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SAND2022-11815C

Sandia National Laboratories

What's new in Tpetra & Data Services?

TRILINOS

Presented by: Chris Siefert, Tpetra Package Lead

EuroTUG 2022, September 13, 2022

U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

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Outline

- What’s new in Zoltan2?
- What’s new in SEACAS/IOSS/Exodus?
- What’s new in STK?
- What’s new in Tpetra?
- Other new developments!

Note: I will be repeating “new” developments from TUG ’21, more detail on those can be found here: https://trilinos.github.io/trilinos_user-developer_group_meeting_2021.html

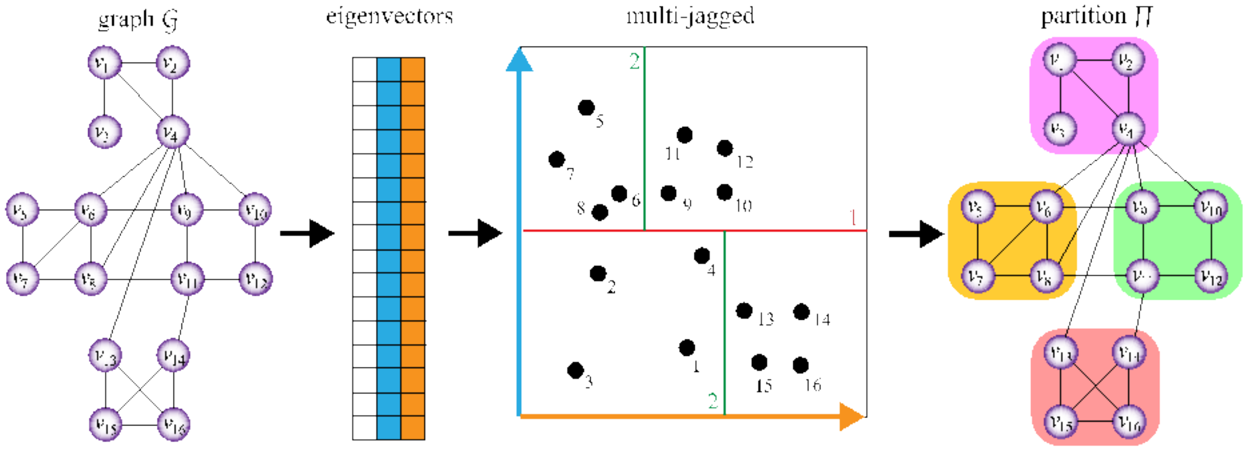
What’s new in Zoltan2? [TUG ‘21 and newer]

- Hybrid distributed/shared memory graph coloring
  - Uses MPI + KokkosKernels coloring
  - Runs on CPU and GPU (Nvidia/CUDA and AMD/HIP)
  - Supports dist-1, dist-2, and partial dist-2 coloring

- Sphynx: New graph partitioner
  - Algorithm based on spectral partitioning
  - Runs on both CPU and GPU (via Kokkos)
  - First multi-GPU graph partitioner!

- In progress:
  - Kokkos-based API for input adapters so users can provide data on either host or device
  - Multilevel graph partitioner for GPU

Sphynx partitioner pipeline:


graph G
eigenvectors
multi-jagged
partition Π
v_1 v_2 v_3 v_4 v_5 v_6 v_7 v_8 v_9 v_{10} v_{11} v_{12} v_{13} v_{14} v_{15} v_{16}
1
2
2
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16

Slide courtesy of Erik Boman, Zoltan2 lead.

What’s new in SEACAS/IOSS/Exodus? [TUG ‘21]

- 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

What’s new in STK? [TUG ‘21]

- 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
- STK Balance: improving work-flow and performance of Balance and BalanceM2N coming soon.

What's new in Tpetra?

- A *lot* has changed since EuroTUG 2019!
- The *big* ones are that Tpetra (and thus the derived linear solver stack) now supports…
  - NVIDIA CUDA w/o UVM.
  - AMD GPUs w/ HIP.
  - Intel GPUs w/ SYCL (Warning: Not yet regularly tested.)
- As of Trilinos 13.4 over 27,000 lines of deprecated code/interfaces were removed.
- There are other new features (on-node graph assembly, simultaneous communications, BlockCrs capabiltities, etc.) as well. We'll get to those in time.

Dynamic Profile Removal [TUG ‘19]

- For better portability to GPUs, we have removed the `DynamicProfile` option for matrix/graph assembly.

- You now need at least an upper bound on storage to build the Graph (like the old `StaticProfile` option).

- Off-processor assembly is still supported (and there is some resizing support for off-rank imports).

FECrs[Graph|Matrix|Vector] [TUG '19]

- For folks interested in finite elements, we have a FE-centric assembly layer.

- Much better performance than using off-rank calls to `insertGlobalEntries`.

