Implicit-Explicit Multirate Time Integration Methods

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Outline

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1. Background
2. IMEX-MRI Methods
3. MRI Time Adaptivity
4. Software
5. Conclusions, etc.

Multiphysics Simulations

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

Climate:

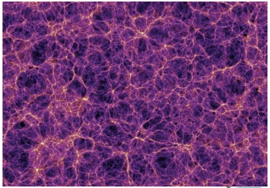
- Atmospheric simulations combine fluid dynamics with local "physics" models for chemistry, condensation, ...
- Atmosphere is coupled at interfaces to myriad other processes (ocean, land/sea ice, . . .), each using distinct models.

Above: https://e3sm.org.

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

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.



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.

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, $i = 1, \dots, s$ [Ascher et al., 1997; Kennedy & Carpenter, 2003; ...]

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).

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 arising from NB-trees (along with stability, high stage order, ...).

Multitrate Infinitesimal (MIS/MRI) methods

[Schlegel et al., 2009; Sandu, 2019; . . .]

MRI methods provide a flexible approach to "subcycling" and support up to $\mathcal{O}(h^4)$ 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 defined by an "outer" RK method, while the fast component is advanced between slow stages by solving a modified IVP with a subcycled "inner" RK method.
- Extremely 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 $\tau \in [c_{i-1}H, c_i H]$, $v(c_{i-1}H) = z_{i-1}$.
   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 the "outer" Runge–Kutta method.
- MRI: $\gamma_{i,j}(\theta)$ is polynomial in θ, coefficients satisfy GARK-based order conditions [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.
- Implicitness at the slow scale depends on $\gamma_{i,i}(\theta) \neq 0$, only used when $c_i = c_{i-1}$ ("solve-decoupled").

Outline

Implicit-Explicit Multirate Infinitesimal GARK Methods

[Chinomona & R., *SISC*, 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 forcing function

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

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

- 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.

IMEX-MRI-GARK Construction

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

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 (s^2 conditions), internal consistency ($2(k_{max} + 1)s$ conditions), plus order conditions:
  - $\mathcal{O}(H^1)$ and $\mathcal{O}(H^2)$: no additional order conditions,
  - $\mathcal{O}(H^3)$: 2 additional order conditions,
  - $\mathcal{O}(H^4)$: 16 additional order conditions.
- With any additional degrees of freedom, we maximized "joint linear stability" (next slide).

Note: we found it challenging to construct embedded IMEX-MRI-GARK methods, largely due to our reliance on IMEX-ARK base methods and the "sorted" abscissa requirement.

IMEX-MRI-GARK Joint Linear Stability

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

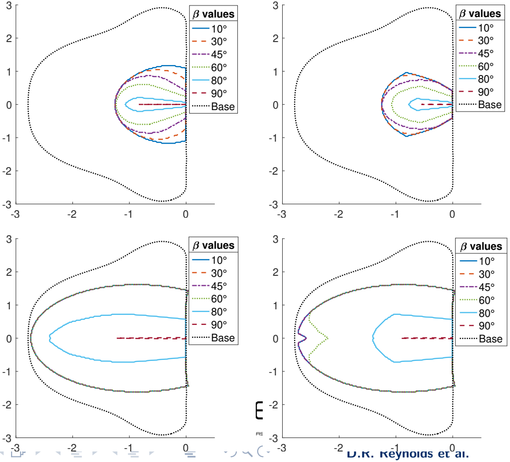
Multirate method stability is currently difficult to analyze. Examining "joint stability" [Zharovsky et al., 2015] for the Dahlquist-like test problem $\dot{y} = \lambda^I y + \lambda^E y + \lambda^F y$:

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

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

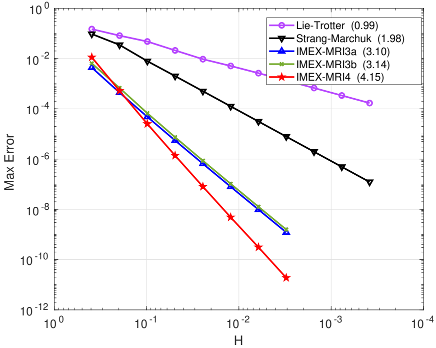
- IMEX-MRI-GARK3a (↑)
- IMEX-MRI-GARK3b (↓)
- fast $\alpha = 10^o$ (←)
- fast $\alpha = 45^o$ (→)

