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USING KOKKOS IN TPETRA FINITE ELEMENT ASSEMBLY

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2:30 PM Wednesday November 1st, 2023,

Trilinos User Group Meeting

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SAND2023-11162PE

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TPETRA'S FINITE ELEMENT ASSEMBLY EXAMPLE

- Background on Kokkos: Kokkos Tutorial on Monday
  - or: Kokkos Lectures & Slides (https://kokkos.github.io/kokkos-core-wiki/videolectures.html)
  - Single code for all CPUs, GPUs, and whatever else Kokkos supports

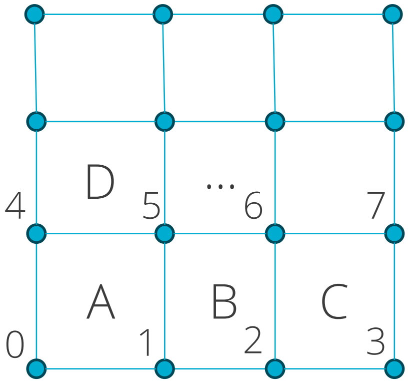
- Trilinos/packages/tpetra/core/example/Finite-Element-Assembly

- Application provides (our example mocks these)
  - Map of elements to nodes in global indices
  - Methods for computing element matrices

- Type-1 assembly
  - Local elements contribute to off-rank FE matrix rows for off-rank nodes

- No worksetting

FE ASSEMBLY IN BRIEF



app. discretization

varies per element, fixed in this example

$$\begin{bmatrix} 2 & -1 & & -1 \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ -1 & & -1 & 2 \end{bmatrix}$$

app. element matrix

A → {0, 1, 5, 4}

B → {1, 2, 6, 5}

C → {2, 3, 7, 6}

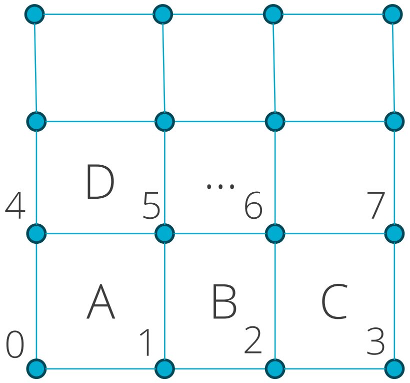
…

app. element-to-node map

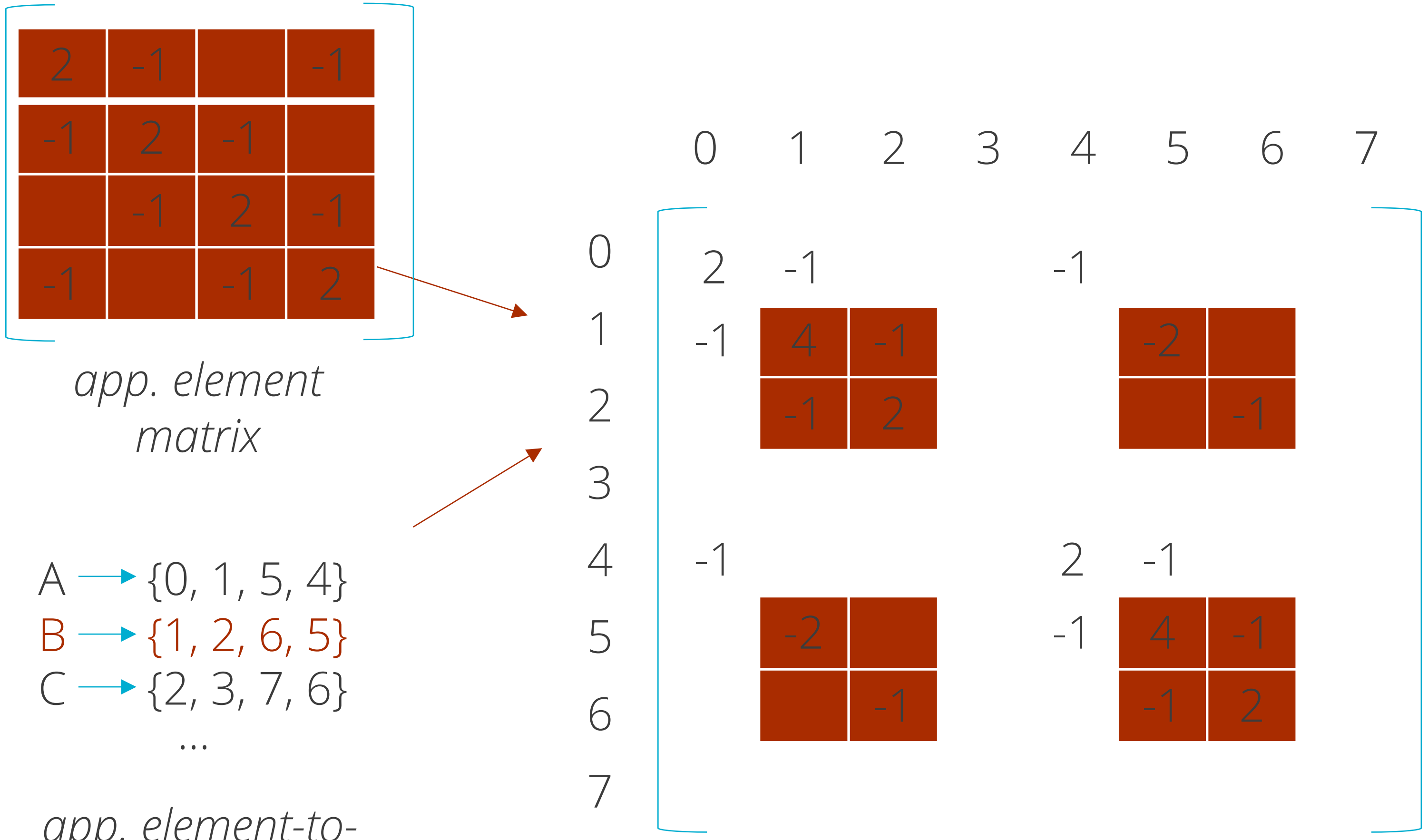
$$\begin{array}{c|ccccccccc} & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & \cdots \\ \hline 0 & 2 & -1 & & & -1 & & & & \\ 1 & -1 & 2 & & & & -1 & & & \\ 2 & & & & & & & & & \\ 3 & & & & & & & & & \\ 4 & -1 & & & & 2 & -1 & & & \\ 5 & & -1 & & & -1 & 2 & & & \\ 6 & & & & & & & & & \\ 7 & & & & & & & & & \\ \vdots & & & & & & & & & \end{array}$$

