Flexible time integration methods for multiphysics PDE systems

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Outline

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Multiphysics Simulations [Keyes et al. 2013]

Multiphysics simulations couple different models either in the bulk or across interfaces.

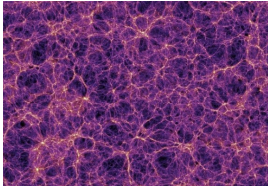
Climate:

- Atmospheric simulations combine fluid dynamics with local "physics" models for chemistry, condensation, ...
- Atmosphere is coupled at interfaces to myriad other processes (ocean, land/sea ice, ...), each using distinct models.

[https://e3sm.org]

Astrophysics/cosmology:

- Dark matter modeled using particles that give rise to large-scale gravitational structures (at right).
- Baryonic matter modeled by combining fluid dynamics, gravity, radiation transport, and reaction networks for chemical ionization states.



[http://svs.gsfc.nasa.gov/cgi-bin/details.cgi?aid=10118]

Multiphysics Challenges [Keyes et al. 2013]

These model combinations can challenge traditional numerical methods:

- "Multirate" processes evolve on different time scales but prohibit analytical reformulation.
- Stiff components disallow fully explicit methods.
- Nonlinearity and insufficient differentiability challenge fully implicit methods.
- Parallel scalability demands optimal algorithms – while robust/scalable algebraic solvers exist for parts (e.g., FMM for particles, multigrid for diffusion), none are optimal for the whole.

We may consider a prototypical problem as having m coupled evolutionary processes:

$$\dot{y}(t) = f^{\{1\}}(t,y) + \cdots + f^{\{m\}}(t,y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0.$$

Each component $f^{\{k\}}(t,y)$:

- may act on all of y (in the bulk), or on only a subset of y (within a subdomain),
- may evolve on a different characteristic time scale,
- may be "stiff" or "nonstiff," thereby desiring implicit or explicit treatment.

Legacy Multiphysics Method 1: Lie–Trotter

"Operator-splitting" approaches have historically been used for multiphysics applications.

Lie–Trotter computes $y_n \to y_{n+1}$ (here, $y_n \approx y(t_n)$) via

$$\begin{aligned}
\dot{y}^{\{1\}}(t) &= f^{\{1\}}\left(t, y^{\{1\}}\right), && t \in [t_n, t_{n+1}], && y^{\{1\}}(t_n) = y_n, \\
\dot{y}^{\{2\}}(t) &= f^{\{2\}}\left(t, y^{\{2\}}\right), && t \in [t_n, t_{n+1}], && y^{\{2\}}(t_n) = y^{\{1\}}(t_{n+1}), \\
&\vdots \\
\dot{y}^{\{m\}}(t) &= f^{\{m\}}\left(t, y^{\{m\}}\right), && t \in [t_n, t_{n+1}], && y^{\{m\}}(t_n) = y^{\{m-1\}}(t_{n+1}),
\end{aligned}$$

and sets $y_{n+1} = y^{\{m\}}(t_{n+1})$. Each IVP tackled independently using different "standard" approaches (e.g., implicit Euler, ERK-4, subcycling, ...).

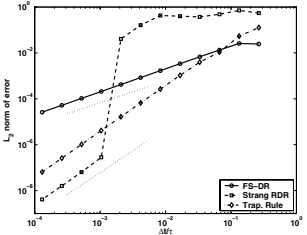
Legacy Multiphysics Method 2: Strang–Marchuk

$$
\begin{aligned}
\dot{y}^{\{1\}}(t) &= f^{\{1\}}\left(t, y^{\{1\}}\right), && t \in [t_n, t_{n+1/2}], && y^{\{1\}}(t_n) = y_n, \\
&\vdots \\
\dot{y}^{\{m-1\}}(t) &= f^{\{m-1\}}\left(t, y^{\{m-1\}}\right), && t \in [t_n, t_{n+1/2}], && y^{\{m-1\}}(t_n) = y^{\{m-2\}}(t_{n+1/2}), \\
\dot{y}^{\{m\}}(t) &= f^{\{m\}}\left(t, y^{\{m\}}\right), && t \in [t_n, t_{n+1}], && y^{\{m\}}(t_n) = y^{\{m-1\}}(t_{n+1/2}), \\
\dot{y}^{\{m-1\}}(t) &= f^{\{m-1\}}\left(t, y^{\{m-1\}}\right), && t \in [t_{n+1/2}, t_{n+1}], && y^{\{m-1\}}(t_{n+1/2}) = y^{\{m\}}(t_{n+1}), \\
&\vdots \\
\dot{y}^{\{1\}}(t) &= f^{\{1\}}\left(t, y^{\{1\}}\right), && t \in [t_{n+1/2}, t_{n+1}], && y^{\{1\}}(t_{n+1/2}) = y^{\{2\}}(t_{n+1}), \\
y_{n+1} &= y^{\{1\}}(t_{n+1}).
\end{aligned}
$$

