Accelerating Time-Stepping Methods with Surrogate Models

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Goal: solve large-scale initial value problems

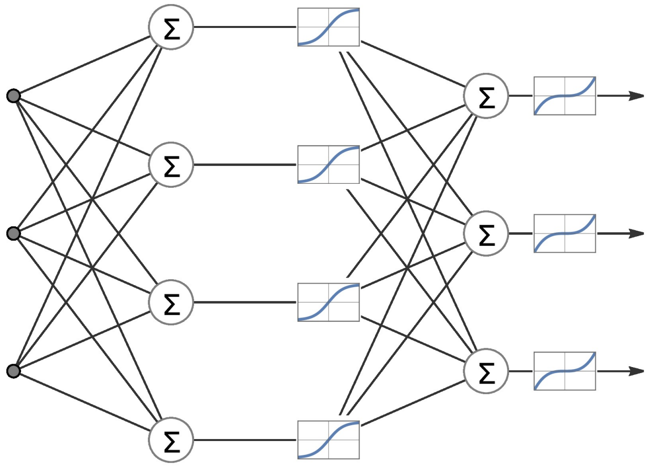
- Consider the initial value problem

$$y' = f(y), \quad y(t_0) = y_0 \in \mathbb{C}^N, \quad t \in [t_0, t_f].$$

- We will focus on explicit methods for nonstiff problems.
- In scientific applications, the dimension N can be intractably large and evaluations of f prohibitively expensive.
- How can we reduce the number of evaluations of f without sacrificing
  - Accuracy
  - Stability
  - Convergence

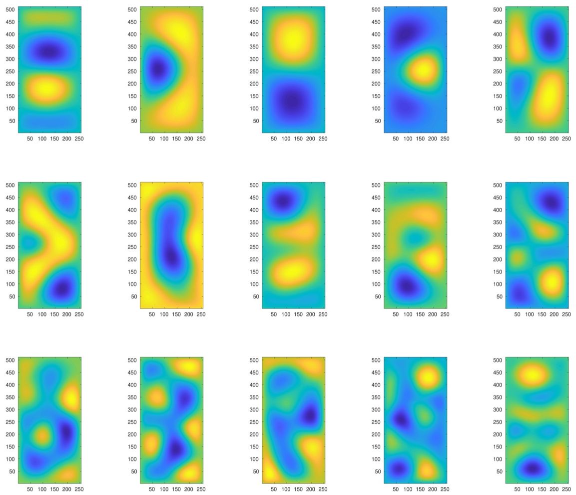
What about surrogate models?

- For many problems, it is possible to produce a cheap but approximate surrogate model.



Machine Learning

Coarser Mesh



Reduced-Order Model

- For complex problems, surrogate models cannot outright replace the full model f.

How can we combine full and surrogate models?

- For convergence, we cannot escape evaluating the full model.
- An ideal hybrid approach would use the surrogate model to substantially reduce evaluations of the full model.
- Surrogate models have been successfully incorporated into optimization algorithms.
- There are some related ideas in the context of time integration
  - Rosenbrock-W methods
  - Coupling a reduced order model and multirate method[1]
  - Defect correction
  - Heterogeneous multiscale method[2]

1. Hachtel, Christoph, et al. "Multirate DAE/ODE-simulation and model order reduction for coupled field-circuit systems." Scientific Computing in Electrical Engineering. Springer, Cham, 2018. 91-100.
2. Abdulle, Assyr, et al. "The heterogeneous multiscale method." Acta Numerica 21 (2012): 1-87.

Defining the surrogate model

- Recall the full model we want to integrate is

$$y' = f(y), \quad y(t) \in \mathbb{C}^N.$$

- The surrogate model is also posed as an ODE:

$$y'_{sur} = f_{sur}(y_{sur}), \quad y_{sur}(t) \in \mathbb{C}^S.$$

- The surrogate model may evolve in a lower-dimensional space: $S < N$.
- Transformations between the full and surrogate spaces are realized by $V, W \in \mathbb{C}^{N \times S}$:

$$y_{sur} = W^* y, \quad y \approx V y_{sur}, \quad W^* V = I_{S \times S}.$$

Surrogate acceleration with multirate methods

- The original, full ODE can be rewritten in the equivalent form

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

- 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 error and is treated with a large timestep.
- The surrogate model is evaluated often to guide the solution trajectory while the expensive full model is evaluated infrequently to correct for surrogate errors.
- Accuracy, stability, and convergence properties are based on the underlying multirate method.