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

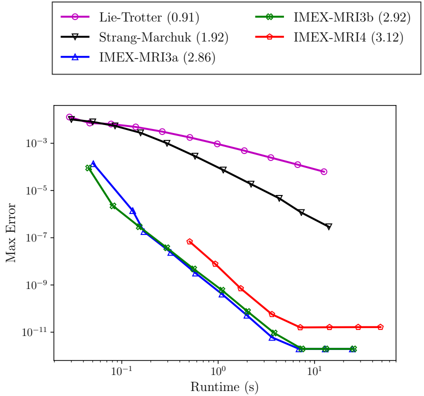


IMEX-MRI-GARK Convergence/Efficiency

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



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.

Implicit-Explicit Multirate Infinitesimal Stage-Restart Methods [Fish, R., & Roberts, 2023]

IMEX-MRI-SR methods consider the same problem as IMEX-MRI-GARK, but circumvent their restriction that $c_i \le c_{i+1}$ by assuming a different 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: $r_i(\tau) = \frac{1}{c_i} \sum_{j=1}^{i-1} \omega_{i,j}\left(\frac{\tau}{c_i H}\right)\left(f_j^E + f_j^I\right)$, with $\omega_{i,j}(\theta) = \sum_{k=0}^{n_\Omega - 1} \omega_{i,j}^{\{k\}} \theta^k$.
   b) Evolve: $\dot{v}(\tau) = f^F(t_n + \tau, v) + r_i(\tau)$, for $\tau \in [0, c_i H]$, $v(0) = y_n$.
   c) Solve: $z_i = v(c_i H) + H \sum_{j=1}^{i} \gamma_{i,j} f_j^I$.
3. Let: $y_{n+1} = z_s$.

- We denote $f_j^E := f^E(t_n + c_j H, z_j)$ and $f_j^I := f^E(t_n + c_j H, z_j)$.
- The embedding has an identical structure as the last stage, z_s.
- There is no "hidden" dependence on $\Delta c_i = 0$ for the algorithm structure, and no "padding" is required when deriving IMEX-MRI-SR methods from IMEX-ARK.

IMEX-MRI-SR Construction

[Fish, R., & Roberts, 2023]

Again begin with an IMEX-ARK pair $\{A^I, b^I, c^I; A^E, b^E, c^E\}$ where $c^I = c^E \equiv c$ (but with any $c_i \neq 0$, $i = 2, \ldots, s$).

- 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 Γ and $\Omega^{(k)}$ for $k = 0, \ldots, n_\Omega$, to satisfy IMEX-ARK consistency (s^2 conditions), internal consistency ($s(2 + n_\Omega)$ conditions), plus order conditions:
  - $\mathcal{O}(H^1)$ and $\mathcal{O}(H^2)$: no additional order conditions,
  - $\mathcal{O}(H^3)$: 1 additional order condition,
  - $\mathcal{O}(H^4)$: 6 additional order conditions.
- With remaining degrees of freedom, maximize joint linear stability for method and minimize next-order error term for embedding.

IMEX-MRI-SR Joint Linear Stability

[Fish, R., & Roberts, 2023]

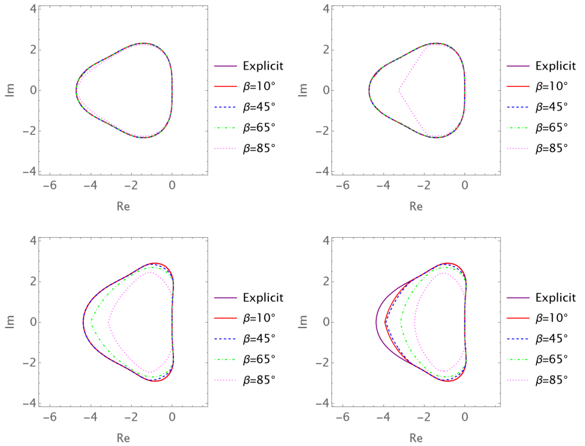
We again analyze joint linear stability for the Dahlquist-like test problem $\dot{y} = \lambda^I y + \lambda^E y + \lambda^F y$:

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

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

- IMEX-MRI-SR2(1) ($\uparrow$)
- IMEX-MRI-SR3(2) ($\downarrow$)
- fast $\alpha = 10^o$ ($\leftarrow$)
- fast $\alpha = 45^o$ ($\rightarrow$)

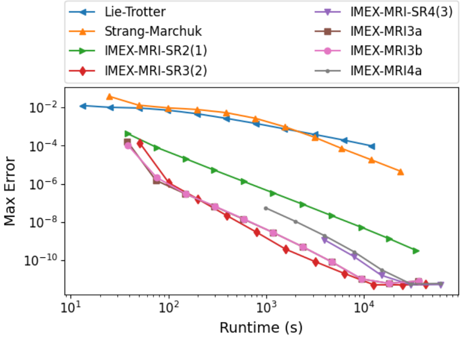
We have an $\mathcal{O}(H^4)$ IMEX-MRI-SR4(3) table for convergence verification, though it again has relatively poor joint stability.



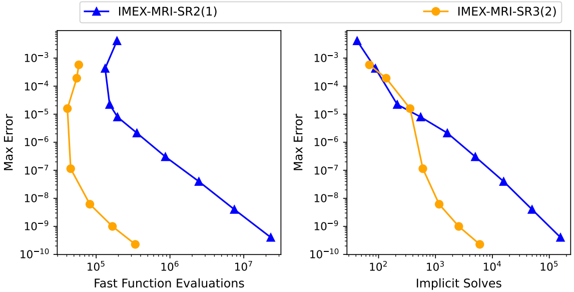
IMEX-MRI-SR Convergence/Efficiency – "Stiff" Brusselator PDE

[Fish, R., & Roberts, 2023]

Runtime efficiency of IMEX-MRI-SR, IMEX-MRI-GARK, and IMEX-MRI versions of Lie–Trotter and Strang–Marchuk splittings:



Modified problem with time-dependent advection, diffusion and reaction coefficients, we explore adaptive IMEX-MRI-SR efficiency using tolerances 10^{-k} with $k = 1, \ldots, 9$ (more on MRI adaptivity in a moment):



Outline

Multirate Infinitesimal Time Step Adaptivity

[Fish & R., *SISC*, 2023]

As with single-rate IVPs, robustness, accuracy, and efficiency hinge on appropriate selection of time step sizes. In the MRI setting, this is complicated:

- We now have separate control parameters at each time scale (H and h):
- The overall solution error is not simply the sum of errors at fast and slow time scales, since errors may propagate between them.
- With two control parameters, we need separate estimates of temporal errors that arise at each scale.
- Although significant work has been performed on single-rate controllers, multirate control has received little investigation (particularly higher-order controller methods).

Multirate control

[Fish & R., *SISC*, 2023]

Denoting the overall error in an MRI time step solution as ε_{n+1}, we estimate

$$\begin{aligned}\varepsilon_{n+1} &= \|y(t_{n+1}) - y_{n+1}\| \le \|y(t_{n+1}) - y^*_{n+1}\| + \|y^*_{n+1} - y_{n+1}\| = \varepsilon^s_{n+1} + \varepsilon^f_{n+1} \\ &= \left(\phi^s_n H_n^P + \mathcal{O}\left(H_n^{P+1}\right)\right) + \left(\phi^f_n \left(\frac{H_n}{M_n}\right)^p H_n + \mathcal{O}\left(\left(\frac{H_n}{M_n}\right)^{p+1} H_n\right)\right),\end{aligned}$$

where

- y^*_{n+1} is the imagined solution wherein each fast IVP is solved exactly,
- P and p are the global orders of accuracy for the MRI method embedding and fast solver embedding, resp.,
- ϕ^s and ϕ^f are the principal error functions for each scale (these depend on method and IVP, but not on H_n or M_n).