Shorcomings of loose "initial condition" coupling

Generally poor accuracy:

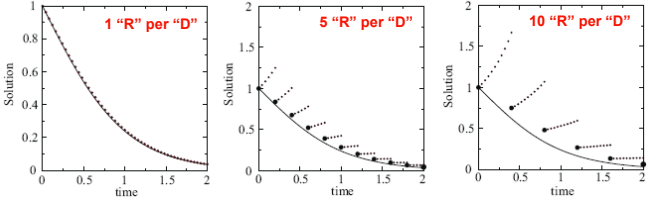
- *No matter the accuracy of each component solver*, Lie–Trotter is $\mathcal{O}(H)$ and Strang–Marchuk is $\mathcal{O}(H^2)$.
- Extrapolation or deferred correction can improve this but at significant cost.



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

Poor stability:

- Even "stable" step sizes for each part can result in unstable modes.



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

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Additive Runge–Kutta (ARK) Methods [Ascher et al. 1997; Araújo et al. 1997; Kennedy & Carpenter 2003; . . .]

ARK methods allow high-order adaptive implicit-explicit time integration for additively-split *single rate* simulations:

$$M(t)\,\dot{y}(t) = f^E(t,y) + f^I(t,y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0,$$

- M is any nonsingular linear operator (mass matrix, typically $M = I$, as used below),
- $f^E(t,y)$ contains the nonstiff terms to be treated explicitly,
- $f^I(t,y)$ contains the stiff terms to be treated implicitly.

Combine two s-stage RK methods; denoting $h_n = t_{n+1} - t_n$, $t^E_{n,j} = t_n + c^E_j h_n$, $t^I_{n,j} = t_n + c^I_j h_n$:

$$z_i = y_n + h_n \sum_{j=1}^{i-1} a^E_{i,j} f^E(t^E_{n,j}, z_j) + h_n \sum_{j=1}^{i} a^I_{i,j} f^I(t^I_{n,j}, z_j), \quad i = 1, \ldots, s,$$

$$y_{n+1} = y_n + h_n \sum_{j=1}^{s} \left[b^E_j f^E(t^E_{n,j}, z_j) + b^I_j f^I(t^I_{n,j}, z_j) \right] \quad \text{(solution)}$$

$$\tilde{y}_{n+1} = y_n + h_n \sum_{j=1}^{s} \left[\tilde{b}^E_j f^E(t^E_{n,j}, z_j) + \tilde{b}^I_j f^I(t^I_{n,j}, z_j) \right] \quad \text{(embedding)}$$

Solving each stage z_i, $i = 1, \ldots, s$

Per-stage cost is commensurate with implicit Euler for $\dot{y}(t) = f^I(t, y)$ – solve a root-finding problem:

$$0 = G_i(z) = \left[z - h_n a^I_{i,i} f^I(t^I_{n,i}, z)\right] - \left[y_n + h_n \sum_{j=1}^{i-1} \left(a^E_{i,j} f^E(t^E_{n,j}, z_j) + a^I_{i,j} f^I(t^I_{n,j}, z_j)\right)\right]$$

- If $f^I(t, y)$ is *linear* in y then this is a large-scale linear system for each z_i.
- Else this requires an iterative solver (e.g., Newton, accelerated fixed-point, or problem-specific).
- All operators in $f^E(t, y)$ are treated explicitly (do not affect algebraic solvers).

