SAND2022-5414D

Trilinos for Exascale

EXASCALE COMPUTING PROJECT

Trilinos Overview

Trilinos is part of the Sake ECP project.

The Trilinos Community

The Trilinos Project is a community of developers, users and user-developers focused on collaborative creation of algorithms and enabling technologies within an object-oriented software framework for the solution of large-scale, complex multi-physics engineering and scientific problems on new and emerging high-performance computing (HPC) architectures.

Trilinos Software

Trilinos is also a collection of reusable scientific software libraries, known in particular for linear solvers, non-linear solvers, transient solvers, optimization solvers, and uncertainty quantification (UQ) solvers.

Parallel Computing Using Trilinos

Most Trilinos algorithms and software are built upon its abilities to construct and solve sparse problems, using sparse linear solvers. These solvers rely on a collection of data structure classes and functions (kernels) for parallel linear algebra, especially parallel sparse kernels.

Trilinos Portable Parallel Execution

Trilinos is targeted for all major parallel architectures, including distributed memory using the Message Passing Interface (MPI), multicore using a variety of common approaches, accelerators using common and emerging approaches, and vectorization.

Trilinos parallel functionality is written on top of libraries that support compile-time polymorphism, such that, as long as a given algorithm and problem size contain enough latent parallelism, the same Trilinos source code can be compiled and execution on any reasonable combination of distributed, multicore, accelerator and vectorizing computing devices.

Trilinos Packages

Trilinos is organized around fundamental software elements called packages. The Trilinos package architecture enables simultaneous development of many new capabilities in a federated system. Each package has its own name and identity within the research community, giving the package team recognition outside of Trilinos itself.

PEEKS solvers research

The PEEKS subproject is focused on developing new algorithms that improve upon the state-of-art in preconditioners and solvers. Recent highlights:

- A new polynomial preconditioner based on the GMRES polynomial (Loe & Morgan, 2021) has been implemented in the Belos package. It is currently used in the spectral partitioner Sphynx (by the ExaGraph ECP project) to precondition the LOBPCG eigensolver. The MueLu multilevel preconditioner was the preferred preconditioner. The new polynomial preconditioner made the eigensolver run 3X faster on highly irregular graphs.
- In collaboration with CU Denver (Bielich, Langou) and NREL (Thomas), we have developed low-synchronization orthogonalization methods that speed up QR factorization. The primary use case is to orthogonalize the Arnoldi basis in GMRES.We have implemented the novel Delayed Classical Gram-Schmidt times 2 (DCGS2) method in Trilinos/Belos. The code is parallel and runs on multiple GPU. Results on Summit (30 nodes, 180 GPUs) show speedup up to 3X compared to the previous (standard) CGS method.

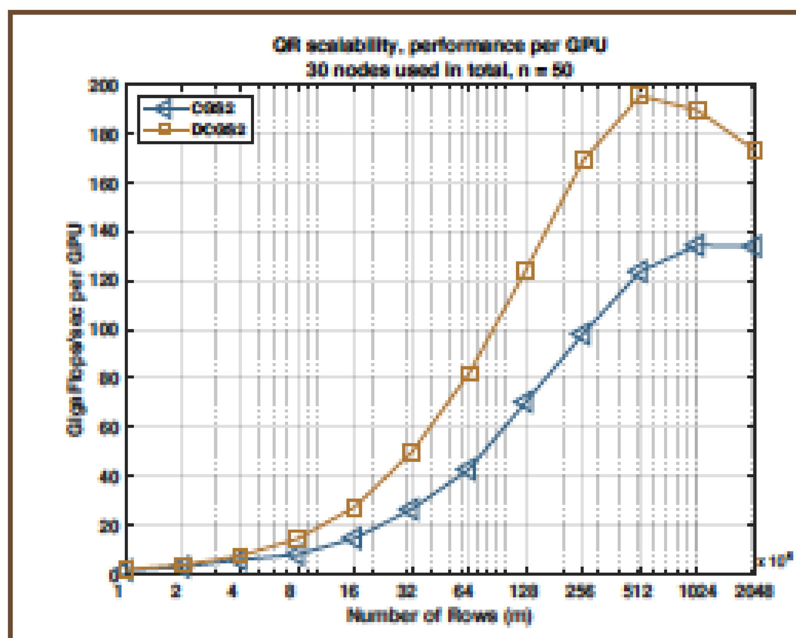


Figure 13: Execution rate per node (30 nodes, 6 GPUs per node).

