Flexible and High Order Time Integration for Multiphysics PDEs

Daniel R. Reynolds

Along with many collaborators, whose contributions will be noted in-line.

Department of Mathematics & Statistics, University of Maryland Baltimore County

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Outline

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Multiphysics Simulations

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

Climate:

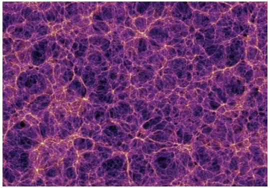
- Atmospheric simulations combine fluid dynamics with local "physics" models for chemistry, condensation, ...
- Atmosphere is coupled at interfaces to myriad other processes (ocean, land/sea ice, . . .), each using distinct models.

Above: 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.

Below: http://svs.gsfc.nasa.gov.



"Standard Practice"

Scientific simulations for evolving processes are typically posed as 1st-order systems of differential equations, e.g.

$$\dot{y}(t) = f(t, y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0,$$

where $y \in \mathbb{R}^N$ (or $\mathbb{C}^N$) contains discrete solution values/weights throughout the computational domain.

Numerical methods typically compute approximations $y_n \approx y(t_n)$ at discrete times, $t_0 < t_1 < \cdots < t_{N_t} = t_f$, "marching" from one step to the next using a prescribed update formula, Φ.

Denoting $h_n := t_{n+1} - t_n$ and $y_n \approx y(t_n)$, "textbook" approaches cluster into two categories:

- Explicit methods: $y_{n+1} = \Phi(t_n, t_{n+1}, y_n, y_{n-1}, \ldots)$.
  To ensure numerical stability, these generally require that $h_n < h_{stab}$, where h_{stab} depends on f.
- Implicit methods: $y_{n+1} = \Phi(t_n, t_{n+1}, y_{n+1}, y_n, y_{n-1}, \ldots)$.
  While these may not have stability limitations, they generally require a nonlinear algebraic solver of the form $0 = \mathbf{F}(y) := y - \Phi\left(t_n, t_{n+1}, y, y_n, y_{n-1}, \ldots\right)$.
- If h_{acc} would give an accurate solution, then we call a simulation "stiff" if $h_{stab} \ll h_{acc}$.

Multiphysics Challenges

[Keyes et al., 2013]

Multiphysics simulations can challenge these textbook methods:

- "Multirate" processes evolve on different time scales but prohibit analytical reformulation.
- Stiff components disallow fully explicit methods.
- Nonlinearity and low differentiability challenge fully implicit methods.
- Parallel scalability demands optimal algorithms – while robust/scalable algebraic solvers exist for parts (e.g., FMM for particles, MG 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 $y_n \to y_{n+1}$ 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 is tackled independently using different "standard" approaches (e.g., implicit Euler, ERK-4, subcycling, ...).

Legacy Multiphysics Method 2: Strang–Marchuk

$$\dot{y}^{\{1\}}(t) = f^{\{1\}}\left(t, y^{\{1\}}\right), \qquad t \in \left[t_n, t_n + \tfrac{h_n}{2}\right], \qquad y^{\{1\}}(t_n) = y_n,$$

$$\vdots$$

$$\dot{y}^{\{M-1\}}(t) = f^{\{M-1\}}\left(t, y^{\{M-1\}}\right), \qquad t \in \left[t_n, t_n + \tfrac{h_n}{2}\right], \qquad y^{\{M-1\}}(t_n) = y^{\{M-2\}}\left(t_n + \tfrac{h_n}{2}\right),$$

$$\dot{y}^{\{M\}}(t) = f^{\{M\}}\left(t, y^{\{M\}}\right), \qquad t \in [t_n, t_{n+1}], \qquad y^{\{M\}}(t_n) = y^{\{M-1\}}\left(t_n + \tfrac{h_n}{2}\right),$$

$$\dot{y}^{\{M-1\}}(t) = f^{\{M-1\}}\left(t, y^{\{M-1\}}\right), \qquad t \in \left[t_n + \tfrac{h_n}{2}, t_{n+1}\right], \qquad y^{\{M-1\}}\left(t_n + \tfrac{h_n}{2}\right) = y^{\{M\}}(t_{n+1}),$$

$$\vdots$$

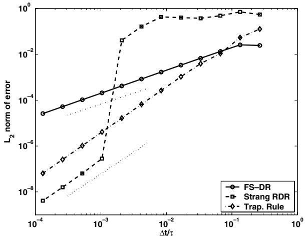
$$\dot{y}^{\{1\}}(t) = f^{\{1\}}\left(t, y^{\{1\}}\right), \qquad t \in \left[t_n + \tfrac{h_n}{2}, t_{n+1}\right], \qquad y^{\{1\}}\left(t_n + \tfrac{h_n}{2}\right) = y^{\{2\}}(t_{n+1}),$$

$$y_{n+1} = y^{\{1\}}(t_{n+1}).$$

Shorcomings of loose "initial condition" coupling

Generally poor accuracy:

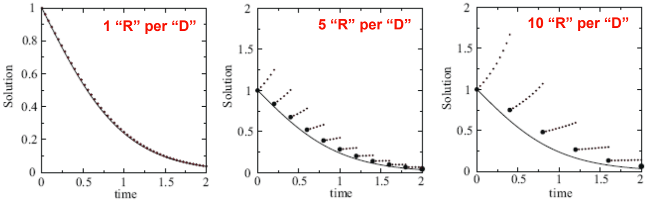
- *No matter the accuracy of each sub-solver,* Lie–Trotter is at best $\mathcal{O}(h_n)$ and Strang–Marchuk is $\mathcal{O}(h_n^2)$.
- Higher-order "fractional-step" methods are possible, but requre backwards-in-time integration [Goldman & Kaper, 1996].
- Extrapolation or deferred correction can also improve accuracy 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].

Implicit-Explicit Additive Runge–Kutta Methods [Ascher et al., 1997; Kennedy & Carpenter, 2003; ...]

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

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

- $f^E(t,y)$ 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, $i = 1, \ldots, s$

[Ascher et al., 1997; Kennedy & Carpenter, 2003; . . .]

At each stage ARK methods must solve a root-finding problem:

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

- If $f^I(t, y) = J(t)y$ (i.e., f^I is *linear* in y) then this is a large-scale linear system for each z_i:

$$\left(I - h_n a^I_{i,i} J(t_{n,i})\right) z_i = rhs_i.$$

- Else this requires an iterative solver (e.g., Newton, accelerated fixed-point, or problem-specific), that itself may require solution of multiple linear systems.

- All operators in $f^E(t, y)$ are treated explicitly (do not affect algebraic solver convergence).

ImEx-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. These are derived in unison to satisfy order conditions, stability, . . .

Multirate Infinitesimal Step (MIS) methods

[Knoth & Wolke, 1998; Schlegel et al., 2009]

MIS methods provide a flexible approach for higher-order "subcycling" in multirate applications:

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

- $f^S(t,y)$ contains the "slow" dynamics, evolved with large step H_n.
- $f^F(t,y)$ contains the "fast" dynamics, evolved with small steps $h_{n,m} \ll H_n$.
- The slow component is similar to an ERK method, while the fast component is advanced between slow stages by solving a modified IVP with a subcycled "inner" method.
- Extremely efficient – achieves second order using *a single traversal* of $[t_n, t_{n+1}]$ for all suitable ERK tables (order 2, and **sorted** $\mathbf{0 = c_1 < \cdots < c_s = 1}$); achieves $\mathcal{O}\left(h_n^3\right)$ if the table satisfies

$$\sum_{i=2}^{s} (c_i - c_{i-1})(\mathbf{e}_i + \mathbf{e}_{i-1})^T Ac + (1 - c_s)\left(\frac{1}{2} + \mathbf{e}_s^T Ac\right) = \frac{1}{3}.$$

MIS Algorithm Outline

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: $t_{n,i} = t_n + c_i H_n$, $\Delta c_i = c_i - c_{i-1}$, and $r_i = \frac{1}{\Delta c_i} \sum_{j=1}^{i-1} \left(a_{i,j} - a_{i-1,j}\right) f_j^S$.
   b) Evolve: $\dot{v}_i(\tau) = f^F(\tau, v_i) + r_i$, for $\tau \in [t_{n,i-1}, t_{n,i}]$, $v(t_{n,i-1}) = z_{i-1}$.
   c) Let: $z_i = v(t_{n,i})$, and $f_i^S = f^S(t_{n,i}, z_i)$.
3. Let: $y_{n+1} = z_s$.

Notes:

- Step 2b may use any sufficiently accurate solver (including another MIS method), hence the "flexibility" mentioned earlier.
- Improved accuracy results from including r_i in solving the fast IVP, naturally serving to propagate information from the slow to fast time scale.

