The Kokkos Lectures

Module 4: Hierarchical Parallelism

August 7, 2020

Online Resources:

- https://github.com/kokkos:
  - Primary Kokkos GitHub Organization
- https://github.com/kokkos/kokkos-tutorials/wiki/Kokkos-Lecture-Series:
  - Slides, recording and Q&A for the Lectures
- https://github.com/kokkos/kokkos/wiki:
  - Wiki including API reference
- https://kokkosteam.slack.com:
  - Slack channel for Kokkos.
  - Please join: fastest way to get your questions answered.
  - Can whitelist domains, or invite individual people.

Lecture Series Outline

- 07/17 Module 1: Introduction, Building and Parallel Dispatch
- 07/24 Module 2: Views and Spaces
- 07/31 Module 3: Data Structures + MultiDimensional Loops
- **08/07 Module 4: Hierarchical Parallelism**
- 08/14 Module 5: Tasking, Streams and SIMD
- 08/21 Module 6: Internode: MPI and PGAS
- 08/28 Module 7: Tools: Profiling, Tuning and Debugging
- 09/04 Module 8: Kernels: Sparse and Dense Linear Algebra
- 09/11 Reserve Day

MDRangePolicy

- Tightly nested loops (similar to OpenMP collapse clause)
- Available with `parallel_for` and `parallel_reduce`
- Tiling strategy over the iteration space
- Control iteration pattern at compile time

```
View<double**,LayoutLeft> A("A",N0,N1);
parallel_for("Label",
  MDRangePolicy<Rank<2,Iterate::Left,Iterate::Left>>(
        {0,0},{N0,N1}),
  KOKKOS_LAMBDA(int i, int j) {
    A(i,j) = 1000.0 * i + 1.0*j;
});
```

Subviews

- Taking slices of Views
- Similar capability as provided by Matlab, Fortran, or Python
- Prefer the use of `auto` for the type

```
View<int ***> v("v", N0, N1, N2);
auto sv = subview(v, i0, ALL, make_pair(start,end));
```

Unmanaged Views

- Interoperability with externally allocated arrays
- No reference counting, memory not deallocated at destruction
- User is responsible for insuring proper dynamic and/or static extents, MemorySpace, Layout, etc.

```
View<float**, LayoutRight, HostSpace>
  v_unmanaged(raw_ptr, N0, N1);
```

Atomic operations

- Atomic functions available on the host or the device (e.g. `Kokkos::atomic_add`)
- Use `Atomic` memory trait for atomic accesses on Views

```
View<int*> v("v", N0);
View<int*, MemoryTraits<Atomic>> v_atomic = v;
```

- Use `ScatterView` for scatter-add parallel pattern

Dual Views

- For managing data synchronization between host and device
- Helps in codes with no holistic view of data flow
  - In particular when porting codes incrementally

Hierarchical Parallelism

- How to leverage more parallelism through nested loops.
- The concept of Thread-Teams and Vectorlength.

Scratch Space

- Getting temporary workspace in kernels.
- Leveraging GPU Shared Memory.

Unique Token

- How to acquire safely per-thread resources.

Hierarchical parallelism

Finding and exploiting more parallelism in your computations.

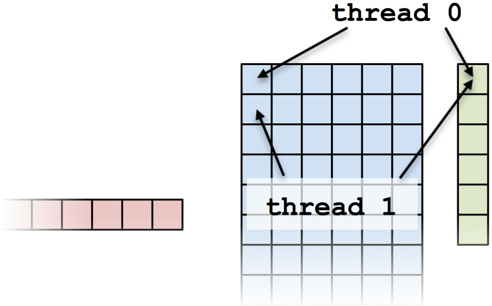
Learning objectives:

- Similarities and differences between outer and inner levels of parallelism
- Thread teams (league of teams of threads)
- Performance improvement with well-coordinated teams

Example: inner product (0)

(Flat parallel) Kernel:

```
Kokkos::parallel_reduce("yAx",N,
  KOKKOS_LAMBDA (const int row, double & valueToUpdate) {
    double thisRowsSum = 0;
    for (int col = 0; col < M; ++col) {
      thisRowsSum += A(row,col) * x(col);
    }
    valueToUpdate += y(row) * thisRowsSum;
  }, result);
```

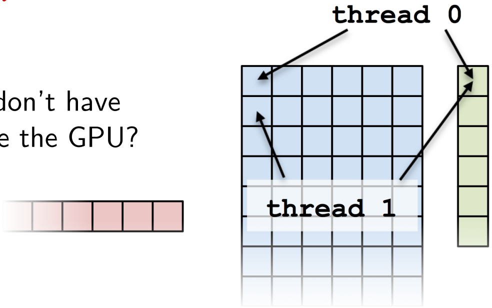


Example: inner product (0)

(Flat parallel) Kernel:

```
Kokkos::parallel_reduce("yAx",N,
  KOKKOS_LAMBDA (const int row, double & valueToUpdate) {
    double thisRowsSum = 0;
    for (int col = 0; col < M; ++col) {
      thisRowsSum += A(row,col) * x(col);
    }
    valueToUpdate += y(row) * thisRowsSum;
  }, result);
```

Problem: What if we don't have enough rows to saturate the GPU?



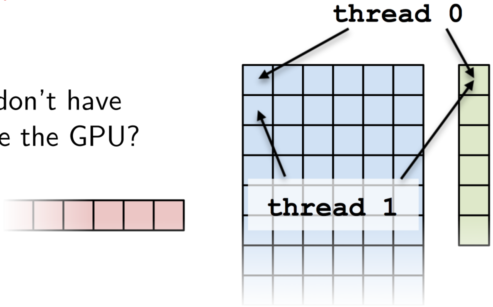
Example: inner product (0)

(Flat parallel) Kernel:

```
Kokkos::parallel_reduce("yAx",N,
  KOKKOS_LAMBDA (const int row, double & valueToUpdate) {
    double thisRowsSum = 0;
    for (int col = 0; col < M; ++col) {
      thisRowsSum += A(row,col) * x(col);
    }
    valueToUpdate += y(row) * thisRowsSum;
  }, result);
```

Problem: What if we don't have enough rows to saturate the GPU?

Solutions?



Example: inner product (0)

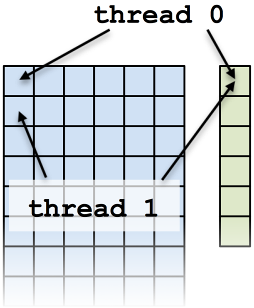
(Flat parallel) Kernel:

```
Kokkos::parallel_reduce("yAx",N,
  KOKKOS_LAMBDA (const int row, double & valueToUpdate) {
    double thisRowsSum = 0;
    for (int col = 0; col < M; ++col) {
      thisRowsSum += A(row,col) * x(col);
    }
    valueToUpdate += y(row) * thisRowsSum;
  }, result);
```

Problem: What if we don't have enough rows to saturate the GPU?