Global FE matrix

ELEMENT B’S CONTRIBUTION



app. discretization



$$\begin{bmatrix} 2 & -1 & & -1 \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ -1 & & -1 & 2 \end{bmatrix}$$

app. element matrix

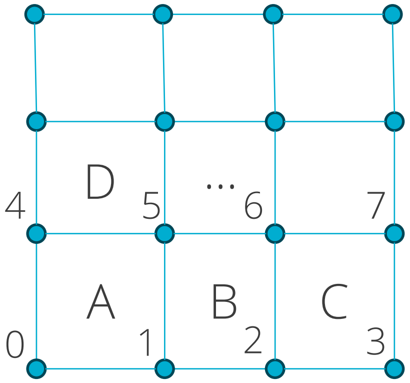
A → {0, 1, 5, 4}
B → {1, 2, 6, 5}
C → {2, 3, 7, 6}
…

app. element-to-node map

$$\begin{array}{c|cccccccc} & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ \hline 0 & 2 & -1 & & & -1 & & & \\ 1 & -1 & 4 & -1 & & & -2 & & \\ 2 & & -1 & 2 & & & & -1 & \\ 3 & & & & & & & & \\ 4 & -1 & & & & 2 & -1 & & \\ 5 & & -2 & & & -1 & 4 & -1 & \\ 6 & & & -1 & & & -1 & 2 & \\ 7 & & & & & & & & \end{array}$$

Global FE matrix

ELEMENT C'S CONTRIBUTION



app. discretization

$$\begin{bmatrix} 2 & -1 & & -1 \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ -1 & & -1 & 2 \end{bmatrix}$$

app. element matrix

A → {0, 1, 5, 4}
B → {1, 2, 6, 5}
C → {2, 3, 7, 6}
…

app. element-to-node map

$$\begin{array}{c|cccccccc} & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ \hline 0 & 2 & -1 & & & -1 & & & \\ 1 & -1 & 4 & -1 & & & -2 & & \\ 2 & & -1 & 4 & -1 & & & -2 & \\ 3 & & & -1 & 2 & & & & -1 \\ 4 & -1 & & & & 2 & -1 & & \\ 5 & & -2 & & & -1 & 4 & -1 & \\ 6 & & & -2 & & & -1 & 4 & -1 \\ 7 & & & & -1 & & & -1 & 2 \end{array}$$

Global FE matrix

FIVE CHANGES TO WATCH OUT FOR

- Bare for-loops

→

- Kokkos::parallel_for
  - Allow device execution
  - Supports CPU execution too

- Host allocations

→

- Kokkos::View

- Functions

→

- KOKKOS_FUNCTION annotation

- Tpetra::[…]::getHostView()
  - Convenient use of global indices

→

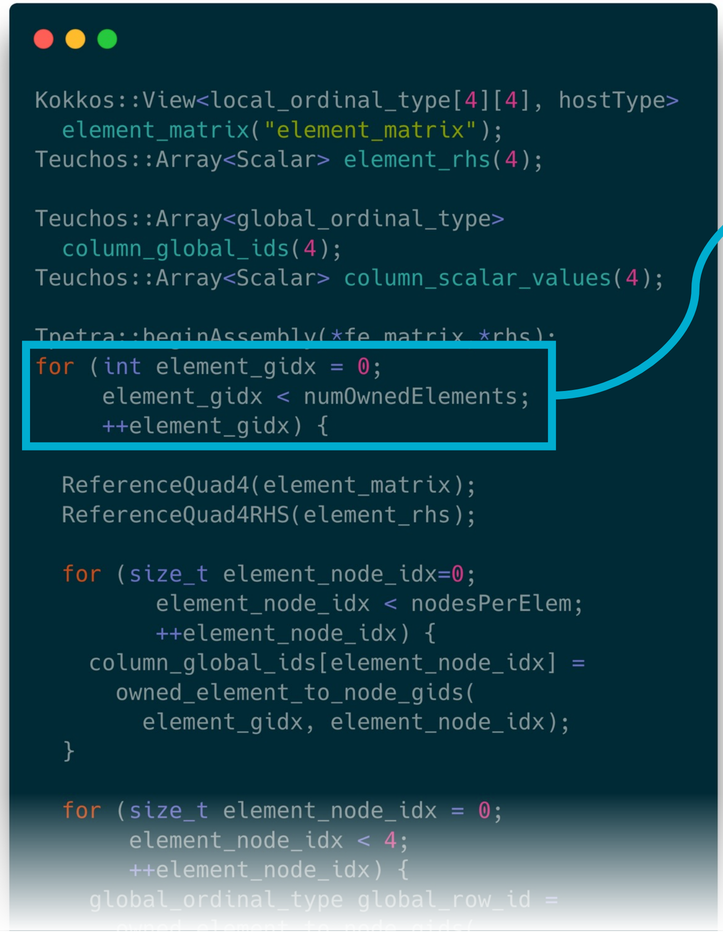
- Tpetra::[]::getDeviceView()
  - Have to use local indices “on device”

- Normal addition

→

- Atomic addition

HOST LOOP -> KOKKOS::PARALLEL_FOR



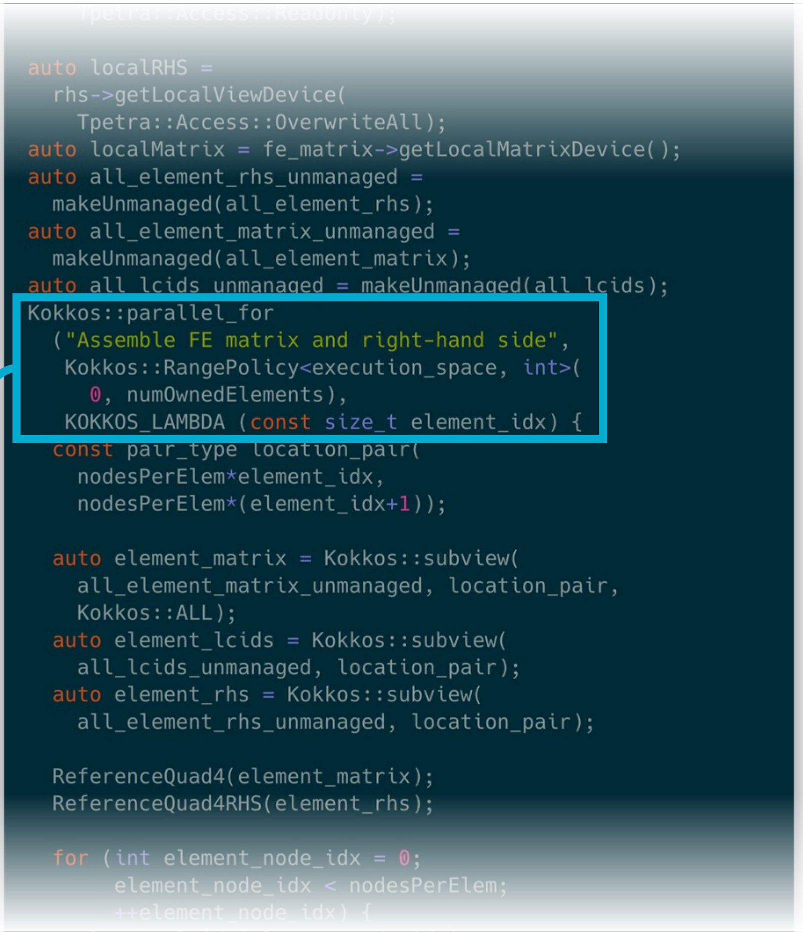
```
Kokkos::View<local_ordinal_type[4][4], hostType>
  element_matrix("element_matrix");
Teuchos::Array<Scalar> element_rhs(4);

Teuchos::Array<global_ordinal_type>
  column_global_ids(4);
Teuchos::Array<Scalar> column_scalar_values(4);

Tpetra::beginAssembly(*fe_matrix,*rhs);
for (int element_gidx = 0;
     element_gidx < numOwnedElements;
     ++element_gidx) {

  ReferenceQuad4(element_matrix);
  ReferenceQuad4RHS(element_rhs);

  for (size_t element_node_idx=0;
         element_node_idx < nodesPerElem;
         ++element_node_idx) {
    column_global_ids[element_node_idx] =
      owned_element_to_node_gids(
        element_gidx, element_node_idx);
  }

  for (size_t element_node_idx = 0;
        element_node_idx < 4;
        ++element_node_idx) {
    global_ordinal_type global_row_id =
      owned_element_to_node_gids(
```