Multirate controllers

[Fish & R., *SISC*, 2023]

Ignoring higher-order terms, setting the desired fast and slow errors to separate fast and slow tolerances ($\varepsilon^f_{n+1} = \texttt{TOL}^f$ and $\varepsilon^s_{n+1} = \texttt{TOL}^s$), solving for $\log(H_n)$ and $\log(M_n)$, and following Gustafsson [*ACM TOMS*, 1994] to approximate the principal error functions $\log(\phi^f_n)$ and $\log(\phi^s_n)$ using piecewise polynomials, we obtain the *constant-constant* controller

$$H_{n+1} = H_n \left(\frac{\texttt{TOL}^s}{\varepsilon^s_{n+1}}\right)^{\alpha}, \qquad M_{n+1} = M_n \left(\frac{\texttt{TOL}^s}{\varepsilon^s_{n+1}}\right)^{\beta_1} \left(\frac{\texttt{TOL}^f}{\varepsilon^f_{n+1}}\right)^{\beta_2},$$

and the *linear-linear* controller

$$H_{n+1} = H_n \left(\frac{H_n}{H_{n-1}}\right) \left(\frac{\texttt{TOL}^s}{\varepsilon^s_{n+1}}\right)^{\alpha_1} \left(\frac{\texttt{TOL}^s}{\varepsilon^s_{n}}\right)^{\alpha_2},$$

$$M_{n+1} = M_n \left(\frac{M_n}{M_{n-1}}\right) \left(\frac{\texttt{TOL}^s}{\varepsilon^s_{n+1}}\right)^{\beta_{11}} \left(\frac{\texttt{TOL}^s}{\varepsilon^s_{n}}\right)^{\beta_{12}} \left(\frac{\texttt{TOL}^f}{\varepsilon^f_{n+1}}\right)^{\beta_{21}} \left(\frac{\texttt{TOL}^f}{\varepsilon^f_{n}}\right)^{\beta_{22}}.$$

Multirate controllers (continued)

[Fish & R., *SISC*, 2023]

We additionally consider two additional controllers:

- *PIMR* is a multirate extension of the PI single-rate controller:

$$H_{n+1} = H_n \left(\frac{\text{TOL}^s}{\varepsilon^s_{n+1}}\right)^{\alpha_1} \left(\frac{\text{TOL}^s}{\varepsilon^s_n}\right)^{\alpha_2},$$

$$M_{n+1} = M_n \left(\frac{\text{TOL}^s}{\varepsilon^s_{n+1}}\right)^{\beta_{11}} \left(\frac{\text{TOL}^s}{\varepsilon^s_n}\right)^{\beta_{12}} \left(\frac{\text{TOL}^f}{\varepsilon^f_{n+1}}\right)^{\beta_{21}} \left(\frac{\text{TOL}^f}{\varepsilon^f_n}\right)^{\beta_{22}}.$$

- *PIDMR* is a multirate extension of the PID single-rate controller:

$$H_{n+1} = H_n \left(\frac{\text{TOL}^s}{\varepsilon^s_{n+1}}\right)^{\alpha_1} \left(\frac{\text{TOL}^s}{\varepsilon^s_n}\right)^{\alpha_2} \left(\frac{\text{TOL}^s}{\varepsilon^s_{n-1}}\right)^{\alpha_3},$$

$$M_{n+1} = M_n \left(\frac{\text{TOL}^s}{\varepsilon^s_{n+1}}\right)^{\beta_{11}} \left(\frac{\text{TOL}^s}{\varepsilon^s_n}\right)^{\beta_{12}} \left(\frac{\text{TOL}^s}{\varepsilon^s_{n-1}}\right)^{\beta_{13}} \left(\frac{\text{TOL}^f}{\varepsilon^f_{n+1}}\right)^{\beta_{21}} \left(\frac{\text{TOL}^f}{\varepsilon^f_n}\right)^{\beta_{22}} \left(\frac{\text{TOL}^f}{\varepsilon^f_{n-1}}\right)^{\beta_{23}}.$$

MRI error estimation

[Fish & R., *SISC*, 2023]

All controllers require accurate/cheap estimates for ε_n^s and ε_n^f. Assuming the MRI method provides an embedding, $\tilde{y}_n$, then $\varepsilon_n^s \approx \|y_n - \tilde{y}_n\|$. However, estimation of $\varepsilon_n^f = \|y_n^* - y_n\|$ is less obvious.