Solutions?

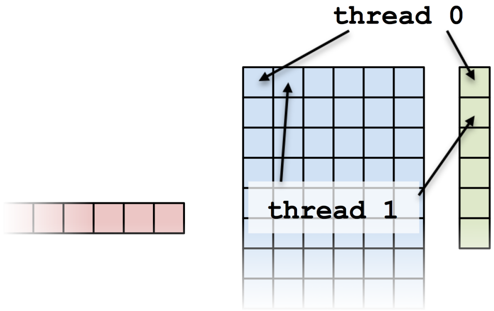
- Atomics
- Thread teams



Example: inner product (1)

Atomics kernel:

```
Kokkos::parallel_for("yAx", N*M,
  KOKKOS_LAMBDA (const size_t index) {
    const int row = extractRow(index);
    const int col = extractCol(index);
    atomic_add(&result, y(row) * A(row,col) * x(col));
  });
```

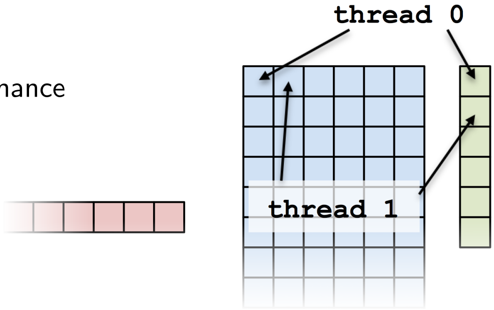


Example: inner product (1)

Atomics kernel:

```
Kokkos::parallel_for("yAx", N*M,
  KOKKOS_LAMBDA (const size_t index) {
    const int row = extractRow(index);
    const int col = extractCol(index);
    atomic_add(&result, y(row) * A(row,col) * x(col));
  });
```

Problem: Poor performance



Example: inner product (2)

Using an atomic with every element is doing scalar integration with atomics. (See module 3)

Instead, you could envision doing a large number of `parallel_reduce` kernels.

```
for each row
  Functor functor(row, ...);
  parallel_reduce(M, functor);
}
```

Example: inner product (2)

Using an atomic with every element is doing scalar integration with atomics. (See module 3)

Instead, you could envision doing a large number of `parallel_reduce` kernels.

```
for each row
  Functor functor(row, ...);
  parallel_reduce(M, functor);
}
```

This is an example of *hierarchical work*.

Important concept: Hierarchical parallelism

Algorithms that exhibit hierarchical structure can exploit hierarchical parallelism with **thread teams**.

Example: inner product (3)

Important concept: Thread team

A collection of threads which are guaranteed to be executing **concurrently** and **can synchronize**.

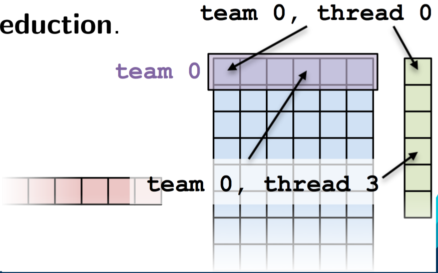
Example: inner product (3)

Important concept: Thread team

A collection of threads which are guaranteed to be executing **concurrently** and **can synchronize**.

High-level **strategy**:

1. Do **one parallel launch** of `N` teams.
2. Each team handles a row.
3. The threads within **teams perform a reduction**.
4. The thread teams **perform a reduction**.



Example: inner product (4)

The final hierarchical parallel kernel:

```
parallel_reduce("yAx",
  team_policy(N, Kokkos::AUTO),

  KOKKOS_LAMBDA (const member_type & teamMember, double & update)
    int row = teamMember.league_rank();

    double thisRowsSum = 0;
    parallel_reduce(TeamThreadRange(teamMember, M),
      [=] (int col, double & innerUpdate) {
        innerUpdate += A(row, col) * x(col);
      }, thisRowsSum);

    if (teamMember.team_rank() == 0) {
      update += y(row) * thisRowsSum;
    }
  }, result);
```

TeamPolicy (0)

Important point

Using teams is changing the execution *policy*.

"**Flat** parallelism" uses `RangePolicy`:

We specify a *total amount of work*.

```
// total work = N
parallel_for("Label",
  RangePolicy<ExecutionSpace>(0,N), functor);
```

TeamPolicy (0)

Important point

Using teams is changing the execution *policy*.

"**Flat** parallelism" uses `RangePolicy`:

We specify a *total amount of work*.

```
// total work = N
parallel_for("Label",
  RangePolicy<ExecutionSpace>(0,N), functor);
```

"**Hierarchical** parallelism" uses `TeamPolicy`:

We specify a *team size* and a *number of teams*.

```
// total work = numberOfTeams * teamSize
parallel_for("Label",
  TeamPolicy<ExecutionSpace>(numberOfTeams, teamSize), functor);
```

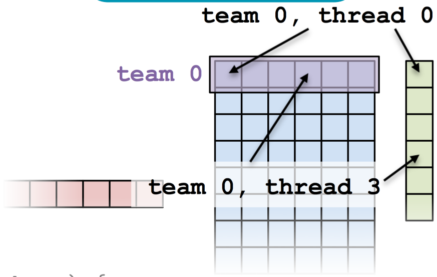
TeamPolicy (1)

Important point

When using teams, functor operators receive a *team member*.

```
typedef typename TeamPolicy<ExecSpace>::member_type member_type;

void operator()(const member_type & teamMember) {
  // How many teams are there?
  const unsigned int league_size = teamMember.league_size();

  // Which team am I on?
  const unsigned int league_rank = teamMember.league_rank();

  // How many threads are in the team?
  const unsigned int team_size = teamMember.team_size();

  // Which thread am I on this team?
  const unsigned int team_rank = teamMember.team_rank();

  // Make threads in a team wait on each other:
  teamMember.team_barrier();
}
```

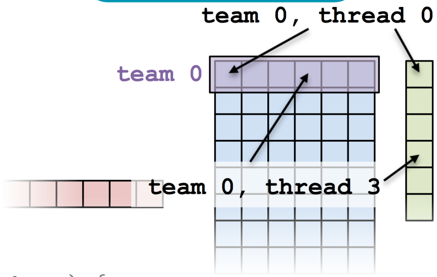
TeamThreadRange (0)



First attempt at exercise:

```
operator() (member_type & teamMember ) {
  const size_t row = teamMember.league_rank();
  const size_t col = teamMember.team_rank();
  atomic_add(&result,y(row) * A(row,col) * x(entry));
}
```

TeamThreadRange (0)



First attempt at exercise:

```
operator() (member_type & teamMember ) {
  const size_t row = teamMember.league_rank();
  const size_t col = teamMember.team_rank();
  atomic_add(&result,y(row) * A(row,col) * x(entry));
}
```

- When team size $\neq$ number of columns, how are units of work mapped to team's member threads? Is the mapping architecture-dependent?

