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Tpetra and Data Services

Karen Devine, October 24, 2018

Tpetra team

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

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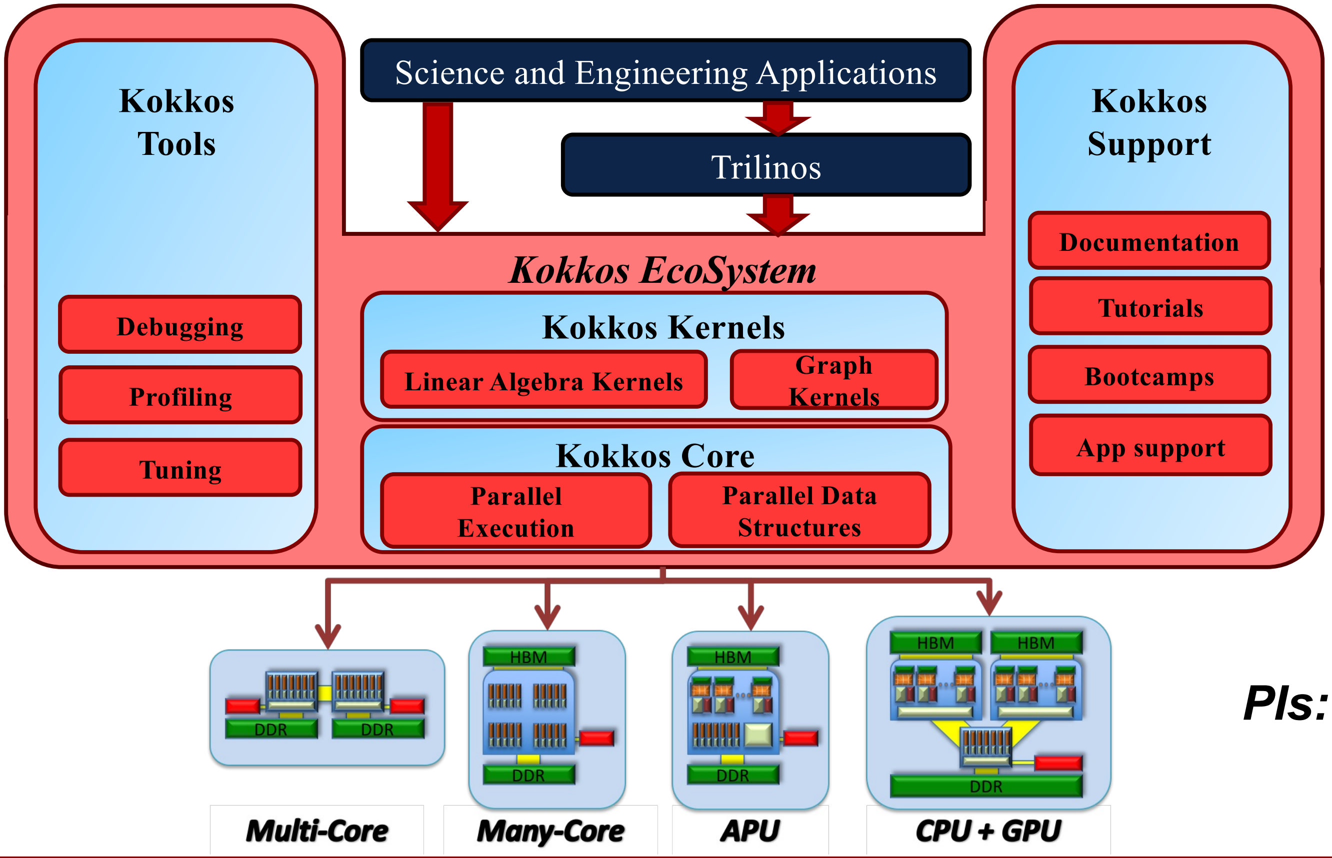
Tpetra FY18 efforts

- New Tpetra team
  - Define high-performance path through Tpetra
  - Reduce complexity of Tpetra code base
  - Increase robustness and usability of Tpetra
- Finite Element Assembly (see talk by Tim Fuller, Chris Siefert)
  - Interfaces, performance optimizations, FEMultiVector, deprecation of DynamicProfile
- Deprecations (see talk by Mark Hoemmen)
  - Template parameters (Global/local ordinal, Node); defaultPlatform
- Documentation
  - User's guide, examples for finite element assembly
- Benchmark performance tests
- https://github.com/trilinos/Trilinos/wiki/Tpetra-Information-Page