Tpetra

Tpetra: a single active thread, loops over each local element

Kokkos: operate on local elements in parallel

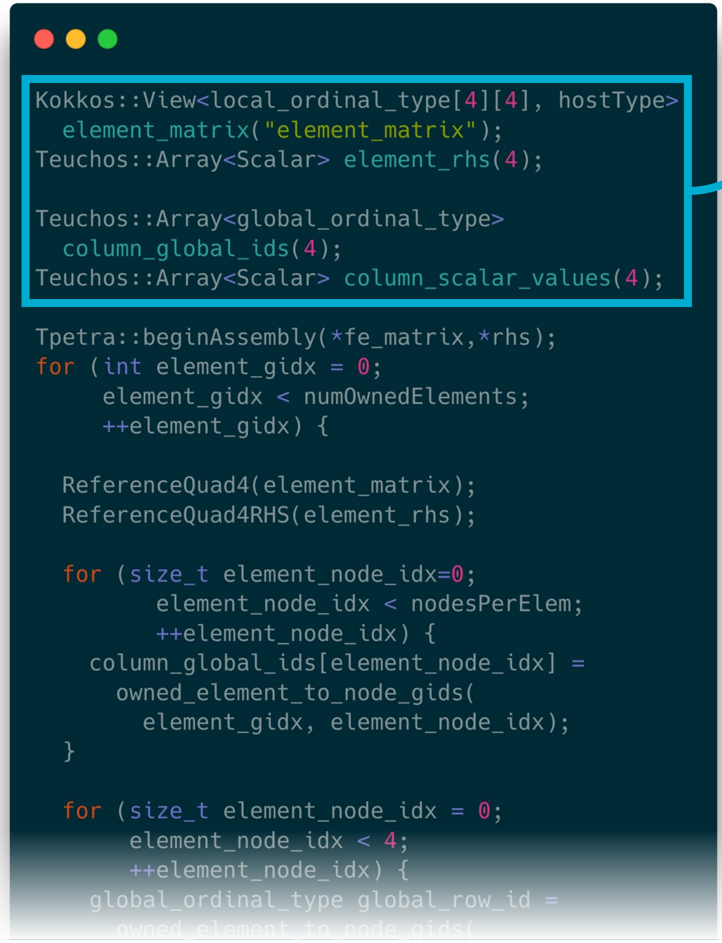
Also works on host, single-threaded (`Kokkos::Serial`) or multi-threaded (`::OpenMP`, `::Threads`)



```
    Tpetra::Access::ReadOnly);

auto localRHS =
  rhs->getLocalViewDevice(
    Tpetra::Access::OverwriteAll);
auto localMatrix = fe_matrix->getLocalMatrixDevice();
auto all_element_rhs_unmanaged =
  makeUnmanaged(all_element_rhs);
auto all_element_matrix_unmanaged =
  makeUnmanaged(all_element_matrix);
auto all_lcids_unmanaged = makeUnmanaged(all_lcids);
Kokkos::parallel_for
  ("Assemble FE matrix and right-hand side",
   Kokkos::RangePolicy<execution_space, int>(
     0, numOwnedElements),
   KOKKOS_LAMBDA (const size_t element_idx) {
  const pair_type location_pair(
    nodesPerElem*element_idx,
    nodesPerElem*(element_idx+1));

  auto element_matrix = Kokkos::subview(
    all_element_matrix_unmanaged, location_pair,
    Kokkos::ALL);
  auto element_lcids = Kokkos::subview(
    all_lcids_unmanaged, location_pair);
  auto element_rhs = Kokkos::subview(
    all_element_rhs_unmanaged, location_pair);

  ReferenceQuad4(element_matrix);
  ReferenceQuad4RHS(element_rhs);

  for (int element_node_idx = 0;
       element_node_idx < nodesPerElem;
       ++element_node_idx) {
```

Tpetra + Kokkos

HOST ALLOCATIONS -> KOKKOS VIEW



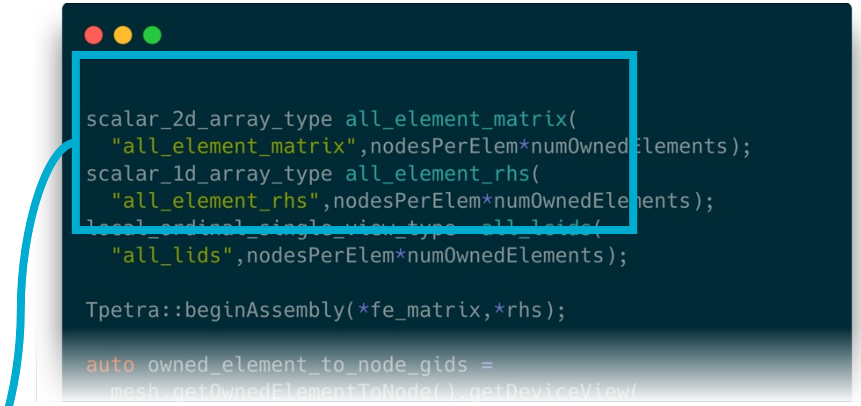
```
Kokkos::View<local_ordinal_type[4][4], hostType>
  element_matrix("element_matrix");
Teuchos::Array<Scalar> element_rhs(4);

Teuchos::Array<global_ordinal_type>
  column_global_ids(4);
Teuchos::Array<Scalar> column_scalar_values(4);

Tpetra::beginAssembly(*fe_matrix,*rhs);
for (int element_gidx = 0;
     element_gidx < numOwnedElements;
     ++element_gidx) {

  ReferenceQuad4(element_matrix);
  ReferenceQuad4RHS(element_rhs);

  for (size_t element_node_idx=0;
        element_node_idx < nodesPerElem;
        ++element_node_idx) {
    column_global_ids[element_node_idx] =
      owned_element_to_node_gids(
        element_gidx, element_node_idx);
  }

  for (size_t element_node_idx = 0;
       element_node_idx < 4;
       ++element_node_idx) {
    global_ordinal_type global_row_id =
      owned_element_to_node_gids(
```