We tested a variety of strategies:

- *Full-Step (FS)* – compute each fast solve twice using fast integrators of different orders, with forcing functions $r_i(\tau)$ that use separate $f^S(t,y)$ evaluations, to obtain $\varepsilon_n^f = \|y_n - \hat{y}_n\|$.
- *Stage-Aggregate (SA)* – compute each fast solve twice using fast integrators of different orders, but with forcing functions $r_i(\tau)$ that use shared $f^S(t,y)$ evaluations, and aggregate stage differences to obtain $\varepsilon_n^f = \text{aggregate}\left(\|z_i - \hat{z}_i\|, i = 2,\ldots,s\right)$.
- *Local-Accumulation-Stage-Aggregate (LASA)* – compute each fast solve once using an embedded method, and accumulate sub-step error estimates $d_{i,j}$ into an overall estimate $\varepsilon_n^f = \text{aggregate}\left(\sum_{j=1}^{M} d_{i,j}, i = 2,\ldots,s\right)$.

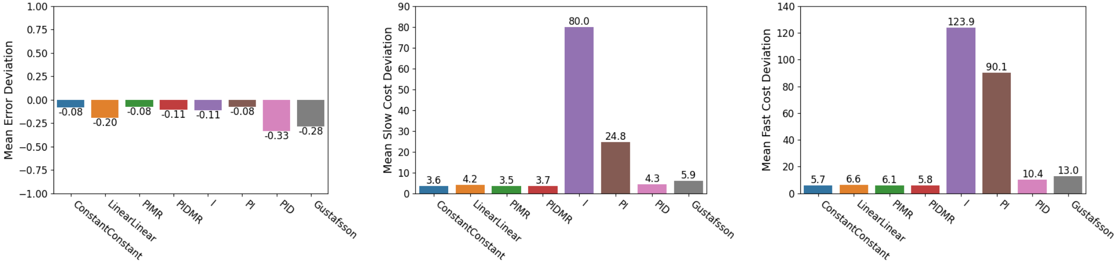
In the end, the "LASA" strategies proved sufficiently accurate (with the least expense).

MRI controller performance

[Fish & R., *SISC*, 2023]

Tested 4 MRI controllers along with 4 single-rate H controllers (each used a fixed $M = 10$), across a test suite of 7 test problems, 4 IVP methods, and 3 tolerances.

- Left: controller overall ability to achieve desired tolerance ($0 \Rightarrow$ perfect, $< 0 \Rightarrow$ overly accurate)
- Center: controller overall f^S cost as multiple of "best possible" (i.e., $1 \Rightarrow$ perfect)
- Right: controller overall f^F cost as multiple of "best possible"



Outline

Software: ARKODE and SUNDIALS

[R. et al., *ACM TOMS*, 2023]

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`: multirate infinitesimal time stepping module.
  - Includes explicit MIS methods $\mathcal{O}(H^3)$, explicit or implicit MRI-GARK methods of $\mathcal{O}(H^2)$ to $\mathcal{O}(H^4)$, IMEX-MRI-GARK methods of $\mathcal{O}(H^3)$ and $\mathcal{O}(H^4)$.
  - Supports user-provided MRI-GARK tables $\Gamma^{\{k\}}$ or IMEX-MRI-GARK tables $\{\Gamma^{\{k\}}, \Omega^{\{k\}}\}$.
  - Currently requires a user-defined H that can be varied between steps. Fast time scale evolved using `ARKStep` or any viable user-supplied IVP solver.
  - *Will soon include embedded IMEX-MRI-SR methods of $\mathcal{O}(H^2)$ to $\mathcal{O}(H^4)$, and multirate time adaptivity controllers.*

Multirate reacting flow demonstration problem

[R. et al., *ACM TOMS*, 2023]

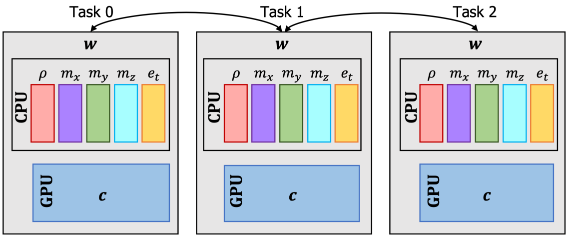
3D nonlinear compressible Euler equations combined with stiff chemical reactions for a low-density primordial gas (molecular & ionization states of H and He, free electrons, and internal gas energy), present in models of the early universe.

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

$\mathbf{w}$: 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.



