

COMPUTATIONAL LIBRARIES OPTIMIZED VIA EXASCALE RESEARCH

Software libraries are powerful means of sharing verified, optimized algorithms and their implementations. Applied research, development, and support are needed to extend existing DOE mathematical software libraries to make better use of exascale architectural features. DOE-supported libraries encapsulate the latest results from mathematics and computer science R&D; many DOE mission-critical applications rely on these numerical libraries and frameworks to incorporate the most advanced technologies available.

The CLOVER merged projects consisting of SLATE, PEEKS, FFT and Kokkos Kernels will ensure the healthy functionality of the numerical software libraries on which the ECP applications will depend. The DOE mathematical software libraries used by computational science and engineering applications span the range from lightweight collections of subroutines with simple APIs to more “end-to-end” integrated environments and provide access to a wide range of algorithms for complex problems.

SLATE

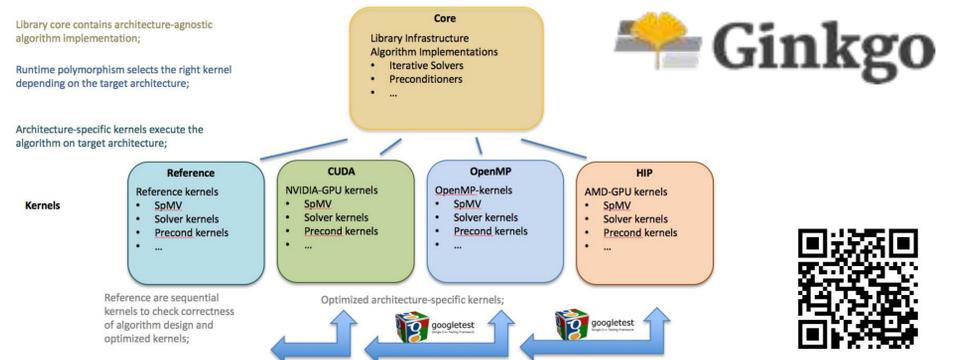
SLATE will offer a modern replacement for ScaLAPACK and will facilitate the development and advancement of multi-core and accelerator capabilities by leveraging recent progress and ongoing efforts in mainstream programming models (e.g., MPI 3+, OpenMP 4+, OpenACC). SLATE provides basic dense matrix operations (e.g., matrix multiplication, rank-k update, triangular solve), linear systems solvers, least square solvers, singular value and eigenvalue solvers.

SLATE ARCHITECTURE



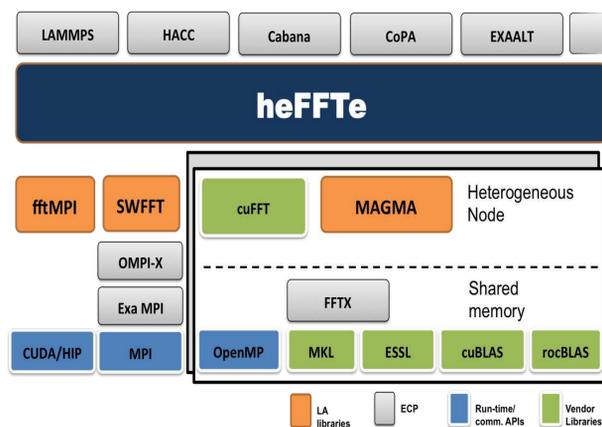
PEEKS

The PEEKS Project part of ECP's CLOVER umbrella project aimed at delivering production-ready high performance preconditioned Krylov solvers for Exascale Computing. For these solvers to efficiently exploit extreme-scale hardware, both the solver algorithms and the implementations must be redesigned to address challenges like extreme concurrency, complex memory hierarchies, costly data movement, and heterogeneous node architectures. One important aspect is the implementation-readiness for GPU accelerators that are expected to provide a significant performance share in Exascale Computing. Products of the PEEKS project are the Trilinos/Belos package and the Ginkgo library, which addresses the efficient use of GPU technology.



FFT

Considered one of the top 10 algorithms of the 20th century, the Fast Fourier Transform (FFT) is widely used by applications in science and engineering. Large scale parallel applications targeting exascale, such as those part of the Exascale Computing Project (ECP), are designed for heterogeneous architectures and, currently, some of them rely on efficient state-of-the-art FFT libraries built as CPU kernels. A product of the FFT project is the *Highly Efficient FFTs for Exascale* (heFFTe), a hybrid highly-scalable and robust library for multidimensional FFT computations targeting exascale.



Kokkos Kernels

Kokkos Kernels is a library in the Kokkos ecosystem for performance portable sparse/dense linear algebra and graph kernels. Both the performance and the portability aspects are key to the stakeholders of the product. Kokkos Kernels deliver sparse and dense linear algebra kernels, BLAS/LAPACK interfaces, graph algorithms and machine learning kernels. All of these kernels are tuned for the architectures of interest to ECP. Kokkos Kernels currently supports solvers for applications such as Exawind, SPARC and EMPIRE (ATDM/SNL).

