Trilinos Users Group
Data Services Update

November 30, 2021
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with contributions from
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Siva Rajamanickam (KokkosKernels team)
Erik Boman (Zoltan2 team)
Alan Williams (STK team)
SEACAS / IOSS / Exodus
(POC: Greg Sjaardema)

• New Features
  • Assemblies – hierarchical groups of blocks/sets/assemblies
  • Blobs -- store arbitrarily-sized objects in an exodus file
  • Entity Attributes -- “provenance” or annotation data on entities and fields
  • Aprepro – Arrays, Exodus integration
  • Exodus.py – python3, improved capabilities, testing

• New Integrations – FAODEL, Catalyst2, ADIOS2, TextMesh

• In progress:
  • Discontinuous Galerkin Fields
  • HDF5 VOL
  • Compression (lossy and lossless)

• Others: windows, scalability, code quality
Kokkos Core 3.4
(POC: Christian Trott)

• HIP Backend works in previous release
  • Performance Improvements for HIP backend
• SYCL Backend Almost Feature Complete
  • Trilinos Tpetra and LAMMPS work now
  • Ongoing issues: Fine grained tasking, and arbitrary sized atomics.
• OpenMPTarget Backend Almost Feature Complete
  • OpenMPTarget still has issues with some custom reduction stuff in addition.
• Require CMake 3.16 or newer

See Brian Kelley’s talk at 11am:
Trilinos Support on AMD and Intel GPUs
Kokkos Kernels 3.4
(POC: Siva Rajamanickam)

• Added full support for HIP
  • Integration with Trilinos is complete and tested on Spock
• Initial support for SYCL
  • Most features functional (coloring algorithms and some batched algorithm still disabled)
  • Integration in Trilinos has started

• Improved support for half precision
• ArmPL library support in specific kernels
• Distance 2 Maximal Independent Set (MIS-2)
• Partial coloring as input for coloring algorithms
• Improved two-stage Gauss-Seidel performance (added damping)
• Supernodal SpTRSV improvements (use batched algorithms internally)

See Brian Kelley’s talk at 11am:
Trilinos Support on AMD and Intel GPUs
Zoltan2
(POC: Erik Boman)

• First multi-GPU graph partitioner for distributed-memory systems: Sphynx
  • Sphynx: Spectral Partitioning for HYbrid aNd aXelerator-based systems
  • Uses several Trilinos packages (Tpetra, Anasazi, Ifpack2, MueLu)
  • Uses Kokkos for performance portability
  • Compared to ParMETIS, Sphynx is faster on irregular graphs and obtains similar quality partitions on regular graphs

• New Multi-GPU graph coloring:
  • Distance-1, Distance-2 and Partial Distance-2 coloring
  • Uses Teuchos::Comm and Kokkos to run with MPI+GPU
  • Zoltan2 TpetraCrsColorer interface accepts Tpetra matrix as input
STK
(POC: Alan Williams)

• GPU: Improving the performance of synchronizing Fields between CPU and GPU memory spaces.
  • Primarily for Sierra SM

• AMD/HIP: stk-mesh unit-tests now build and run on AMD platforms, using ROCM 4.3.
  • Primarily for Exawind