Multirate time integration with ARKode/SUNDIALS

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(significant contributions from C.J. Balos[2], J. Loffeld[2], and C.S. Woodward[2])

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Multiphysics Problems

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

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

Multiphysics simulation challenges include:

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

Historical approaches rely on lowest-order time step splittings, may suffer from:

- Low accuracy – typically $\mathcal{O}(h)$-accurate; symmetrization/extrapolation may improve this but at significant cost [Ropp, Shadid & Ober 2005].
- Poor/unknown stability – even when each part utilizes a 'stable' step size, the combined problem may admit unstable modes [Estep et al., 2007].

Need for Flexible Time Integration Libraries

Multiphysics time integration needs:

- Stability/accuracy for each component, as well as inter-physics couplings
- Custom/flexible step sizes for distinct components
- Robust temporal error estimation & adaptivity of step size(s)
- Built-in support for spatial adaptivity
- Ability to apply optimal solver algorithms for individual components
- Support for testing a variety of methods and solution algorithms

Legacy software frameworks enforce overly-rigid standards on applications:

- Fully implicit or fully explicit, without IMEX flexibility.
- Inflexible data structures for vectors, matrices, (non)linear solvers.
- Hard-coded parameters – good for most problems, but rarely optimal.

SUNDIALS: SUite of Nonlinear and DIfferential-ALgebraic equation Solvers

Software library of ODE and DAE time integrators and nonlinear solvers

- Consists of six packages: CVODE(S), ARKode, IDA(S), and KINSOL
- Written in C with interfaces to Fortran
- Designed to be easily incorporated into existing codes

Modular implementation

- Data use is fully encapsulated by vector and matrix APIs
- Nonlinear and linear solvers are fully encapsulated from the integrators
- All parallelism is encapsulated in vectors, solvers, and user-supplied functions
- Vector, matrix, and solver modules can all be user-supplied

Availability and support

- Freely available; BSD 3-Clause license; $> 25,000$ downloads in 2018
- Detailed user manuals and an active user community email list

More information: `https://computing.llnl.gov/casc/sundials`

- 11:30 Friday: talk by Carol Woodward (MS GH-3-5-9)
- Monday/Tuesday: poster by David Gardner (PA-041)

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

ARKode was initially designed to implement adaptive ARK methods for initial value problems (IVPs), supporting up to two split components: *explicit* and *implicit*,

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

- M is any nonsingular linear operator (mass matrix, typically $M = I$),
- $f^E(t,y)$ contains the explicit terms,
- $f^I(t,y)$ contains the implicit terms.

Combine two s-stage RK methods; denoting $t^*_{n,j} = t_n + c^*_j h_n$, $h_n = t_{n+1} - t_n$:

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

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

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

ARKode Flexibility Enhancements

ARKode includes several enhancements for multiphysics codes, including:

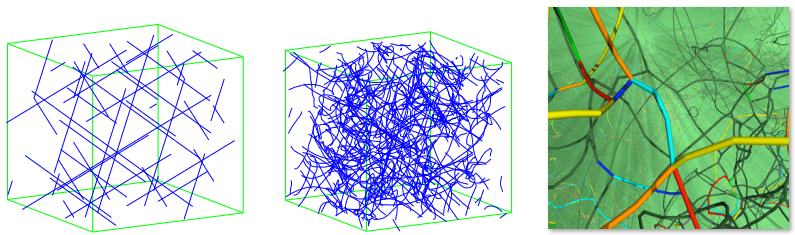
- Variety of built-in Butcher tables (ERK, DIRK, IMEX ARK); supports user-supplied.
- Variety of built-in temporal adaptivity functions; supports user-supplied.
- Variety of built-in implicit predictor algorithms.
- Ability to specify that problem is linearly implicit.
- Ability to resize data structures based on changing IVP size.
- All internal solver parameters are user-modifiable.

