FASTMath: Time Integration Activities

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The FASTMath time integrator team is focused on delivering highly efficient time integration methods and software for DOE applications. Work is focused on methods that provide support for multirate systems, that address the bottleneck of sequential time stepping, and that allow for efficient optimization of time-dependent systems.

Overview

Many DOE applications are taking advantage of increasing compute power through addition of multiple physics modules resulting in the need to take advantage of new time integration software and methods.

FASTMath is delivering new time integration capabilities through:

- ***SUNDIALS:*** multistep and multistage methods for ODEs and DAEs with forward and adjoint sensitivity analysis
- ***PETSc:*** multistage methods for ODEs and DAEs with advanced sensitivity capabilities enabling dynamic optimization
- ***AMReX:*** structured adaptive mesh refinement framework – being adapted to include higher-order semi- and multi-implicit temporal integrators based on multi-level spectral deferred corrections

Multirate Integrators in SUNDIALS

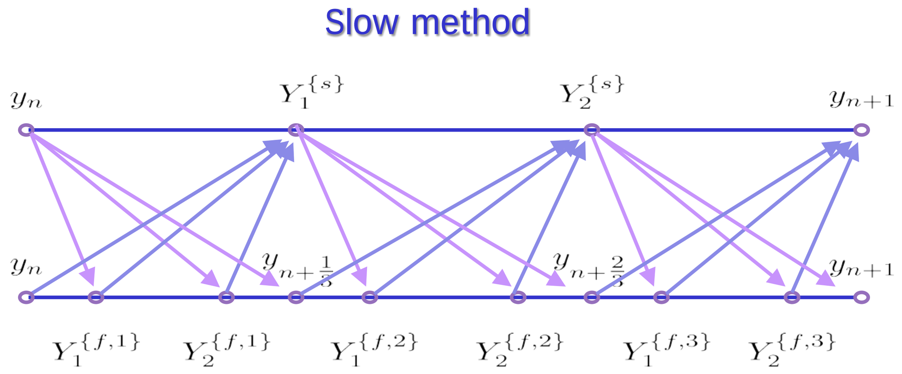
To support complex multiphysics SciDAC applications, we are working to derive and implement highly efficient additive multirate integrators into SUNDIALS.

Multirate methods allow distinct step sizes per physical process, enabling optimal methods for each component, based on physically-relevant decompositions.

Approach:

- Develop production-level software for flexible 3rd and 4th-order explicit+explicit multirate integrators, based off of one-step GARK methods.
- Investigate optimal algorithms for error-based adaptivity of both the macroscale step size and time-scale separation factor.
- Derive high-order mixed implicit/explicit two-rate methods.
- Explore three-rate ImEx methods

Time line showing the coupling between fast (bottom) and slow (top) stages and steps in a 3rd-order two-rate explicit multirate method. The most recent slow stage solution is held constant over the fast substeps between the slow stages. Fast stage solutions are then used to update the next slow stage value.