Tpetra

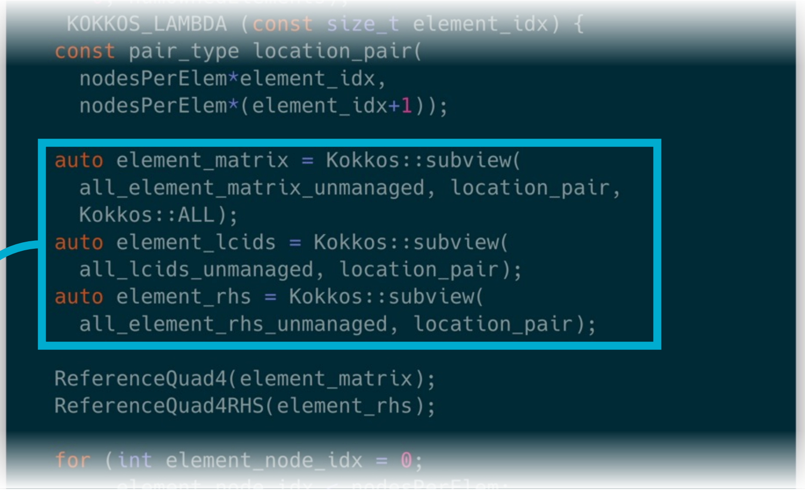
Tpetra: allocate some scratch space on the stack. Reused for each iteration of element loop

Kokkos: allocate enough device memory for all active threads

Kokkos: each thread gets its own piece of the preallocated scratch space



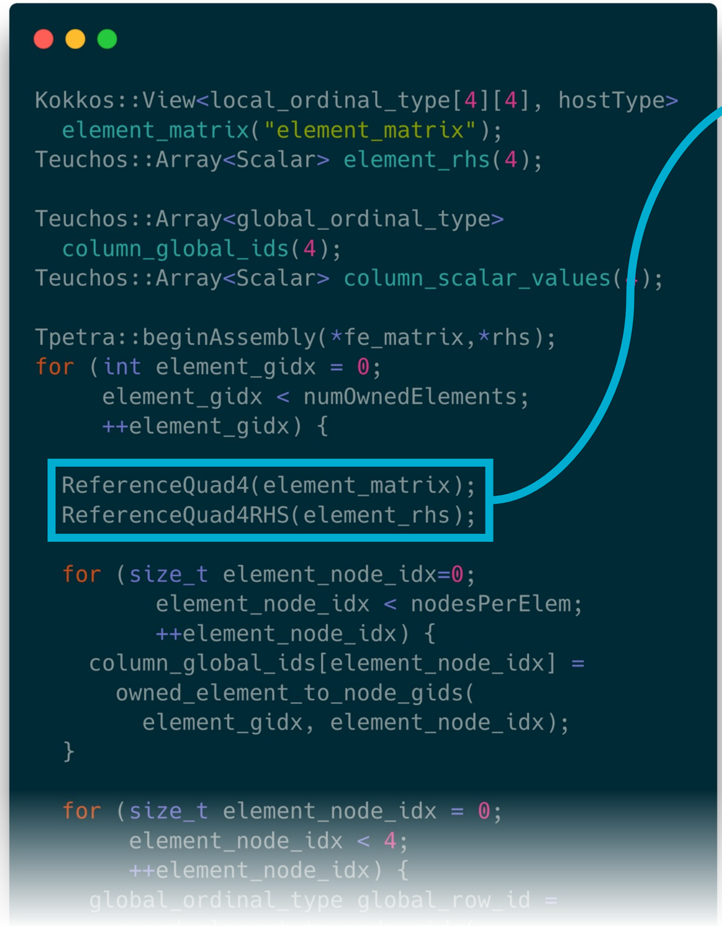
```
scalar_2d_array_type all_element_matrix(
  "all_element_matrix",nodesPerElem*numOwnedElements);
scalar_1d_array_type all_element_rhs(
  "all_element_rhs",nodesPerElem*numOwnedElements);
local_ordinal_single_view_type  all_lcids(
  "all_lids",nodesPerElem*numOwnedElements);

Tpetra::beginAssembly(*fe_matrix,*rhs);

auto owned_element_to_node_gids =
  mesh.getOwnedElementToNode().getDeviceView(
```



```
 KOKKOS_LAMBDA (const size_t element_idx) {
const pair_type location_pair(
  nodesPerElem*element_idx,
  nodesPerElem*(element_idx+1));

auto element_matrix = Kokkos::subview(
  all_element_matrix_unmanaged, location_pair,
  Kokkos::ALL);
auto element_lcids = Kokkos::subview(
  all_lcids_unmanaged, location_pair);
auto element_rhs = Kokkos::subview(
  all_element_rhs_unmanaged, location_pair);

ReferenceQuad4(element_matrix);
ReferenceQuad4RHS(element_rhs);

for (int element_node_idx = 0;
```