Tpetra FY19 Efforts

- New capability to allow run-time decisions about which execution and memory spaces to use during operations
  - Related to Node deprecation
- Application support: performance portability of matrix assembly for GPU and KNL
  - Performance evaluation/remediation in applications; FECrsMatrix
- Removal of deprecated features
  - Targeting Q3 removal; work with applications
- Improved communication performance of Tpetra
  - Import/Export/Distributor

Kokkos and KokkosKernels Ecosystem



Coordinated integration testing, releases, snapshots into Trilinos

PIs: Christian Trott
Siva Rajamanickam

STK Highlights

- STK: Mesh database developed in SIERRA, snapshotted into Trilinos
- Working on improved GPU support in NGP-Mesh (built on Kokkos) this year
  - Integrating into SIERRA-TF, SIERRA-SM, Nalu-Wind
- Trying to be responsive to Trilinos issues as well
  - Recent GPU warnings issues are taking longer than expected to resolve
- Using STK Balance (built on Zoltan2) in SIERRA-TF and SIERRA-SM for dynamic load balancing
  - If others are interested in using this capability, STK team would be happy to partner
- PI: Kendall Pierson

Have you noticed? (Probably not)

- Package deprecations to remove obsolete, unsupported, untested code
- MeshingGenie package – removed
  - Vorocrust (Mohamed Ebeida)
- Stk_classic subpackage – removed
  - STK
- ThreadPool package – PR #3725
  - Kokkos
- Suggestions for others?

Trilinos-wide topics for Developer Day discussion

- UVM / CUDA_LAUNCH_BLOCKING usage throughout Trilinos
  - Currently required in several packages, including Tpetra
  - If not needed in Tpetra, would other packages still need it?
  - Cost/benefit/requirements?
- Deprecation and release schedule
- Developer documentation (doxygen? wiki?)
- Separation of Tpetra and Epetra stacks
- Testing requirements on test-bed platforms (regarding MPI and compiler versions)
- Use of boost in Trilinos – how necessary is it? how remove warnings?

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Tpetra Finite Element Assembly

Tim Fuller and Chris Siefert, October 24, 2018

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Tpetra Finite Element Assembly

- Motivation:
  - Provide matrix/vector construction that supports variety of application scenarios
  - Provide high-performance path on new architectures
  - Reduce maintenance costs within Tpetra code base
- Deprecation of Dynamic Profile
- User interfaces:
  - Type 1: Simple global insertions
  - Type 2: Two-map insertions
  - Type 3: Applications with ghosted elements
- Other optimizations
- Other deprecations

Deprecation of Dynamic Profile

- CrsGraph/CrsMatrix default for construction: DynamicProfile
  - User did not have to provide correct information on number of nonzeros per row before inserting nonzeros