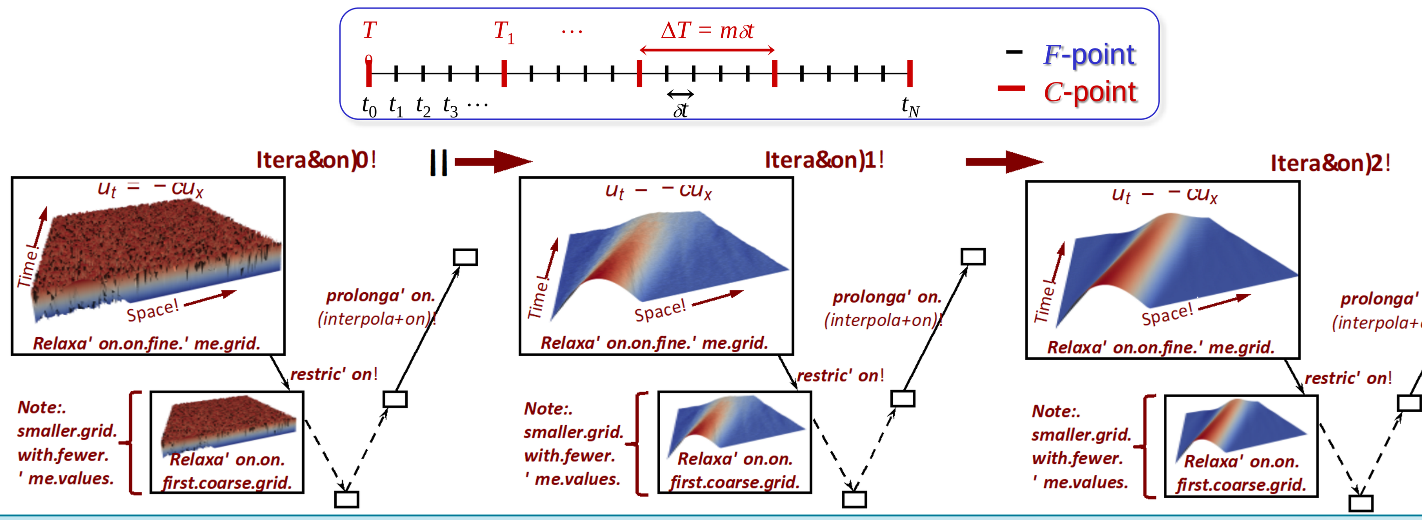


Parallel in Time Capabilities in SUNDIALS

- To expose additional concurrency in time dependent simulations we are adding parallel in time capabilities to SUNDIALS adaptive integrators through the XBraid package

sundials + XBRAID

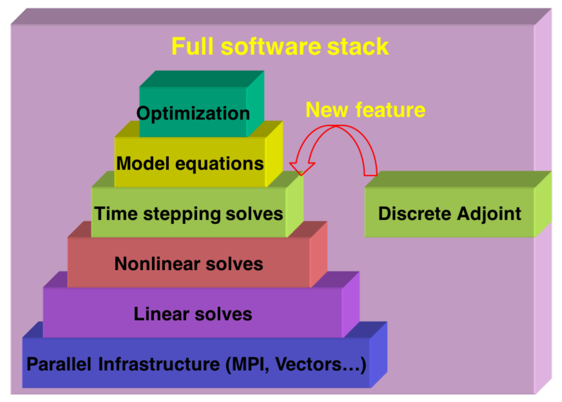
- An interface between ARKode and XBraid is planned:
  - ARKode – adaptive step implicit, explicit, and additive (IMEX) Runge-Kutta methods for stiff, non-stiff, and mixed systems
  - XBraid – multigrid reduction in time (MGRIT) iteratively computes the solution at multiple times simultaneously



Discrete Adjoint Sensitivity Analysis for PETSc

We are improving support for PDE-constrained optimization in PETSc

www.mcs.anl.gov/petsc

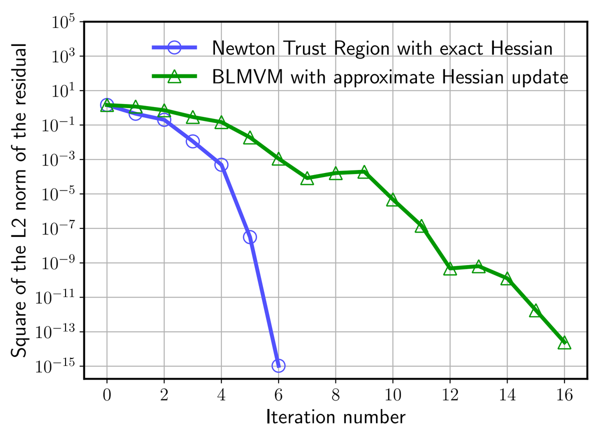


Approach

- Develop 2nd-order discrete adjoints for sensitivity analysis of time-dependent simulations
- Enable derivative-based optimization, data assimilation, and optimal control