ARK methods are defined by compatible *explicit* $\left\{c^E, A^E, b^E, \tilde{b}^E\right\}$ and *implicit* $\left\{c^I, A^I, b^I, \tilde{b}^I\right\}$ tables.

- Derived in unison to satisfy order conditions arising from NB-trees (see Sandu's talk this morning).
- By selecting $A^I = 0$ and $f^I(t, y) = 0$, or $A^E = 0$ and $f^E(t, y) = 0$, ARK methods reduce to standard ERK or DIRK.

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Multirate Infinitesimal Step (MIS/MRI) methods [Schlegel et al. 2009; Sandu 2019; ...]

MRI methods arose in the numerical weather prediction community. This generic infrastructure supports up to $\mathcal{O}(h^4)$ methods for multirate problems:

$$\dot{y}(t) = f^S(t,y) + f^F(t,y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0.$$

- $f^S(t,y)$ contains the "slow" dynamics, evolved with time step H.
- $f^F(t,y)$ contains the "fast" dynamics, evolved with time steps $h \ll H$
- The slow component is integrated using an "outer" RK method, while the fast component is advanced between slow stages by solving a modified IVP with a subcycled "inner" RK method.
- Highly efficient – high order attainable with *only a single traversal* of $[t_n, t_{n+1}]$.

MIS/MRI Algorithm [Schlegel et al. 2009; Sandu 2019; ...]

Denoting $y_n \approx y(t_n)$ and $H = t_{n+1} - t_n$, a single step $y_n \to y_{n+1}$ proceeds as follows:

1. Let: $z_1 = y_n$.
2. For each slow stage z_i, $i = 2, \ldots, s$:
   a) Define: $r_i(\tau) = \sum_{j=1}^{i} \gamma_{i,j}\left(\frac{\tau}{(c_i - c_{i-1})H}\right) f^S\left(t_n + c_j H, z_j\right)$.
   b) Evolve: $\dot{v}(\tau) = f^F\left(t_n + \tau, v\right) + r_i(\tau)$, 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: $y_{n+1} = z_s$.

- MIS: $\gamma_{i,j}(\theta)$ is independent of θ, with coefficients computed from a base "outer" Runge–Kutta method.
- MRI: $\gamma_{i,j}(\theta)$ is polynomial in θ, with coefficients that satisfy order conditions arising from GARK methods [Sandu & Günther, 2015].
- Step 2b may use any applicable algorithm of sufficient accuracy (including another MRI method).
- When $c_i = c_{i-1}$, step 2b reduces to a standard ERK/DIRK Runge–Kutta stage update.

Other high-order infinitesimal methods

In the last few years multiple groups have also progressed on higher-order MRI-like methods:

- *extMIS* [Bauer & Knoth 2019] slightly modifies their MIS algorithm, and develops $\mathcal{O}(H^4)$ conditions.
- *RMIS* [Sexton & R. 2019] follows basic MIS stages by computing updated step y_{n+1} as $\sum_{j=1}^{s} b_j \left(f^S(t_n + c_j H, z_j) + f^F(t_n + c_j H, z_j)\right)$, enabling $\mathcal{O}(H^4)$ and conserv. linear invariants.
- *MERK* [Luan, Chinomona & R., 2020] constructs $r_i(\tau)$ to approximate the action of matrix φ-functions from Exponential Runge–Kutta methods, inheriting up to $\mathcal{O}(H^5)$ from base ExpRK method.
- *MERB* [Luan, Chinomona & R., 2021] constructs $r_i(\tau)$ to approximate the action of matrix φ-functions from Exponential Rosenbrock methods, inheriting up to $\mathcal{O}(H^6)$ from base ExpRB method.

All of these methods focus on explicit treatment of slow time scale $f^S(t, y)$.

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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:

$$\dot{y}(t) = f^I(t,y) + f^E(t,y) + f^F(t,y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0.$$

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

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

where $\gamma_{i,j}(\theta) := \sum_{k=0}^{k_{max}} \gamma_{i,j}^{\{k\}} \theta^k$ and $\omega_{i,j}(\theta) := \sum_{k=0}^{k_{max}} \omega_{i,j}^{\{k\}} \theta^k$.