TeamThreadRange (1)

Second attempt at exercise:

Divide row length among team members.

```
operator() (member_type & teamMember ) {
  const size_t row = teamMember.league_rank();

  int begin = teamMember.team_rank();
  for(int col = begin; col < M; col += teamMember.team_size()) {
    atomic_add(&result, y(row) * A(row,col) * x(entry));
  }
}
```

TeamThreadRange (1)

Second attempt at exercise:

Divide row length among team members.

```
operator() (member_type & teamMember ) {
  const size_t row = teamMember.league_rank();

  int begin = teamMember.team_rank();
  for(int col = begin; col < M; col += teamMember.team_size()) {
    atomic_add(&result, y(row) * A(row,col) * x(entry));
  }
}
```

- Still bad because `atomic_add` performs badly under high contention, how can team's member threads performantly cooperate for a nested reduction?
- On CPUs you get a bad data access pattern: this hardcodes coalesced access, but not caching.

We shouldn't be hard-coding the work mapping...

```
operator() (member_type & teamMember, double & update) {
  const int row = teamMember.league_rank();
  double thisRowsSum;
  ``do a reduction''(``over M columns'',
    [=] (const int col) {
      thisRowsSum += A(row,col) * x(col);
    });
  if (teamMember.team_rank() == 0) {
    update += (row) * thisRowsSum;
  }
}
```

TeamThreadRange (2)

We shouldn't be hard-coding the work mapping...

```
operator() (member_type & teamMember, double & update) {
  const int row = teamMember.league_rank();
  double thisRowsSum;
  ''do a reduction''(''over M columns'',
    [=] (const int col) {
      thisRowsSum += A(row,col) * x(col);
    });
  if (teamMember.team_rank() == 0) {
    update += (row) * thisRowsSum;
  }
}
```

If this were a parallel execution,

we'd use `Kokkos::parallel_reduce`.

We shouldn't be hard-coding the work mapping...

```
operator() (member_type & teamMember, double & update) {
  const int row = teamMember.league_rank();
  double thisRowsSum;
  ``do a reduction''(``over M columns'',
    [=] (const int col) {
      thisRowsSum += A(row,col) * x(col);
    });
  if (teamMember.team_rank() == 0) {
    update += (row) * thisRowsSum;
  }
}
```

If this were a parallel execution,

we'd use `Kokkos::parallel_reduce`.

Key idea: this *is* a parallel execution.

TeamThreadRange (2)

We shouldn't be hard-coding the work mapping...

```
operator() (member_type & teamMember, double & update) {
  const int row = teamMember.league_rank();
  double thisRowsSum;
  ''do a reduction''(''over M columns'',
    [=] (const int col) {
      thisRowsSum += A(row,col) * x(col);
    });
  if (teamMember.team_rank() == 0) {
    update += (row) * thisRowsSum;
  }
}
```

If this were a parallel execution,

we'd use `Kokkos::parallel_reduce`.

Key idea: this *is* a parallel execution.

$\Rightarrow$ **Nested parallel patterns**

TeamThreadRange (3)

TeamThreadRange:

```
operator() (const member_type & teamMember, double & update ) {
  const int row = teamMember.league_rank();
  double thisRowsSum;
  parallel_reduce(TeamThreadRange(teamMember, M),
    [=] (const int col, double & thisRowsPartialSum ) {
      thisRowsPartialSum += A(row, col) * x(col);
    }, thisRowsSum );
  if (teamMember.team_rank() == 0) {
    update += y(row) * thisRowsSum;
  }
}
```

TeamThreadRange (3)

TeamThreadRange:

```
operator() (const member_type & teamMember, double & update ) {
  const int row = teamMember.league_rank();
  double thisRowsSum;
  parallel_reduce(TeamThreadRange(teamMember, M),
    [=] (const int col, double & thisRowsPartialSum ) {
      thisRowsPartialSum += A(row, col) * x(col);
    }, thisRowsSum );
  if (teamMember.team_rank() == 0) {
    update += y(row) * thisRowsSum;
  }
}
```

- The **mapping** of work indices to threads is **architecture-dependent**.
- The **amount of work** given to the TeamThreadRange **need not be a multiple** of the team_size.
- Intrateam **reduction handled** by Kokkos.

Anatomy of nested parallelism:

```
parallel_outer("Label",
  TeamPolicy<ExecutionSpace>(numberOfTeams, teamSize),
  KOKKOS_LAMBDA (const member_type & teamMember[, ...]) {
    /* beginning of outer body */
    parallel_inner(
      TeamThreadRange(teamMember, thisTeamsRangeSize),
      [=] (const unsigned int indexWithinBatch[, ...]) {
        /* inner body */
      }[, ...]);
    /* end of outer body */
  }[, ...]);
```

- `parallel_outer` and `parallel_inner` may be any combination of `for` and/or `reduce`.
- The inner lambda may capture by reference, but capture-by-value is recommended.
- The policy of the inner lambda is always a `TeamThreadRange`.
- `TeamThreadRange` cannot be nested.

What should the team size be?

In practice, you can **let Kokkos decide**:

```
parallel_something(
  TeamPolicy<ExecutionSpace>(numberOfTeams, Kokkos::AUTO),
  /* functor */);
```

What should the team size be?

In practice, you can **let Kokkos decide**:

```
parallel_something(
  TeamPolicy<ExecutionSpace>(numberOfTeams, Kokkos::AUTO),
  /* functor */);
```

GPUs

- Special hardware available for coordination within a team.
- Within a team 32 (NVIDIA) or 64 (AMD) threads execute "lock step."
- Maximum team size: **1024**; Recommended team size: **128/256**

What should the team size be?

In practice, you can **let Kokkos decide**:

```
parallel_something(
  TeamPolicy<ExecutionSpace>(numberOfTeams, Kokkos::AUTO),
  /* functor */);
```

GPUs

- Special hardware available for coordination within a team.
- Within a team 32 (NVIDIA) or 64 (AMD) threads execute "lock step."
- Maximum team size: **1024**; Recommended team size: **128/256**

Intel Xeon Phi:

- Recommended team size: # hyperthreads per core
- Hyperthreads share entire cache hierarchy
  a well-coordinated team avoids cache-thrashing