Which multirate methods should we use?

- With 6 decades of development, there are many options!

- Multirate infinitesimal (MRI) methods have gain traction in recent years.
  - Fast dynamics are evolved by solving ODEs with any consistent integrator.
  - Very flexible

- MRI methods based on Runge-Kutta methods
  - Knoth, Oswald, and Ralf Wolke. "Implicit-explicit Runge-Kutta methods for computing atmospheric reactive flows." *APNUM* (1998)
  - Sandu, Adrian. "A class of multirate infinitesimal GARK methods." *SINUM* (2019)
  - Roberts, Steven, Arash Sarshar, and Adrian Sandu. "Coupled multirate infinitesimal GARK schemes for stiff systems with multiple time scales." *SISC* (2020)

- MRI methods based on linear multistep methods
  - Demirel, Abdullah, et al. "Efficient multiple time-stepping algorithms of higher order." *JCP* (2015)

Multirate Euler method example

- Our multirate ODE is

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

- Consider the simple multirate infinitesimal method

$$\begin{aligned} v(0) &= y_n, \\ v'(\theta) &= f^{\{f\}}\big(v(\theta)\big) + f^{\{s\}}(y_n), \\ y_{n+1} &= v(H). \end{aligned}$$

- There is one evaluation of $f^{\{s\}}$ per step.
- $f^{\{f\}}$ is evaluated as many times as it takes to integrate v to $\theta = H$.

Multirate Euler method example

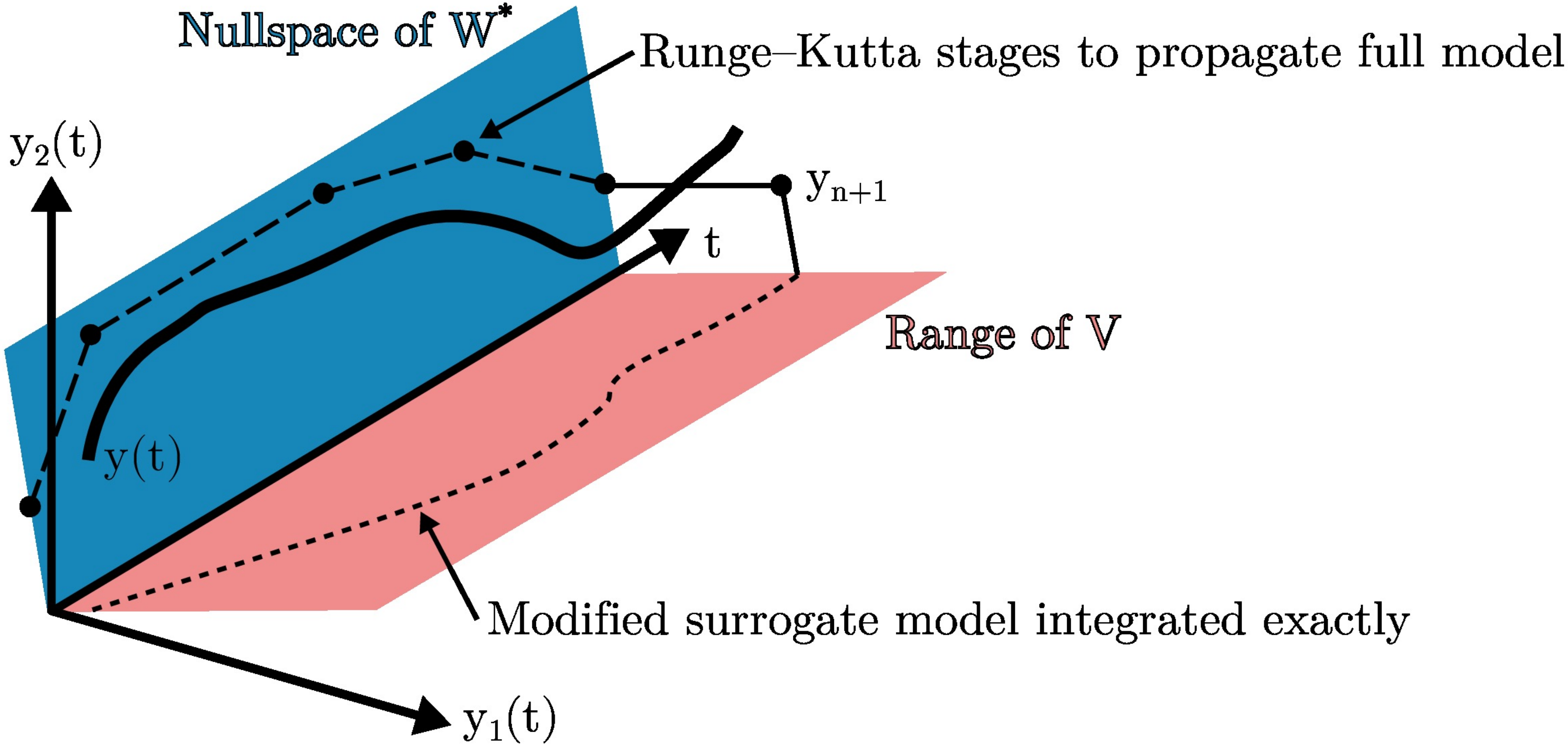
$y' = V f_{sur}(W^* y) + f(y) - V f_{sur}(W^* y)$