Results

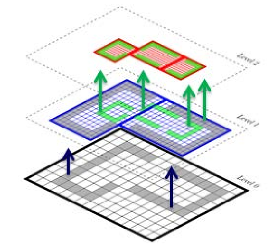
- Implemented 2nd-order adjoint for implicit time integration methods; explicit methods in progress
- Experimented with an inverse initial value (IIV) problem



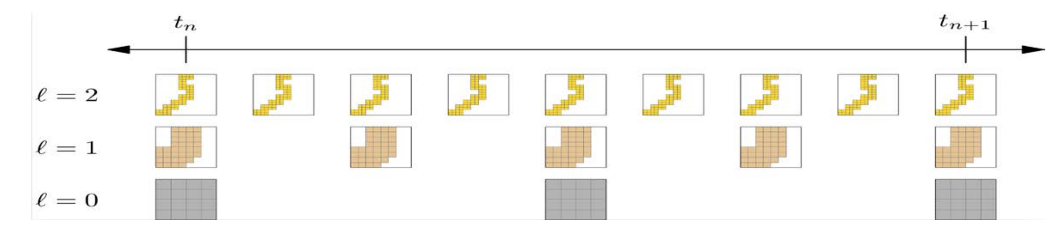
The Hessian-vector product computed with 2nd-order adjoint leads to faster convergence in a simple IIV problem

Synergistic Activities with Structured Mesh

The FASTMath time integration team is working with the AMReX structured mesh discretization team to provide support for higher-order temporal integration of PDEs posed on AMR meshes.



Spectral Deferred Corrections (SDC): methods and software support for multi-level SDC methods where the AMR grid levels correspond to the SDC levels providing time-space coarsening.



Space-time hierarchy of structured grids for multi-level SDC with AMR (Emmett, et. al. 2018)

Multirate Integrators: methods and software for multiscale problems posed on block-structured AMR grids

Approach:

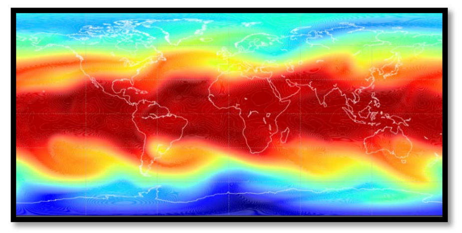
- Develop and test two-rate explicit and three-rate IMEX methods on low Mach combustion on locally refined grids
- Explore multirate coupling strategies for multiple implicit components to allow efficient solves
- Investigate constraint enforcement

Applications

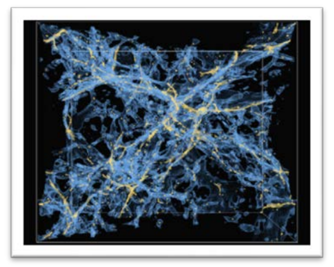
Our FASTMath Time Integration tools are used in numerous DOE applications

- Climate
- Materials science
- Power grids
- Combustion
- Superconductors
- Cosmology
- Computational Fluids
- Subsurface flow
- Fusion

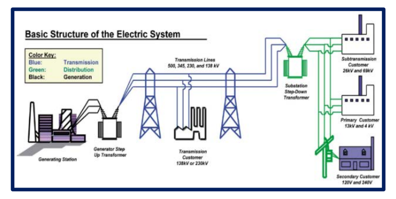
Dislocation dynamics



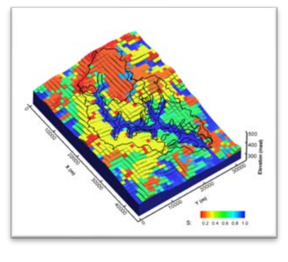
Atmospheric Dynamics



Cosmology



Power Grid Dynamics



Subsurface flow

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