Exercise: TeamPolicy

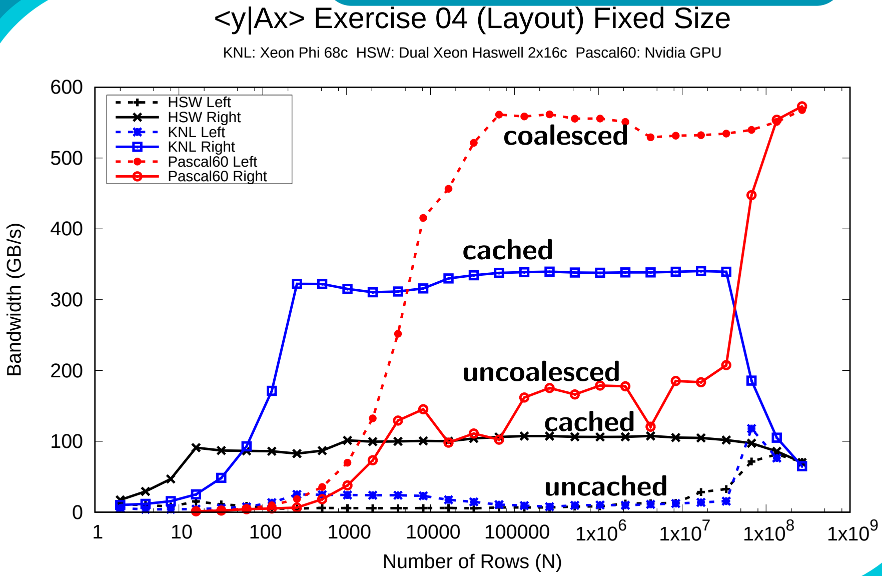
Details:

- Location: `Exercises/team_policy/`
- Replace `RangePolicy<Space>` with `TeamPolicy<Space>`
- Use `AUTO` for `team_size`
- Make the inner loop a `parallel_reduce` with `TeamThreadRange` policy
- Experiment with the combinations of `Layout`, `Space`, `N` to view performance
- Hint: what should the layout of `A` be?

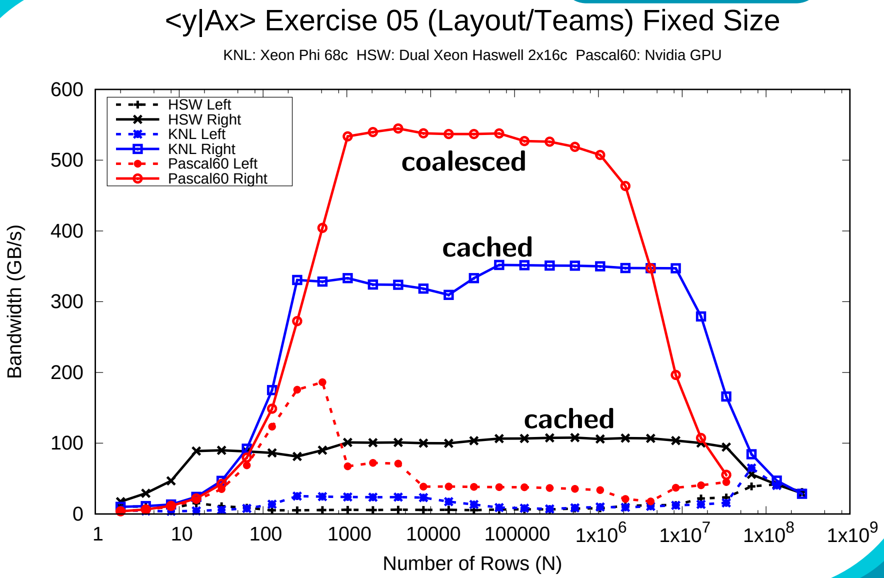
Things to try:

- Vary problem size and number of rows (-S ...; -N ...)
- Compare behavior with Exercise 4 for very non-square matrices
- Compare behavior of CPU vs GPU

Reminder, Exercise #4 with Flat Parallelism



Exercise: TeamPolicy



Exposing Vector Level Parallelism

- Optional **third level** in the hierarchy: `ThreadVectorRange`
  - Can be used for `parallel_for`, `parallel_reduce`, or `parallel_scan`.
- Maps to vectorizable loop on CPUs or (sub-)warp level parallelism on GPUs.
- Enabled with a **runtime** vector length argument to `TeamPolicy`
- There is **no** explicit access to a vector lane ID.
- Depending on the backend the full global parallel region has active vector lanes.
- `TeamVectorRange` uses both **thread** and **vector** parallelism.

Anatomy of nested parallelism:

```
parallel_outer("Label",
  TeamPolicy<>(numberOfTeams, teamSize, vectorLength),
  KOKKOS_LAMBDA (const member_type & teamMember[, ...]) {
    /* beginning of outer body */
    parallel_middle(
      TeamThreadRange(teamMember, thisTeamsRangeSize),
      [=] (const int indexWithinBatch[, ...]) {
        /* begin middle body */
        parallel_inner(
          ThreadVectorRange(teamMember, thisVectorRangeSize),
          [=] (const int indexVectorRange[, ...]) {
            /* inner body */
          }[, ....);
        /* end middle body */
      }[, ...]);
    parallel_middle(
    TeamVectorRange(teamMember, someSize),
      [=] (const int indexTeamVector[, ...]) {
        /* nested body */
      }[, ...]);
    /* end of outer body */
  }[, ...]);
```

Sum sanity checks (0)

Question: What will the value of `totalSum` be?

```
int totalSum = 0;
parallel_reduce("Sum", RangePolicy<>(0, numberOfThreads),
  KOKKOS_LAMBDA (size_t& index, int& partialSum) {
    int thisThreadsSum = 0;
    for (int i = 0; i < 10; ++i) {
      ++thisThreadsSum;
    }
    partialSum += thisThreadsSum;
}, totalSum);
```

Sum sanity checks (0)

Question: What will the value of `totalSum` be?

```
int totalSum = 0;
parallel_reduce("Sum", RangePolicy<>(0, numberOfThreads),
  KOKKOS_LAMBDA (size_t& index, int& partialSum) {
    int thisThreadsSum = 0;
    for (int i = 0; i < 10; ++i) {
      ++thisThreadsSum;
    }
    partialSum += thisThreadsSum;
}, totalSum);
```

`totalSum = numberOfThreads * 10`

Sum sanity checks (1)

Question: What will the value of `totalSum` be?

```
int totalSum = 0;
parallel_reduce("Sum", TeamPolicy<>(numberOfTeams, team_size),
  KOKKOS_LAMBDA (member_type& teamMember, int& partialSum) {
    int thisThreadsSum = 0;
    for (int i = 0; i < 10; ++i) {
      ++thisThreadsSum;
    }
    partialSum += thisThreadsSum;
}, totalSum);
```

Sum sanity checks (1)

Question: What will the value of `totalSum` be?

```
int totalSum = 0;
parallel_reduce("Sum", TeamPolicy<>(numberOfTeams, team_size),
  KOKKOS_LAMBDA (member_type& teamMember, int& partialSum) {
    int thisThreadsSum = 0;
    for (int i = 0; i < 10; ++i) {
      ++thisThreadsSum;
    }
    partialSum += thisThreadsSum;
}, totalSum);
```

`totalSum = numberOfTeams * team_size * 10`

Sum sanity checks (2)