- When we apply the multirate Euler method to our ODE, we arrive at

$$
\begin{aligned}
z(0) &= W^* y_n, \\
z'(\theta) &= f_{sur}\big(z(\theta)\big) + W^* f(y_n) - f_{sur}(W^* y_n), \\
y_{n+1} &= V\, z(H) + (I_{N\times N} - V W^*)\big(y_n + H\, f(y_n)\big).
\end{aligned}
$$

- $z(\theta) \in \mathbb{C}^S$ is integrated in the range of V.
- An Euler step is taken in the nullspace of W^*.
- There is one evaluation of the full model per step and many for the surrogate model.

Illustration of the time-stepping approach



SM-MRI-GARK

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

- Let's replace multirate Euler with MRI-GARK to achieve higher orders.
- A surrogate model MRI-GARK (SM-MRI-GARK)[1] method is given by

$$
\begin{aligned}
Y_1 &= y_n, \\
z_i(0) &= W^* Y_i \in \mathbb{C}^S, \\
z_i'(\theta) &= \Delta c_i^{\{s\}} f_{sur}\big(z_i(\theta)\big) + \sum_{j=1}^{i+1} \gamma_{i,j}\left(\frac{\theta}{H}\right)\Big(W^* f\big(Y_j\big) - f_{sur}\big(W^* Y_j\big)\Big), \\
Y_{i+1} &= V\, z_i(H) + (I_{N \times N} - V W^*)\left(Y_i + H \sum_{j=1}^{i+1} \bar{\gamma}_{i,j} f\big(Y_j\big)\right), \quad i = 1, \dots, s^{\{s\}}, \\
y_{n+1} &= Y_{s^{\{s\}}+1}.
\end{aligned}
$$

1. Roberts, Steven, et al. "A Fast Time-Stepping Strategy for Dynamical Systems Equipped with a Surrogate Model." *SIAM Journal on Scientific Computing* 44.3 (2022): A1405-A1427.

SM-SPC-MRI-GARK

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

- If instead we base our method on SPC-MRI-GARK we have the class of surrogate model SPC-MRI-GARK (SM-SPC-MRI-GARK)[1]:

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

$$z(0) = W^* y_n \in \mathbb{C}^S,$$

$$z'(\theta) = f_{sur}\left(z(\theta)\right) + \sum_{j=1}^{s^{\{s\}}} \gamma_j \left(\frac{\theta}{H}\right) \left(W^* f\left(Y_j\right) - f_{sur}\left(W^* Y_j\right)\right),$$

$$y_{n+1} = V\, z(H) + (I_{N \times N} - V W^*) \left(y_n + H \sum_{j=1}^{s^{\{s\}}} b_j f\left(Y_j\right) \right)$$

