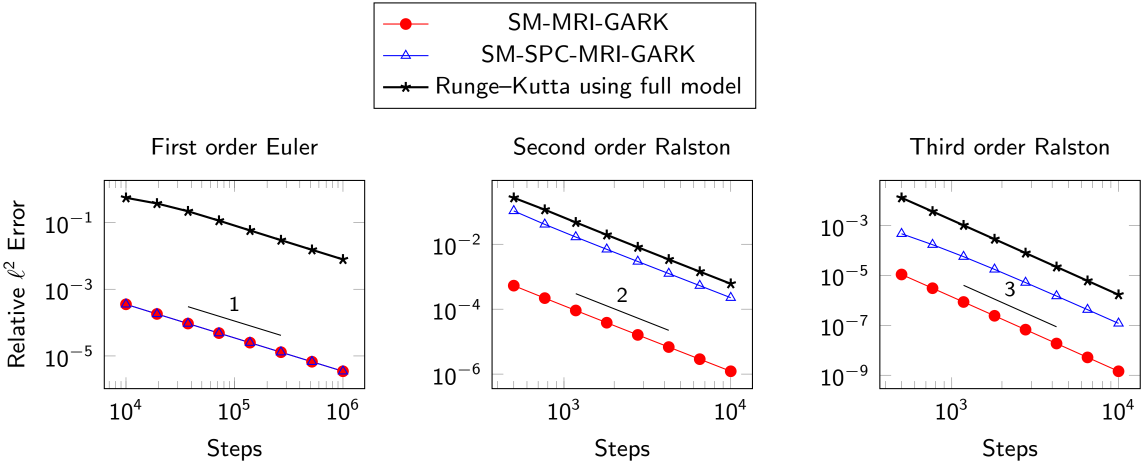
$$\frac{\mathrm{d}}{\mathrm{d}t} X_k = -X_{k-2} X_{k-1} + X_{k-1} X_{k+1} - X_k + F,$$

for $k = 1, 2, \dots, 40$.

- In an offline phase, 5000 snapshots of the state and its derivative were generated over the timespan $[2, 10]$.
- A 3-layer neural network was trained on this data to learn the right-hand side function.
- The neural network is used as f_{sur} and $\mathrm{V} = \mathrm{W} = \mathrm{I}_{40 \times 40}$.



Numerical experiment: Lorenz ’96 II



Numerical experiment: DG advection I

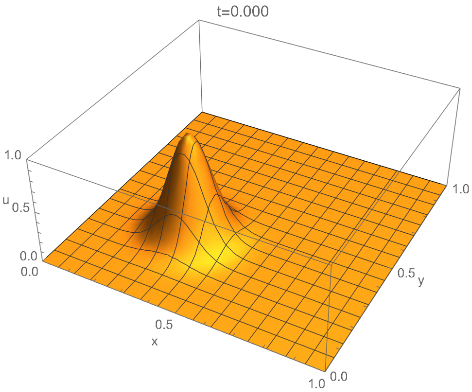
- Consider the Molenkamp–Crowley problem

$$\frac{\partial u}{\partial t} + a \cdot \nabla u = 0, \quad \text{on } \Omega = [0,1] \times [0,1],$$
$$u = 0, \quad \text{on } \partial\Omega,$$