Tpetra + Kokkos

HOST FUNCTIONS -> KOKKOS_FUNCTION



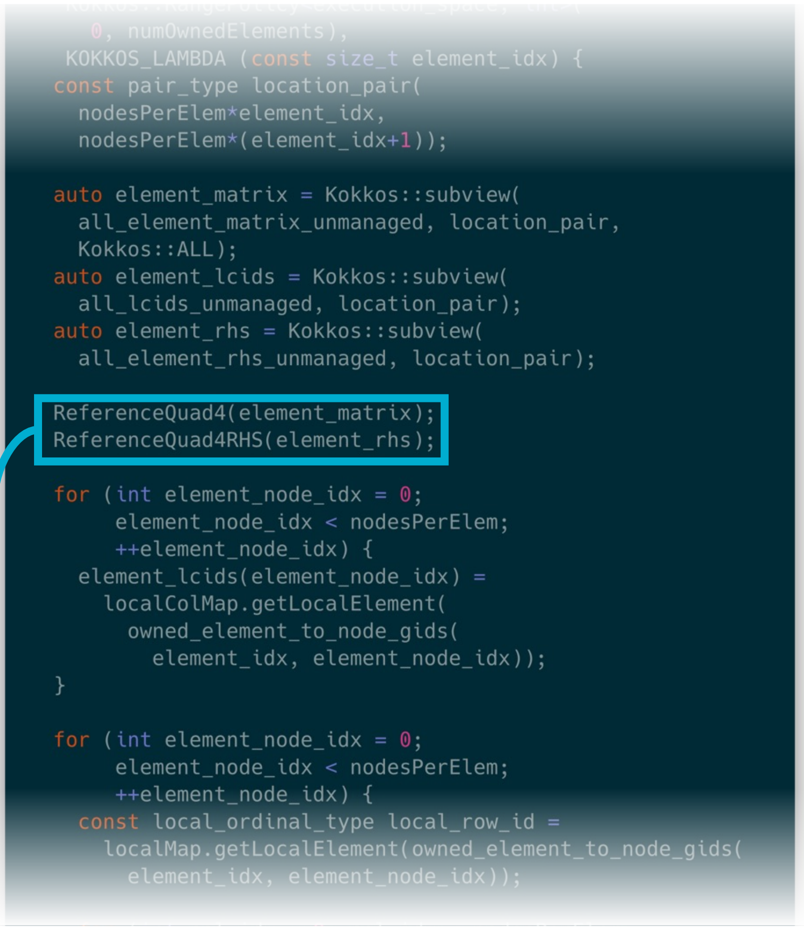
```
Kokkos::View<local_ordinal_type[4][4], hostType>
  element_matrix("element_matrix");
Teuchos::Array<Scalar> element_rhs(4);

Teuchos::Array<global_ordinal_type>
  column_global_ids(4);
Teuchos::Array<Scalar> column_scalar_values(4);

Tpetra::beginAssembly(*fe_matrix,*rhs);
for (int element_gidx = 0;
     element_gidx < numOwnedElements;
     ++element_gidx) {

  ReferenceQuad4(element_matrix);
  ReferenceQuad4RHS(element_rhs);

  for (size_t element_node_idx=0;
         element_node_idx < nodesPerElem;
         ++element_node_idx) {
    column_global_ids[element_node_idx] =
      owned_element_to_node_gids(
        element_gidx, element_node_idx);
  }

  for (size_t element_node_idx = 0;
        element_node_idx < 4;
        ++element_node_idx) {
    global_ordinal_type global_row_id =
```

Tpetra: fill scratch space with matrix for this element

Kokkos: each thread fills scratch space in parallel

These functions must be allowed to execute on the device

```
KOKKOS_FUNCTION
void Reference4Quad(...) {
  ...
};
```

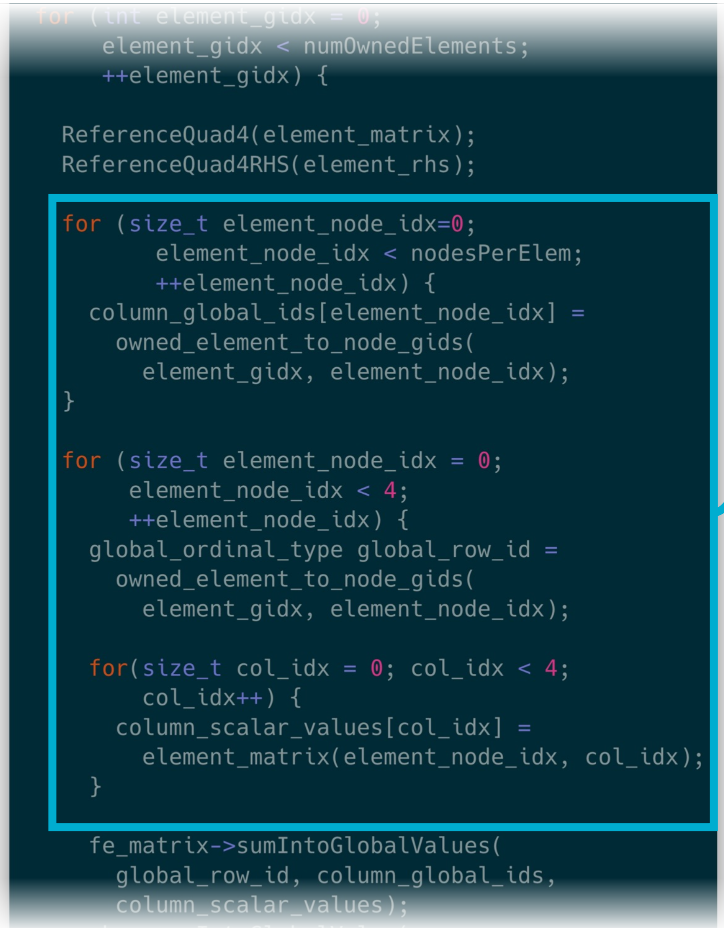


```
  Kokkos::RangePolicy<execution_space, int>(
    0, numOwnedElements),
  KOKKOS_LAMBDA (const size_t element_idx) {
 const pair_type location_pair(
   nodesPerElem*element_idx,
   nodesPerElem*(element_idx+1));

 auto element_matrix = Kokkos::subview(
   all_element_matrix_unmanaged, location_pair,
   Kokkos::ALL);
 auto element_lcids = Kokkos::subview(
   all_lcids_unmanaged, location_pair);
 auto element_rhs = Kokkos::subview(
   all_element_rhs_unmanaged, location_pair);

 ReferenceQuad4(element_matrix);
 ReferenceQuad4RHS(element_rhs);

 for (int element_node_idx = 0;
      element_node_idx < nodesPerElem;
      ++element_node_idx) {
   element_lcids(element_node_idx) =
     localColMap.getLocalElement(
       owned_element_to_node_gids(
         element_idx, element_node_idx));
 }

 for (int element_node_idx = 0;
      element_node_idx < nodesPerElem;
      ++element_node_idx) {
   const local_ordinal_type local_row_id =
     localMap.getLocalElement(owned_element_to_node_gids(
       element_idx, element_node_idx));
```

Tpetra

Tpetra + Kokkos

GLOBAL INDICES -> LOCAL INDICES



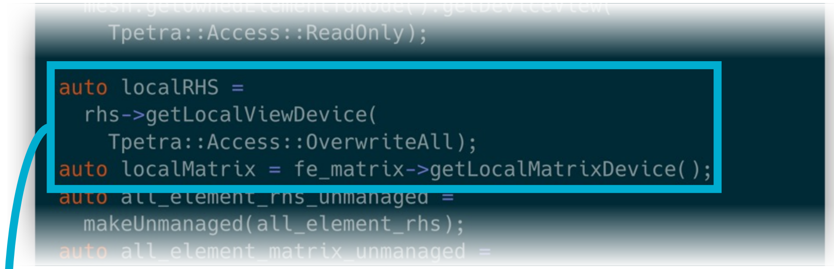
```
for (int element_gidx = 0;
     element_gidx < numOwnedElements;
     ++element_gidx) {

  ReferenceQuad4(element_matrix);
  ReferenceQuad4RHS(element_rhs);

  for (size_t element_node_idx=0;
         element_node_idx < nodesPerElem;
         ++element_node_idx) {
    column_global_ids[element_node_idx] =
      owned_element_to_node_gids(
        element_gidx, element_node_idx);
  }

  for (size_t element_node_idx = 0;
       element_node_idx < 4;
       ++element_node_idx) {
    global_ordinal_type global_row_id =
      owned_element_to_node_gids(
        element_gidx, element_node_idx);

    for(size_t col_idx = 0; col_idx < 4;
        col_idx++) {
      column_scalar_values[col_idx] =
        element_matrix(element_node_idx, col_idx);
    }

    fe_matrix->sumIntoGlobalValues(
      global_row_id, column_global_ids,
      column_scalar_values);
```

