Flexible time integration methods for multiphysics PDE systems

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   - Infinitesimal Multirate Methods

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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.

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.

[https://e3sm.org]

[http://svs.gsfc.nasa.gov/cgi-bin/details.cgi?aid=10118]
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 $y_n \rightarrow y_{n+1}$ (here, $y_n \approx y(t_n)$) via

\[
\dot{y}^{\{1\}}(t) = f^{\{1\}} \left( t, y^{\{1\}} \right), \quad t \in [t_n, t_{n+1}], \quad y^{\{1\}}(t_n) = y_n,
\]

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

\[
\vdots
\]

\[
\dot{y}^{\{m\}}(t) = f^{\{m\}} \left( t, y^{\{m\}} \right), \quad t \in [t_n, t_{n+1}], \quad y^{\{m\}}(t_n) = y^{\{m-1\}}(t_{n+1}),
\]

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

\[ \dot{y}^{(1)}(t) = f^{(1)} \left( t, y^{(1)} \right), \quad t \in [t_n, t_{n+1/2}], \quad y^{(1)}(t_n) = y_n, \]

\[ \vdots \]

\[ \dot{y}^{(m-1)}(t) = f^{(m-1)} \left( t, y^{(m-1)} \right), \quad t \in [t_n, t_{n+1/2}], \quad y^{(m-1)}(t_n) = y^{(m-2)}(t_{n+1/2}), \]

\[ \dot{y}^{(m)}(t) = f^{(m)} \left( t, y^{(m)} \right), \quad t \in [t_n, t_{n+1}], \quad y^{(m)}(t_n) = y^{(m-1)}(t_{n+1/2}), \]

\[ \dot{y}^{(m-1)}(t) = f^{(m-1)} \left( t, y^{(m-1)} \right), \quad t \in [t_{n+1/2}, t_{n+1}], \quad y^{(m-1)}(t_{n+1/2}) = y^{(m)}(t_{n+1}), \]

\[ \vdots \]

\[ \dot{y}^{(1)}(t) = f^{(1)} \left( t, y^{(1)} \right), \quad t \in [t_{n+1/2}, t_{n+1}], \quad y^{(1)}(t_{n+1/2}) = y^{(2)}(t_{n+1}), \]

\[ y_{n+1} = y^{(1)}(t_{n+1}). \]
Shorcomings of loose “initial condition” coupling

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

Poor stability:
- Even “stable” step sizes for each part can result in unstable modes.

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

Subcycling stability (reaction-diffusion) [Estep et al. 2008].
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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 \( h_n = t_{n+1} - t_n \), \( t^E_{n,j} = t_n + c^E_j h_n \), \( t^I_{n,j} = t_n + c^I_j h_n \):

\[
\begin{align*}
z_i &= y_n + h_n \sum_{j=1}^{i-1} a^E_{i,j} f^E(t^E_{n,j}, z_j) + h_n \sum_{j=1}^{i} a^I_{i,j} f^I(t^I_{n,j}, z_j), \quad i = 1, \ldots, s, \\
y_{n+1} &= y_n + h_n \sum_{j=1}^{s} \left[ b^E_j f^E(t^E_{n,j}, z_j) + b^I_j f^I(t^I_{n,j}, z_j) \right] \quad \text{(solution)} \\
\tilde{y}_{n+1} &= y_n + h_n \sum_{j=1}^{s} \left[ \tilde{b}^E_j f^E(t^E_{n,j}, z_j) + \tilde{b}^I_j f^I(t^I_{n,j}, z_j) \right] \quad \text{(embedding)}
\end{align*}
\]
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 $\{c^E, A^E, b^E, \tilde{b}^E\}$ and implicit $\{c^I, A^I, b^I, \tilde{b}^I\}$ 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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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 $[t_n, t_{n+1}]$. 

[Schlegel et al. 2009; Sandu 2019; ...]
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 \( y_n \rightarrow y_{n+1} \) 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 \( \theta \), with coefficients computed from a base “outer” Runge–Kutta method.
- MRI: \( \gamma_{i,j}(\theta) \) is polynomial in \( \theta \), 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 $O(H^4)$ 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 $O(H^4)$ and conserv. linear invariants.

- **MERK** [Luan, Chinomona & R., 2020] constructs $r_i(\tau)$ to approximate the action of matrix $\varphi$-functions from Exponential Runge–Kutta methods, inheriting up to $O(H^5)$ from base ExpRK method.

- **MERB** [Luan, Chinomona & R., 2021] constructs $r_i(\tau)$ to approximate the action of matrix $\varphi$-functions from Exponential Rosenbrock methods, inheriting up to $O(H^6)$ from base ExpRB method.

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

\[ r_i(\tau) = \sum_{j=1}^{i} \gamma_{i,j}(\frac{\tau}{(c_i - c_i-1)H}) f^I(t_n + c_j H, z_j) + \sum_{j=1}^{i-1} \omega_{i,j}(\frac{\tau}{(c_i - c_i-1)H}) f^E(t_n + c_j H, z_j), \]

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

\[ J_{\alpha,\beta} = \{ z^E \in \mathbb{C}^- : \left| R(z^F, z^E, z^I) \right| \leq 1, \forall z^F \in S^F_{\alpha}, \forall z^I \in S^I_{\beta} \}, \quad S^\sigma_{\alpha} = \{ z^\sigma \in \mathbb{C}^- : |\arg(z^\sigma) - \pi| \leq \alpha \} \]

\( J_{\alpha,\beta} \) regions for various implicit sector angles \( \beta \):

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

We have an initial \( O(H^4) \) IMEX-MRI-GARK4 table for convergence tests, though it has poor joint stability.
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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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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 $O(H^3)$.
  - Includes explicit or solve-decoupled implicit MRI-GARK methods of $O(H^2)$ to $O(H^4)$.
  - Includes IMEX-MRI-GARK methods of $O(H^3)$ to $O(H^4)$.
  - 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.

\[
\partial_t w = -\nabla \cdot F(w) + R(w), \quad w(t_0) = w_0,
\]

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

\(w\) 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.
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 \(\Omega\), parallelized using standard 3D MPI domain decomposition.

- \(O(\Delta x^5)\) 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, \(O(H^3)\) ARK-IMEX method from ARKStep: \(f_1\) explicit and \(f_2\) implicit,
  - (b) fixed-step, \(O(H^3)\) 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

~10x speedup with multirate

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).

90% weak scaling efficiency using 80 to 138,240 CPU cores of OLCF Summit
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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-splitting remains standard, new & flexible methods are catching up:

- Explicit $f^S(t, y)$ allow $O(H^3)$-$O(H^6)$ MIS, MRI-GARK, extMIS, RMIS, MERK, & MERB.
- Implicit $f^S(t, y)$ allow $O(H^3)$-$O(H^4)$ MIS & MRI-GARK.
- ImEx $f^S(t, y) = f^I(t, y) + f^E(t, y)$ allow $O(H^3)$-$O(H^4)$ 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, . . .
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 $O(H^3)$-$O(H^4)$ MRI-GARK and IMEX-MRI-GARK methods (and order conditions for $O(H^5)$ or higher).

- Support for additional infinitesimal multirate methods (e.g., MERK, MERB, etc.) within ARKODE’s MRIStep module.
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References (all link to web versions)

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