On the development and implementation of optimized, high-order time integrators for multi-physics problems

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Outline

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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.

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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 $t^*_{n,j} = t_n + c^*_j h_n$, $h_n = t_{n+1} - t_n$:

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

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

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

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

Each stage is implicitly defined via a root-finding problem:

$$
\begin{aligned}
0 &= G_i(z) \\
&= Mz - My_n - h_n \left[A^I_{i,i} f^I(t^I_{n,i}, z) + \sum_{j=1}^{i-1} \left(A^E_{i,j} f^E(t^E_{n,j}, z_j) + A^I_{i,j} f^I(t^I_{n,j}, z_j) \right) \right]
\end{aligned}
$$

- if $f^I(t, y)$ is *linear* in y then we must solve a linear system for each z_i,
- else G_i is nonlinear, requiring an iterative solver – options include
  - modified Newton,
  - inexact Newton,
  - Anderson-accelerated fixed point,
  - user-supplied.

Linear Solvers and Vector Data Structures

Linear solver options:

- Direct – dense/band/sparse solvers (incl. LAPACK, KLU & SuperLU)
- Krylov – GMRES, FGMRES, BiCGStab, TFQMR or PCG
    - support user-supplied preconditioning (left/right/both)
    - support residual/solution scaling for "unit-aware" stopping criteria
    - support "matrix-free" methods through approximation of product Jv, where $J \equiv \frac{\partial}{\partial y} f^I(t, y)$
- External solvers may be "plugged in" by providing a `SUNLinearSolver` implementation

All solvers (except for direct linear) formulated via generic vector operations:

- Numerous supplied vector implementations: serial, MPI, OpenMP, PETSc, *hypre*, CUDA, Raja, Trilinos, ...
- Application-specific vectors may be supplied

ARKode Flexibility Enhancements

Additionally, ARKode includes enhancements for multi-physics codes, including:

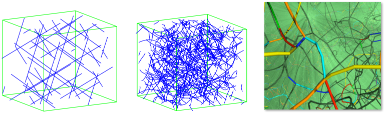
- Variety of built-in RK tables; supports user-supplied
- Variety of built-in adaptivity functions; supports user-supplied
- Variety of built-in implicit predictor algorithms
- Ability to specify that problem is linearly implicit
- Ability to resize data structures based on changing IVP size
- All internal solver parameters are user-modifiable

ARKode Usage

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

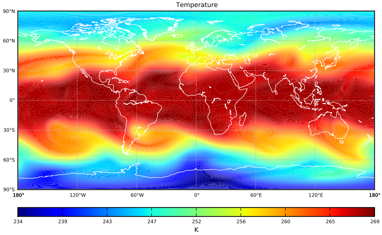
ParaDiS – large-scale simulations of dislocation growth/propagation (material strain hardening) [Gardner et al., *MSMSE*, 2015]

- Examined high-order adaptive DIRK methods.
- Examined nonlinear solvers and options.



Tempest & *HOMME-NH* – non-hydrostatic 3D dynamical cores for atmospheric simulations [Gardner et al., *GMD*, 2018; Vogl et al, *in prep.*]

- Examined ImEx splittings & fixed-step ARK methods for accuracy/stability
- Examined nonlinear/linear solver algorithms for implicit components



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Reconfiguring ARKode into an infrastructure

Over the last year, 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 SUNDIALS' generic matrix/solver structures ($\mathcal{A}x = b$) and IVP-specific linear systems ($\mathcal{A} \approx M - \gamma \frac{\partial f^I}{\partial y}(t, y)$),
  - time-step adaptivity controllers: PID, PI, I, *user-supplied*,
  - ...

Continued support for ARK, DIRK and ERK methods

All functionality from previous ARKode versions has been retained:

- *ARKStep* 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* is a leaner module that provides more optimal support for ERK-specific methods applied to the standard IVP form,

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

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

MIS/RFSMR 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:

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

- $f^{\{f\}}(t,y)$ 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 $c_i \le c_{i+1}$, $i = 1, \ldots, s$;
- the fast component is advanced between slow stages by solving 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 $y_n \to y_{n+1}$ has the generic form:

Set $z_1 = y_n$,

For $i = 1, \ldots, s$:

Let $t_{n,i} = t_n + c_i h_s$ and $v(t_{n,i}) = z_i$, then for $\tau \in [t_{n,i}, t_{n,i+1}]$ solve:

$$\dot{v}(\tau) = f^{\{f\}}(\tau, v) + \sum_{j=1}^{i} \alpha_{i+1,j} f^{\{s\}}(t_{n,j}, z_j),$$

Set $z_{i+1} = v(t_{n,i+1})$

Set $y_{n+1} = z_{s+1}$,

where the coefficients $\alpha_{i,j}$ are defined appropriately.

