High-order multirate time integration for multiphysics systems

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SIAM/CAIMS Annual Meeting
8 July 2020

Outline

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Multiphysics/Multirate Problems

"Multiphysics" problems typically involve a variety of interacting processes:

- System of components coupled in the bulk [cosmology, combustion]
- System of components coupled across interfaces [climate, tokamak fusion]

Multiphysics simulation challenges include:

- Multirate processes, but too close to analytically reformulate.
- Optimal solvers may exist for some pieces, but not for the whole.
- Mixing of stiff/nonstiff processes, a challenge for standard algorithms.

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 splittings and subcycling, e.g.,

$$y_n^{(1)} = y_n + H f^S(t_n, y_n),$$

$$\text{Evolve: } v'(\theta) = f^F(t_n + \theta, v), \quad \text{for } \theta \in [0, H], \; v(0) = y_n^{(1)},$$

$$y_{n+1} = v(H),$$

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

$$y_n^{(1)} = y_n + \frac{H}{4} f^S(t_n, y_n) + \frac{H}{4} f^S\left(t_n + \frac{H}{2}, y_n + \frac{H}{2} f^S(t_n, y_n)\right),$$

$$\text{Evolve: } v'(\theta) = f^F(t_n + \theta, v), \quad \text{for } \theta \in [0, H], \; v(0) = y_n^{(1)}$$

$$y_n^{(2)} = v(H),$$

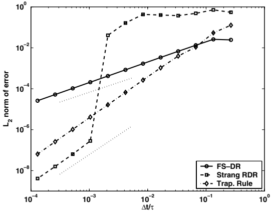
$$y_{n+1} = y_n^{(2)} + \frac{H}{4} f^S\left(t_n + \frac{H}{2}, y_n^{(2)}\right) + \frac{H}{4} f^S\left(t_{n+1}, y_n^{(2)} + \frac{H}{2} f^S\left(t_n + \frac{H}{2}, y_n^{(2)}\right)\right).$$

Legacy Multirate Approaches

Unfortunately, these simplistic splittings may suffer from:

Low accuracy:

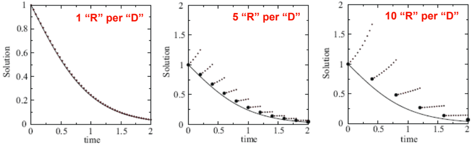
- typically $\mathcal{O}(H)$-accurate
- symmetrization & extrapolation may improve but at significant cost.



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

Poor/unknown stability:

- Even when each part utilizes a ‘stable’ step size, the combined problem may admit unstable modes



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:

- 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 $\mathcal{O}(H^3)$
- Extrapolation / deferred correction techniques[2]:
  - $+$ potential for arbitrarily-high accuracy
  - $-$ require many traversals of the step $[t_n, t_{n+1}]$

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

Sharpening our focus

Although there are a wide range of areas for additional research on multirate integration, we further narrow our focus.

- We consider only methods that require a small number of traversals of each step $[t_n, t_{n+1}]$, as these offer the potential for increased order and stability without excessive computational cost.

- We consider only methods that allow freedom in how the fast time scale is integrated (similarly to the simplistic methods outlined earlier).*

*Many higher-order approaches require a fixed fast method and/or a fixed relationship between H and h in order to interleave interpolation operations between scales.

Multitrate Infinitesimal Step (MIS) methods [Knoth & Wolke 1998; Schlegel et al. 2009; ...]

MIS/RFSMR methods arose in the numerical weather prediction community. This generic infrastructure supports $\mathcal{O}(h^2)$ and $\mathcal{O}(h^3)$ methods for multirate problems:

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

- 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 be the 'exact' solution to 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:

$$
\begin{aligned}
& z_1 = y_n, \\
& \text{For } i = 2, \ldots, s: \\
& \qquad \text{Let } r = \sum_{j=1}^{i-1} \alpha_{i,j} f^S\left(t_n + c_j H, z_j\right) \\
& \qquad \text{Evolve: } v'(\theta) = f^F(t_n + \theta, v) + r, \quad \text{for } \theta \in [c_{i-1}H, c_i H], \ v(0) = z_i, \\
& \qquad z_i = v(c_i H) \\
& y_{n+1} = z_s,
\end{aligned}
$$

where $\alpha_{i,j}$ are uniquely defined from 'slow' coefficients T_O.

