STRUMPACK/SuperLU/FFTX

Many simulation and data analysis codes need to solve sparse systems of equations. The high-fidelity simulations being solved by exascale application teams involve large-scale multiphysics and multiscale modeling problems that generate highly ill-conditioned and indefinite systems, for which iterative methods struggle. The STRUMPACK/SuperLU/FFTX project is delivering robust and scalable factorization-based algorithms that are indispensable building blocks for solving these numerically challenging problems and a Fourier transform package that is applicable to spectral-based methods used by exascale applications.

Scalable factorization-based methods are important components in solvers for ill-conditioned and indefinite systems of equations that arise in many exascale applications, while performant Fourier transforms are required by applications using certain spectral-based methods. The STRUMPACK/SuperLU/FFTX project is producing robust and scalable factorization-based methods and preconditioners for systems of equations and is providing a Fourier transform software stack suitable for obtaining the highest possible performance on exascale systems.

The team is delivering factorization-based sparse solvers encompassing two widely used algorithm variants, the supernodal SuperLU library and the multifrontal STRUMPACK library. The team is also adding scalable preconditioning functionality using hierarchical matrix algebra to the STRUMPACK library. Both libraries are applicable to a large variety of application domains. These scalable libraries are being enhanced to ensure that they will be performant on the pre-exascale and exascale architectures.

The team will also provide the FFTX library to address the need for Fourier transforms by certain spectral-based methods. This library will use symbolic transformation tools, code generation techniques, and autotuning to create exascale-ready high-level Fourier transform packages for multiple applications that will support multi-GPU and multi-node parallelism.

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Progress to date

- The team released SuperLU DIST version 6.1.0, with improvements in the strong scaling of the triangular solve—up to 4.4× faster than version 5.x on 4000+ cores—and on-node threading optimization, providing up to a 3× speedup on a Cori-KNL node.
- The team released STRUMPACK version 3.1.0, with improvements in the scalability of the hierarchical matrix algorithms—the dense hierarchical matrix compression is up to 4.7× faster on eight nodes of Cori-Haswell and 2.4× faster on Cori-NKL, while the hierarchical sparse factorization is up to 2.2× faster on eight Cori-KNL nodes—and improvements in the hierarchical solve to reduce communication and more OpenMP support, leading to a 7× faster matrix redistribution and 1.4× faster solve.
- The team specified an initial set of FFTX applications use cases, designed the FFTX API version 1.0, and provided a reference implementation targeting FFTW.