High-order multirate time integration for multiphysics PDE systems

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Outline

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Multiphysics/Multirate Problems [Keyes et al. 2013]

"Multiphysics" problems couple models together either in the bulk (cosmology, combustion) or across interfaces (climate, tokamak fusion), challenging traditional numerical methods.

- "Multirate": processes evolve on different time scales, may not admit analytical reformulation.
- Existence of stiff components prohibits fully explicit methods.
- Nonlinearity and insufficient differentiability challenge fully implicit methods.
- Parallel scalability demands optimal algorithms – while robust/scalable algebraic solvers exist for some pieces (e.g., FMM for particles, multigrid for diffusion), none are optimal for the full problem.

Here we'll consider the prototypical problem

$$y'(t) = f^S(t,y) + f^F(t,y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0 \in \mathbb{R}^n.$$

- $f^S(t,y)$ contains "slow" components that evolve with time scale H, and
- $f^F(t,y)$ contains "fast" components that evolve with time scale $h \ll H$.
- f^S or f^F may be further decomposed into stiff/nonstiff or fast/slow parts.

Legacy Multirate Approaches

Historical approaches for the time step $y_n \approx y(t_n) \to y_{n+1} \approx y(t_n + H)$ include first-order Lie–Trotter splittings and subcycling, e.g.,

1. Compute: $y_n^{(1)} = y_n + H f^S(t_n, y_n)$
2. Evolve: $v'(\tau) = f^F(t_n + \tau, v)$, for $\tau \in [0, H]$, $v(0) = y_n^{(1)}$, and let $y_{n+1} = v(H)$.

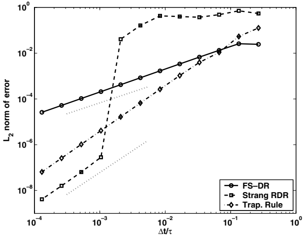
or potentially "Strang–Marchuk" splitting, e.g.,

1. Compute: $y_n^{(1)} = y_n + \frac{H}{4} f^S(t_n, y_n) + \frac{H}{4} f^S\left(t_n + \frac{H}{2}, y_n + \frac{H}{2} f^S(t_n, y_n)\right)$
2. Evolve: $v'(\tau) = f^F(t_n + \tau, v)$, for $\tau \in [0, H]$, $v(0) = y_n^{(1)}$ and let: $y_n^{(2)} = v(H)$
3. Compute: $y_{n+1} = y_n^{(2)} + \frac{H}{4} f^S\left(t_n + \frac{H}{2}, y_n^{(2)}\right) + \frac{H}{4} f^S\left(t_{n+1}, y_n^{(2)} + \frac{H}{2} f^S\left(t_n + \frac{H}{2}, y_n^{(2)}\right)\right)$

Legacy Multirate Approaches – Shortcomings

Low accuracy due to loose "initial condition" coupling:

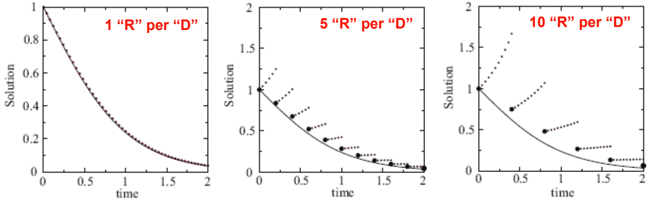
- Lie-Trotter is $\mathcal{O}(H)$ and Strang-Marchuk is $\mathcal{O}(H^2)$.
- Extrapolation can improve this but at significant cost.



Convergence of splitting approaches (brusselator) [Ropp & Shadid 2005].

Poor stability:

- Even with "stable" step sizes for each part, unstable modes may arise.



Subcycling stability (reaction-diffusion) [Estep et al. 2008].

Multirate Improvements

In recent decades, improvements to accuracy and stability for multirate numerical methods have generally taken one of two forms:

A. Tighter slow $\leftrightarrow$ fast coupling[1]:

- \+ typically only require a single traversal of the step $[t_n, t_{n+1}]$ by each operator
- − typically only enable $\mathcal{O}(H^2)$ or $\mathcal{O}(H^3)$

B. Extrapolation / deferred correction techniques[2]:

- \+ potential for arbitrarily-high accuracy
- − require many traversals of the step $[t_n, t_{n+1}]$

In this work we pursue approach A.