Question: What will the value of `totalSum` be?

```
int totalSum = 0;
parallel_reduce("Sum", TeamPolicy<>(numberOfTeams, team_size),
  KOKKOS_LAMBDA (member_type& teamMember, int& partialSum) {
    int thisTeamsSum = 0;
    parallel_reduce(TeamThreadRange(teamMember, team_size),
      [=] (const int index, int& thisTeamsPartialSum) {
      int thisThreadsSum = 0;
      for (int i = 0; i < 10; ++i) {
        ++thisThreadsSum;
      }
      thisTeamsPartialSum += thisThreadsSum;
    }, thisTeamsSum);
    partialSum += thisTeamsSum;
}, totalSum);
```

Sum sanity checks (2)

Question: What will the value of `totalSum` be?

```
int totalSum = 0;
parallel_reduce("Sum", TeamPolicy<>(numberOfTeams, team_size),
  KOKKOS_LAMBDA (member_type& teamMember, int& partialSum) {
    int thisTeamsSum = 0;
    parallel_reduce(TeamThreadRange(teamMember, team_size),
      [=] (const int index, int& thisTeamsPartialSum) {
      int thisThreadsSum = 0;
      for (int i = 0; i < 10; ++i) {
        ++thisThreadsSum;
      }
      thisTeamsPartialSum += thisThreadsSum;
    }, thisTeamsSum);
    partialSum += thisTeamsSum;
}, totalSum);
```

`totalSum = numberOfTeams * team_size * team_size * 10`

Restricting Execution: single pattern

The `single` pattern can be used to restrict execution

- Like parallel patterns it takes a policy, a lambda, and optionally a broadcast argument.
- Two policies: `PerTeam` and `PerThread`.
- Equivalent to OpenMP **single** directive with **nowait**

```
// Restrict to once per thread
single(PerThread(teamMember), [&] () {
  // code
});

// Restrict to once per team with broadcast
int broadcastedValue = 0;
single(PerTeam(teamMember), [&] (int& broadcastedValue_local) {
        broadcastedValue_local = special value assigned by one;
}, broadcastedValue);
// Now everyone has the special value
```

The previous example was extended with an outer loop over “Elements” to expose a third natural layer of parallelism.

Details:

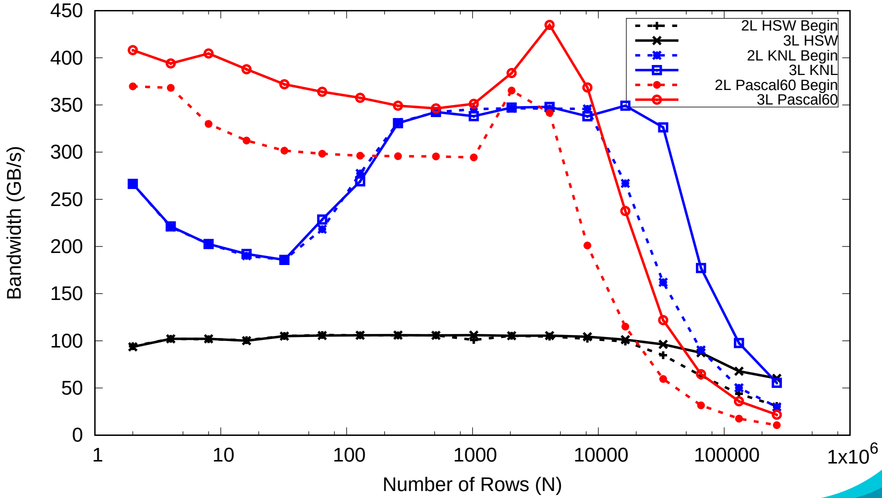
- Location: `Exercises/team_vector_loop/`
- Use the `single` policy instead of checking team rank
- Parallelize all three loop levels.

Things to try:

- Vary problem size and number of rows (-S ...; -N ...)
- Compare behavior with TeamPolicy Exercise for very non-square matrices
- Compare behavior of CPU vs GPU

<y|Ax> Exercise 06 (Three Level Parallelism) Fixed Size

KNL: Xeon Phi 68c HSW: Dual Xeon Haswell 2x16c Pascal60: Nvidia GPU



Section Summary

- **Hierarchical work** can be parallelized via hierarchical parallelism.
- Hierarchical parallelism is leveraged using **thread teams** launched with a `TeamPolicy`.
- Team "worksets" are processed by a team in nested `parallel_for` (or `reduce` or `scan`) calls with a `TeamThreadRange`, `ThreadVectorRange`, and `TeamVectorRange` policy.
- Execution can be restricted to a subset of the team with the `single` pattern using either a `PerTeam` or `PerThread` policy.

Scratch memory

Learning objectives:

- Understand concept of **team** and **thread** private **scratch pads**
- Understand how scratch memory can **reduce global memory accesses**
- Recognize **when to use** scratch memory
- Understand **how to use** scratch memory and when barriers are necessary

Types of Scratch Space Uses

Two Levels of Scratch Space

- Level 0 is limited in size but fast.
- Level 1 allows larger allocations but is equivalent to High Bandwidth Memory in latency and bandwidth.

Team or Thread private memory

- Typically used for per work-item temporary storage.
- Advantage over pre-allocated memory is aggregate size scales with number of threads, not number of work-items.

Manually Managed Cache

- Explicitly cache frequently used data.
- Exposes hardware specific on-core scratch space (e.g. NVIDIA GPU Shared Memory).

Types of Scratch Space Uses

Two Levels of Scratch Space

- Level 0 is limited in size but fast.
- Level 1 allows larger allocations but is equivalent to High Bandwidth Memory in latency and bandwidth.

Team or Thread private memory

- Typically used for per work-item temporary storage.
- Advantage over pre-allocated memory is aggregate size scales with number of threads, not number of work-items.

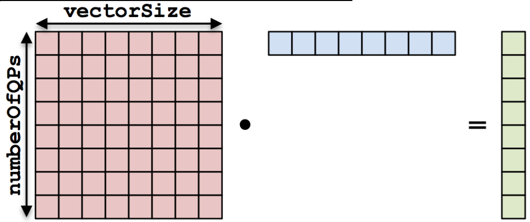
Manually Managed Cache

- Explicitly cache frequently used data.
- Exposes hardware specific on-core scratch space (e.g. NVIDIA GPU Shared Memory).

Now: Discuss Manually Managed Cache Usecase.