- Coefficients matrices $\Gamma^{\{k\}}, \Omega^{\{k\}} \in \mathbb{R}^{s\times s}$ are lower and strictly lower triangular, respectively.
- Order conditions up to $\mathcal{O}(H^4)$ leverage *GARK* framework (see Rujeko's lightning talk tomorrow).
- While theory supports "solve-coupled" methods; our current tables are solve-decoupled.

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

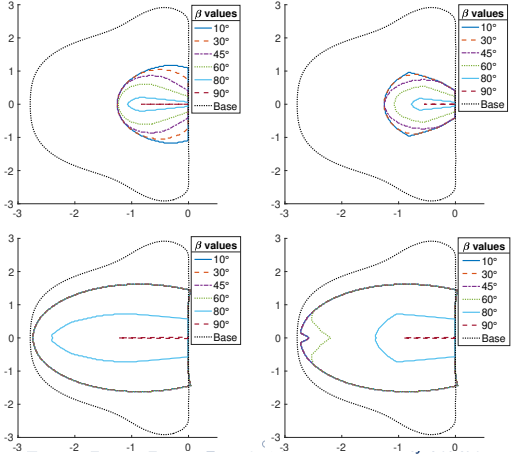
Multirate method stability is currently difficult to analyze. Examining "joint stability" [Zharovsky et al. 2015] for the Dahlquist-like test problem $\dot{y} = \lambda^I y + \lambda^E y + \lambda^F y$:

$$\mathcal{J}_{\alpha,\beta} = \left\{ z^E \in \mathbb{C}^- : \left| R\left(z^F, z^E, z^I\right) \right| \leq 1, \forall z^F \in \mathcal{S}_\alpha^F, \forall z^I \in \mathcal{S}_\beta^I \right\}, \quad \mathcal{S}_\alpha^\sigma = \left\{ z^\sigma \in \mathbb{C}^- : |\arg(z^\sigma) - \pi| \leq \alpha \right\}$$

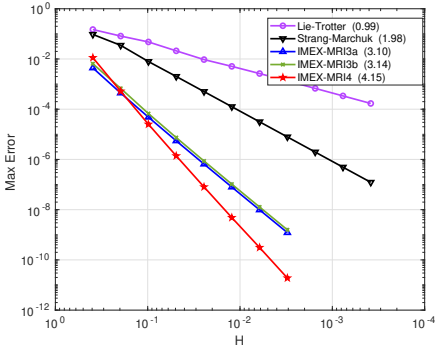
$\mathcal{J}_{\alpha,\beta}$ regions for various implicit sector angles β:

- IMEX-MRI-GARK3a (↑)
- IMEX-MRI-GARK3b (↓)
- fast $\alpha = 10^o$ (←)
- fast $\alpha = 45^o$ (→)

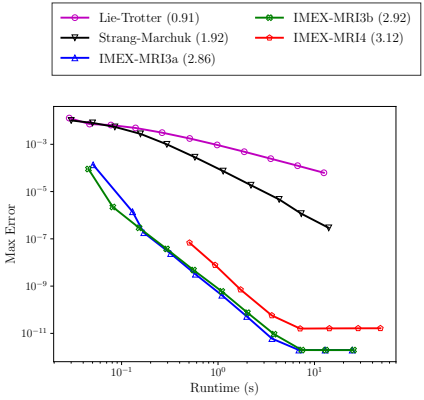
We have an initial $\mathcal{O}(H^4)$ IMEX-MRI-GARK4 table for convergence tests, though it has poor joint stability.



IMEX-MRI-GARK Convergence/Efficiency Results



Nonlinear Kværnø-Prothero-Robinson test problem convergence.



Stiff brusselator PDE test runtime efficiency.

$H = \left\{\frac{1}{40}, \frac{1}{80}\right\}$ runs were unstable for IMEX-MRI4.