[1] Gear & Wells 1984; Günther, Kværnø & Rentrop 1999-2002; Constantinescu & Sandu 2007-09; Fok 2016; Arnold, Galant, Knoth, Schlegel, Wensch & Wolke 2009-14

[2] Engstler, Hairer, Lubich, Ostermann 1990-97; Constantinescu & Sandu 2010-13, Bouzarth & Minion 2010

"Infinitesimal" Multirate Methods (MIS, RFSMR) [Knoth & Wolke 1998; Schlegel et al. 2009; ...]

The infinitesimal family of multirate methods allow up to $\mathcal{O}(H^3)$ accuracy, through more tightly coupling the fast and slow operators. Returning to our prototypical problem:

$$y'(t) = f^S(t,y) + f^F(t,y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0 \in \mathbb{R}^n.$$

- the slow component is integrated using an explicit "outer" RK method, $T_O = \{A, b, c\}$, where $0 = c_1 \le c_2 \le \ldots \le c_s \le 1$;
- the fast component is assumed to *exactly* solve a modified IVP (next slide);
- practically, this fast solution is subcycled using an "inner" RK method.

MIS Algorithm

A single MIS step $y_n \to y_{n+1}$ has the form:

1. Let: $z_1 = y_n$
2. For $i = 2, \ldots, s$:
   a. Define: $r = \sum_{j=1}^{i-1} \alpha_{ij} f^S\left(t_n + c_j H, z_j\right)$
   b. Evolve: $v'(\tau) = f^F(t_n + \tau, v) + r$, for $\tau \in [c_{i-1}H, c_i H]$, $v(c_{i-1}H) = z_i$
   c. Let: $z_i = v(c_i H)$
3. Let $y_{n+1} = z_s$

Here, the constants α_{ij} are uniquely defined from the "slow" Butcher table, T_O.

- When $c_i = c_{i-1}$, the IVP "solve" reduces to a standard RK update.
- The "fast" IVP in step 2b may be solved using any viable algorithm.

MIS Properties

MIS methods satisfy a number of desirable properties:

- $\mathcal{O}(H^2)$ if both inner/outer methods are at least $\mathcal{O}(H^2)$.
- $\mathcal{O}(H^3)$ if both inner/outer methods are at least $\mathcal{O}(H^3)$, and T_O satisfies

$$\sum_{i=2}^{s} (c_i - c_{i-1})(e_i + e_{i-1})^T Ac + (1 - c_s)\left(\frac{1}{2} + e_s^T Ac\right) = \frac{1}{3}.$$

- The inner method may be a subcycled T_O, enabling a *telescopic* multirate method (i.e., n-rate problems supported via recursion).
- Both inner/outer methods can utilize problem-specific tables (SSP, etc.).
- Highly efficient – only a single traversal of $[t_n, t_{n+1}]$ is required. To our knowledge, MIS are the most efficient $\mathcal{O}(H^3)$ multirate methods available.

Higher-order MIS-like methods [Sandu 2019; Bauer & Knoth 2019; Sexton & R. 2019]

In the last few years groups have worked to extend the MIS approach to $\mathcal{O}(H^4)$ accuracy:

- *MRI-GARK* modifies the fast IVP:

$$r \quad \to \quad r(\tau) = \sum_{j=1}^{i} \gamma_{i,j}\left(\frac{\tau}{(c_i - c_{i-1})H}\right) f^S\left(t_n + c_j H, z_j\right),$$

  and supports "solve-decoupled" implicit methods at the slow time scale (i.e., alternate between DIRK-like solves and fast IVP evolution).

- *extMIS* relaxes the MIS structure slightly, and then develops additional order conditions on T_O.

- *RMIS* computes y_{n+1} as a linear combination of $\left\{f^S(t_n + c_i H, z_i) + f^F(t_n + c_i H, z_i)\right\}_{i=1}^{s}$, additionally enabling conservation of linear invariants.

