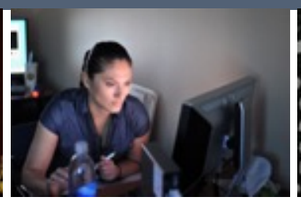
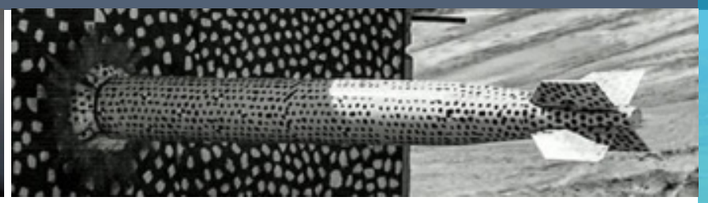
SAND2024-14271PE
UUR

Trilinos Core Product Area Update


PRESENTED BY

Roger Pawlowski

Current Package Owners: R. Bartlett, L. Berger-Vergiat, E. Boman, C. Glusa, C. Siefert, G. Sjaardema, C. Trott

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Trilinos Core Product Area

- Teuchos: Common Trilinos utilities
- Tpetra: Parallel sparse linear algebra
- Xpetra: Petra abstraction layer
- PyTrilinos2: Python wrappers
- Pamgen: Inline mesh generation utility
- RTOp: Reduction/transformation operators
- Thyra: Abstraction layer for Trilinos

- Snapshotted Packages:
  - Kokkos: Performance portability
  - KokkosKernels: Performance portable linear algebra
  - SEACAS: Finite Element tools for Exodus database format

- Deprecated Packages:
  - Epetra
  - EpetraExt
  - Isorropia
  - TriUtils
  - PyTrilinos

Kokkos Core Updates

Focused on continuous improvement in capability, ease-of-use and robustness.

- New Features
  - Multi-GPU support for CUDA
  - Improved half precision support (e.g. numeric traits, math functions)
  - Team level std::algorithms
  - SIMD improvements
  - SYCL is non-experimental
  - MI300A unified memory support (Kokkos 4.3.1: opt-in; 4.5 default)
  - View – mdspan interoperability
- Robustness Improvements
  - Thread-safety for most Kokkos operations => dispatch parallel operations from multiple (non-Kokkos) threads
  - Better checks for valid iteration ranges and out of bounds accesses
  - Deprecation of dangerous implicit conversions (e.g. int to execution space instances)
  - Better support for non-default constructible View element types
- Ease-of-Use Enhancements
  - Initial introduction of C++ deduction guides (CTAD support) for Kokkos classes
  - Improved ISO C++ conformance of Array and complex

Attention: C++20 will be required with Kokkos 5.0 in late summer 2025.

Teuchos and Zoltan2

Teuchos

- Improved YAML Parser Support
  - Native yaml parser covers 99% of users.
  - Enabling yaml-cpp TPL for full yaml support: Tabs as errors, list of lists, line continuation lists, Unicode in comments, …
- Trilinos Leadership: discussions on what we can clean up and remove
  - Keep common look and feel (e.g. ParameterLists, scalar_traits, …)
  - New c++ standards (e.g. Teuchos::any → std:any)
  - RCPs/memory management tools (RCP → shared_ptr, Array→std::vector)?
  - Test harness (Teuchos → gtest)?

Zoltan2

- Jet is a new multilevel graph partitioner based on Kokkos so runs on GPU
- The partition quality is slightly better than Metis/ParMetis
- Jet is currently limited to a single GPU but multi-GPU version is in progress
- Jet is currently stand-alone code but will be integrated into Trilinos/Zoltan2

[1] Gilbert, Madduri, Boman, Rajamanickam: “Jet: Multilevel Partitioning on GPUs”, SISC, to appear.

SEACAS

Exodus/IOSS new capabilities:

- Discontinuous Galerkin / Enhanced Field Metadata support.
  - Eliminates need for conventions; explicitly specifies field types
  - Permits Bases and Quadrature Rule definitions in file
- Support for Advanced Compression Capabilities
  - Lossy compression
  - Zstd, BZip
- Beginnings of Dynamic Topology support
  - Store multiple model topology changes in a single file.

Embedded Visualization

- Catalyst2 improvements and refactoring

General SEACAS Improvements

- General improvements in many applications
- Better compression support
- Improved Assembly capabilities