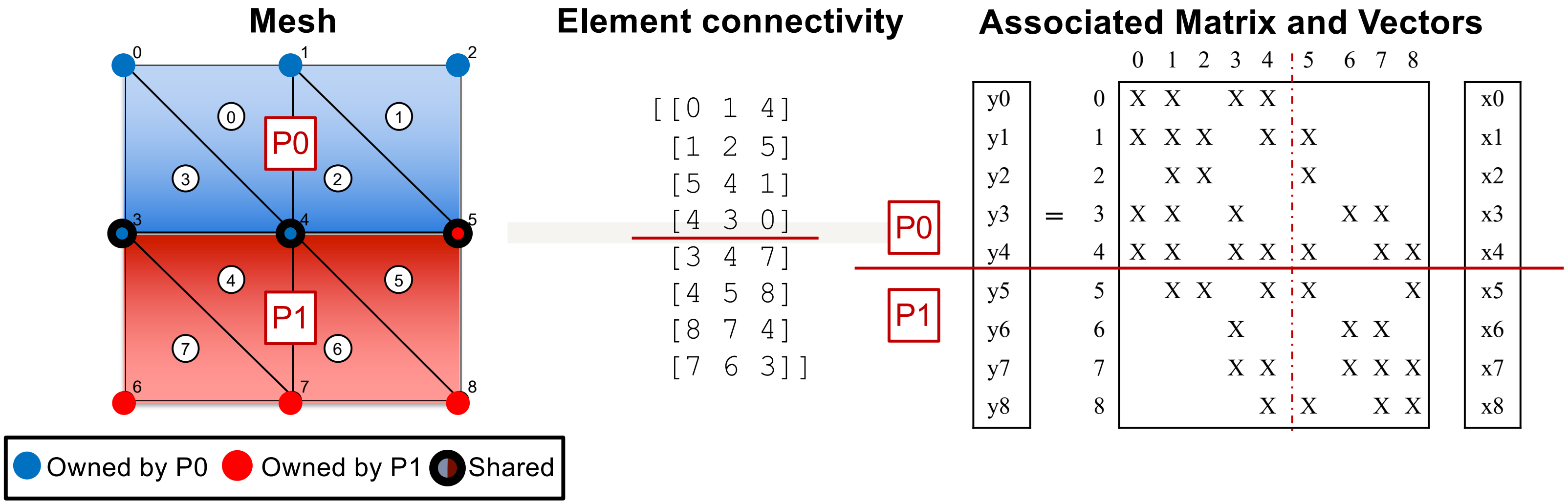
```
CrsMatrix (const Teuchos::RCP<const map_type>& rowMap,
           size_t maxNumEntriesPerRow,
           ProfileType pftype = DynamicProfile,
           const Teuchos::RCP<Teuchos::ParameterList>& params = Teuchos::null);
```

- DynamicProfile requires dynamic memory allocation in Tpetra
  - Higher execution time
  - Current interface is infeasible on GPUs
- DynamicProfile option is being removed now; Trilinos tests being updated.

Use StaticProfile

- StaticProfile is already an option in Tpetra: Applications can use it NOW
  - User provides either *accurate* max number of nonzeros per row OR actual number of nonzeros in each row
  - Tpetra allocates memory once before insertions
  - Tpetra will throw error if counts are insufficient; applications can then increase counts and try again
- Application conversion:
  - Many applications already have needed nonzeros counts; give them to Graph/Matrix constructor with StaticProfile flag
  - Otherwise, applications need to compute nonzero counts and provide them to Graph/Matrix constructor with StaticProfile flag
- Schedule: all Tpetra code changes in place FY19 Q1; DynamicProfile removed Q3.
- Examples in Tpetra repository; will post to wiki

Assumptions for this discussion



- Element-based partition of mesh (i.e., elements owned uniquely by processes)
- DOFs associated with mesh nodes
- Mesh nodes have unique owner but may be copied (“shared”) on many processes
- 1D partition of matrix by rows

Type 1 assembly: Global insertions

- Processor *p* can insert nonzeros into any processor's rows
  - insertGlobalValues(…)
- Tpetra uses map to build directory and send nonzeros to owning processors
  - globalAssemble(…) in fillComplete(…)

- Advantages:
  - Simplest use-case for applications
- Disadvantages:
  - Most expensive path for Tpetra – much off-processor discovery needed