Outline

Multirate Exponential Runge–Kutta (MERK) & Rosenbrock (MERB) Methods [Luan, Chinomona & R., *SISC* 2020 & *arXiv* 2021]

We consider multirate IVP splittings of the form

$$y'(t) = F(t,y) = \mathcal{J}_n y + \mathcal{V}_n t + \mathcal{N}_n(t,y), \quad t \in [t_n, t_n + H], \quad y(t_n) = y_n \in \mathbb{R}^n.$$

- "Fast" scale corresponds to $\mathcal{J}_n y$: for MERK $\mathcal{J}_n$ may be arbitrary, for MERB $\mathcal{J}_n = \frac{\partial F}{\partial y}(t_n, u_n)$.
- "Slow" scale corresponds to $\mathcal{V}_n t + \mathcal{N}_n(t,y)$ with $\mathcal{V}_n = \frac{\partial F}{\partial t}(t_n, y_n)$ and $\mathcal{N}_n(t,y) = F(t,y) - \mathcal{J}_n y - \mathcal{V}_n t$.
- MERK, and MERB for autonomous systems, have $\mathcal{V}_n = 0$, allowing some simplifications.

This problem has the same structure assumed by ExpRK and ExpRB methods, that approximate y_{n+1} via:

$$z_i = y_n + c_i H \varphi_1(c_i H \mathcal{J}_n)\, F(t_n, y_n) + c_i^2 H^2 \varphi_2(c_i H \mathcal{J}_n) V_n + H \sum_{j=2}^{i-1} a_{ij}(H\mathcal{J}_n)\, D_{nj}, \quad 1 \le 2 \le s,$$

$$y_{n+1} = y_n + H\varphi_1(H\mathcal{J}_n)\, F(t_n, y_n) + H^2 \varphi_2(H\mathcal{J}_n) V_n + H \sum_{i=2}^{s} b_i(H\mathcal{J}_n)\, D_{ni},$$

where $D_{ni} = \mathcal{N}_n(t_n + c_i H, z_i) - \mathcal{N}_n(t_n, y_n)$, and $a_{ij}(z)$, $b_i(z)$ are typically linear combinations of $\varphi_k(c_i z)$ and $\varphi_k(z)$, with $\varphi_k(z) = \frac{1}{H^k} \int_0^H e^{(1-\tau/H)z} \frac{\tau^{k-1}}{(k-1)!}\, \mathrm{d}\tau, \; k \ge 1$.

MERK & MERB Construction

Theorem (Luan, Chinomona & R., 2020 & 2021)

Assuming that $a_{ij}(H\mathcal{J}_n)$, $b_i(H\mathcal{J}_n)$ are strictly linear combinations of $\varphi_k(c_iH\mathcal{J}_n)$ and $\varphi_k(H\mathcal{J}_n)$, respectively:

$$a_{ij}(H\mathcal{J}_n) = \sum_{k=1}^{l_{ij}} \alpha_{ij}^{(k)} \varphi_k(c_iH\mathcal{J}_n), \qquad b_i(H\mathcal{J}_n) = \sum_{k=1}^{m_i} \beta_i^{(k)} \varphi_k(H\mathcal{J}_n),$$

then z_i and y_{n+1} are the exact solutions of the "fast" IVPs

$$\begin{aligned} v_{n,i}'(\tau) &= \mathcal{J}_n v_{n,i}(\tau) + p_{ni}(\tau), \quad v_n(0) = y_n, \quad i = 1, \dots, s, \\ v_{n+1}'(\tau) &= \mathcal{J}_n v_{n+1}(\tau) + q_n(\tau), \quad v_{n+1}(0) = y_n \end{aligned}$$

at $\tau = c_iH$ and $\tau = H$, respectively, where

$$p_{n,i}(\tau) = \mathcal{N}_n(t_n, y_n) + (t_n + \tau)\mathcal{V}_n + \sum_{j=2}^{i-1} \left(\sum_{k=1}^{l_{ij}} \frac{\alpha_{ij}^{(k)}}{c_i^k H^{k-1}(k-1)!} \tau^{k-1} \right) D_{nj},$$

$$q_n(\tau) = \mathcal{N}_n(t_n, y_n) + (t_n + \tau)\mathcal{V}_n + \sum_{j=2}^{s} \left(\sum_{k=1}^{m_i} \frac{\beta_i^{(k)}}{H^{k-1}(k-1)!} \tau^{k-1} \right) D_{ni}.$$

MERK & MERB Convergence

Theorem (Luan, Chinomona & R., 2020 & 2021)

Assuming that a MERK or MERB method is constructed from an ExpRK or ExpRB method of global order p, with the associated "fast" IVPs integrated with a step $h = H/m$ using methods with global orders q and r, respectively, then:

$$\|y_n - y(t_n)\| \leq C_1 H^p + C_2 H h^q + C_3 h^r$$

on $t_0 \leq t_n = t_0 + nH \leq t_f$. Here C_1 depends on $t_f - t_0$ but is independent of n and H; C_2 and C_3 depend on the global order error constants of the chosen IVP solvers.