- When $c_i = c_{i-1}$, the IVP "solve" reduces to a standard RK update.
- The 'fast' IVP for $v(\theta)$ may be solved using any applicable algorithm.

MIS Properties

MIS methods satisfy a number of desirable multirate method 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 table (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

Very recently, groups have worked to extend the MIS approach to higher order:

- A. Sandu's *MRI-GARK* [SIAM J. Numer. Anal., 2019] modifies the fast IVP:

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

  supporting $\mathcal{O}(H^4)$ accuracy and implicit methods at the slow time scale.

- Bauer & Knoth's *extMIS* [J. Comput. Appl. Math., 2019] relaxes the MIS structure slightly, and then develops additional order conditions on T_O to guarantee up to $\mathcal{O}(H^4)$.

- J.M. Sexton's *RMIS* [arXiv:1808.03718, 2019] computes y_{n+1} as a linear combination of $\{f^S(t_n + c_i H, z_i) + f^F(t_n + c_i H, z_i)\}$, enabling $\mathcal{O}(H^4)$ accuracy and conservation of linear invariants.

Outline

Multirate Exponential Runge–Kutta (MERK) [Luan, Chinomona & R., *SISC*, 2020]

We consider the class of multirate IVPs

$$y'(t) = Ay + g(t,y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0 \in \mathbb{R}^n,$$

- The 'fast' time scale corresponds to the *linear* operator Ay.
- The 'slow' time scale corresponds to $g(t,y)$.

The <u>same</u> structure assumed by exponential Runge–Kutta (ExpRK) methods, that may be written [Luan & Ostermann, JCAM, 2014]:

$$z_i = y_n + c_i H \varphi_1(c_i H A)\, F(t_n, y_n) + H \sum_{j=2}^{i-1} a_{i,j}(HA)\, D_{n,j}, \quad 1 \le i \le s,$$

$$y_{n+1} = y_n + H\varphi_1(HA)\, F(t_n, y_n) + H \sum_{i=2}^{s} b_i(HA)\, D_{n,i},$$

where $F(t,y) = Ay + g(t,y)$, $D_{n,i} = g(t_n + c_i H, z_i) - g(t_n, y_n)$, and $a_{i,j}(z)$, $b_i(z)$ are linear combinations of $\varphi_k(c_i z)$ and $\varphi_k(z)$, with

$$\varphi_k(z) = \int_0^1 e^{(1-\theta)z} \frac{\theta^{k-1}}{(k-1)!}\, d\theta, \quad k \ge 1.$$

MERK Construction

Theorem (Luan, Chinomona & R., 2020)

Assuming that $a_{i,j}(HA)$, $b_i(HA)$ *are* *strictly* *linear combinations of* $\varphi_k(c_i HA)$ *and* $\varphi_k(HA)$, *respectively:*

$$a_{i,j}(HA) = \sum_{k=1}^{l_{i,j}} \alpha_{i,j}^{(k)} \varphi_k(c_i HA), \qquad b_i(HA) = \sum_{k=1}^{m_i} \beta_i^{(k)} \varphi_k(HA),$$

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

$$\begin{aligned} v_{n,i}'(\theta) &= A v_{n,i}(\theta) + p_{n,i}(\theta), \quad v_{n,i}(0) = y_n \quad (2 \le i \le s), \\ v_n'(\theta) &= A v_n(\theta) + q_{n,s}(\theta), \quad v_n(0) = y_n \end{aligned}$$

at $\theta = c_i H$ *and* $\theta = H$, *respectively, where*

$$p_{n,i}(\theta) = g(t_n, y_n) + \sum_{j=2}^{i-1} \left(\sum_{k=1}^{l_{i,j}} \frac{\alpha_{i,j}^{(k)}}{c_i^k H^{k-1} (k-1)!} \theta^{k-1} \right) D_{n,j},$$

$$q_{n,s}(\theta) = g(t_n, y_n) + \sum_{j=2}^{s} \left(\sum_{k=1}^{m_i} \frac{\beta_i^{(k)}}{H^{k-1} (k-1)!} \theta^{k-1} \right) D_{n,i}.$$

MERK Convergence

Theorem (Luan, Chinomona & R., 2020)

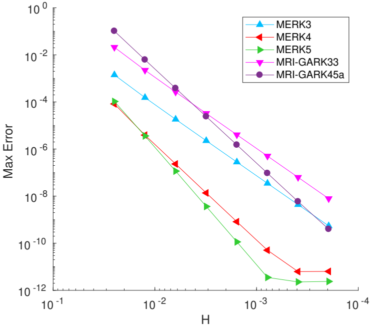
Assuming that a MERK method is constructed from an ExpRK method of global order p, with the associated 'fast' IVPs integrated with a step $h = H/m$ using methods with global orders q and r, respectively, then:

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

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.