Type 1 assembly: Global insertions

- **Procedure:**

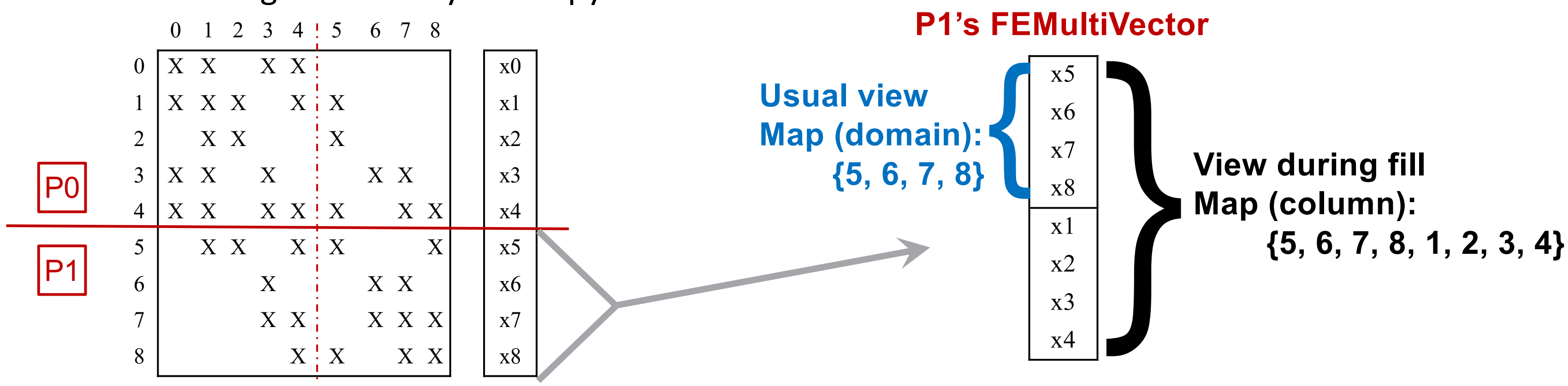
```
1. Construct map
   owned_map = {owned DOFs}
   domain_map = owned_map
   range_map = owned_map

2. Construct graph
   owned_graph = Graph(owned_map)
   for each element e
       for each DOF n of e
           owned_graph.insertGlobalIndices(n, {all DOFs of e})
   owned_graph.fillComplete(domain_map, range_map)

3. Construct matrices
   owned_mat = Matrix(owned_graph)
   for each element e
       for each DOF n of e
           owned_mat.sumIntoGlobalValues(n, {all DOFs of e}, vals)
   owned_mat.fillComplete(domain_map, range_map)
```

MultiVector Assembly:: FEMultiVector

- MultiVector's sumIntoGlobalValue works only for global IDs in MultiVector's map
- But right-hand-side assembly contributes to shared DOF's MultiVector values
- User could manage with multiple maps & multivectors and Export
- Easier alternative: Tpetra::FEMultiVector
- Implementation may or may not have two copies of vector data
  - If maps align, same storage used for both owned and owned+shared
  - Potential savings in memory and copy costs



FEMultiVector Assembly

- **Procedure**:

  1. Build and fillComplete owned_graph CrsGraph as before

  2. Construct FEMultiVector

  ```
  Tpetra::FEMultiVector femv(domain_map, owned_graph.getImporter())
  ```

  3. Fill FEMultiVector

  ```
  femv.beginFill  // enables access to shared DOFs
  for each element e
      for each DOF n of e
          femv.sumIntoGlobalValue(n, val)
  femv.endFill    // exports with ADD; disables access to shared DOFs
  ```

- Notes:
  - Can use with Type 2 assembly as well
  - Coming soon: FECrsGraph, FECrsMatrix

Type 2 assembly: Two maps/graphs/matrices

- I.e., Local Element loop
- FEMultiVector exploited two maps; can do same with matrices

- Build two graphs & two matrices
  - Owned graph and matrix for owned DOFs
  - Shared graph & matrix for shared DOFs
- Export shared graph & matrix to owned graph & matrix

- Advantages:
  - Less discovery needed in Tpetra, so more efficient
- Disadvantages:
  - More complex for user (goal is to alleviate complexity with FECrsGraph, FECrsMatrix)

Type 2 Assembly: Two maps/graphs/matrices

1. Construct two maps and exporter between them

```
owned_map = {Owned DOFs};
shared_map = {Shared DOFs}
exporter = Export(shared_map, owned_map)
```

2. Construct two graphs

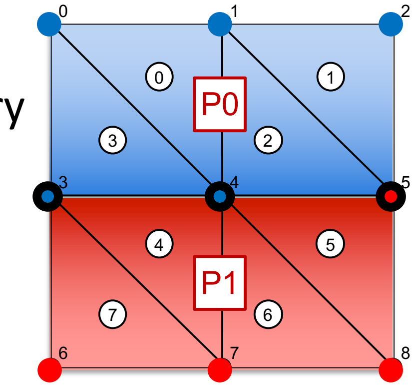
```
owned_graph = Graph(owned_map);
shared_graph = Graph(shared_map)
for each element e
    for each DOF n of e
        if (n is owned) owned_graph.insertGlobalIndices(n, {all DOFs of e})
        else shared_graph.insertGlobalIndices(n, {all DOFs of e})
shared_graph.fillComplete(domain_map, range_map)
owned_graph.doExport(shared_graph, exporter, INSERT)
owned_graph.fillComplete(domain_map, range_map)
```