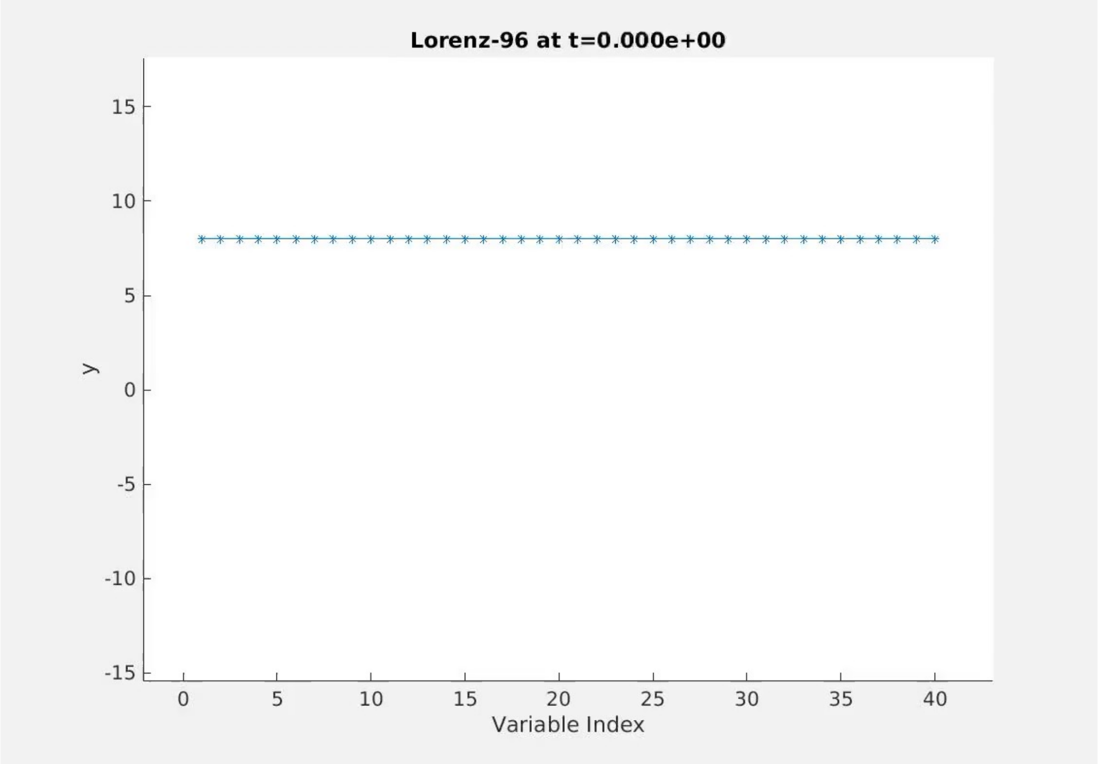
1. Roberts, Steven, et al. "A Fast Time-Stepping Strategy for Dynamical Systems Equipped with a Surrogate Model." *SIAM Journal on Scientific Computing* 44.3 (2022): A1405-A1427.