Example: contractDataFieldScalar (1)

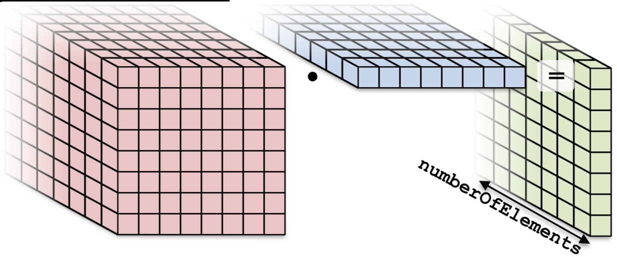
One slice of contractDataFieldScalar:



```
for (qp = 0; qp < numberOfQPs; ++qp) {
  total = 0;
  for (i = 0; i < vectorSize; ++i) {
    total += A(qp, i) * B(i);
  }
  result(qp) = total;
}
```

Example: contractDataFieldScalar (2)

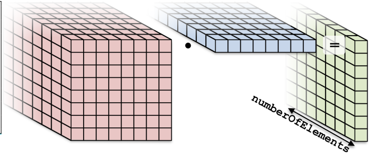
contractDataFieldScalar:



```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```

Example: contractDataFieldScalar (3)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```

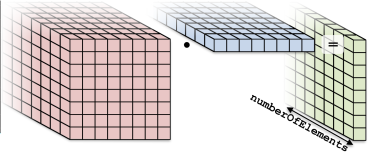


Parallelization approaches:

- Each thread handles an `element`.
  Threads: `numberOfElements`

Example: contractDataFieldScalar (3)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```

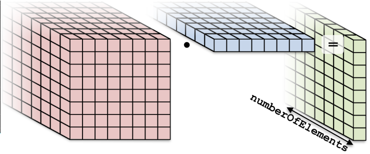


Parallelization approaches:

- Each thread handles an `element`.
  Threads: `numberOfElements`
- Each thread handles a `qp`.
  Threads: `numberOfElements * numberOfQPs`

Example: contractDataFieldScalar (3)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```



Parallelization approaches:

- Each thread handles an `element`.

  Threads: `numberOfElements`
- Each thread handles a `qp`.

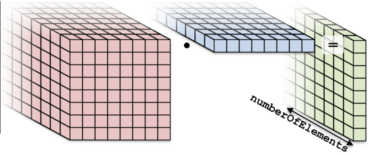
  Threads: `numberOfElements * numberOfQPs`
- Each thread handles an `i`.

  Threads: `numElements * numQPs * vectorSize`

  Requires a `parallel_reduce`.

Example: contractDataFieldScalar (3)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```

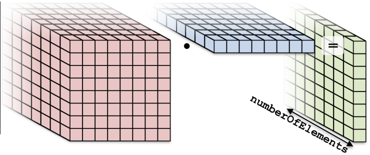


Parallelization approaches:

- Each thread handles an `element`.
  Threads: `numberOfElements`
- Each thread handles a `qp`.
  Threads: `numberOfElements * numberOfQPs`
- Each thread handles an `i`.
  Threads: `numElements * numQPs * vectorSize`
  Requires a `parallel_reduce`.

Example: contractDataFieldScalar (4)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```

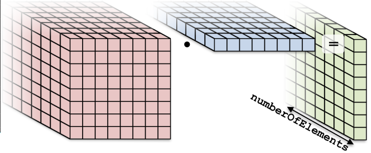


Flat kernel: Each thread handles a quadrature point

```
parallel_for("L",MDRangePolicy<Rank<2>>({0,0},{numE,numQP}),
  KOKKOS_LAMBDA(int element, int qp) {
  double total = 0;
  for (int i = 0; i < vectorSize; ++i) {
    total += A(element, qp, i) * B(element, i);
  }
  result(element, qp) = total;
}
```

Example: contractDataFieldScalar (6)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```

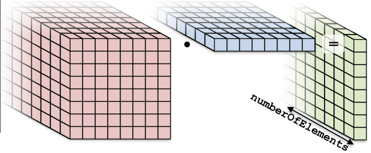


Teams kernel: Each team handles an element

```
operator()(member_type teamMember) {
  int element = teamMember.league_rank();
  parallel_for(
    TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * B(element, i);
      }
      result(element, qp) = total;
    });
}
```

Example: contractDataFieldScalar (6)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```



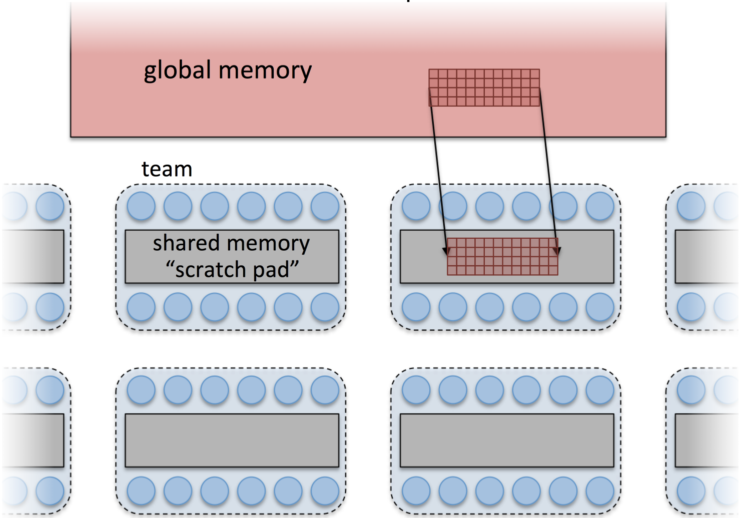
Teams kernel: Each team handles an element

```
operator()(member_type teamMember) {
  int element = teamMember.league_rank();
  parallel_for(
    TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * B(element, i);
      }
      result(element, qp) = total;
    });
}
```

No real advantage (yet)

Scratch memory (0)

Each team has access to a "scratch pad".



Scratch memory (scratch pad) as manual cache:

- Accessing data in (level 0) scratch memory is (usually) **much faster** than global memory.
- **GPUs** have separate, dedicated, small, low-latency scratch memories (*NOT subject to coalescing requirements*).
- **CPUs** don't have special hardware, but programming with scratch memory results in cache-aware memory access patterns.
- Roughly, it's like a *user-managed* L1 cache.

Scratch memory (1)

Scratch memory (scratch pad) as manual cache:

- Accessing data in (level 0) scratch memory is (usually) **much faster** than global memory.
- **GPUs** have separate, dedicated, small, low-latency scratch memories (*NOT subject to coalescing requirements*).
- **CPUs** don't have special hardware, but programming with scratch memory results in cache-aware memory access patterns.
- Roughly, it's like a *user-managed* L1 cache.

Important concept

When members of a team read the same data multiple times, it's better to load the data into scratch memory and read from there.

Scratch memory (2)

Scratch memory for temporary per work-item storage:

- Scenario: Algorithm requires temporary workspace of size W.
- **Without scratch memory:** pre-allocate space for N work-items of size N x W.
- **With scratch memory:** Kokkos pre-allocates space for each Team or Thread of size T x W.
- `PerThread` and `PerTeam` scratch can be used concurrently.
- Level 0 and Level 1 scratch memory can be used concurrently.

Scratch memory (2)

Scratch memory for temporary per work-item storage:

- Scenario: Algorithm requires temporary workspace of size W.
- **Without scratch memory:** pre-allocate space for N work-items of size N x W.
- **With scratch memory:** Kokkos pre-allocates space for each Team or Thread of size T x W.
- `PerThread` and `PerTeam` scratch can be used concurrently.
- Level 0 and Level 1 scratch memory can be used concurrently.

Important concept

If an algorithm requires temporary workspace for each work-item, then use Kokkos' scratch memory.

Scratch memory (3)

To use scratch memory, you need to:

1. **Tell Kokkos how much** scratch memory you'll need.
2. **Make** scratch memory **views** inside your kernels.

Scratch memory (3)

To use scratch memory, you need to:

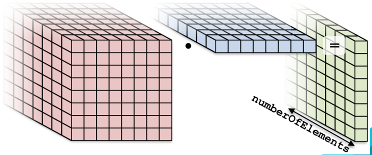
1. **Tell Kokkos how much** scratch memory you'll need.
2. **Make** scratch memory **views** inside your kernels.