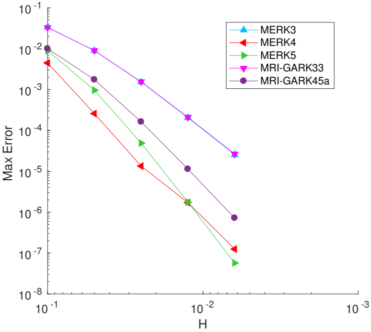
- Note the extra H in the second term: for a global method of order p we require inner solvers for z_i and y_{n+1} of orders $q \geq p-1$ and $r \geq p$.
- We evolve each of the s stages over $[0, c_i H]$ for $i = 2, \ldots, s$, thus the overall 'traversal time' is $\left(1 + \sum_{i=1}^{s} c_i\right) H$ (typically smaller than $3H$).

MERK Results



Bi-directional coupling conv. rates:
MERK3 3.05, MRI-GARK33 3.06,
MERK4 4.11, MRI-GARK45a 4.10,
MERK5 4.97.

$m = 100$ fixed, H and h are varied.



Stiff brusselator conv. rates:
MERK3 2.62, MRI-GARK33 2.60,
MERK4 3.75, MRI-GARK45a 3.48,
MERK5 4.36.

$h = 0.001$ fixed, H and m are varied.

Multirate Exponential Rosenbrock (MERB) [Luan, Chinomona & R., *in progress*]

We consider the class of multirate IVPs

$$y'(t) = F(t,y) = \mathcal{J}_n y + \mathcal{V}_n t + \mathcal{N}(t,y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0 \in \mathbb{R}^n.$$

- 'Fast' scale corresponds to $\mathcal{J}_n y$ with $\mathcal{J}_n = \frac{\partial F}{\partial y}(t_n, u_n)$.
- 'Slow' scale corresponds to $\mathcal{V}_n t + \mathcal{N}(t,y)$ with $\mathcal{V}_n = \frac{\partial F}{\partial t}(t_n, y_n)$ and $\mathcal{N}(t,y) = F(t,y) - \mathcal{J}_n y - \mathcal{V}_n t$
- Autonomous systems ($\mathcal{V}_n = 0$) admit simpler methods.

The same structure as assumed by exponential Rosenbrock (ExpRB) methods, that approximate each stage and step similarly to ExpRK. However, the additional structure ($\nabla\mathcal{N} = 0$) simplifies the order conditions immensely.

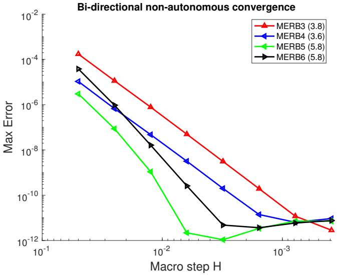
- We have constructed MERB methods of orders 2 through **6**
- Even MERB6 only has a 'traversal time' of $1.254H$

MERB Results – Non-autonomous bi-directional coupling test

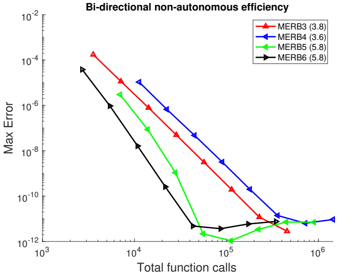
For $t \in (0,1)$, $x(0) = 2$, $y(0) = 20$, $z(0) = 2005$, and $\beta = 10^{-4}$:

$$x' = 100y - z - \beta t, \qquad y' = -100x,$$

$$z' = -5z - 5\beta t - \beta\left(x - \frac{1}{2005}z - \frac{\beta}{2005}t\right)^2 - \beta\left(y - \frac{20}{2005}z - \frac{20\beta}{2005}t\right)^2$$



Convergence rate comparisons.



'Efficiency' comparisons.