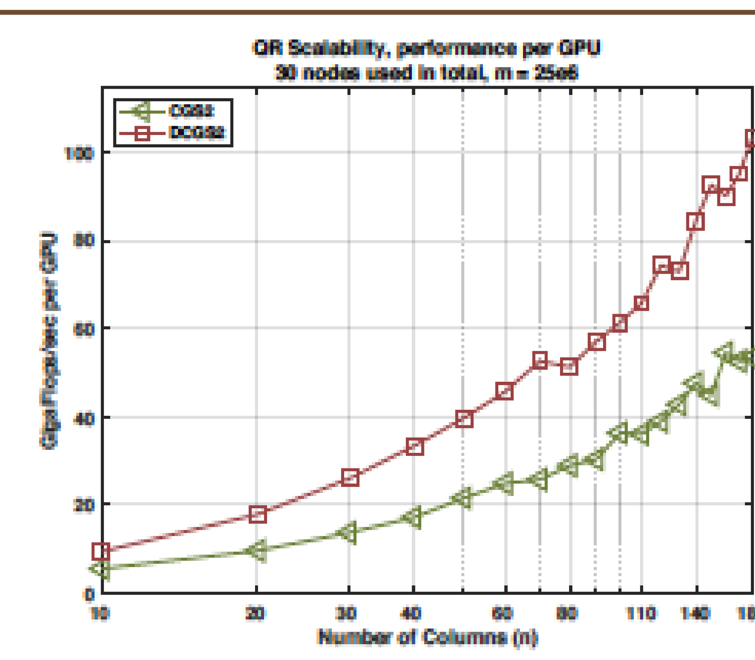
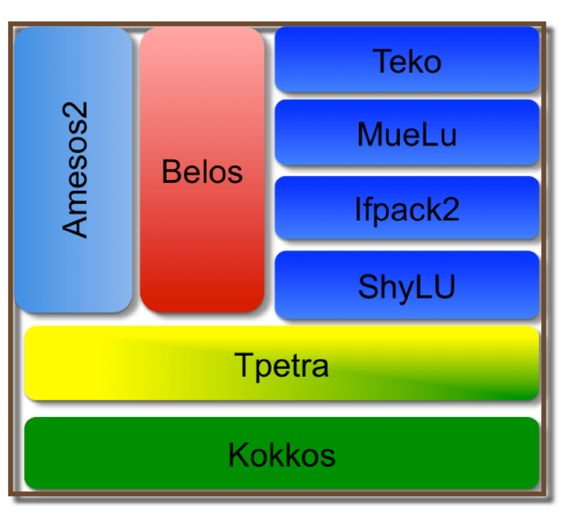


Figure 14: Execution rate per node (30 nodes, 6 GPUs per node).

Exascale solvers in Trilinos

Trilinos solver subproject is focused on preparing the Trilinos solver software stack for the ECP machines. For this year, to prepare the solvers for Frontier and El Captain, we have updated the software stack to support HIP backend for the AMD GPUs. These packages include:

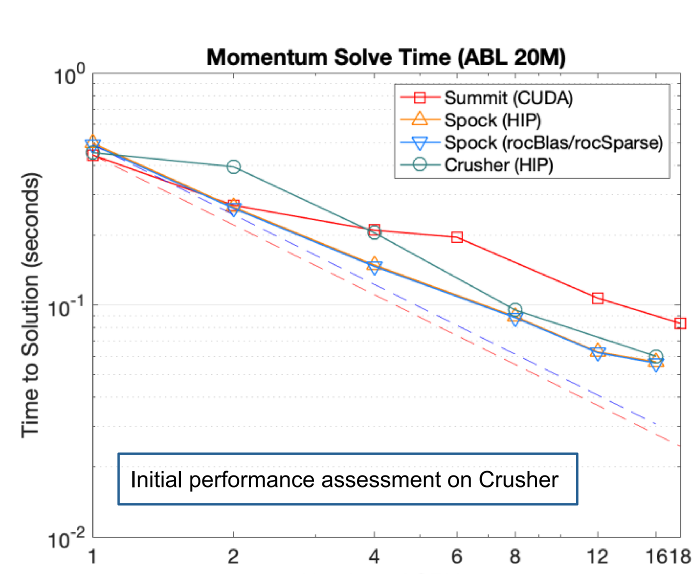
- Tpetra and Xpetra
  - distribued sparse and dense matrix operations (e.g., SpMV, SpGEMM, dot-products)
- Belos
  - Krylov solvers (including s-step/pipelined solvers from PEEKS subproject)
- Ifpack2
  - algebraic preconditioners/smoothers (e.g., relaxation, domain-decomposition, incomplete factorization)
- Amesos2
  - direct solver interface (e.g., SuperLU, KLU2)



