FASTMath Nonlinear and ODE Solver Technologies

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FASTMath is developing next-generation nonlinear solvers and time integrators within robust library frameworks, and working with applications to integrate these technologies within scientific codes.

Overview

As scientific models improve in physical fidelity, simulations increasingly couple large-scale, stiff and temporally disparate interacting processes. FASTMath efforts have therefore focused on next-generation solvers for challenging multi-physics and multi-rate problems:

- New solver libraries for stable and accurate split time integration
- New nonlinear solvers for simplified prototyping and increased robustness
- Solvers including sensitivity information for enhanced uncertainty quantification
- Enhancements to support state-of-the-art architectures
- Collaboration with simulation scientists to incorporate new technologies within application codes

Adaptive Implicit/Explicit Time Integrators

To better capture the multi-rate and multi-physics nature of science applications, we have developed a highly flexible ImEx time integration solver, ARKode:

- Single-step, adaptive, additive Runge-Kutta methods
- Explicit, implicit or mixed implicit/explicit options
- Stable and high-order-accurate (Δt^3 to Δt^5)
- Interfaces in C, C++, Fortran
- Designed for space-time adaptivity:
  - Built-in adaptive temporal error control; user-modifiable
  - Supports adaptive problem resizing between time steps
  - Native support for multiple discretization types via non-identity mass matrix

$$M\dot{y} = f_E(t,y) + f_I(t,y),$$

Leverages SUNDIALS' wide variety of implicit solver algorithms:

- Nonlinear: Modified Newton, Inexact Newton, Fixed-point, Anderson-accelerated Fixed-point
- Linear:
  - Direct: Dense, Band, Sparse
  - Preconditioned Krylov: GMRes, FGMRes, BiCGStab, TFQMR, CG

Accelerated Fixed-Point Nonlinear Solvers

To better handle nonlinear problems with reduced differentiability, or arising within time-adaptive implicit simulations, we have developed robust Anderson-accelerated fixed-point solvers:

- Jacobian-free methods enable fast prototyping of implicit application codes
- Robust fixed-point iteration is accelerated using Krylov subspace techniques (a.k.a. "nonlinear GMRES")
- Implemented in SUNDIALS (KINSOL, ARKode) and Trilinos (NOX)

Architecture-Aware Enhancements

Incorporating Threading within SUNDIALS:

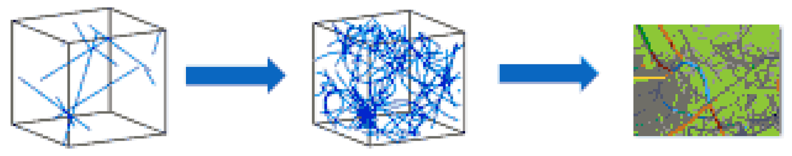
- New OpenMP and Pthreads vector kernels for threaded solves
- Interface with SuperLU_MT for threaded linear solvers, enabling simplified construction of hybrid MPI+thread preconditioners

Trilinos/NOX refactored for new solver stack: updated interfaces to allow for global ordinals above 32-bit limit.

Implicit Simulations of Dislocation Dynamics

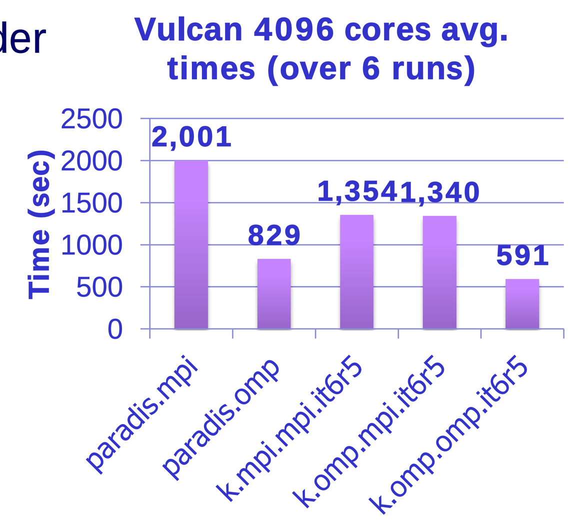
The ParaDiS code performs large-scale simulations of dislocation dynamics models of strain-hardening within a crystal lattice

Simulations begin with a small number of segments, which multiply, collide, join and separate, resulting in rapid configuration changes throughout a simulation.