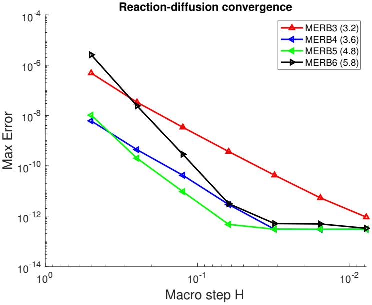
Subcycling factors (H/h): MERB3: 40, MERB4: 80, MERB5: 20, MERB6: 10

SMU FASTMATH sundials

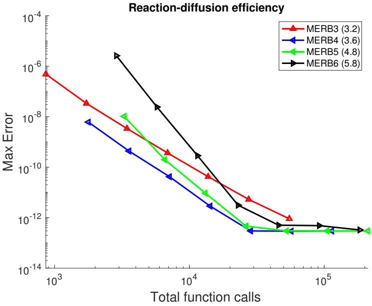
MERB Results – Reaction-Diffusion test (autonomous)

For $u_x(0,t) = u_x(1,t) = 0$, $u(x,0) = (1 + e^{\lambda(x-1)})^{-1}$, $\lambda = \frac{1}{2}\sqrt{2\gamma/\epsilon}$, and $\gamma = \epsilon = 10^{-2}$:

$$u_t = \epsilon u_{xx} + \gamma u^2 (1-u), \quad x \in (0,5), \quad t \in (0,3)$$



Convergence rate comparisons.



'Efficiency' comparisons.

All methods use a subcycling factor of $H/h = 25$.

Implicit-Explicit Multirate Infinitesimal Step (IMEX-MRI) [Chinomona & R., *in progress*]

We have extended Sandu's MRI-GARK methods to support mixed 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

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

We provide order conditions on coefficients for $\gamma_{i,j}$ and $\omega_{i,j}$ up to $\mathcal{O}(H^4)$, relying on Sandu & Günther's *GARK* framework [SIAM J. Numer. Anal., 2015].

IMEX-MRI Construction

IMEX-MRI methods 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 $0 = c_1 \le \cdots \le c_s \le 1$.

- Transform tables to 'solve-decoupled' form by inserting redundant stages: each stage i may have *either* $A^I_{i,i} \neq 0$ *or* $c_i - c_{i-1} \neq 0$.
- Extend A^I, A^E and c to ensure 'stiffly-accurate' condition: $c_{\tilde{s}} = 1$, $A^I_{\tilde{s},:} = b^I$, $A^E_{\tilde{s},:} = b^E$.
- Generate coefficients $\Gamma^{(k)} \in \mathbb{R}^{\tilde{s}\times\tilde{s}}$ and $\Omega^{(k)} \in \mathbb{R}^{\tilde{s}\times\tilde{s}}$ for $k = 0, \ldots, K$, to satisfy ARK consistency, internal consistency, order conditions, and maximize 'joint stability' [Zharovsky et al., SINUM 2015; Sandu, SINUM 2019]:

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

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

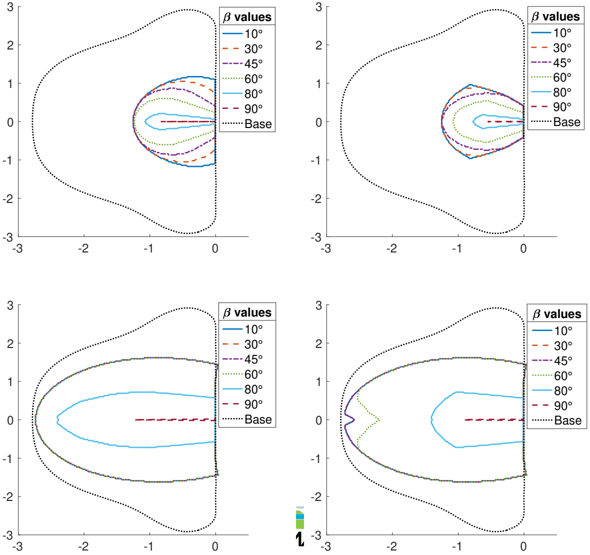
  - $\mathcal{O}\left(H^3\right)$ – $\tilde{s}^2 + 2(K+1)\tilde{s} + 2$ algebraic conditions (plus stability opt.)
  - $\mathcal{O}\left(H^4\right)$ – $\tilde{s}^2 + 2(K+1)\tilde{s} + 16$ algebraic conditions (plus stability opt.)