Outline

1. Background
2. Unifying Theory
3. Method development
4. Open-source scientific software
5. Conclusions, Etc.

Generalized Structure Additive Runge–Kutta Theory [Sandu & Günther, 2015]

In 2015, Adrian Sandu and Michael Günther introduced a theory to analyze all of the aforementioned multiphysics methods. Assigning a separate set of internal stages, $\left\{z_i^{\{q\}}\right\}_{i=1}^{s^{\{q\}}}$, for each RHS partition $\left\{f^{\{q\}}\right\}_{q=1}^{M}$, they write a single step $y_n \to y_{n+1}$ as

$$z_i^{\{q\}} = y_n + h_n \sum_{m=1}^{M} \sum_{j=1}^{s^{\{m\}}} a_{i,j}^{\{q,m\}} f^{\{m\}}\left(z_j^{\{m\}}\right), \quad i = 1, \ldots, s^{\{q\}}, \quad q = 1, \ldots, M,$$

$$y_{n+1} = y_n + h_n \sum_{q=1}^{M} \sum_{j=1}^{s^{\{q\}}} b_j^{\{q\}} f^{\{q\}}\left(z_j^{\{q\}}\right).$$

The coefficients form a *generalized Butcher tableau*

$$\begin{array}{cccc} A^{\{1,1\}} & A^{\{1,2\}} & \cdots & A^{\{1,M\}} \\ A^{\{2,1\}} & A^{\{2,2\}} & \cdots & A^{\{2,M\}} \\ \vdots & \vdots & & \vdots \\ A^{\{M,1\}} & A^{\{M,2\}} & \cdots & A^{\{M,M\}} \\ \hline b^{\{1\}} & b^{\{2\}} & \cdots & b^{\{M\}} \end{array}$$

GARK Order Conditions

[Sandu & Günther, 2015]

Assuming internal consistency between tables, $c^{\{q\}} := A^{\{q,1\}}\mathbf{1}^{\{1\}} = \cdots = A^{\{q,M\}}\mathbf{1}^{\{M\}}$ for $q = 1, \ldots, M$, and leveraging NB-tree theory [Araujo et al., 1997], they derived conditions up to order 4:

$$
\begin{aligned}
b^{\{\sigma\}}\mathbf{1}^{\{\sigma\}} &= 1 && \forall\sigma && \text{(order 1)},\\
b^{\{\sigma\}}c^{\{\sigma\}} &= \tfrac{1}{2} && \forall\sigma && \text{(order 2)},\\
b^{\{\sigma\}}C^{\{\sigma\}}c^{\{\sigma\}} &= \tfrac{1}{3} && \forall\sigma && \text{(order 3)},\\
b^{\{\sigma\}}A^{\{\sigma,\nu\}}c^{\{\nu\}} &= \tfrac{1}{6} && \forall\sigma,\nu && \text{(order 3)},\\
b^{\{\sigma\}}C^{\{\sigma\}}C^{\{\sigma\}}c^{\{\sigma\}} &= \tfrac{1}{4} && \forall\sigma && \text{(order 4)},\\
b^{\{\sigma\}}C^{\{\sigma\}}A^{\{\sigma,\nu\}}c^{\{\nu\}} &= \tfrac{1}{8} && \forall\sigma,\nu && \text{(order 4)},\\
b^{\{\sigma\}}A^{\{\sigma,\nu\}}C^{\{\nu\}}c^{\{\nu\}} &= \tfrac{1}{12} && \forall\sigma,\nu && \text{(order 4)},\\
b^{\{\sigma\}}A^{\{\sigma,\nu\}}A^{\{\nu,\mu\}}c^{\{\mu\}} &= \tfrac{1}{24} && \forall\sigma,\nu,\mu && \text{(order 4)},
\end{aligned}
$$

where $\mathbf{1}^{\{\nu\}} \in \mathbb{R}^{s^{\{\nu\}}}$ is a vector of all ones, and $C^{\{\sigma\}} = \operatorname{diag}\left(c^{\{\sigma\}}\right)$.