Tpetra

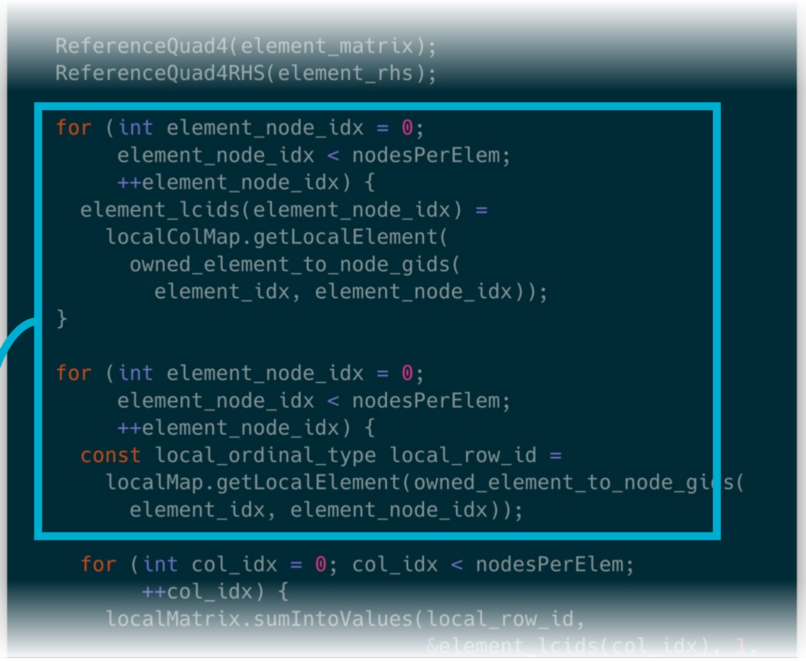
Tpetra: interact with FE matrix and RHS through global indices. Simpler interface, made possible by dynamic memory allocation

Kokkos: need device views of the local FE matrix and RHS to operate on.

Kokkos: local FE matrix and RHS only understands local indices. Use `Tpetra::Map`s to translate between local and global



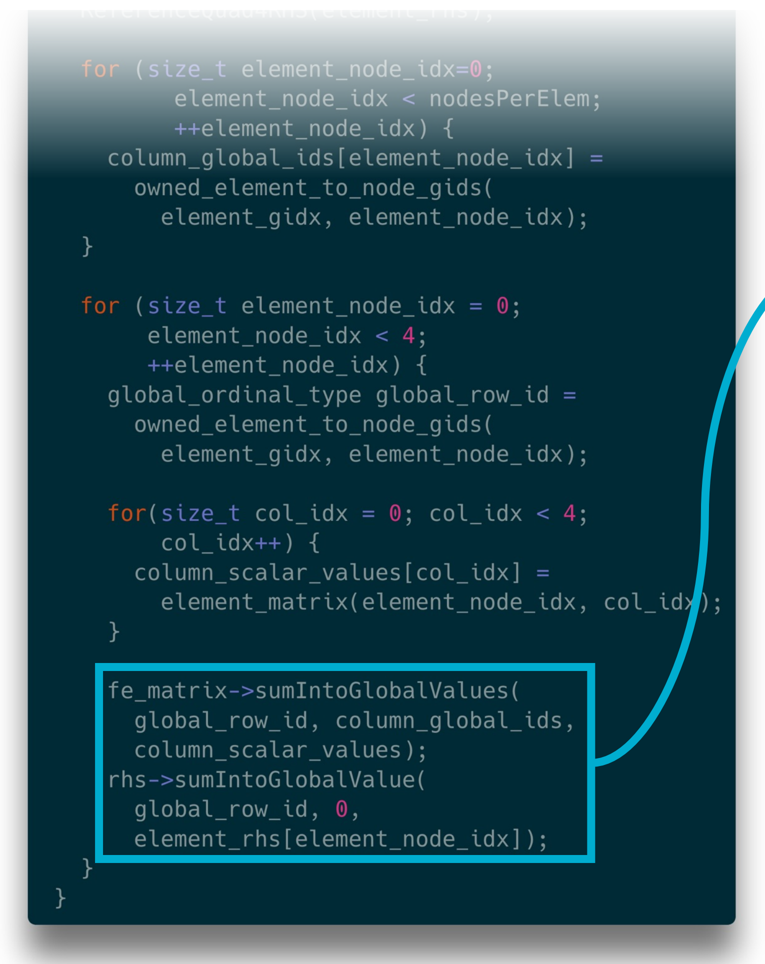
```
  mesh.getOwnedElementToNode().getDeviceView(
    Tpetra::Access::ReadOnly);

auto localRHS =
  rhs->getLocalViewDevice(
    Tpetra::Access::OverwriteAll);
auto localMatrix = fe_matrix->getLocalMatrixDevice();
auto all_element_rhs_unmanaged =
  makeUnmanaged(all_element_rhs);
auto all_element_matrix_unmanaged =
```



```
  ReferenceQuad4(element_matrix);
  ReferenceQuad4RHS(element_rhs);

  for (int element_node_idx = 0;
         element_node_idx < nodesPerElem;
         ++element_node_idx) {
    element_lcids(element_node_idx) =
      localColMap.getLocalElement(
        owned_element_to_node_gids(
          element_idx, element_node_idx));
  }

  for (int element_node_idx = 0;
         element_node_idx < nodesPerElem;
         ++element_node_idx) {
    const local_ordinal_type local_row_id =
      localMap.getLocalElement(owned_element_to_node_gids(
        element_idx, element_node_idx));

    for (int col_idx = 0; col_idx < nodesPerElem;
         ++col_idx) {
      localMatrix.sumIntoValues(local_row_id,
                                &element_lcids(col_idx), 1,
```