- Note the second term: for an order p method a "fast" solver for z_i need only have order $q = p - 1$.
- Evolve each stage over $[0, c_i H]$ – overall "fast traversal time" is $\left(1 + \sum_{i=1}^{s} c_i\right) H$ (typically $< 3H$).
- Since MERB methods may assume $\nabla \mathcal{N}_n = 0$ they have dramatically fewer order conditions, resulting in fewer fast solves and reduced fast traversal time.

MERK & MERB Methods

Comparison of MERK and MERB methods against Sandu's explicit MRI-GARK methods of comparable order.

- "Slow stages" corresponds to the number of evaluations of $\mathcal{N}_n$
- "Modified IVPs" corresponds to the number of fast IVP solves

Type	Order	Slow stages	Modified IVPs	Fast traversal time
MERK	3	3	3	$2.17H$
	4	6	4	$2.83H$
	5	10	5	$3.2H$
MERB	3	2	2	$1.5H$
	4	2	2	$1.75H$
	5	4	3	$2.08H$
	6	7	3	$1.25H$
MRI-GARK	3	3	3	H
	4	5	5	H

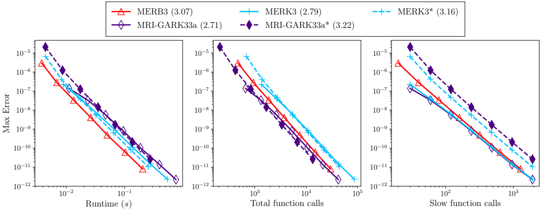
$\star\star\star$ *MERK5, MERB5 and MERB6 are the first-ever infinitesimal methods with order* > 4 $\star\star\star$

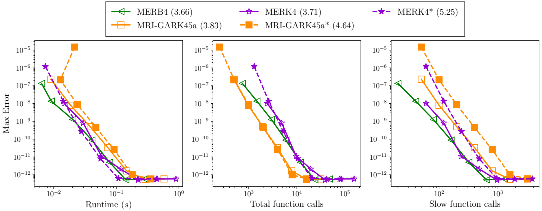
MERK & MERB Results – Reaction-Diffusion PDE test

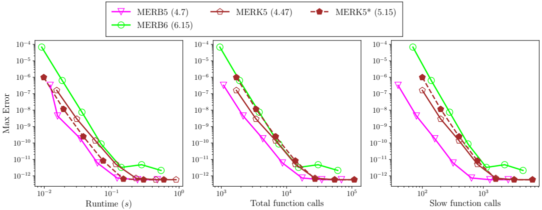
Problem: $u_t = \epsilon u_{xx} + \gamma u^2(1-u), \; x \in (0,5), \; t \in [0,5]$,
with $\gamma = 0.1$, $\epsilon = 10^{-2}$, $\lambda = \sqrt{5}$, $u(x,0) = (1+\exp(\lambda(x-1)))^{-1}$, and $u_x(0,t) = u_x(5,t) = 0$.

Efficiency plots (runtime, total RHS calls, $\mathcal{N}_n$ calls):

- Top-right: $\mathcal{O}(H^3)$ methods
- Bottom-left: $\mathcal{O}(H^4)$ methods
- Bottom-right: $\mathcal{O}(H^5)$ and $\mathcal{O}(H^6)$ methods
- Methods* use a "natural" splitting; others use dynamic linearization.







Outline

Implicit-Explicit Multirate Infinitesimal GARK Methods [Chinomona & R., *SIAM J. Sci. Comput.*, 2021]

To better support the flexibility needs of multiphysics problems, we have extended Sandu's MRI-GARK methods to support implicit-explicit treatment of the slow time scale, for problems of the form:

$$y'(t) = f^I(t,y) + f^E(t,y) + f^F(t,y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0 \in \mathbb{R}^n.$$

These follow the same basic approach as the previous MIS algorithm, but with

$$r(\tau) = \sum_{j=1}^{i} \gamma_{ij}\left(\tfrac{\tau}{\Delta c_i H}\right) f^I(t_n + c_j H, z_j) + \sum_{j=1}^{i-1} \omega_{ij}\left(\tfrac{\tau}{\Delta c_i H}\right) f^E(t_n + c_j H, z_j),$$

where $\Delta c_i = c_i - c_{i-1}$, $\gamma_{ij}(\theta) := \sum_{k=0}^{k_{max}} \gamma_{ij}^{\{k\}} \theta^k$ and $\omega_{ij}(\theta) := \sum_{k=0}^{k_{max}} \omega_{ij}^{\{k\}} \theta^k$.