Numerical experiment: Lorenz ‘96

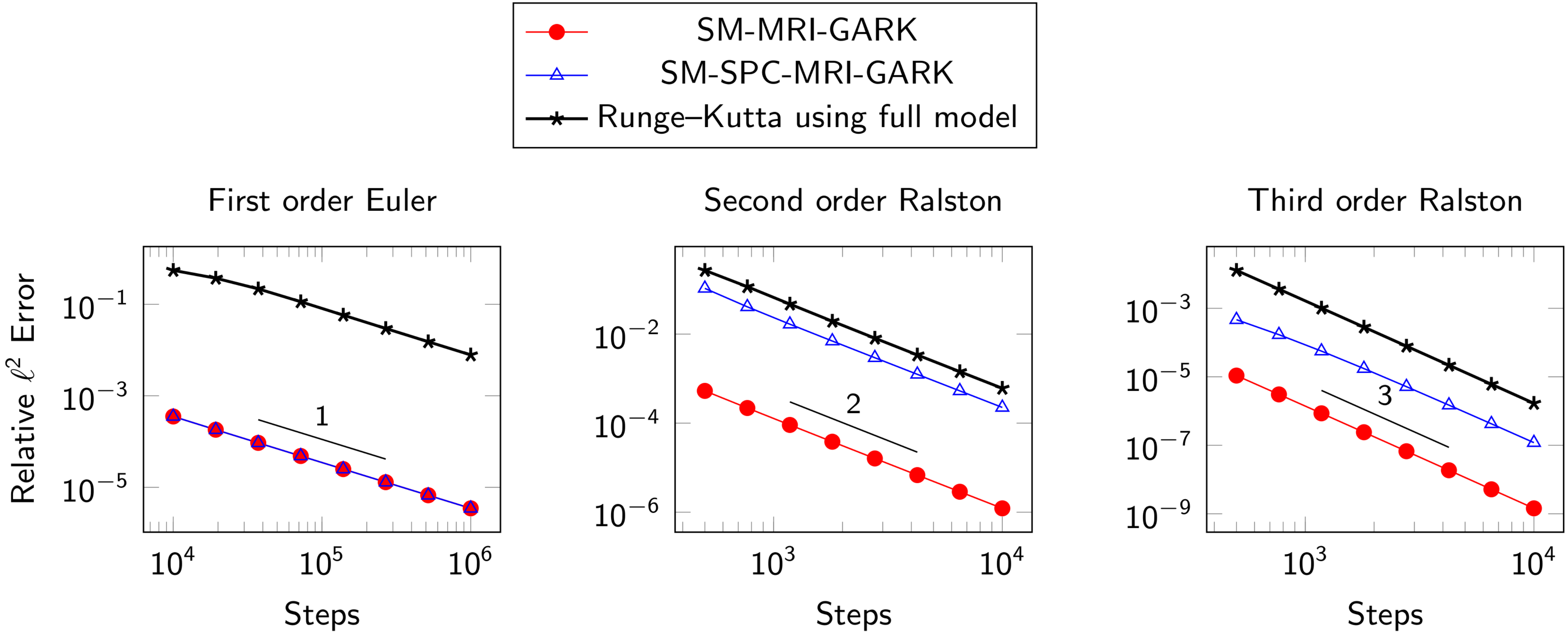
- The Lorenz ‘96 is a 40 variable ODE

$$\frac{dX_k}{dt} = -X_{k-2}X_{k-1} + X_{k-1}X_{k+1} - X_k + F.$$

- In an offline phase, 5000 snapshots of the trajectory and its derivative were generated over the timespan $[2, 10]$.
- A 3-layer neural network was trained on the data to approximate the RHS function f.
- The neural network acts as f_{sur}, and $V = W = I_{40\times 40}$.



