SUNDIALS-*hypre*

Time integrators are at the core of every time-dependent simulation application. In addition, many applications require the solution of linear algebraic systems of equations, whether through use of an implicit approach for integrating the time dependence or for solution of steady state systems. The SUNDIALS-*hypre* project is enhancing the SUNDIALS library of numerical software packages for integrating differential systems in time using state-of-the-art adaptive time step technologies and the *hypre* library for solving large systems of linear equations both for use on exascale systems.

Many exascale applications depend on efficient time integrators and linear solvers yet do not use state-of-the-art algorithms and are not able to easily take advantage of algorithmic advances. Through flexible and efficient libraries, applications can more easily take advantage of new algorithms and more efficient implementations that will allow for easier adaptations to exascale architectures. The SUNDIALS-*hypre* project is enhancing the SUNDIALS and *hypre* libraries, which collectively deliver time integrators, nonlinear solvers, linear solvers, and preconditioners, for use in scientific applications running on exascale systems.

SUNDIALS provides both adaptive multistep and multistage time integrators designed to evolve systems of ordinary differential equations and differential algebraic equations. This suite also includes both Newton and fixed-point nonlinear solvers and scaled Krylov methods with hooks for user-supplied data structures and solvers. The SUNDIALS team is extending SUNDIALS to include an efficient time-dependent mass matrix mechanism, a new GPU-enabled approach for solving multiple ODE systems in parallel, a rewrite of an ordinary differential equation integrator that projects solutions on constraint manifolds, integration into ECP applications, and performance assessments and improvements on pre-exascale and exascale systems.

hypre is a software library of high-performance preconditioners and solvers for the solution of large, sparse linear systems of equations on massively parallel computers. The library includes parallel multigrid solvers for both structured and unstructured grid problems and features conceptual interfaces, which include a structured, a semi-structured interface, and a traditional linear-algebra-based interface. The *hypre* team is adding both CUDA and OpenMP 4.x ports of the *hypre* library and is assessing the performance of these ports, examining performance bottlenecks, and developing new variants of algorithms or new algorithms that are better suited for pre-exascale and exascale architectures.

Progress to date

- The SUNDIALS team released new versions of the SUNDIALS suite that include new linear and nonlinear solver APIs that allow easier interfacing with external packages, a new set of optional fused vector kernels which can result in an over 90% reduction in run time for reduction operations, and a new many-vector capability allowing the underlying data structures to be vectors of vectors. The team also supported ECP applications through the development of CUDA vectors with managed memory, optional streams, and more flexibility in memory management from the application.

- The *hypre* team released new versions of the *hypre* library that include a new GMRES solver with improved communication properties, a new integer type for 64-bit integers allowing for a mixed-integer option that uses less memory and is about 20–25% faster than the 64-bit integer version, and GPU-enabled AMG setup components.

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