The IVP for $v(\tau)$ may be solved using any applicable algorithm.

MIS Properties

MIS methods satisfy a number of desirable multirate method properties:

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

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

- 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 table (SSP, etc.).
- Highly efficient – only a single traversal of $[t_n, t_n + h]$ is required. To our knowledge, MIS are the most efficient $\mathcal{O}(h^3)$ multirate methods available.

MRIStep ARKode stepper

David Gardner has implemented a new *MRIStep* module to support $\mathcal{O}(h^2)$ and $\mathcal{O}(h^3)$ MIS-like methods [released Dec. 2018].

- Currently requires user-defined h_s and h_f (may be varied between outer steps). *We are currently expanding this to support temporal adaptivity*.
- Slow time scale is integrated with an ERK method. *We are currently exploring methods with an implicit slow component*.
- Fast scale is advanced by calling the ARKStep module. Current release requires ERK fast scale, but *implicit and ImEx will be released soon*.
- Extensions to $\mathcal{O}(h^4)$ and higher are under investigation:
  - J.M. Sexton's *RMIS* computes y_{n+1} as a combination of $\{f(t_{n,i}, z_i)\}$;
  - V.T. Luan's *MERK* constructs fast IVP using exponential integrators;
  - A. Sandu's *MRI-GARK* modifies the fast IVP:

$$\dot{v}(\tau) = f^{\{f\}}(\tau, v) + \sum_{j=1}^{i+1} \gamma_{i,j}\left(\frac{\tau - t_{n,i}}{h_s}\right) f^{\{s\}}(t_{n,j}, z_j).$$

Generalized Additive Runge-Kutta (GARK) stepper [Sandu & Günther, SINUM 2015]

David has also implemented a new *IMEXGARKStep* module to support ImEx GARK methods for problems with two partitions:

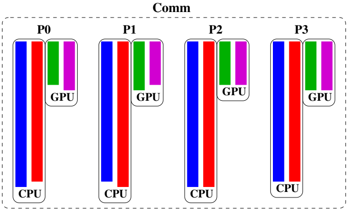
$$\dot{y} = f^{\{E\}}(t, y) + f^{\{I\}}(t, y), \quad t \in [t_0, t_f], \quad y(t_0) = y_0.$$

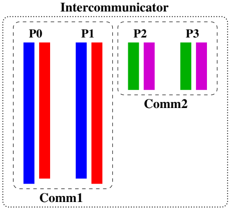
- Users supply Butcher table components $A^{\{E,E\}}$, $A^{\{I,I\}}$, $A^{\{E,I\}}$ and $A^{\{I,E\}}$, corresponding to E-E, I-I, E-I and I-E couplings, respectively; coefficients $b^{\{E\}}$ and $b^{\{I\}}$ define the timestep solution.
- $A^{\{E,E\}}$ and $A^{\{E,I\}}$ must be explicit.
- $A^{\{I,I\}}$ and $A^{\{I,E\}}$ can be diagonally implicit.
- Currently assumes that all tables have the same number of stages.

This module will be included in an upcoming release.

"ManyVector" for multi-physics data partitioning

We are also finishing a new vector kernel for SUNDIALS that will support multi-physics data partitioning, $y = \begin{bmatrix} y_1 & y_2 & \cdots & y_m \end{bmatrix}$, $y_j \in \mathbb{R}^{n_j}$:





Multi-rate or data partitioning: subvectors utilize distinct processing elements within each node, allowing optimal hardware for each component.

Multi-physics decompositions: one physical system utilizes `Comm1` while another utilizes `Comm2`; inter-physics coupling is handled with an MPI intercommunicator.

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Conclusions

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

- Numerous built-in ERK, DIRK, and ARK methods; supports user-supplied.
- Numerous vector/matrix data structures, support for user-supplied and data partitioned.
- Numerous algebraic solver algorithms, support for user-supplied.
- Actively developing state-of-the-art flexible time integration methods for multi-physics applications:
  - Additive partitioning – break apart physical processes based on stiffness (implicit/explicit/IMEX) or time scale (fast/slow).
  - Variable partitioning – break apart solution based on time scales (fast/slow) or solvers (algebraic, computing hardware).
  - Focus on ease-of-use and support for user-supplied components, so that critical methods can be highly optimized for a given problem.

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Software:

- ARKode – http://faculty.smu.edu/reynolds/arkode
- SUNDIALS – https://computation.llnl.gov/casc/sundials

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