- Does *not* require ghosted elements
  - Key assumption: If you own an element, you own at least one dof associated with that element.
  - Requires an `ownedRowMap` and an `ownedPlusSharedRowMap` (any dof into which you will be inserting entries. Not quite the column map).

- All indexing can be done locally and both owned and ghost rows are pre-allocated.

WrappedDualView and UVM-free Code [TUG'21]

- UVM = CUDA Vinified Memory (can be addressed both on Host & GPU)
- Tpetra has Kokkos::DualViews of matrix and vector data
- Kokkos::DualView provides the *means* for tracking host/device views.
  - Sync/modify mechanics.
  - Correct use has to be enforced by the user.
- Tpetra::WrappedDualView manages the sync / modify flags between host and device
  - A little like SYCL buffers.
  - Users no longer sync / modify explicitly.
  - Users cannot hold both host and device pointers concurrently.
  - Affects MultiVector, CrsMatrix, CrsGraph, and Block variants.

Example: Vector fill with UVM is straightforward [TUG ‘21]

```
// Without UVM, this code will fail
multivector_t mv(…);
auto mvData =
     mv.getLocalViewHost();



for (j = 0; j < numData; j++)
   mvData(j,0) = rhs(j);


myDeviceFunction(mv);
```

Code worked with UVM

but failed without UVM

Non-UVM requires careful management of host and device views [TUG ‘21]

Without UVM, explicit modify/syncs were needed – messy and error-prone

```
multivector_t mv(…);
auto mvData =
     mv.getLocalViewHost();
mv.clear_sync_state();
mv.modify_host();
for (j = 0; j < numData; j++)
   mvData(j,0) = rhs(j);
mv.sync_device();
myDeviceFunction(mv);
```

Tpetra host/device management issues easier [TUG '21]

Without UVM, explicit modify/syncs were needed – messy and error-prone

```
multivector_t mv(…);
auto mvData =
     mv.getLocalViewHost();
mv.clear_sync_state();
mv.modify_host();
for (j = 0; j < numData; j++)
   mvData(j,0) = rhs(j);
mv.sync_device();
myDeviceFunction(mv);
```

Tpetra now manages the sync/modify state for users

```
multivector_t mv(…);
{ auto mvData =
       mv.getLocalViewHost(
          Tpetra::Access::OverwriteAll);

  for (j = 0; j < numData; j++)
    mvData(j,0) = rhs(j);
}
myDeviceFunction(mv);
```

Key changes for Tpetra::MultiVector users [TUG '21]

1. Capture host and device views in separate scopes
   - Don't hold raw pointers to multivector's data
   - Let views go out of scope as soon as you're done working with them

2. Separate scope for local operations and Trilinos operations on an object
   - Trilinos operations can choose where to access data

3. Indicate intended usage of views
   - ReadOnly, ReadWrite, OverwriteAll

4. Reduce switching between host and device accesses
   - Be aware of data synchronization

Key changes for Tpetra::CrsGraph/CrsMatrix users [TUG '21]

Same as MultiVector

1. Capture host and device views in separate scopes
   - Don't hold raw pointers to data
   - Let views go out of scope as soon as you're done working with them
2. Separate scope for local operations and Trilinos operations on an object
   - Trilinos operations can choose where to access data
3. Indicate intended usage of views
   - ReadOnly, ReadWrite, OverwriteAll
4. Reduce switching between host and device accesses
   - Be aware of data synchronization
5. getLocalMatrix*() and getLocalGraph*() build Kokkos' matrix and graph ON DEMAND now (rather than returning stored data structures); use wisely
6. Functions returning Teuchos::ArrayView of CrsMatrix/CrsGraph data are dangerous and <u>have been removed</u>.
7. Functions returning raw pointers to CrsMatrix/CrsGraph data are dangerous and <u>have been removed</u>.

Indicate intended usage of views [TUG '21]

Tpetra syncs as needed for type of access

- Tpetra::Access::ReadOnly
  - Tpetra syncs if needed
- Tpetra::Access::ReadWrite
  - Tpetra syncs if needed
  - Tpetra marks modified
- Tpetra::Access::OverwriteAll
  - Tpetra syncs only if view is a subview
  - Tpetra marks modified
  - Use only if writing ALL entries of view

```
// Use access tags to indicate intent
{
  auto read_h =
       mv.getLocalViewHost(
            Tpetra::Access::ReadOnly);
  auto readwrite_h =
       mv.getLocalViewHost(
            Tpetra::Access::ReadWrite);
  auto write_h =
       mv.getLocalViewHost(
            Tpetra::Access::OverwriteAll);

}
```

Access tags allow Tpetra to manage sync/modify status for users

MultiVector: Update code to remove old interfaces [TUG '21]