- The coefficients $\Gamma^{\{k\}}, \Omega^{\{k\}} \in \mathbb{R}^{s \times s}$ are lower and strictly lower triangular, respectively.
- We provide order conditions up to $\mathcal{O}(H^4)$, relying on *GARK* framework [Sandu & Günther 2015].
- While theory supports "solve-coupled" methods; our current tables are solve-decoupled.

IMEX-MRI-GARK Construction

Begin with an IMEX-ARK pair $\{A^I, b^I, c^I; A^E, b^E, c^E\}$ where $c^I = c^E \equiv c$ with $0 = c_1 \le \cdots \le c_{\tilde{s}} \le 1$.

- Convert to solve-decoupled form: insert redundant stages such that $\Delta c_i A^I_{ii} = 0$ for $i = 1, \ldots, s$.
- Extend A^I, A^E and c to ensure "stiffly-accurate" condition: $c_s = 1$, $A^I_{s,:} = b^I$, $A^E_{s,:} = b^E$.
- Generate $\Gamma^{(k)}$ and $\Omega^{(k)}$ for $k = 0, \ldots, k_{max}$, to satisfy ARK consistency, internal consistency, order conditions, and maximize "joint stability" [Zharovsky et al. SINUM 2015; Sandu SINUM 2019]:

$$\mathcal{J}_{\alpha,\beta} := \left\{ z^E \in \mathbb{C}^- \ : \ \left| R\left(z^F, z^E, z^I\right)\right| \le 1, \ \ \forall z^F \in \mathcal{S}^F_\alpha, \ \ \forall z^I \in \mathcal{S}^I_\beta \right\}$$

$$\mathcal{S}^\sigma_\alpha := \left\{ z^\sigma \in \mathbb{C}^- \ : \ |\arg(z^\sigma) - \pi| \le \alpha \right\}$$

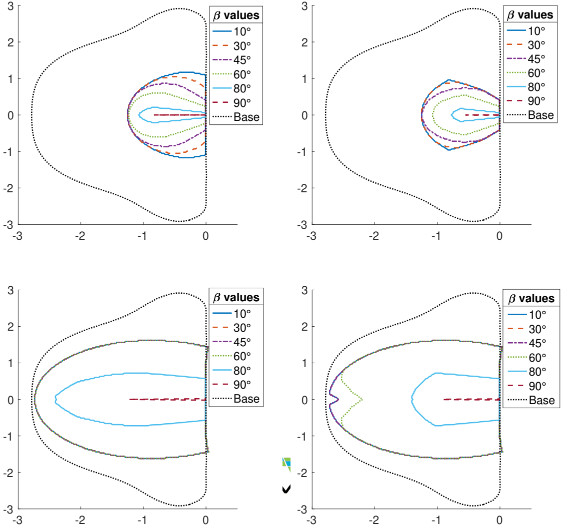
  - $\mathcal{O}(H^3)$: $s^2 + 2(k_{max}+1)s + 2$ algebraic conditions (plus stability opt.)
  - $\mathcal{O}(H^4)$: $s^2 + 2(k_{max}+1)s + 16$ algebraic conditions (plus stability opt.)

IMEX-MRI-GARK Stability – IMEX-MRI-GARK3a & IMEX-MRI-GARK3b (stab. opt.)