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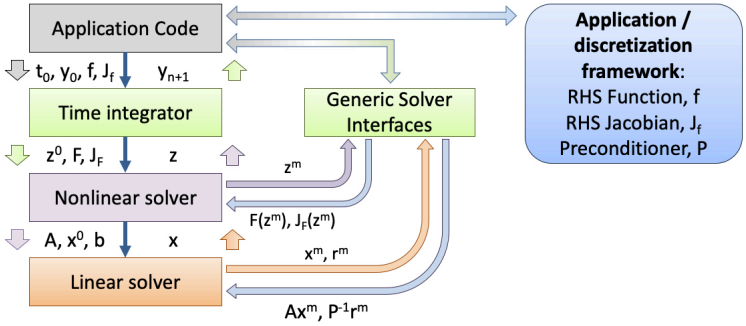
Software: ARKODE and SUNDIALS (see Carol Woodward's talk on Wednesday)

ARKODE's initial release within SUNDIALS in 2014 provided adaptive IMEX-ARK methods. Since then we have enhanced ARKODE to include a variety of "steppers":

- `ARKStep`: supports all of ARKODE's original functionality (adaptive ARK, ERK, DIRK methods); includes an interface to XBraid for PinT (work by D. Gardner).
- `ERKStep`: tuned for highly efficient explicit Runge–Kutta methods.
- `MRIStep`: infinitesimal multirate time stepping module.
  - Includes explicit MIS method of $\mathcal{O}(H^3)$.
  - Includes explicit or solve-decoupled implicit MRI-GARK methods of $\mathcal{O}(H^2)$ to $\mathcal{O}(H^4)$.
  - Includes IMEX-MRI-GARK methods of $\mathcal{O}(H^3)$ to $\mathcal{O}(H^4)$.
  - Supports user-provided MRI-GARK tables $\Gamma^{\{k\}}$ or IMEX-MRI-GARK tables $\{\Gamma^{\{k\}}, \Omega^{\{k\}}\}$.
  - Slow time scale uses a user-defined H that can be varied between steps. Fast time scale evolved using `ARKStep` or any viable user-supplied IVP solver.
  - *Multirate temporal adaptivity (H and h) in progress (current PhD work of A. Fish @ SMU).*

ARKODE leverages SUNDIALS' Modular Design & Control Inversion

Control passes between integrator, solvers, and application code as the integration progresses:



Time integrators are agnostic of vector data layout and specific algebraic solvers used.

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Multirate reacting flow demonstration problem

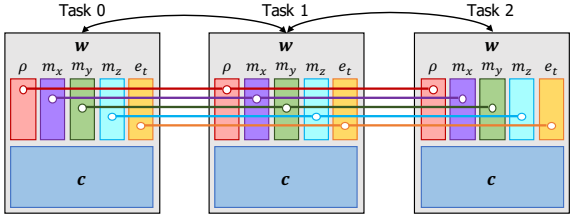
3D nonlinear compressible Euler equations combined with stiff chemical reactions for a low-density primordial gas (molecular & ionization states of H and He, free electrons, and internal gas energy), present in models of the early universe.

$$\partial_t \mathbf{w} = -\nabla \cdot \mathbf{F}(\mathbf{w}) + \mathbf{R}(\mathbf{w}), \quad \mathbf{w}(t_0) = \mathbf{w}_0,$$

$\mathbf{w}$: density, momenta, total energy, and chemical densities (10)
$\mathbf{F}$: advective fluxes (nonstiff/slow); and $\mathbf{R}$: reaction network (stiff/fast)

$\mathbf{w}$ is stored as an `MPIManyVector`:

- Software layer treating collection of vector objects as a single cohesive vector.
- Does not touch any vector data directly.
- Simplifies partitioning of data among computational resources (e.g., CPU vs GPU).
- May also combine distinct MPI intracommunicators together in a multiphysics simulation.

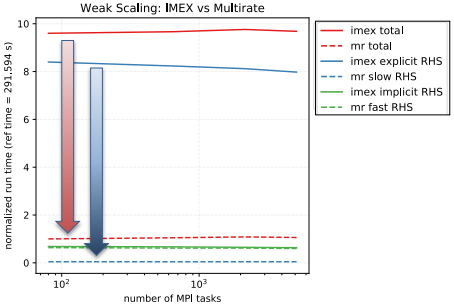


$\mathbf{w}$ is a collection of distributed vectors (density ρ, momentum m_i, and total energy e_T), and local vectors $\mathbf{c}$ (chemical densities).