GARK Linear Stability

[Sandu & Günther, 2015]

Linear stability is more challenging – assuming simultaneous diagonalizability, they consider the Dahlquist-like test problem

$$\dot{y}(t) = \sum_{\ell=1}^{M} \lambda^{\{\ell\}} y, \quad y(0) = 1, \quad \Re\left(\lambda^{\{\ell\}}\right) < 0.$$

Denoting $z^{\{\ell\}} = h\lambda^{\{\ell\}}$, the GARK stability function may be written as

$$\mathcal{R}\left(z^{\{1\}}, \ldots, z^{\{M\}}\right) = 1 + \mathbf{b}Z\left(I_{s\times s} - AZ\right)^{-1}\mathbf{1}_{s\times 1},$$

where $s = \sum_{q=1}^{M} s^{\{q\}}, \quad \mathbf{b} = \begin{bmatrix} b^{\{1\}} & \cdots & b^{\{M\}} \end{bmatrix},$

$$\mathbf{A} = \begin{bmatrix} A^{\{1,1\}} & \cdots & A^{\{1,M\}} \\ & \ddots & \\ A^{\{M,1\}} & \cdots & A^{\{M,M\}} \end{bmatrix}, \quad \text{and} \quad Z = \begin{bmatrix} z^{\{1\}} \otimes I_{s^{\{1\}}\times s^{\{1\}}} & & \\ & \ddots & \\ & & z^{\{M\}} \otimes I_{s^{\{M\}}\times s^{\{M\}}} \end{bmatrix}.$$

However, plotting the stability region $\left\{\mathbf{z} \in \mathbb{C}^M \;:\; |\mathcal{R}(\mathbf{z})| < 1\right\}$ is considerably less straightforward than with traditional non-partitioned methods.

Outline

Multirate Infinitesimal GARK (MRI-GARK) methods [Sandu, 2019]

Soon after inventing GARK theory, Sandu extended MIS methods to implicit and higher-order accuracy. The only change from the MIS algorithm is in his definition of the forcing function,

$$r_i(\tau) = \frac{1}{\Delta c_i} \sum_{j=1}^{i} \gamma_{i,j}(\tau) f_j^S, \quad \text{where} \quad \gamma_{i,j}(\tau) = \sum_{\ell=1}^{n_\Gamma} \Gamma_{i,j}^{\{\ell\}} \tau^{\ell-1}.$$

Notes:

- Fourth order is attainable, again with *only a single traversal* of $[t_n, t_{n+1}]$.
- The coefficients $\left\{\Gamma^{\{\ell\}}\right\}_{\ell=1}^{n_\Gamma}$ satisfy order conditions derived from GARK theory *(next slide)*.
- Implicitness depends on $\gamma_{i,i}(\tau) \neq 0$. It is only allowed when $\Delta c_i = 0$ (i.e., "solve-decoupled"), in which case the "fast IVP" becomes a DIRK-like implicit solve

$$0 = F_i(z) := \left[z - h_n \left(\sum_{\ell=1}^{n_\Gamma} \frac{\Gamma_{i,i}^{\{\ell\}}}{\ell}\right) f^S\left(t_{n,i}, z\right)\right] - \left[z_{i-1} + h_n \sum_{j=1}^{i-1} \left(\sum_{\ell=1}^{n_\Gamma} \frac{\Gamma_{i,j}^{\{\ell\}}}{\ell}\right) f_j^S\right].$$

- **As with MIS, derivation requires sorted abscissae: $\mathbf{0 = c_1 \leq c_2 \leq \cdots \leq c_s = 1}$.**

Infinitesimal "order conditions"

MIS/MRI methods of order $\mathcal{O}(h_n^p)$ couple time scales via the forcing function $r_i(\tau) = \frac{1}{\Delta c_i}\sum_j \gamma_{ij}(\tau) f_j^S$,

that is used in solving the fast IVP

$$\dot{v}_i(\tau) = f^F(\tau, v_i) + r_i(\tau), \quad \tau \in [\tau_{i,0}, \tau_{i,f}], \quad v_i(\tau_0) = v_{i,0}$$

$$\Leftrightarrow$$

$$v_i(\tau_{i,f}) = \Phi(\tau_{i,0}, \tau_{i,f}, v_{i,0}).$$

MIS/MRI methods do not care how Φ operates, only that it also has global accuracy $\mathcal{O}(h_n^p)$. Thus to $\mathcal{O}\left(h_n^{p+1}\right)$ it is equivalent to an $s^{\{f\}}$-stage RK method $\{A^{\{f,f\}}, b^{\{f\}}, c^{\{f\}}\}$ that satisfies

$$\begin{aligned} b^{\{f\}}\mathbf{1}^{\{f\}} &= 1 && \text{(order 1)}, \\ b^{\{f\}}c^{\{f\}} &= \tfrac{1}{2} && \text{(order 2)}, \\ b^{\{f\}}C^{\{f\}}c^{\{f\}} &= \tfrac{1}{3} && \text{(order 3)}, \\ b^{\{f\}}A^{\{f\}}c^{\{f\}} &= \tfrac{1}{6} && \text{(order 3)}, \\ &\vdots \end{aligned}$$

These are then combined with the GARK theory to derive conditions on $\gamma_{ij}(\tau)$, and thus $\Gamma_{ij}^{\{\ell\}}$.