Numerical experiment: Lorenz '96

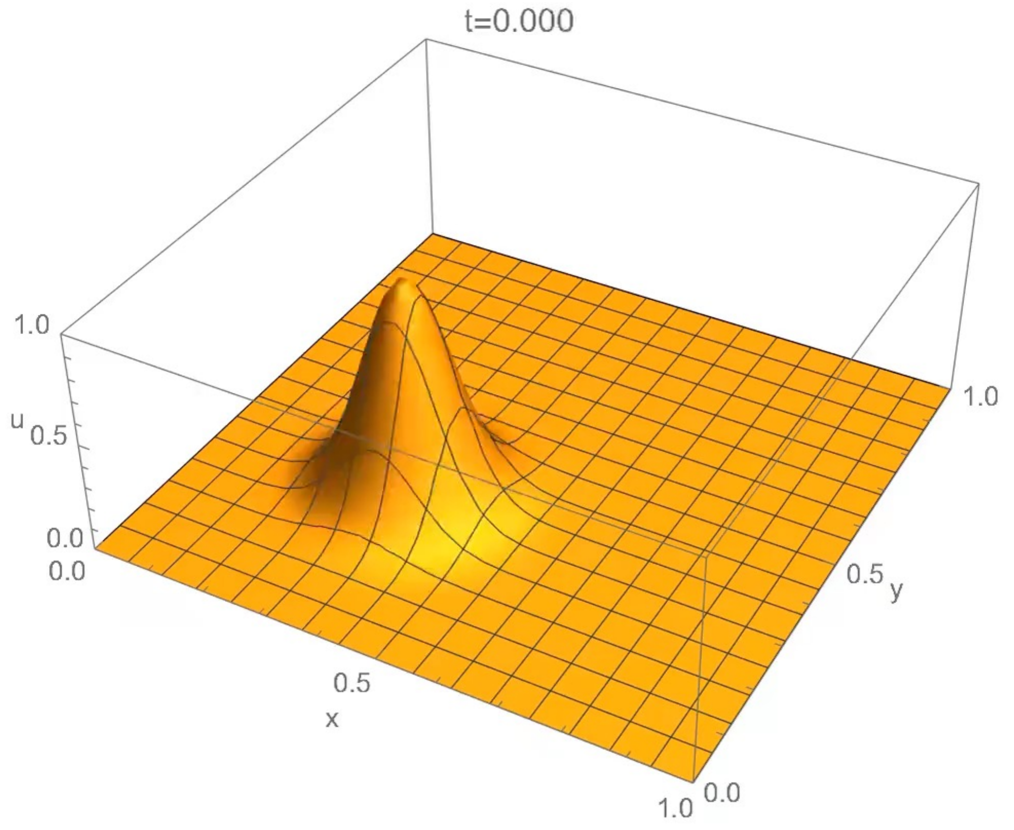


Numerical experiment: DG advection

- Consider the Molenkamp-Crowley problem

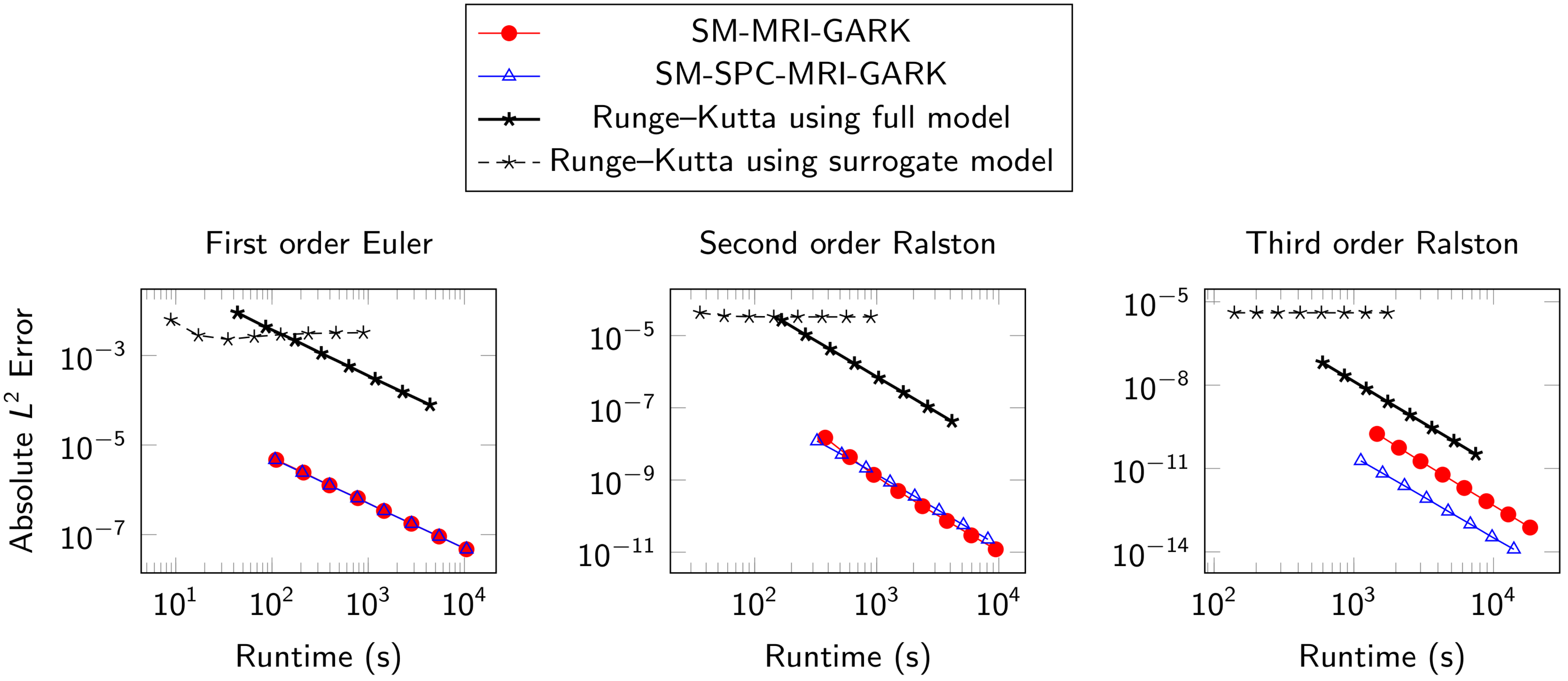
$$\frac{\partial u}{\partial t} + a \cdot \nabla u = 0, \quad \text{on } \Omega = [0,1]^2,$$
$$u = 0, \quad \text{on } \partial\Omega,$$

  with the circular wind profile $a(x, y)$.



- 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



Conclusions

- New methods extend traditional Runge-Kutta and linear multistep methods to incorporate information from a surrogate model.
- This work broadens the scope and applicability of multirate methods.
- The quality of the surrogate model does not affect the order of convergence.
- Experiments show large speedups over traditional integrators, especially when V, W^*, and f_{sur} are inexpensive.
- Future work
  - Additional testing of methods based on linear multistep methods
  - Support for surrogate models that are flow maps instead of ODEs

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Questions?

See my website for additional details
https://people.llnl.gov/roberts115