IMEX-MRI Stability – 3rd-order IMEX-MRI3a & IMEX-MRI3b (stab. opt.)

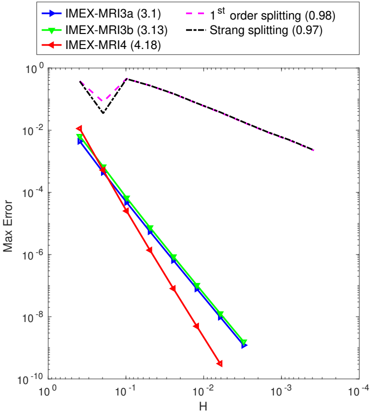
$\mathcal{J}_{\alpha,\beta}$ regions for various implicit sector angles β:

- IMEX-MRI3a ($\uparrow$)
- IMEX-MRI3b ($\downarrow$)
- fast $\alpha = 10^o$ ($\leftarrow$)
- fast $\alpha = 45^o$ ($\rightarrow$)

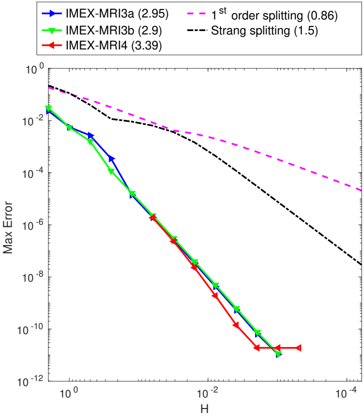
We have a simple $\mathcal{O}(H^4)$ IMEX-MRI4 for convergence tests, but it lacks sufficient joint stability for general use.



IMEX-MRI Results



Nonlinear KPR test problem
(measured convergence rates)



Stiff brusselator test problem
(measured convergence rates)

Outline

Conclusions

Pervasive in multiphysics computations, simplistic operator-spliting & subcycling remain the norm. New, flexible methods may soon break their monopoly:

- Problems allowing explicit slow treatment may benefit from new approaches:
  - $\mathcal{O}(H^3)$: MIS, MRI-GARK, MERK (fast linear), MERB (fast ∼linear)
  - $\mathcal{O}(H^4)$: MRI-GARK, ExtMIS, RMIS, MERK (fast linear), MERB (fast ∼linear)
  - $\mathcal{O}(H^5)$: MERK (fast linear), MERB (fast ∼linear)
  - $\mathcal{O}(H^6)$: MERB (fast ∼linear)
- Problems that require implicit slow treatment may utilize novel $\mathcal{O}(H^3)$ MIS & MRI-GARK, or $\mathcal{O}(H^4)$ MRI-GARK.
- Problems that require mixed implicit-explicit slow treatment may utilize novel $\mathcal{O}(H^3)$ or $\mathcal{O}(H^4)$ IMEX-MRI.

All of the methods discussed here allow:

- Nearly arbitrary treatment of the fast time scale (explicit, implicit, IMEX, further multirate) through definition of *modified 'fast' IVPs*.
- May be extended to allow temporal adaptivity of both H and h.

Future Work

Much work remains to be done:

- Robust temporal controllers for both H and h (or even m-level multirating, $h_1 > h_2 > \cdots > h_m$).
- Advanced algorithms for 'solve-coupled' MRI-GARK and IMEX-MRI (i.e., a stage i may have *both* $A^I_{i,i} \neq 0$ and $c_i - c_{i-1} \neq 0$).
- 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 for $\mathcal{O}(H^4)$ MRI-GARK and IMEX-MRI methods (and theory for order conditions at $\mathcal{O}(H^5)$ and higher).
- Robust and efficient software to facilitate use by multiphysics practitioners.

Thanks & Acknowledgements

Collaborators/Students:

- David J. Gardner [LLNL]
- Carol S. Woodward [LLNL]
- John Loffeld [LLNL]
- Jean M. Sexton [LBL]

Current Grant/Computing Support:

- DOE SciDAC & ECP Programs
- SMU Center for Scientific Computation

Software:

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

Support for this work was provided by the Department of Energy, Office of Science project "Frameworks, Algorithms and Scalable Technologies for Mathematics (FASTMath)," under Lawrence Livermore National Laboratory subcontract B626484.

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