Implicit-Explicit Multirate Infinitesimal GARK Methods

[Chinomona & R., *SISC*, 2021]

My student Rujeko Chinomona extended Sandu's MRI-GARK methods to support implicit-explicit treatment of the slow time scale:

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

These define an ImEx forcing function

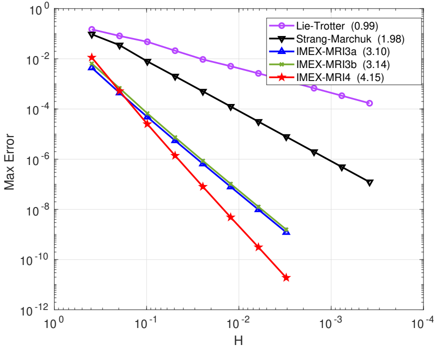
$$r_i(\tau) = \frac{1}{\Delta c_i} \sum_{j=1}^{i} \gamma_{i,j}(\tau) f_j^I + \frac{1}{\Delta c_i} \sum_{j=1}^{i-1} \omega_{i,j}(\tau) f_j^E,$$

where $\gamma_{i,j}(\tau)$ and $\omega_{i,j}(\tau)$ are defined similarly as for MRI-GARK.

- Order conditions up to $\mathcal{O}(h_n^4)$ again leverage the GARK framework.
- Derived $\mathcal{O}(h_n^3)$ methods with optimized linear stability, and a candidate $\mathcal{O}(h_n^4)$ method.
- *However, due to sorted abscissae requirement, we were unable to derive embedded $\mathcal{O}(h_n^3)$ ImEx-MRI-GARK methods, and struggled to optimize linear stability at $\mathcal{O}(h_n^4)$.*

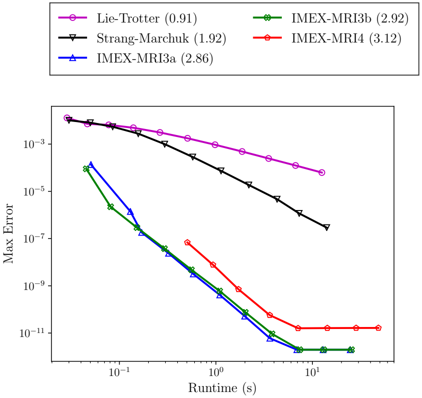
ImEx-MRI-GARK Convergence/Efficiency

[Chinomona & R., *SISC*, 2021]



Nonlinear Kværnø-Prothero-Robinson ODE test problem convergence.

All methods exhibit expected convergence rate; ImEx-MRI are far more accurate than OS.



1D stiff Brusselator PDE test runtime efficiency.

Similar story for stiff PDE test, but the largest two step sizes were unstable for ImEx-MRI4.

Implicit-Explicit Multirate Infinitesimal Stage-Restart Methods

[Fish, R., & Roberts, *JCAM*, 2024]

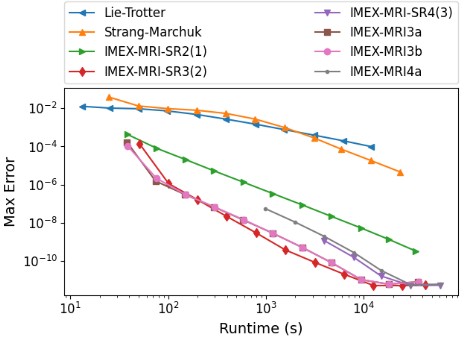

To circumvent the sorted abscissae requirement, my student Alex Fish, collaborator Steven Roberts, and I developed ImEx-MRI-SR methods by assuming a simpler structure for the step $y_n \to y_{n+1}$:

1. Let: $z_1 = y_n$.
2. For each slow stage z_i, $i = 2, \ldots, s$:
   a) Define: $r_i(\tau) = \frac{1}{c_i} \sum_{j=1}^{i-1} \omega_{i,j} \left(\frac{\tau}{c_i h_n}\right) \left(f_j^E + f_j^I\right)$, with $\omega_{i,j}(\theta) = \sum_{\ell=1}^{n_\Omega} \omega_{i,j}^{\{\ell\}} \theta^{\ell-1}$.
   b) Evolve: $\dot{v}(\tau) = f^F(t_n + \tau, v) + r_i(\tau)$, for $\tau \in [0, c_i h_n]$, $v(0) = y_n$.
   c) Solve: $0 = \left[z_i - h_n \gamma_{i,i} f^I(t_{n,i}, z_i)\right] - \left[v(c_i h_n) + h_n \sum_{j=1}^{i-1} \gamma_{i,j} f_j^I\right]$.
3. Let: $y_{n+1} = z_s$.

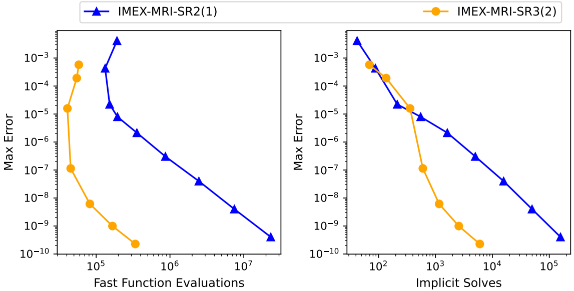
- Structure is independent of $\Delta c_i = 0$; no "padding" is required to derive ImEx-MRI-SR from ImEx-ARK.
- The embedding has an identical structure as the last stage, z_s.
- Derived embedded methods from $\mathcal{O}(h_n^2) - \mathcal{O}(h_n^4)$; linear stability at $\mathcal{O}(h_n^4)$ again challenging to optimize.

ImEx-MRI-SR Convergence/Efficiency – 1D Stiff Brusselator PDE [Fish, R., & Roberts, *JCAM*, 2024]

1D Stiff Brusselator PDE results: fixed-step runtime efficiency (left), and adaptive-step efficiency measured via f^F evaluations or f^I solves.



ImEx-MRI-SR have similar accuracy to ImEx-MRI-GARK (far better than OS); reduced linear stability at $\mathcal{O}(h_n^4)$ again visible..

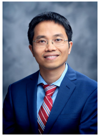


Both methods can adaptively track multirate dynamics (more on adaptivity in a few slides);
$\mathcal{O}(h_n^3)$ more efficient at tighter accuracy;
$\mathcal{O}(h_n^2)$ competive wrt implicit solves at loose accuracy.

Multirate Exponential Runge–Kutta (MERK) and Rosenbrock (MERB) Methods

[Luan, Chinomona & R., *SISC*, 2020; Luan, Chinomona & R., *SISC*, 2022]

To circumvent the explosion in GARK order conditions, with collaborator Vu Thai Luan, Rujeko and I leveraged exponential method theory to replace the action of the φ_j functions with "infinitesimal" IVP solves *(next slide)*.



We consider multirate IVP of the form

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

- "Fast" scale corresponds to $\mathcal{J}_n y$: for MERK $\mathcal{J}_n$ may be arbitrary, for MERB $\mathcal{J}_n = \frac{\partial F}{\partial y}(t_n, y_n)$.
- "Slow" scale corresponds to $f^S(t,y)$; must be treated explicitly in MERK and MERB methods.
- Their implementations are nearly identical to ImEx-MRI-SR, albeit without any implicit solves.
- Provide embedded MERK up to $\mathcal{O}(h_n^5)$, and non-embedded MERB up to $\mathcal{O}(h_n^6)$.

Multirate Exponential "Idea"

[Luan, Chinomona & R., *SISC*, 2020]

A single exponential Euler time step $y_n \to y_{n+1}$ has the form

$$y_{n+1} = \varphi_0(h_n \mathcal{J}_n) y_n + h_n \varphi_1(h_n \mathcal{J}_n) f^S(t_n, y_n),$$

where $\varphi_0(z) = e^z$, and $\varphi_1(z) = \frac{e^z - 1}{z}$.

Instead of approximating these matrix functions, we note that this method exactly solves a *modified IVP*

$$\dot{v}(\tau) = \mathcal{J}_n v + r, \quad \tau \in [0, h_n], \quad v(0) = y_n, \quad r := f^S(t_n, y_n).$$

Thus, to $\mathcal{O}(h_n^2)$, we can replace the action of $\varphi_j(h_n \mathcal{J}_n)$ with an "infinitesimal" IVP solve.