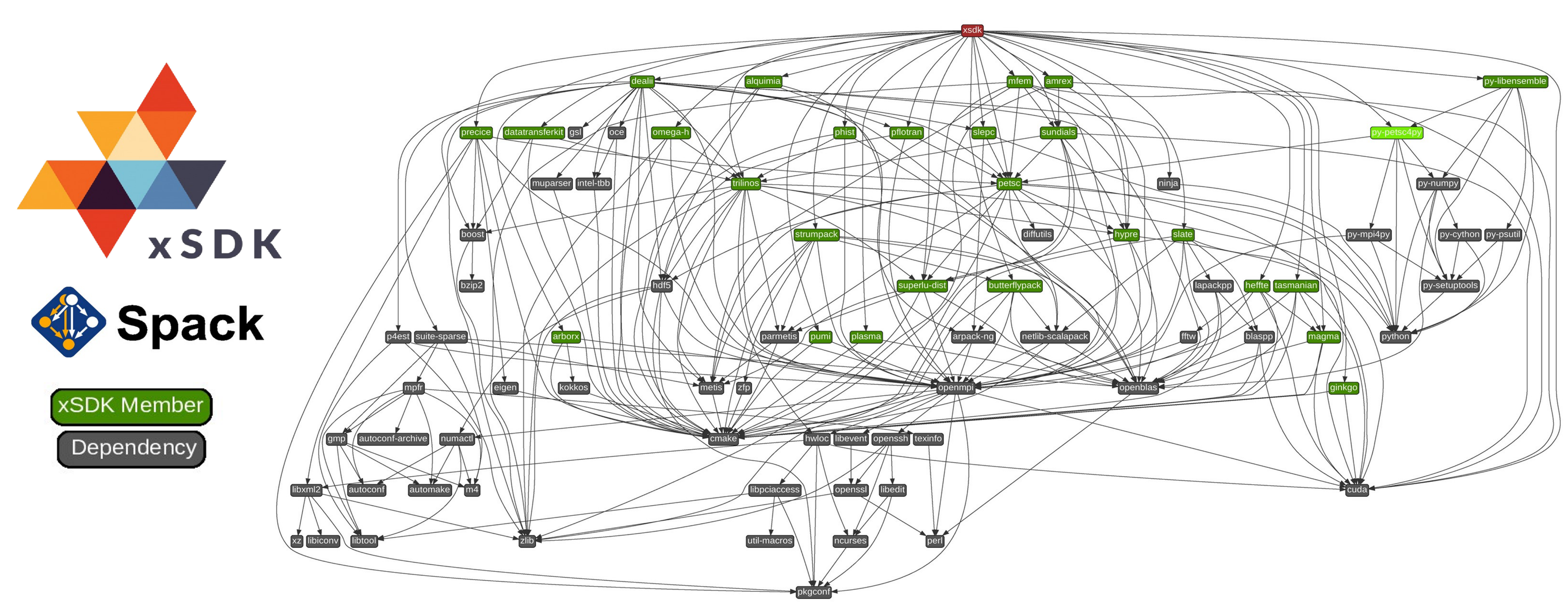
Though outside of the Sake project scope, other solver packages, such as Zoltan2 (graph partitioners) and MueLu (AMG), have been also updated to support HIP backend.

We are actively assessing and improving the performance on Spock and Crusher at ORNL.

We plan to support SYCL backend for Aurora by the end of fiscal year '22 (2022-09-30)



xSDK and Trilinos



The Extreme-Scale Scientific Software Development Kit (xSDK) is to provide a cohesive collection of 24 scientific libraries and reusable domain components that provide building blocks for application codes throughout the extreme-scale computational science community. In xSDK, Trilinos has been one of the member packages from its genesis and serves multiple capabilities for other xSDK packages in the latest version (0.7.0) including:

- PRECICE
- Data Transfer Toolkit (DTK)
- omega-h
- phist
- deal-II
- SUNDIALS

In xSDK 0.7.0, Trilinos improves its interoperability with other packages including new Amesos-2 interfaces for STRUMPACK and ButterflyPack.

The future version of Trilinos will have its build system (TriBITS) compatible with the modern CMake (3.20 or later) to serve "target" based package integrations.

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This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.

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