We incorporated the SUNDIALS KINSOL and ARKode solvers for faster nonlinear solvers and adaptive/higher-order time integrators:

- Accelerated fixed point (AA) in KINSOL and 3rd order integrator from ARKode showed significant speedups over original solver on 16 cores w/ BCC lattice:
  - Early time: 40% with AA, 30% with 3rd order
  - Late time: 60% with AA, 70% with 3rd order
- New solvers gave speedups and robustness for large array of strains
- Developed hybrid MPI/OpenMP vector kernels; tested AA
  - 35% speedup on 4,096 cores of LLNL Vulcan machine
  - 12% speedup on 262,000 cores of LLNL Sequoia machine



Collaboration with T. Arsenlis (LLNL), S. Aubry (LLNL), G. Hommes (LLNL), K. Mohror (LLNL), and D. Gardner (SMU & LLNL)

Adjoint Capabiliies in Albany

An adjoint-based gradient capability is being developed in the Albany application code. This is motivated by inversion and UQ milestones of the PISCEES Ice Sheet application, but is being written as a general purpose capability.

This capability makes use of automatic differentiation, nonlinear and linear solvers, and parallel data structures from the Trilinos suite.

Direct Sensitivities

$$\frac{dg}{dp} = \frac{\partial g}{\partial x}^T \frac{\partial f}{\partial x}^{-1} \frac{\partial f}{\partial p} + \frac{\partial g}{\partial p}$$

Adjoint Sensitivities

Time Integration of Coupled Climate Physics

We are investigating time integration and nonlinear solution strategies within atmospheric physics

- Physics effects are operator split
- Order of application can change solution

We are developing an implicit reference solution to help measure error

- Kinematic driver framework -- full CAM microphysics but idealized fluid motions
- Assessing time step convergence
- Applying an explicit prediction

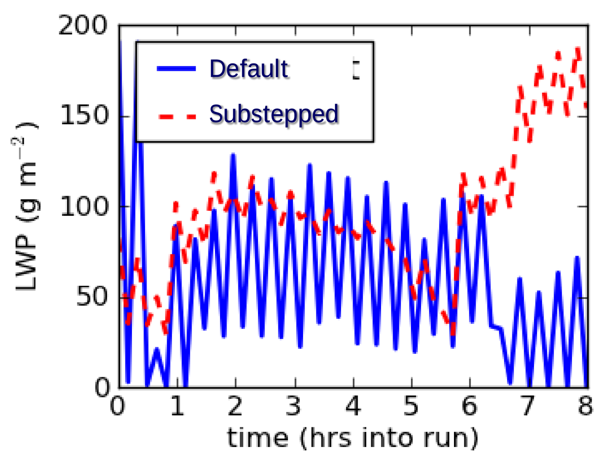


Fig: Splitting causes oscillations in liquid water path (LWP), with large values before microphysics and low values after. From a single-column simulation of Arctic stratus (MPACE-B)

Collaboration with P. Caldwell (LLNL)

Future Plans

Simplified interaction between solver libraries:

- We are constructing interfaces between SUNDIALS' solvers and both HYPRE and PETSc for scalable preconditioning.

Continued development of solvers for LCF architectures:

- Investigation of communication-avoiding techniques within SUNDIALS solvers, for increased performance at large scales.
- Development of MPI+Thread vector kernels for hybrid solvers.

Working to derive/develop new stable and high-order-accurate methods for time-subcycled multiphysics applications.

More Information: http://www.fastmath-scidac.org or contact Lori Diachin, LLNL, diachin2@llnl.gov, 925-422-7130

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