Higher-order MERK and MERB methods are derived similarly, so long as the internal stages and time step solution of the exponential method may be written as linear combinations of φ_k functions,

$$\sum_{k=1}^{\ell_i} \alpha_{i,j}^{(k)} \varphi_k(c_i h_n \mathcal{J}_n),$$

where c_i is the abscissa of the i-th stage, and $\alpha_{i,j}^{(k)}$ are method-specific coefficients.

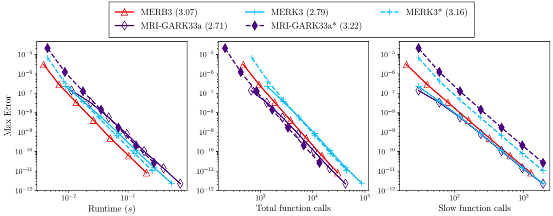
MERK/MERB Efficiency – 1D Reaction-Diffusion PDE

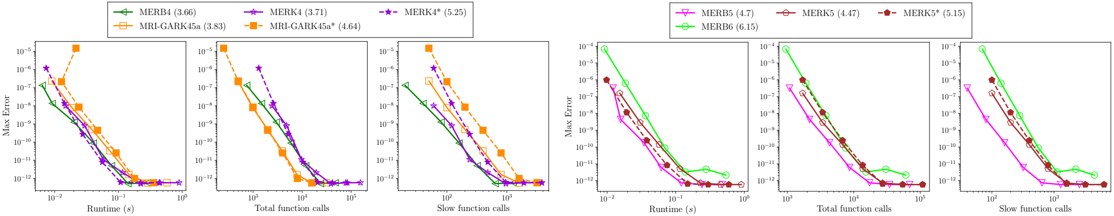
[Luan, Chinomona & R., *SISC*, 2022]

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, RHS calls, f^S 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.



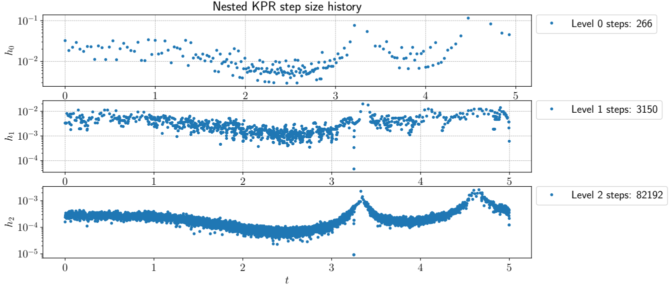


MERK/MERB more efficient than MRI-GARK in both runtime and f^S cost; MRI-GARK more efficient in f^F.

MRI time step adaptivity

[Fish & R., *SISC*, 2023; R., Amihere, Mitchell, & Luan, *JCAM*, 2026]

- For single-rate problems, it is well-known that method robustness, accuracy, and efficiency hinge on appropriate selection of h_n.
- While decades of work have optimized single-rate "controllers", we were the first to establish rigorous methods for time step control of MRI methods.
- In [Fish & R., 2023] we simultaneously select both H_n and h_n for a given time step $y_n \to y_{n+1}$, based on separate estimates of the local truncation error in both the MRI method and the inner integrator.
- In [R. et al., 2026] we instead select both H_n and an inner solver tolerance scaling factor $r_{tol,n}$, using similar local error estimates. These allow the inner solver to adapt *within* the MRI step $y_n \to y_{n+1}$, and enable temporal adaptivity with nested MRI methods.



Outline

SUNDIALS [Hindmarsh et al., *TOMS*, 2005; Balos et al., *ParComp*, 2021; Gardner et al., *TOMS*, 2022; Roberts et al., *TOMS*, 2026]

A primary goal of my research is to impact other fields – I feel can best achieve this through dissemination of modern methods through high-quality open-source software.