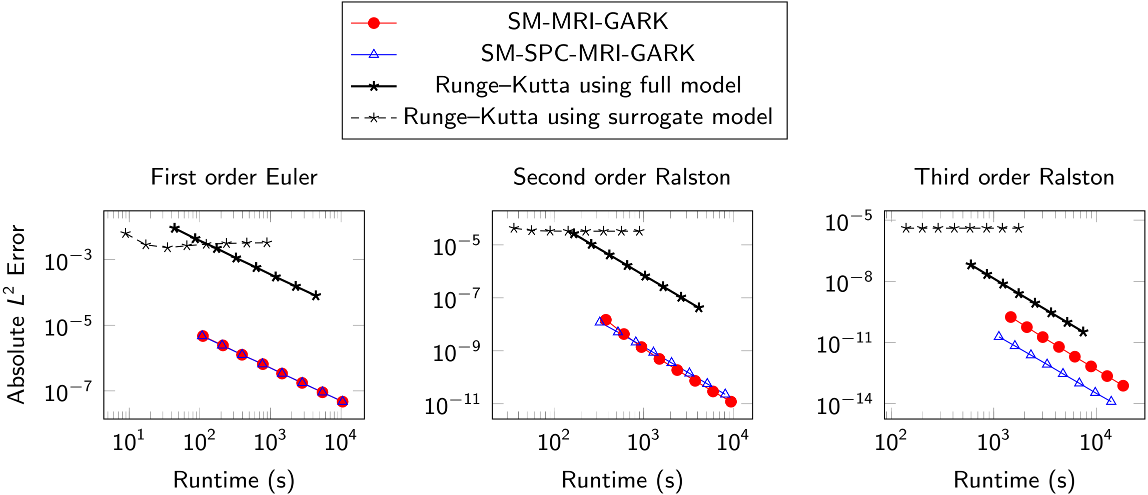
with the circular wind profile

$$a(x,y) = \begin{bmatrix} 2\pi \left(y - \frac{1}{2}\right) \\ -2\pi \left(x - \frac{1}{2}\right) \end{bmatrix}.$$

- f corresponds to a discontinuous Galerkin discretization on a 100×100 uniform, triangular mesh, while f_{sur} uses a 50×50 mesh.
- V and W* are sparse interpolation operators.



Numerical experiment: DG advection II



Conclusions

- Surrogate model MRI-GARK extends traditional Runge–Kutta to incorporate a surrogate model and improve efficiency.
- It combines continuous integration of a surrogate model with discrete evaluations of the full model for error correction.
- Quality of the surrogate model does not affect order of convergence.
- The infinitesimal characteristic allows any method to be applied to the surrogate model.
- Large speedups over traditional Runge–Kutta methods can be achieved, especially when evaluations of V, W*, and f_{sur} are cheap.

References

M.W.F.M. Bannenberg, A. Ciccazzo, and M. Günther. "Coupling of model order reduction and multirate techniques for coupled dynamical systems". In: *Applied Mathematics Letters* 112 (2021), p. 106780. ISSN: 0893-9659. DOI: 10.1016/j.aml.2020.106780.

L. Chacón et al. "Multiscale high-order/low-order (HOLO) algorithms and applications". In: *Journal of Computational Physics* 330 (2017), pp. 21–45. ISSN: 10902716. DOI: 10.1016/j.jcp.2016.10.069.

Christoph Hachtel et al. "Multirate DAE/ODE-Simulation and Model Order Reduction for Coupled Field-Circuit Systems". In: *Scientific Computing in Electrical Engineering*. Ed. by Ulrich Langer, Wolfgang Amrhein, and Walter Zulehner. Cham: Springer International Publishing, 2018, pp. 91–100. ISBN: 978-3-319-75538-0.

O. Knoth and R. Wolke. "Implicit-explicit Runge–Kutta methods for computing atmospheric reactive flows". In: *Applied Numerical Mathematics* 28.327–341 (1998).

Steven Roberts, Arash Sarshar, and Adrian Sandu. "Coupled Multirate Infinitesimal GARK Schemes for Stiff Systems with Multiple Time Scales". In: *SIAM Journal on Scientific Computing* 42.3 (2020), A1609–A1638. DOI: 10.1137/19M1266952.

Steven Roberts et al. "A fast time-stepping strategy for ODE systems equipped with a surrogate model". In: *arXiv preprint arXiv:2011.03688* (2020).

Adrian Sandu. "A Class of Multirate Infinitesimal GARK Methods". In: *SIAM Journal on Numerical Analysis* 57.5 (2019), pp. 2300–2327. DOI: 10.1137/18M1205492.

Jörg Wensch, Oswald Knoth, and Alexander Galant. "Multirate infinitesimal step methods for atmospheric flow simulation". In: *BIT Numerical Mathematics* 49.2 (2009), pp. 449–473. ISSN: 00063835. DOI: 10.1007/s10543-009-0222-3.

Questions?

- Preprint available at:
  https://arxiv.org/abs/2011.03688
- These slides are available on my website:
  https://steven-roberts.github.io