Examples of ARKode Usage

ARKode has been freely-available since 2014. We have specifically worked with applications groups in:

ParaDiS – large-scale simulations of dislocation growth/propagation (material strain hardening)

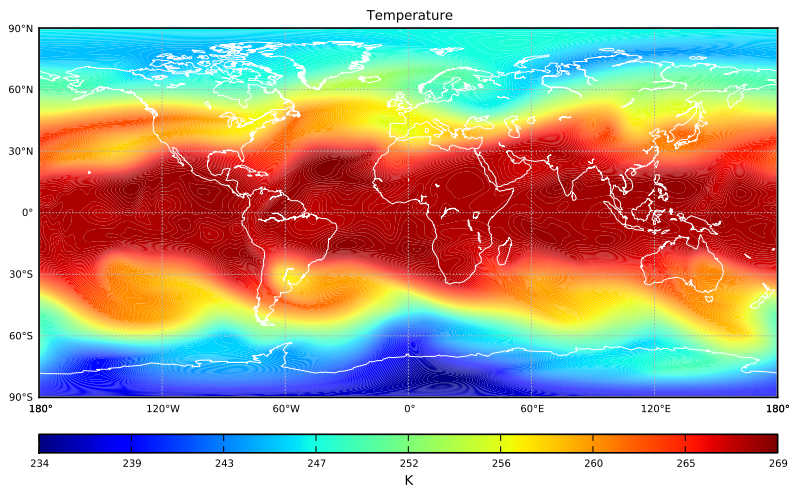
- Examined high-order adaptive DIRK methods.
- Examined nonlinear solvers and options.
- *51%-98% speedup (production/test problems)*



Gardner et al., *MSMSE*, 2015

Tempest & **HOMME-NH** – non-hydrostatic 3D dynamical cores for atmospheric simulations

- Examined IMEX splittings & fixed-step ARK methods for accuracy/stability
- Examined nonlinear/linear solver algorithms for implicit components
- *Identified 'optimal' splitting+solver+ARK; invented new climate-specific ARK methods.*



Gardner et al., *GMD*, 2018; Vogl et al, 2019.

Reconfiguring ARKode into an infrastructure

Over the last 18 months, we have overhauled ARKode to serve as an infrastructure for general, adaptive, one-step time integration methods:

- ARKode provides the outer time integration loop and generic usage modes (interpolation vs "tstop"; one-step versus time interval).
- Time-stepping modules handle problem-specific components: definition of the IVP, algorithm for a single time step.
- Time-stepping modules may leverage shared ARKode infrastructure:
  - SUNDIALS' vector, matrix, linear solver and nonlinear solver objects,
  - translation between generic solvers and IVP-specific algebraic systems,
  - time-step adaptivity controllers: PID, PI, I, *user-supplied*,
  - ...

Increased agility for implementing state-of-the-art algorithms in a production software environment.

ARKode Time-Stepping Modules

The new ARKode structure based on time-stepping modules eases the implementation of new integration schemes:

- **ARKStep** Provides all the functionality from previous ARKode versions. Supports ARK, DIRK and ERK methods for problems of the form

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

- **ERKStep**: A streamlined module that provides more optimal support for ERK-specific methods applied to the standard IVP form

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

- **MRIStep**: Provides support for Multirate Infinitesimal Step (MIS) like methods

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

- **IMEXGARKStep**: Provides support for IMEX Generalized Runge-Kutta methods (currently testing)

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

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

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

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

- $f^F(t,y)$ contains the "fast" terms; $f^S(t,y)$ contains the "slow" terms.
- $h^S > h^F$, with a time scale separation $h^S/h^F \approx m$.
- y is frequently partitioned as well, e.g. $y = \left[y^F\ y^S\right]^T$.
- The slow component may be integrated using an explicit "outer" RK method, $T_O = \{A, b, c\}$, where $c_i \leq c_{i+1}$, $i = 1, \ldots, s-1$.
- The fast component is advanced between slow stages as the exact solution of a modified ODE.
- Practically, this fast solution is subcycled using an "inner" RK method.