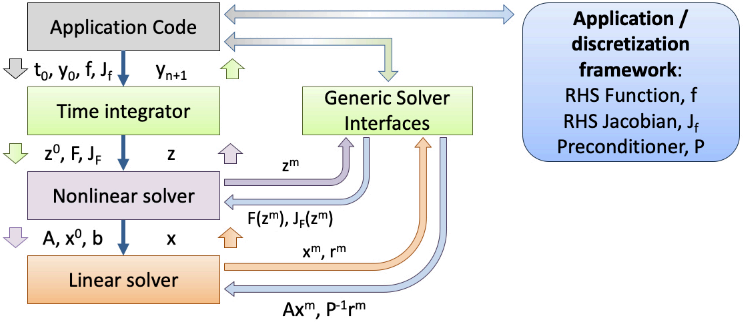
My collaborators and I develop and maintain *SUNDIALS* – the SUite of Nonlinear and DIfferential/ALgebraic Solvers

- Adaptive time integrators for ODEs and DAEs and efficient nonlinear solvers, used throughout research and industry.
- Written in C/C++, natively supports parallel computing:
    - GPUs via CUDA, HIP, SYCL, RAJA and Kokkos
    - Clusters/supercomputers via MPI
    - Threading via OpenMP and Pthreads
- BSD license; available from GitHub or Spack.
- Over 100,000 downloads/year since 2016.
- Runs anywhere from laptops to supercomputers.
- Embedded in MATLAB, Mathematica, Python (scikit), DifferentialEquations.jl, OpenModelica, . . .

- CVODE(S): linear multistep methods for IVPs, fwd/adj sensitivities
- IDA(S): linear multistep methods for DAEs, fwd/adj sensitivities
- ARKODE: multi-stage methods for IVPs
- KINSOL: nonlinear solver

SUNDIALS' Modular Design & Control Inversion [Gardner et al., 2022]

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



Time integrators are agnostic as to the vector data layout and algebraic solvers used, leveraging application-specific implementations where possible, and providing native modules if desired.

SUNDIALS' ARKODE solver

[R. et al., *TOMS*, 2023; Roberts et al., *TOMS*, 2026]

ARKODE has been released as part of SUNDIALS since 2014, providing adaptive ImEx-ARK methods. Since then we have enhanced ARKODE to include a variety of "steppers":

- `ARKStep`: adaptive ARK, ERK, DIRK methods [all]; includes an interface to XBraid for parallel-in-time [D. Gardner]
- `ERKStep`: adaptive explicit RK methods [all]; includes fixed-step discrete FSA/ASA [C. Balos]
- `MRIStep`: adaptive infinitesimal multirate methods (MIS, MRI-GARK, ImEx-MRI-GARK, ImEx-MRI-SR, MERK) [R. Chinomona, D. Gardner]
- `SPRKStep`: fixed-step symplectic RK methods for partitioned Hamiltonian systems [C. Balos]
- `SplittingStep` and `ForcingStep`: fixed-step operator splitting methods (including very high order) [S. Roberts]
- `LSRKStep`: adaptive explicit RK methods with low-storage structure (strong-stability preserving, RKC and RKL "super time stepping") [M. Aggul]

Outline

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, supporting time adaptivity, high order accuracy (up to $\mathcal{O}(h_n^6)$), and multirate/ImEx flexibility.

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, ...

Current projects in my group (all are in collaboration with external partners)

- Construct embedded ImEx and split-explicit super-time-stepping methods [M. Aggul, S. Amihere]
- Construct embedded ImEx-ARK methods with SSP properties [S. Amihere]
- Explore performance of novel ImEx and MRI algorithms for simulating instabilities in magnetic fusion plasmas [M. Aggul, S. Amihere, Y. Hu]
- Examine approaches to leverage data-driven machine learning techniques to accelerate first-principles predictive simulations [D. Mitchell]
- Examine approaches for temporal error estimation and control for application-specific quantities of interest

Future directions (for my group or others)

- Devise constraint-preserving MRI methods – while these naturally conserve linear invariants, are there extensions for energy conservation, asymptotic preserving, SSP?
- Can we extend these "flexible integration" ideas approaches (ImEx & MRI) to large-scale systems of DAEs?
- Can we devise robust and automated approaches for splitting an IVP into stiff/nonstiff or fast/slow partitions, $f(t,y) = \sum_k f^{\{k\}}(t,y)$?
- Can we come up with a more rigorous stability theory for additively-partitioned ODE systems (not just $\dot{y} = \sum_k \lambda_k y$)?
- ?

Thank you for your time and attention!

- For more information on any of our new methods research, please see my webpage: https://drreynolds.github.io.
- For more information on SUNDIALS, please see our
  - Github: https://github.com/llnl/sundials
  - Documentation: https://sundials.readthedocs.io
- For anything else, talk to me at this meeting or send me an email (dreynolds@umbc.edu)

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