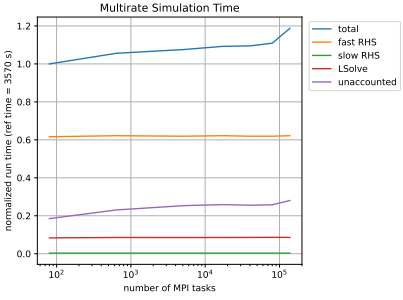
Multirate reacting flow solver strategy

- Method of lines: $(X,t) \in \Omega \times (t_0, t_f]$, with $\Omega = [x_l, x_r] \times [y_l, y_r] \times [z_l, z_r]$.
- Regular $n_x \times n_y \times n_z$ FV grid for Ω, parallelized using standard 3D MPI domain decomposition.
- $\mathcal{O}(\Delta x^5)$ WENO flux reconstruction for $F(w)$ [Shu, 2003].
- Resulting IVP system: $\dot{y}(t) = f_1(y) + f_2(y)$, $y(t_0) = y_0$, where $f_1(y)$ contains $-\nabla \cdot F(w)$, and $f_2(y)$ contains spatially-local reaction network $R(w)$.
- Compare two forms of temporal evolution:
  (a) temporally-adaptive, $\mathcal{O}(H^3)$ ARK-IMEX method from `ARKStep`: f_1 explicit and f_2 implicit,
  (b) fixed-step, $\mathcal{O}(H^3)$ MRI-GARK method from `MRIStep` (multirate factor $H/h = 1000$): f_1 slow/explicit and f_2 fast/DIRK.
- Implicit solves for spatially-local f_2 use unpreconditioned GMRES.

Multirate reacting flow – parallel scalability



$\sim 10x$ speedup with multirate



90% weak scaling efficiency using 80 to 138,240 CPU cores of OLCF Summit

- Multirating allows advection (which requires MPI) to run at a far larger time step size than that required for the single rate IMEX method to maintain stability, leading to significant speedup.
- Multirate cost now dominated by fast RHS (which remains unchanged from ImEx); upturn at largest size due to serialized chemical rate table input (subsequently fixed).

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Conclusions

Large-scale multiphysics problems:

- Nonlinear, interacting models pose key challenges to stable, accurate and scalable simulation.
- Large data requirements require scalable solvers; while individual processes admit "optimal" algorithms & time scales, these rarely agree.
- Most classical methods derived for idealized problems perform poorly on "real world" applications.

Although simple operator-spliting remains standard, new & flexible methods are catching up:

- Explicit $f^S(t,y)$ allow $\mathcal{O}(H^3)$-$\mathcal{O}(H^6)$ MIS, MRI-GARK, extMIS, RMIS, MERK, & MERB.
- Implicit $f^S(t,y)$ allow $\mathcal{O}(H^3)$-$\mathcal{O}(H^4)$ MIS & MRI-GARK.
- ImEx $f^S(t,y) = f^I(t,y) + f^E(t,y)$ allow $\mathcal{O}(H^3)$-$\mathcal{O}(H^4)$ IMEX-MRI-GARK.

Each support (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:

- whether the problem admits a natural and effective ImEx and/or multirate splitting,
- relative costs of $f^S(t,y)$ and $f^F(t,y)$ for multirate; availability of optimal algebraic solvers for $f^I(t,y)$,
- desired solution accuracy, ...

Future Work

Much work remains to be done:

- Robust temporal controllers for both H and h (or even nested multirating, $h_1 > h_2 > \cdots > h_m$).
- Advanced algorithms for "solve-coupled" infinitesimal multirate methods.
- Rigorous stability theory for additively-partitioned ODE systems (not just $\dot{y} = \sum_k \lambda_k y$, that assumes *simultaneous diagonalizability*).
- Robust, or even automated, approaches for determining additive splittings $f(t,y) = \sum_k f^{\{k\}}(t,y)$
- New $\Gamma^{(k)}$ and $\Omega^{(k)}$ tables (with embeddings) for $\mathcal{O}(H^3)$-$\mathcal{O}(H^4)$ MRI-GARK and IMEX-MRI-GARK methods (and order conditions for $\mathcal{O}(H^5)$ or higher).
- Support for additional infinitesimal multirate methods (e.g., MERK, MERB, etc.) within ARKODE's `MRIStep` module.

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