MIS Algorithm

Denoting $y_n \approx y(t_n)$, a single MIS step $y_n \to y_{n+1}$ is as follows:

1. Set $z_1 = y_n$
2. For each outer Runge-Kutta stage $z_i, i = 2, \ldots, s+1$:

   a) Let $v(t_{n,i-1}) = z_{i-1}$ and $r = \sum_{j=1}^{i-1} \left(\frac{A_{i,j} - A_{i-1,j}}{c_i - c_{i-1}} \right) f^S\left(t_{n,j}, z_j\right)$

   b) Solve the fast ODE: $\dot{v}(\tau) = f^F\left(\tau, v\right) + r$, for $\tau \in [t_{n,i-1}, t_{n,i}]$

   c) Set $z_i = v(t_{n,i})$
3. Set $y_{n+1} = z_{s+1}$

where the outer stage times are $t_{n,j} = t_n + c_j h^S$ and $A_{s+1,j} = b_j$.

- When $c_i = c_{i+1}$, the IVP "solve" reduces to a standard Runge–Kutta update.
- Step 2b may use any applicable algorithm of sufficient accuracy.

MIS Properties

MIS methods satisfy a number of desirable multirate method properties:

- The MIS method is $\mathcal{O}\left(h^2\right)$ if both inner/outer methods are at least $\mathcal{O}\left(h^2\right)$.
- The MIS method is $\mathcal{O}\left(h^3\right)$ if both inner/outer methods are at least $\mathcal{O}\left(h^3\right)$, and T_O satisfies

$$\sum_{i=2}^{s} \left(c_i - c_{i-1}\right)\left(e_i + e_{i-1}\right)^T Ac + \left(1 - c_s\right)\left(\frac{1}{2} + e_s^T Ac\right) = \frac{1}{3}.$$

- The inner method may be a subcycled T_O, enabling a *telescopic* multirate method (i.e., n-rate problems supported via recursion).
- Both inner/outer methods can utilize problem-specific tables (SSP, etc.).
- h^F may be varied within a slow step to adapt the multirate structure.
- Highly efficient – only a single traversal of $[t_n, t_{n+1}]$ is required. To our knowledge, MIS are the most efficient $\mathcal{O}\left(h^3\right)$ multirate methods available.

MRIStep Module

The new MRIStep module supports $\mathcal{O}(h^2)$ and $\mathcal{O}(h^3)$ MIS-like methods.

- The slow time scale is integrated with an explicit Runge–Kutta method.
- The slow time scale uses a user-defined h^S that can be varied between slow steps.
- The fast time scale is advanced by calling the ARKStep module, and thus allows for explicit, implicit or IMEX integration.
- The fast time scale can use adaptive or fixed time step sizes.
- Supports user-defined Butcher tables for both time scales.
- Explicit-explicit released in SUNDIALS v4.0, implicit and IMEX fast are available in SUNDIALS v5.0 beta releases.

Currently implementing extensions to $\mathcal{O}(h^4)$ and implicit slow integration.

MRIStep Example – Advection-Reaction

Explicit (slow) advection and implicit (fast) Brusselator reactions:

$$u_t = -cu_x + k_1 A - k_2 Bu + k_3 u^2 v - k_4 u$$
$$v_t = -cv_x + k_2 Bu - k_3 u^2 v$$

Comparison of $\mathcal{O}(h^3)$ MIS vs IMEX (time steps chosen for comparable accuracy):

	IMEX	**MRI**
Time steps	6,805	1,429 / 8,813
Advection evals	29,379	4,288
Reaction evals	98,917	116,949

- MIS requires fewer advection evaluations, lowering MPI communication costs.
- MRIStep benefits depend on an array of factors:
  - separation of time scales (e.g., CFL vs reaction rates)
  - relative cost of f^S vs f^F function evaluations

MRIStep Example in AMReX (from J. Loffeld @ LLNL)

