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HPC NUMERICAL LIBRARIES: SUCCESSES AND NEXT-GENERATION CHALLENGES

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While high-performance architectures provide unprecedented resources for scientific discovery, next-generation scientific applications present daunting challenges. A major difficulty is the increasing complexity of algorithms and computer science techniques needed to model multiphysics and multiscale phenomena and to pursue portable performance in an era of dramatic architectural changes [3, 5].

We believe that well-designed and well-supported scalable numerical software libraries are an important tool to help many high-performance applications address these challenges. There is some evidence to this effect; for example, several Gordon Bell winners and finalists have been implemented using PETSc [1, 2]. Also, various other libraries, including those within the FASTMath institute [4], have been successfully used throughout the high-performance computing (HPC) community. From an application perspective, advantages of using numerical libraries include the ability to focus on research areas of primary interest while not reinventing the wheel for other functionalities, but instead employing well-tested implementations with all the best bells and whistles. Some disadvantages are possibly less flexibility (e.g., what if the library writers didn't incorporate the bell I need?) and risk (e.g., what if the developers stop supporting the library?).

This presentation will highlight practices that have proven effective in PETSc library development and use in large-scale scientific appications. A key feature for achieving efficient, robust, and scalable performance on emerging architectures is full composability of solvers for multiphysics and multilevel methods, including support for arbitrary, dynamic composition of hierarchical methods for coupled problems and customization of all components in composite solvers. We will discuss lessons learned and strategies developed for the combined use of multiple libraries [6]; an important point, which has consequences on suitable programming models and design, is for libraries to be unassuming about control of the overall simulation. We will also consider opportunities that are ripe to enhance high-performance application software productivity.

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