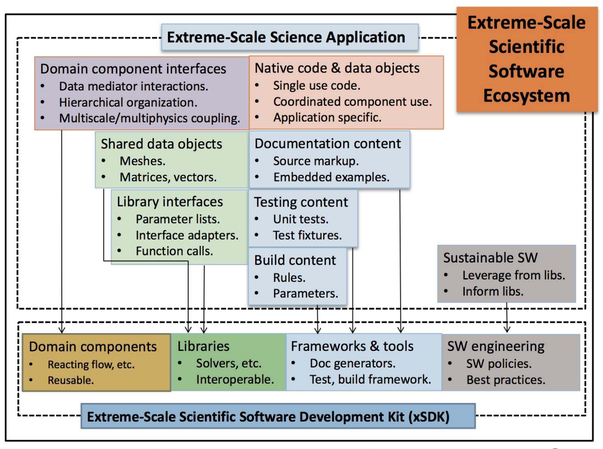
Extreme-scale Scientific Software Development Kit (xSDK) for ECP

xSDK Vision

https://xsdk.info: Building the foundation of a highly effective extreme-scale scientific software ecosystem.



*The vision of the xSDK is to provide infrastructure for and interoperability of a **collection of related and complementary software elements**—developed by diverse, independent teams throughout the high-performance computing (HPC) community—that provide the building blocks, tools, models, processes, and related artifacts for rapid and efficient development of high-quality applications.*

Motivation: Next-generation scientific simulations require combined use of independent packages

- Installing multiple independent software packages is tedious and error prone
  - Need consistency of compiler (+version, options), 3rd-party packages, etc.
  - Namespace and version conflicts make simultaneous build/link of packages difficult
- Multilayer interoperability among packages requires careful design and sustainable coordination

xSDK4ECP Project Overview

https://xsdk.info/ecp: Addressing xSDK challenges for exascale.

Project Scope

Enable seamless combined use of diverse, independently developed software packages as needed by ECP apps

- Coordinated use of on-node resources
- Integrated execution
- Coordinated & sustainable documentation, testing, packaging, distribution

Approach

- Develop **community policies** and **interoperability** layers among xSDK component packages
- Determine xSDK sustainability strategy for ECP
- Work with ECP applications to motivate and test xSDK

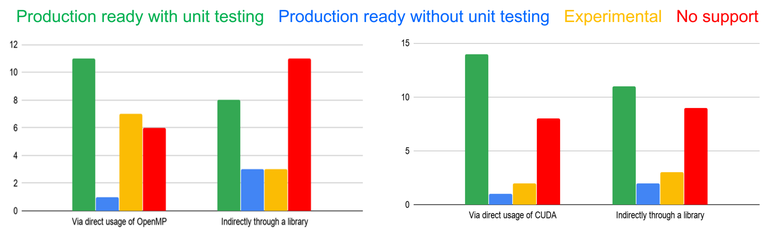
Document on node-level resource management activities within the ECP

Survey status and plans of on-node (and internode) parallel computing capabilities for individual xSDK libraries and prospective additions.

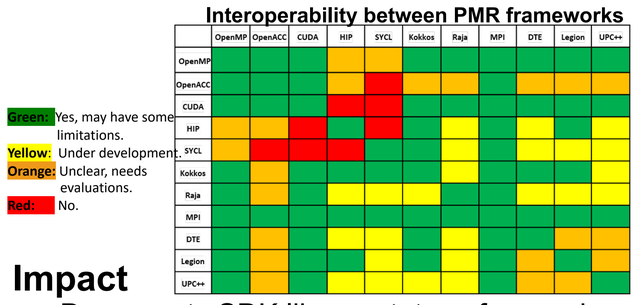
Status of CUDA and OpenMP capabilities of 25 math libraries

Figure 1: Does your library have OpenMP CPU multi-threading capabilities? What is the status?

Figure 3: Does your library have CUDA capabilities? What is the status?



Interoperability between PMR frameworks



Survey programming models and runtime libraries (PMR) projects on status and plans for node-level resource management and other issues that impact mathematical libraries.

Impact

- Document xSDK library status of on-node capabilities, new developments on node-level resource management and its potential impact on xSDK libraries.
- Inform greater ECP community.

Autotuning Parameter Selection for ECP Applications

Objective

Develop autotuning software that learns optimal parameter selection.

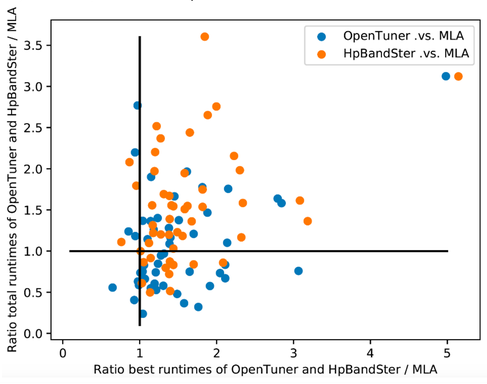
- Enable ECP math libraries and apps to run efficiently on exascale machines.
- New autotuning methods will advance the state of the art in performance optimization research.