Tpetra + Kokkos

ATOMIC ADDITION

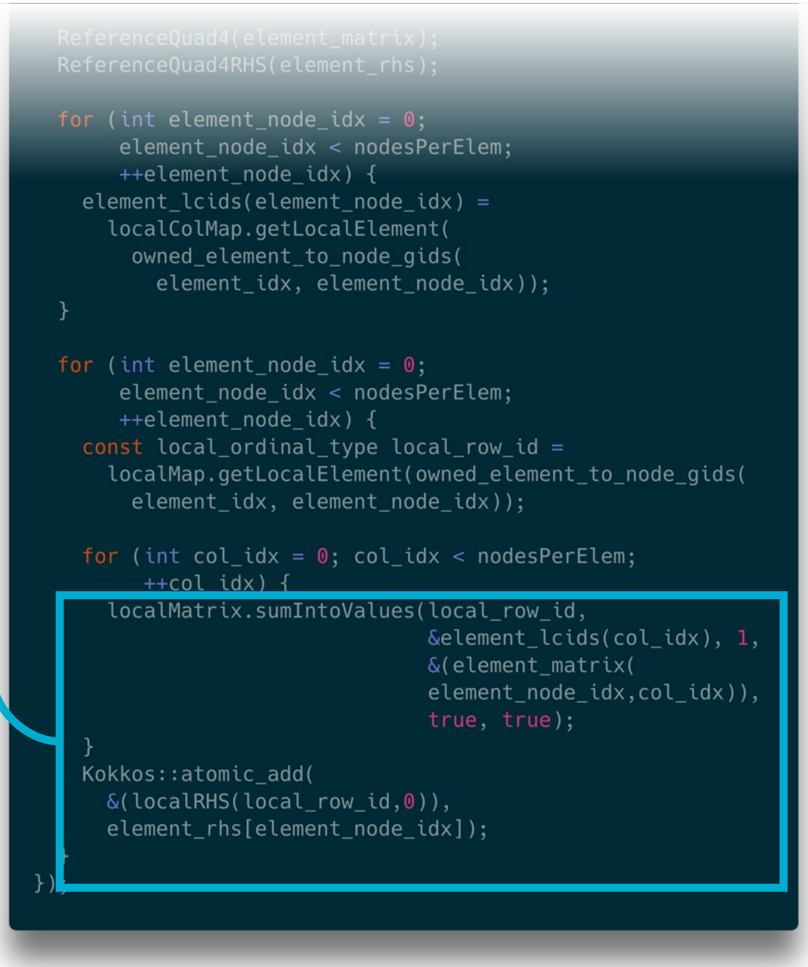


```
  ReferenceQuad4RHS(element_rhs);

  for (size_t element_node_idx=0;
         element_node_idx < nodesPerElem;
         ++element_node_idx) {
    column_global_ids[element_node_idx] =
      owned_element_to_node_gids(
        element_gidx, element_node_idx);
  }

  for (size_t element_node_idx = 0;
       element_node_idx < 4;
       ++element_node_idx) {
    global_ordinal_type global_row_id =
      owned_element_to_node_gids(
        element_gidx, element_node_idx);

    for(size_t col_idx = 0; col_idx < 4;
        col_idx++) {
      column_scalar_values[col_idx] =
        element_matrix(element_node_idx, col_idx);
    }

    fe_matrix->sumIntoGlobalValues(
      global_row_id, column_global_ids,
      column_scalar_values);
    rhs->sumIntoGlobalValue(
      global_row_id, 0,
      element_rhs[element_node_idx]);
  }
}
```

Tpetra

Tpetra: contribute element values to FE matrix and RHS

Kokkos: atomic adds, since each thread (element) may contribute to the same node at the same time



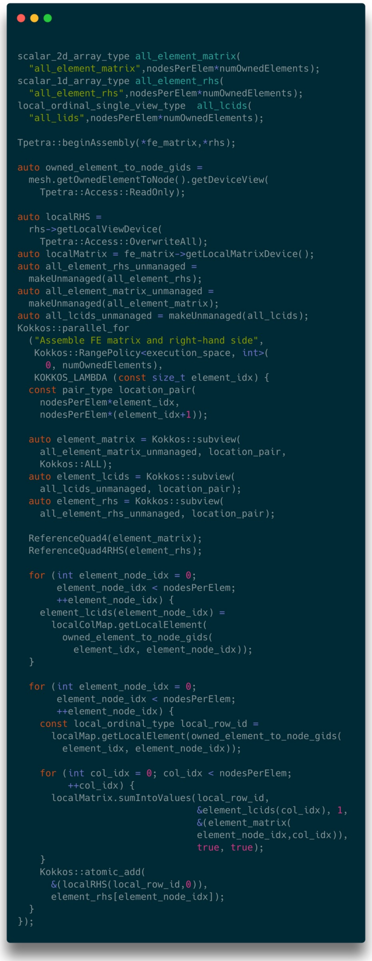
```
  ReferenceQuad4(element_matrix);
  ReferenceQuad4RHS(element_rhs);

  for (int element_node_idx = 0;
       element_node_idx < nodesPerElem;
       ++element_node_idx) {
    element_lcids(element_node_idx) =
      localColMap.getLocalElement(
        owned_element_to_node_gids(
          element_idx, element_node_idx));
  }

  for (int element_node_idx = 0;
       element_node_idx < nodesPerElem;
       ++element_node_idx) {
    const local_ordinal_type local_row_id =
      localMap.getLocalElement(owned_element_to_node_gids(
        element_idx, element_node_idx));

    for (int col_idx = 0; col_idx < nodesPerElem;
         ++col_idx) {
      localMatrix.sumIntoValues(local_row_id,
                                &element_lcids(col_idx), 1,
                                &(element_matrix(
                                element_node_idx,col_idx)),
                                true, true);
    }
    Kokkos::atomic_add(
      &(localRHS(local_row_id,0)),
      element_rhs[element_node_idx]);
  }
});
```