For now, most interfaces remain

- Get an ArrayRCP (1D or 2D):
  - `getData, getDataNonConst`
  - `get1dView, get1dViewNonConst`
  - `get2dView, get2dViewNonConst`
- Get a single column as Vector:
  - `getVector, getVectorNonConst`

Removed before Trilinos 13.4

- `Tpetra::withLocalAccess`
- `Tpetra::for_each`
- `Tpetra::transform`

Removed by Trilinos 13.4

- Accessors without Access tags
  - `getLocalViewHost()`
  - `getLocalViewDevice()`
  - `getLocalView<>()`
  - `getLocalBlock()`
- Sync/modify now handled by MultiVector
  - `mv.sync_host(), mv.sync_device(), mv.sync<>()`
  - `mv.modify_host(), mv.modify_device(), mv.modi()`
  - `mv.clear_sync_state()`

Asynchronous Import/Export [NEW]

- Motivation
  - Import/Export transfer data from one distributed object (`Tpetra::DistObject`) to another
  - Let's say you have many MultiVectors to do import on …
  - What if you want to overlap communication?
    - Launch sends for multiple DistObjects simultaneously
    - Launch sends and do some other computation while you wait
- Synchronous API
  - Do the complete import, don't return until it's finished: `DistObject::doImport`
- New asynchronous API
  - Pack data and kick off sends: `DistObject::beginImport`
  - (Optionally) check if data has arrived and is ready to unpack: `DistObject::transferArrived`
  - Unpack and combine data: `DistObject::endImport`
- Backend improvements mean each DistObject handles communication separately
  - BUT, can still share the same communication plan from the importer (expensive to create)

Lead developer: Timothy Smith

Prototype: On-node graph assembly [NEW]

- For on-node matrix assembly, we've had an interface for quite some time…
    - Grab the Kokkos::SparseCrsMatrix and wok on that directly.

- But how do you assembly a *Graph* on-node?
    - For many apps, host-assembly suffices --- the connectivity never changes.
    - But some apps have Graphs that change over time.

- Brian Kelley has been working on a FEM-centric prototype for graph assembly:

```
RCP<CrsGraph> Tpetra::assembleFEGraph(
    RCP<Map> rowMap,
    View<GO**, Node::memory_space> ownedElements,
    View<GO**, Node::memory_space> ghostElements);
```

- Still in development: Watch for more info at next EuroTUG.

Lead developer: Brian Kelley

Improved BlockCrsMatrix Support [NEW]

- Tpetra::BlockCrsMatrix was designed to support fixed-sized, small, blocks, e.g., 5x5.

- Uses a CrsGraph on *nodes* (groups of dofs) for the blocked problem --- less pointer chasing than CrsGraph for each individual dof.

- New features
  - Transpose operation.
  - Sparse matrix-matrix multiplication.

- Enables blocks-through-the-whole-hierarchy in certain MueLu code-paths.

- Still in development: Should be in Trilinos/develop by end of CY22.

Lead developer: Conrad Clevenger

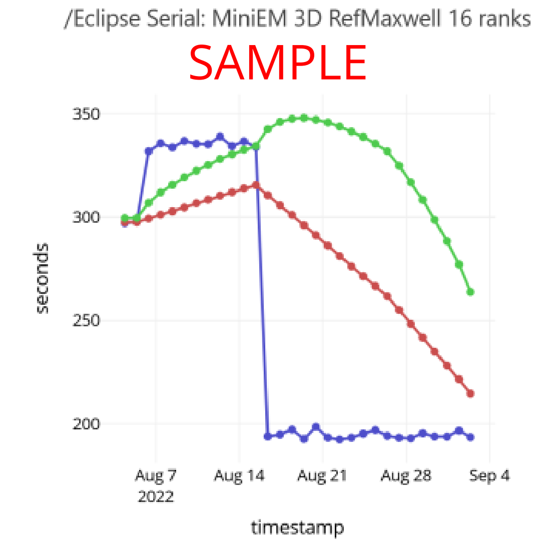
Performance Monitoring [NEW]

- Nightly performance testing on: Intel CPU, ARM CPU, Power9/A100 (NVIDIA), EPYC/MI250 (AMD).

- Performance tests:
  - Tpetra SpMV.
  - Tpetra FE assembly.
  - MiniEM (Maxwell CG+MueLu).
  - Abnormal Energy (GMRES + ILU(3) w/ overlap 2).

- Checked by humans every Tuesday.

- Goals: Work towards automatic changepoint detection, more app-relevant tests.


/Eclipse Serial: MiniEM 3D RefMaxwell 16 ranks

SAMPLE

Lead developers: Brian Kelley / Jonathan Hu

Thank you for your time!

- The last few years in Tpetra have been full of new developments!

- New architectures, UVM-free Cuda, overlapping halo exchanges and more!

- Is there something *you* want to see in Tpetra & Data services? No guarantees, but please feel free to ask (or submit a patch)!