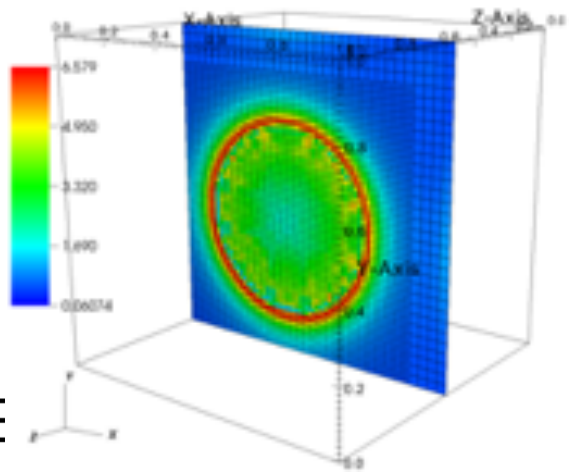
We have integrated SUNDIALS with AMReX, providing a powerful new set of tools for solving multiscale problems posed on block-structured AMR grids.

- `NVector` API enables SUNDIALS to use native AMReX structures for single-level and multi-level problems.
- `SUNLinearSolver` API enables SUNDIALS to use AMReX `MLABecLaplacian` solver for scalable diffusion solves in implicit methods.

3D Brusselator (two-level AMR grid with 2:1 refinement ratio):

- Explicit-explicit MRIStep with $h^S/h^F = 100$.
- MRIStep effectively removes advection cost for similar accuracy requirements.
- At core-counts tested, advection costs 66% more than reactions (will increase at larger scales)

2D slice of 3D Brusselator solution



Results from LLNL's Quartz cluster:

Cores	Fine Grid	Time (s)
64	256^3	335
512	512^3	342
4096	1024^3	368

Extensions to Higher Order and Implicit Slow

We are currently exploring extensions for $\mathcal{O}\left(h^4\right)$ methods in MRIStep:

- MRI-GARK methods [Sandu, 2018] modify the MIS slow forcing term in the fast IVP to have time-dependent coefficients:

$$r(\tau) = \sum_{j=1}^{i-1} \gamma_{i,j}\left(\frac{\tau - t_{n,i-1}}{(c_i - c_{i-1})h^S}\right) f^S\left(t_{n,j}, z_j\right).$$

- MRI-GARK also include *decoupled implicit methods* that do not require solving a fully coupled fast and slow system – these can readily leverage the existing ARKStep solver infrastructure.

- Relaxed MIS methods (RMIS) [Sexton & R., 2018] compute y_{n+1} as a combination of $\{f^F(t_{n,i}, z_i) + f^S(t_{n,i}, z_i)\}$ to produce a $\mathcal{O}\left(h^4\right)$ method with $\mathcal{O}\left(h^3\right)$ MIS embedding.

- Multirate exponential Runge–Kutta methods (MERK) [Luan, Chinomona & R., 2019] are similar to MRI-GARK, constructing time-dependent fast IVP forcing terms $r(\tau)$, but rely on exponential integrator theory (as opposed to GARK).

Conclusions

The ARKode infrastructure flexibly supports extensive studies of optimal algorithms for multiphysics problems:

- Numerous built-in methods; supports user-supplied.
- Numerous vector/matrix data structures, support for user-supplied.
- Numerous algebraic solver algorithms, support for user-supplied.
- Actively developing state-of-the-art flexible time integration methods for multiphysics applications:
  - Additive partitioning – break apart physical processes based on stiffness (implicit/explicit/IMEX) or time scale (fast/slow).
  - New support for explicit slow MIS methods with explicit, implicit or IMEX fast integration, with higher order and implicit slow coming.
  - Focus on ease-of-use and support for user-supplied components, allowing SUNDIALS to reuse previous development of optimal data structures and algebraic solvers.

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- John Loffeld [LLNL]
- Cody J. Balos [LLNL]
- Alan C. Hindmarsh [LLNL]
- DOE SciDAC & ECP Programs
- SMU Center for Scientific Computation

Software:

- ARKode/SUNDIALS – https://computation.llnl.gov/casc/sundials
- AMReX – https://amrex-codes.github.io

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