Tpetra + Kokkos

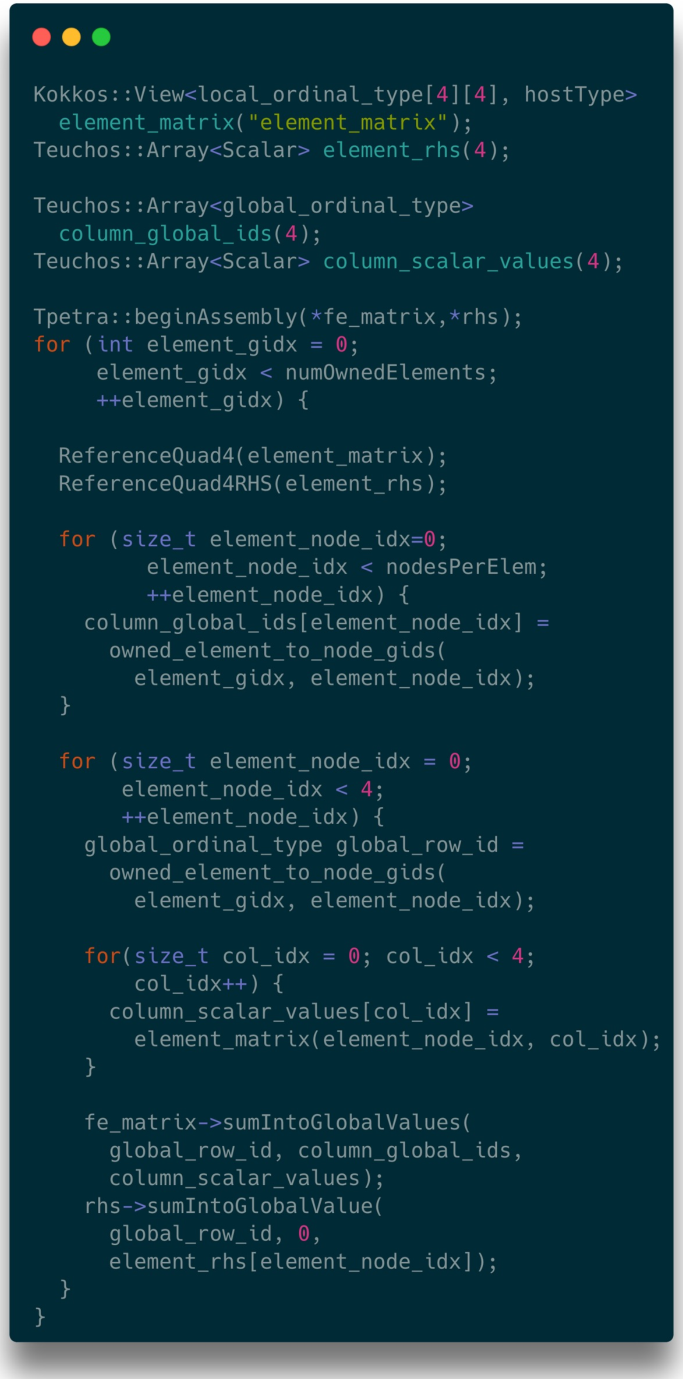
CONCLUSION

- Create parallel execution using `Kokkos::parallel_for`
  - also supports host CPU execution
- `Kokkos::View` for data accessed in parallel regions
  - convert `std::vector`, `Teuchos::Array`, `malloc`, `new`, …
- Functions called in that region must be `KOKKOS_FUNCTION`
  - e.g. producing the element matrix
  - …and any data it requires must be in a `Kokkos::View` (material properties, node coordinates, etc.)
- Use `Tpetra::[]::get*Device()` to get `Kokkos::View` of Tpetra data
  - As a consequence, have to operate with local rather than global indices
- Parallel regions may require atomics for their contributions

EXTRA SLIDES



```
scalar_2d_array_type all_element_matrix(
  "all_element_matrix",nodesPerElem*numOwnedElements);
scalar_1d_array_type all_element_rhs(
  "all_element_rhs",nodesPerElem*numOwnedElements);
local_ordinal_single_view_type  all_lcids(
  "all_lids",nodesPerElem*numOwnedElements);

Tpetra::beginAssembly(*fe_matrix,*rhs);

auto owned_element_to_node_gids =
  mesh.getOwnedElementToNode().getDeviceView(
    Tpetra::Access::ReadOnly);

auto localRHS =
  rhs->getLocalViewDevice(
    Tpetra::Access::OverwriteAll);
auto localMatrix = fe_matrix->getLocalMatrixDevice();
auto all_element_rhs_unmanaged =
  makeUnmanaged(all_element_rhs);
auto all_element_matrix_unmanaged =
  makeUnmanaged(all_element_matrix);
auto all_lcids_unmanaged = makeUnmanaged(all_lcids);
Kokkos::parallel_for
  ("Assemble FE matrix and right-hand side",
   Kokkos::RangePolicy<execution_space, int>(
     0, numOwnedElements),
   KOKKOS_LAMBDA (const size_t element_idx) {
  const pair_type location_pair(
    nodesPerElem*element_idx,
    nodesPerElem*(element_idx+1));

  auto element_matrix = Kokkos::subview(
    all_element_matrix_unmanaged, location_pair,
    Kokkos::ALL);
  auto element_lcids = Kokkos::subview(
    all_lcids_unmanaged, location_pair);
  auto element_rhs = Kokkos::subview(
    all_element_rhs_unmanaged, location_pair);

  ReferenceQuad4(element_matrix);
  ReferenceQuad4RHS(element_rhs);

  for (int element_node_idx = 0;
       element_node_idx < nodesPerElem;
       ++element_node_idx) {
    element_lcids(element_node_idx) =
      localColMap.getLocalElement(
        owned_element_to_node_gids(
          element_idx, element_node_idx));
  }

  for (int element_node_idx = 0;
       element_node_idx < nodesPerElem;
       ++element_node_idx) {
    const local_ordinal_type local_row_id =
      localMap.getLocalElement(owned_element_to_node_gids(
        element_idx, element_node_idx));

    for (int col_idx = 0; col_idx < nodesPerElem;
         ++col_idx) {
      localMatrix.sumIntoValues(local_row_id,
                                &element_lcids(col_idx), 1,
                                &(element_matrix(
                                element_node_idx,col_idx)),
                                true, true);
    }
    Kokkos::atomic_add(
      &(localRHS(local_row_id,0)),
      element_rhs[element_node_idx]);
  }
});
```



```
Kokkos::View<local_ordinal_type[4][4], hostType>
  element_matrix("element_matrix");
Teuchos::Array<Scalar> element_rhs(4);

Teuchos::Array<global_ordinal_type>
  column_global_ids(4);
Teuchos::Array<Scalar> column_scalar_values(4);

Tpetra::beginAssembly(*fe_matrix,*rhs);
for (int element_gidx = 0;
     element_gidx < numOwnedElements;
     ++element_gidx) {

  ReferenceQuad4(element_matrix);
  ReferenceQuad4RHS(element_rhs);

  for (size_t element_node_idx=0;
         element_node_idx < nodesPerElem;
         ++element_node_idx) {
    column_global_ids[element_node_idx] =
      owned_element_to_node_gids(
        element_gidx, element_node_idx);
  }

  for (size_t element_node_idx = 0;
       element_node_idx < 4;
       ++element_node_idx) {
    global_ordinal_type global_row_id =
      owned_element_to_node_gids(
        element_gidx, element_node_idx);

    for(size_t col_idx = 0; col_idx < 4;
        col_idx++) {
      column_scalar_values[col_idx] =
        element_matrix(element_node_idx, col_idx);
    }

    fe_matrix->sumIntoGlobalValues(
      global_row_id, column_global_ids,
      column_scalar_values);
    rhs->sumIntoGlobalValue(
      global_row_id, 0,
      element_rhs[element_node_idx]);
  }
}
```

ABSTRACT

This talk walks through a side-by-side comparison of the Kokkos implementation and traditional implement of the Tpetra finite element assembly example in the Trilinos scientific computing project. It emphasizes five main changes: parallel regions, device allocations, function annotations, atomic operations, and accessing Tpetra data on-device.