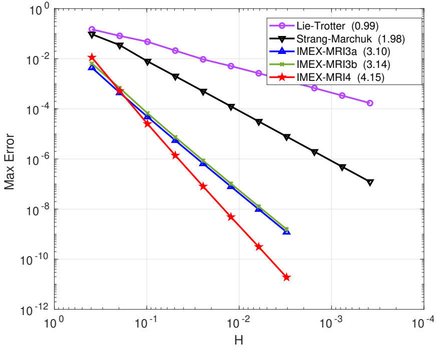
$\mathcal{J}_{\alpha,\beta}$ regions for various implicit sector angles β:

- IMEX-MRI-GARK3a ($\uparrow$)
- IMEX-MRI-GARK3b ($\downarrow$)
- fast $\alpha = 10^o$ ($\leftarrow$)
- fast $\alpha = 45^o$ ($\rightarrow$)

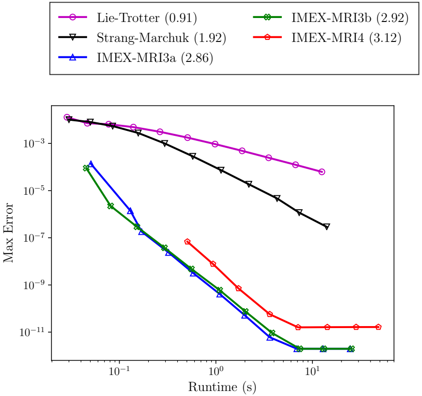
We have a simple $\mathcal{O}(H^4)$ IMEX-MRI-GARK4 table for convergence tests, but it lacks sufficient joint stability for general use.



IMEX-MRI-GARK Results



Nonlinear Kværnø-Prothero-Robinson test problem convergence.



Stiff brusselator PDE test runtime efficiency. $H = \{\frac{1}{40}, \frac{1}{80}\}$ runs were unstable for IMEX-MRI4.

IMEX-MRI-GARK Software

With David Gardner, Cody Balos & Carol Woodward at LLNL, we have implemented support for explicit and solve-decoupled implicit MIS and MRI-GARK methods within the `MRIStep` module of the ARKODE library from SUNDIALS:

- Built-in methods of orders 2, 3, and 4; user-provided MRI-GARK tables $\Gamma^{\{k\}}$ are supported.
- Slow time scale uses a user-defined H that can be varied between steps.
- Fast time scale is evolved using adaptive ARK-IMEX solver (`ARKStep`).

Future updates will include:

- Support for user-supplied fast time scale IVP solver [next minor release, October 2021].
- Support for IMEX-MRI-GARK methods [next major release, late 2021].
- Temporal adaptivity at both the slow and fast time scales [$\sim$1 year off].

Outline

Conclusions

Although simple operator-split subcycling remains standard, new & flexible methods are catching up.

- Problems allowing explicit slow treatment may benefit from higher-order approaches:
  - $\mathcal{O}(H^3)$: MIS, MRI-GARK, MERK, MERB
  - $\mathcal{O}(H^4)$: MRI-GARK, ExtMIS, RMIS, MERK, MERB
  - $\mathcal{O}(H^5)$: MERK, MERB
  - $\mathcal{O}(H^6)$: MERB
- To treat $f^S(t,y)$ implicitly, novel $\mathcal{O}(H^3)$ MIS & MRI-GARK, or $\mathcal{O}(H^4)$ MRI-GARK may be used.
- To split $f^S(t,y) = f^I(t,y) + f^E(t,y)$ we may use novel $\mathcal{O}(H^3)$ or $\mathcal{O}(H^4)$ IMEX-MRI-GARK.

All of these methods allow (a) flexibility for $f^F(t,y)$ via "infinitesimal" structure (explicit, implicit, IMEX, nested multirate), and (b) extension to allow temporal adaptivity of both H and h.

The optimal choice of method depends on a variety of factors:

- the relative costs of $f^S(t,y)$ and $f^F(t,y)$,
- whether the problem admits a good multirate splitting,
- the desired solution accuracy, ...

Future Work

Much work remains to be done:

- Advanced algorithms for "solve-coupled" MRI-GARK and IMEX-MRI-GARK.
- Rigorous stability theory for additively-partitioned ODE systems (not just $y' = \sum_k \lambda_k y$, that assumes *simultaneous diagonalizability*).
- New $\Gamma^{(k)}$ and $\Omega^{(k)}$ tables (with embeddings) for $\mathcal{O}(H^4)$ MRI-GARK and IMEX-MRI-GARK methods (and order conditions for $\mathcal{O}(H^5)$ or higher).
- Improved support for MERK, MERB and other infinitesimal multirate methods within ARKODE's `MRIStep` module.

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Software:

- SUNDIALS – https://computation.llnl.gov/projects/sundials

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