3. Construct two matrices

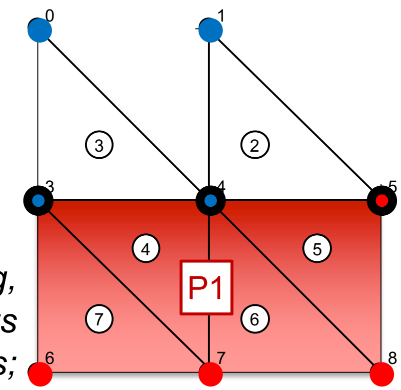
```
owned_mat = Matrix(owned_graph);
shared_mat = Matrix(shared_graph)
<fill owned_mat and shared_mat with values as above>
owned_mat.doExport(shared_mat, exporter, ADD)
owned_mat.fillComplete(domain_map, range_map)
```

Type 3 Assembly: Total element loop

- For applications with a layer of element copies around part boundary
  - Ghost elements, aura, total-element-loop
- All computations for owned DOFs can be done locally
  - No contributions to shared DOFs
- Application needs only owned map
- Application can use local indexing



- Advantage:
  - All insertions are local; no export needed
- Disadvantage:
  - Not all applications have ghost elements



With one layer of ghosting, P1 stores four owned elements and two ghost elements; fills values for DOFs {5, 6, 7, 8}

Type 3 Assembly: Total element loop

- **Procedure**:

```
1. Construct map
   owned_map = {owned DOFs}

2. Construct graph
   owned_graph = Graph(owned_map)
   for each owned and ghost element e
       for each owned DOF n of e
           owned_graph.insertLocalIndices(n, {all DOFs of e})
   owned_graph.fillComplete(domain_map, range_map)

3. Construct matrices
   owned_mat = Matrix(owned_graph)
   for each owned and ghost element e
       for each owned DOF n of e
           owned_mat.sumIntoLocalValues(n, {all DOFs of e}, vals)
   owned_mat.fillComplete(domain_map, range_map)
```

Optimizations: Local indexing and Kokkos::StaticCrsGraph

- Especially easy for Type 3 assembly

- Using local indices to fill graph/matrix/vector
  - avoids conversion from global to local through lookup table
  - E.g., `insertLocalIndices()`, `insertLocalValues()`

- Can provide three Kokkos::Views for CRS arrays (rowOffsets, columnIndices, values) and row/column maps to CrsMatrix constructor
  - See Tpetra tutorial Trilinos/packages/tpetra/core/example/Lesson07-Kokkos-Fill

- Similarly, can provide Kokkos::StaticCrsGraph

Optimizations: exploit mesh info

- Many applications already know owning processor of shared mesh nodes
- Allow Tpetra to use this information when available

```
1. Construct map
   row_map = {owned DOFs}
   Import importer (row_map, {owned+shared DOFs},
                             {processors owning the DOFs})
   column_map = importer.getTargetMap()

2. Construct graph
   owned_graph = Graph(row_map, column_map)
   …
```

- Nalu simulation of a Vestas wind turbine on 12,288 Haswell cores on NERSC's Cori
  - reduced matrix initialization costs from 109 seconds to 84.5 seconds (22.5% reduction)

Optimizations: column map layout

- If specifying column map, Aztec-style layout of column map may be best
  - Owned entries first
  - Followed by shared entries, grouped by owning processor
- Allows fewer copies during MPI communication
  - Communicate directly to/from memory
  - No need to gather into buffers
- May reduce communication time in MatVec
- `makeOptimizedColMapAndImport` creates new column map from row map and old column map

Optimizations: Contiguous DOF numbering

- Tpetra allows arbitrary numbering of owned rows
  - Directory used to lookup off-processor IDs
- Default Trilinos ordering is most efficient
  - Rows 0 to N0 on rank zero
  - Rows N0+1 to N1 on rank one
  - Rows N1+1 to N2 on rank two
  - Etc.
- Enables fast, simple lookup of IDs during Import/Export construction
  - Directory is trivial

Resources

- Tpetra tutorials
  - Trilinos/packages/tpetra/core/examples/tutorial
- Finite-element assembly examples (Types 1, 2, 3)
  - Trilinos/packages/tpetra/core/examples/Finite-Element-Assembly
- Tpetra wiki
  - https://github.com/trilinos/Trilinos/wiki/Tpetra-Information-Page
- FY18 Tpetra team

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