Accomplishments

GPTune: https://github.com/xiaoyeli/GPTune

- **Easy integration** - Easy to use Python interface
- **Collaborated** with Y-TUNE team - Developed a ***common interface*** so users can access both tuners and others easily in the same code.
- **Applied** GPTune for parameter search for ScaLAPACK QR & SVD, hypre, and SuperLU

- 128 nodes Edison, 50 tasks (1< m=n < 20000), 4 parameters (mb, nb, #MPIs, #Threads)



GPTune finds **better parameters** in 42 (84%) and 47 (94%) cases compared to OpenTuner and HyBandSter, resp., for ScaLAPACK QR.

xSDK Community Policies

https://xsdk.info/policies: Addressing challenges in interoperability & sustainability of software developed by diverse, independent teams.

xSDK compatible package: Must satisfy mandatory xSDK policies:

- **M1.** Support xSDK community GNU Autoconf or CMake options.
- **M2.** Provide a comprehensive test suite.
- **M3.** Employ user-provided MPI communicator.
- **M4.** Give best effort at portability to common platforms.
- **M5.** Provide a documented, reliable way to contact the development team.
- **M6.** Respect system resources and settings made by other previously called packages.
- **M7.** Come with an OSI-approved, permissive open source license.
- **M8.** Provide a runtime API to return the current version number of the software.
- **M9.** Use a limited and well-defined symbol, macro, library, and include file name space.
- **M10.** Provide an accessible repository (not necessarily publicly available).
- **M11.** Have no hardwired print or IO statements.
- **M12.** Allow installing, building, and linking against an outside copy of external software.
- **M13.** Install headers and libraries under <prefix>/include/ and <prefix>/lib/.
- **M14.** Be buildable using 64 bit pointers. 32 bit is optional.
- **M15.** All xSDK compatibility changes should be sustainable.
- **M16.** The package must support production-quality installation compatible with the xSDK install tool and xSDK metapackage.

We welcome feedback. What policies make sense for your software?

Also specify recommended policies: Currently encouraged but not required:

- **R1.** Have a public repository.
- **R2.** Possible to run test suite under valgrind in order to test for memory corruption issues.
- **R3.** Adopt and document consistent system for error conditions/exceptions.
- **R4.** Free all system resources it has acquired as soon as they are no longer needed.
- **R5.** Provide a mechanism to export ordered list of library dependencies.
- **R6.** Each package should document the versions of packages with which it can work and on which it depends.
- **R7**. Have README, SUPPORT, LICENSE, and CHANGELOG files in top directory.

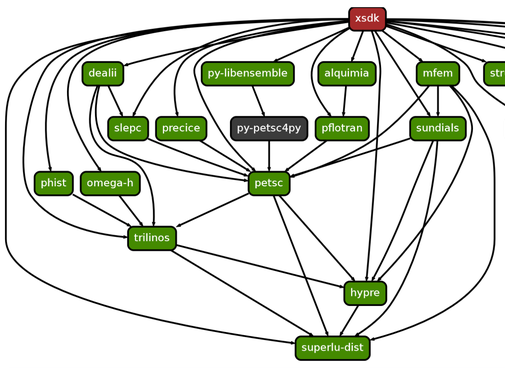
Full version of community policies available on Github: https://github.com/xsdk-project/xsdk-community-policies

New or revised polices can now be proposed with pull requests on Github (https://github.com/xsdk-project/xsdk-community-policies/blob/master/process-for-new-or-revised-policies.md).

xSDK member package: Must be an xSDK-compatible package, *and* it uses or can be used by another package in the xSDK, and the connecting interface is regularly tested for regressions.

xSDK Packages and Releases

https://xsdk.info/packages: Enabling ECP applications to readily access many of the most popular HPC math libraries.



xSDK-0.5.0
released Nov 2019

Tested on key platforms at ALCF, NERSC, and OLCF, also Linux and Mac OS X

Original xSDK math libraries: **hypre, PETSc, SuperLU, Trilinos**

Added Dec 2017: **MAGMA, MFEM, SUNDIALS**

Added Dec 2018: **AMReX, deal.II, DTK, Omega_h, PHIST, PLASMA, PUMI, SLEPc, STRUMPACK, TASMANIAN**

Added Nov 2019: **ButterflyPACK, Ginkgo, libEnsemble, preCICE**

Impact

- Improve access & sustainability of math libraries for ECP
- Lay groundwork for addressing broader issues in software interoperability and performance portability

Spack/Git Workflow

- **Packages**
  - Follow the standard workflow for a Spack package
  - Submit pull requests with the "xSDK" label
  - Provide package candidate and final xSDK release tags
- **xSDK Meta-package**
  - Depends on xSDK member packages: "**spack install xsdk**"
  - Maintain shared Spack branch for release coordination

History and Plans

- Began in ASCR/BER partnership, IDEAS project (Sept 2014), needed for BER multiscale, multiphysics surface-subsurface hydrology models
- Work toward regular xSDK releases with increased formality of release process.
- Collaboration with broader SDK efforts in ECP

ECP 4th Annual Meeting, February 2020

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