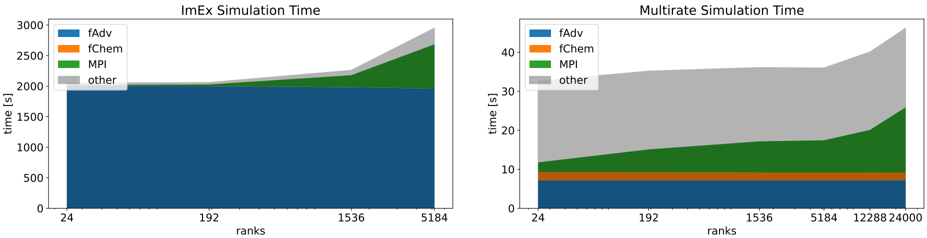
Fluid species (density, momenta, total energy) are stored in main memory, while chemical densities are stored in GPU memory.

Multirate reacting flow solver strategy

[R. et al., *ACM TOMS*, 2023]

- 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 $n_x \times n_y \times n_z$ grid for Ω, parallelized using standard 3D MPI domain decomposition.
- $\mathcal{O}(\Delta x^5)$ FD-WENO flux reconstruction for $\mathbf{F}(\mathbf{w})$ [Shu, 2003].
- Resulting IVP system: $\dot{\mathbf{w}}(t) = f_1(\mathbf{w}) + f_2(\mathbf{w})$, $\mathbf{w}(t_0) = \mathbf{w}_0$, where $f_1(\mathbf{w})$ contains $-\nabla \cdot \mathbf{F}(\mathbf{w})$ and is evaluated on the CPU, while $f_2(\mathbf{w})$ contains spatially-local reaction network $\mathbf{R}(\mathbf{w})$ and is evaluted on the GPU.
- Compare two forms of temporal evolution:
  (a) Temporally-adaptive, $\mathcal{O}(H^3)$ IMEX-ARK method from `ARKStep`: f_1 explicit and f_2 implicit,
  (b) Fixed-step, $\mathcal{O}(H^3)$ MRI-GARK method from `MRIStep` (temporally-adaptive fast step h): f_1 slow/explicit and f_2 fast/DIRK.

Multirate reacting flow – ImEx and multirate results using hybrid CPU+GPU on OLCF Summit.



- Weak scaling runs with 1 MPI rank per GPU.
- Both use robust, GPU-enabled MAGMA batched linear solver.
- Multirate H chosen proportional to CFL condition on f_1.
- Both approaches show excellent algorithmic scalability.
- Huge reduction in f_1 evaluations allows ImEx $\to$ MR speedup of $\sim 70\times$.
- GPU synchronization more severly hinders runtime scalability of ImEx than MR, due to increased frequency (fast vs slow stages).

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 operator-spliting remains standard, new & flexible methods are catching up, supporting high order accuracy (even up to $\mathcal{O}(H^6)$) 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, ...

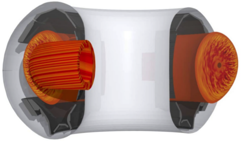
Future Work

Much work remains to be done:

- Improved stability analysis for partitioned Runge–Kutta methods, since assumption of simultaneous diagonalizability for Dahlquist-like problem $y' = \sum_k \lambda_k y$ loses predictive capability.
- Improved [embedded] IMEX-MRI-GARK and IMEX-MRI-SR methods (particulary for $\mathcal{O}(H^4)$).
- Support for a broad range of adaptive MRI methods within open-source software libraries.
- Rigorous testing of MRI methods in "challenging" multirate applications.
- Robust temporal controllers for nested multirating, $h_1 > h_2 > \cdots > h_m$.
- Robust (automated?) approaches for determining additive splittings $f(t,y) = \sum_k f^{\{k\}}(t,y)$.
- Suggestions?

Postdoctoral Positions in Numerical Methods for Fusion Energy

I'm looking to hire two postdocs to work on the development and implementation of advanced time integration methods for large-scale simulations in magnetic fusion energy.



- Looking for candidates with expertise in one or more of:
  - high-performance computing,
  - numerical analysis, and
  - simulation of differential equations.
- Competitive salary (including benefits).
- Initial appointment is for 1 year (renewable annually up to 4).
- Funded by DOE SciDAC partnership program (ASCR & FES).
- Contact me at reynolds@smu.edu with any questions or interest.

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