```
TeamPolicy<ExecutionSpace> policy(numberOfTeams, teamSize);

// Define a scratch memory view type
using ScratchPadView =
    View<double*,ExecutionSpace::scratch_memory_space>;
// Compute how much scratch memory (in bytes) is needed
size_t bytes = ScratchPadView::shmem_size(vectorSize);

// Tell the policy how much scratch memory is needed
int level = 0;
parallel_for(policy.set_scratch_size(level, PerTeam(bytes)),
  KOKKOS_LAMBDA (const member_type& teamMember) {

    // Create a view from the pre-existing scratch memory
    ScratchPadView scratch(teamMember.team_scratch(level),
                           vectorSize);
});
```

Example: contractDataFieldScalar (7)

Kernel outline for teams with scratch memory:

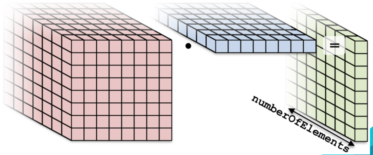
```
operator()(member_type teamMember) {
  ScratchPadView scratch(teamMember.team_scratch(0),
                         vectorSize);
  // TODO: load slice of B into scratch

  parallel_for(
    TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        // total += A(element, qp, i) * B(element, i);
        total += A(element, qp, i) * scratch(i);
      }
      result(element, qp) = total;
    });
}
```



How to populate the scratch memory?

- One thread loads it all?

```
if (teamMember.team_rank() == 0) {
  for (int i = 0; i < vectorSize; ++i) {
    scratch(i) = B(element, i);
  }
}
```



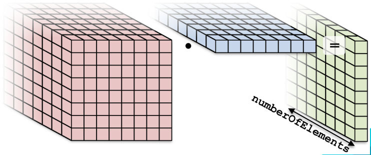
How to populate the scratch memory?

- ~~One thread loads it all?~~ Serial

```
if (teamMember.team_rank() == 0) {
  for (int i = 0; i < vectorSize; ++i) {
    scratch(i) = B(element, i);
  }
}
```

- Each thread loads one entry?

```
scratch(team_rank) = B(element, team_rank);
```



Example: contractDataFieldScalar (8)

How to populate the scratch memory?

- ~~One thread loads it all?~~ Serial

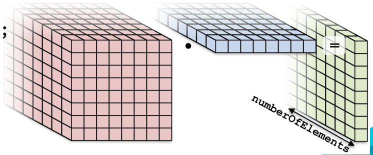
```
if (teamMember.team_rank() == 0) {
  for (int i = 0; i < vectorSize; ++i) {
    scratch(i) = B(element, i);
  }
}
```

- ~~Each thread loads one entry?~~ teamSize $\neq$ vectorSize

```
scratch(team_rank) = B(element, team_rank);
```

- TeamVectorRange

```
parallel_for(
  TeamVectorRange(teamMember, vectorSize),
  [=] (int i) {
    scratch(i) = B(element, i);
  });
```



How to populate the scratch memory?

- ~~One thread loads it all?~~ Serial

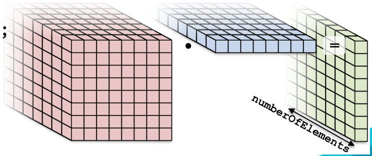
```
if (teamMember.team_rank() == 0) {
  for (int i = 0; i < vectorSize; ++i) {
    scratch(i) = B(element, i);
  }
}
```

- ~~Each thread loads one entry?~~ teamSize $\neq$ vectorSize

```
scratch(team_rank) = B(element, team_rank);
```

- TeamVectorRange

```
parallel_for(
  TeamVectorRange(teamMember, vectorSize),
  [=] (int i) {
    scratch(i) = B(element, i);
  });
```



Example: contractDataFieldScalar (9)

(incomplete) Kernel for teams with scratch memory:

```
operator()(member_type teamMember) {
  ScratchPadView scratch(...);

  parallel_for(TeamVectorRange(teamMember, vectorSize),
    [=] (int i) {
      scratch(i) = B(element, i);
    });
  // TODO: fix a problem at this location

  parallel_for(TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * scratch(i);
      }
      result(element, qp) = total;
    });
}
```

(incomplete) Kernel for teams with scratch memory:

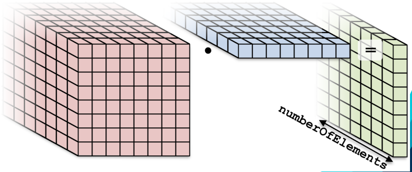
```
operator()(member_type teamMember) {
  ScratchPadView scratch(...);

  parallel_for(TeamVectorRange(teamMember, vectorSize),
    [=] (int i) {
      scratch(i) = B(element, i);
    });
  // TODO: fix a problem at this location

  parallel_for(TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * scratch(i);
      }
      result(element, qp) = total;
    });
}
```

Problem: threads may start to use `scratch` before all threads are done loading.

Example: contractDataFieldScalar (10)

Kernel for teams with scratch memory:

```
operator()(member_type teamMember) {
  ScratchPadView scratch(...);

  parallel_for(ThreadVectorRange(teamMember, vectorSize),
    [=] (int i) {
      scratch(i) = B(element, i);
    });
  teamMember.team_barrier();

  parallel_for(TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * scratch(i);
      }
      result(element, qp) = total;
    });
}
```



Exercise: Scratch Memory

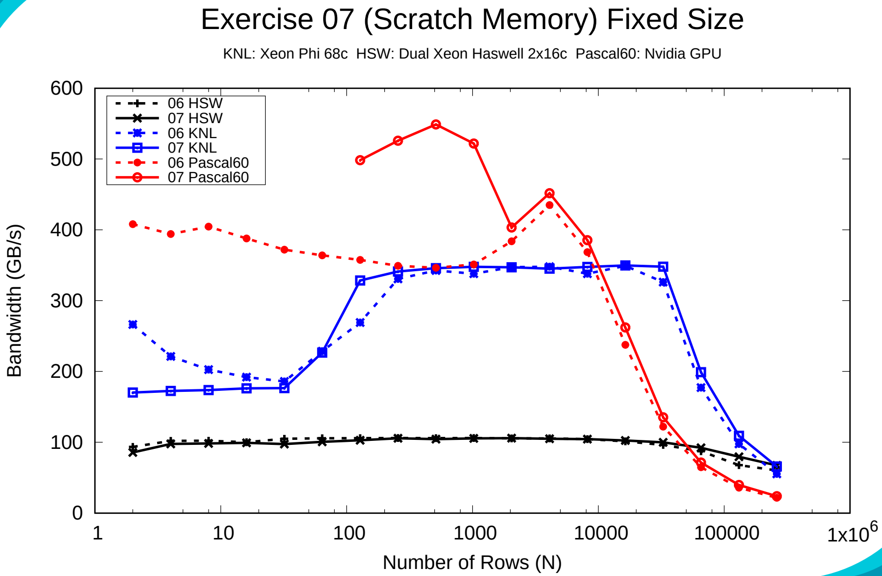
Use Scratch Memory to explicitly cache the x-vector for each element.

Details:

- Location: `Exercises/team_scratch_memory/`
- Create a scratch view
- Fill the scratch view in parallel using a TeamVectorRange

Things to try:

- Vary problem size and number of rows (-S ...; -N ...)
- Compare behavior with Exercise 6
- Compare behavior of CPU vs GPU


Exercise 07 (Scratch Memory) Fixed Size
KNL: Xeon Phi 68c HSW: Dual Xeon Haswell 2x16c Pascal60: Nvidia GPU
06 HSW
07 HSW
06 KNL
07 KNL
06 Pascal60
07 Pascal60
Bandwidth (GB/s)
Number of Rows (N)
0
100
200
300
400
500
600
1
10
100
1000
10000
100000
1x10^6

Scratch Memory: API Details

Allocating scratch in different levels:

```
int level = 1; // valid values 0,1
policy.set_scratch_size(level,PerTeam(bytes));
```

Scratch Memory: API Details

Allocating scratch in different levels:

```
int level = 1; // valid values 0,1
policy.set_scratch_size(level,PerTeam(bytes));
```

Using PerThread, PerTeam or both:

```
policy.set_scratch_size(level,PerTeam(bytes));
policy.set_scratch_size(level,PerThread(bytes));
policy.set_scratch_size(level,PerTeam(bytes1),
                              PerThread(bytes2));
```

Scratch Memory: API Details

Allocating scratch in different levels:

```
int level = 1; // valid values 0,1
policy.set_scratch_size(level,PerTeam(bytes));
```

Using PerThread, PerTeam or both:

```
policy.set_scratch_size(level,PerTeam(bytes));
policy.set_scratch_size(level,PerThread(bytes));
policy.set_scratch_size(level,PerTeam(bytes1),
                              PerThread(bytes2));
```

Using both levels of scratch:

```
policy.set_scratch_size(0,PerTeam(bytes0))
      .set_scratch_size(1,PerThread(bytes1));
```

Note: `set_scratch_size()` returns a new policy instance, it doesn't modify the existing one.

Section Summary

- **Scratch Memory** can be use with the `TeamPolicy` to provide thread or team **private** memory.
- Usecase: per work-item temporary storage or manual caching.
- Scratch memory exposes on-chip user managed caches (e.g. on NVIDIA GPUs)
- The size must be determined before launching a kernel.
- Two levels are available: large/slow and small/fast.

Unique Token

Learning objectives:

- Understand concept of unique tokens and thread-safe resource access.
- Learn how to acquire per-team unique ids.
- Understand the difference between **Global** and **Instance** scope.

Unique Tokens - Motivation

Why do we need a unique token concept?

- Within Functor operator / Lambda there is no portable way to identify the active execution resource (thread id)
- Some algorithms make efficient use of shared resources by dividing based on execution resource (thread id)
- Thread Id is not consistent or portable across all execution environments
- Unique Token provides consistent identifier for resource allocations and work division

Original Example: Random Number Generator Pool

```
int N = 10000000
int K = ...;
RandomGenPool pool(K,seed);
parallel_for("Loop", N, KOKKOS_LAMBDA(int i) {
  int gen_id = ...
  auto gen = pool[gen_id];
});
```

How many generators do we need (`K`)?

Original Example: Random Number Generator Pool

```
int N = 10000000
int K = ...;
RandomGenPool pool(K,seed);
parallel_for("Loop", N, KOKKOS_LAMBDA(int i) {
  int gen_id = ...
  auto gen = pool[gen_id];
});
```

How many generators do we need (`K`)?

How to get a unique one in the loop (`gen_id`)?

Original Example: Random Number Generator Pool

```
int N = 10000000
int K = ...;
RandomGenPool pool(K,seed);
parallel_for("Loop", N, KOKKOS_LAMBDA(int i) {
  int gen_id = ...
  auto gen = pool[gen_id];
});
```

How many generators do we need (`K`)?

How to get a unique one in the loop (`gen_id`)?

In OpenMP we could use the **thread-id** but what in CUDA?

Motivating Example

OpenMP

```
int K = omp_get_max_threads();
Kokkos::parallel_for("L", N, KOKKOS_LAMBDA(int i) {
  int tid = omp_get_thread_num();
});
```

CUDA

```
int K = N; // ??
Kokkos::parallel_for("L", N, KOKKOS_LAMBDA(int i) {
  int tid = threadIdx.x + blockDim.x * blockIdx.x; //i??
});
```

Motivating Example

OpenMP

```
int K = omp_get_max_threads();
Kokkos::parallel_for("L", N, KOKKOS_LAMBDA(int i) {
  int tid = omp_get_thread_num();
});
```

CUDA

```
int K = N; // ??
Kokkos::parallel_for("L", N, KOKKOS_LAMBDA(int i) {
  int tid = threadIdx.x + blockDim.x * blockIdx.x; //i??
});
```

Problem: In **CUDA** there is no way to get **hardware thread-id**.

Motivating Example

OpenMP

```
int K = omp_get_max_threads();
Kokkos::parallel_for("L", N, KOKKOS_LAMBDA(int i) {
  int tid = omp_get_thread_num();
});
```

CUDA

```
int K = N; // ??
Kokkos::parallel_for("L", N, KOKKOS_LAMBDA(int i) {
  int tid = threadIdx.x + blockDim.x * blockIdx.x; //i??
});
```

Problem: In **CUDA** there is no way to get **hardware thread-id**.

Solution: We need a thread-safe and portable way to obtain unique identifier that is per-thread specific.

$\Rightarrow$ **UniqueToken**

UniqueToken is a pool of IDs

- User acquires an ID and releases it again.

```
UniqueToken<ExecutionSpace> token;
int number_of_uniqe_ids = token.size();
RandomGenPool pool(number_of_unique_ids,seed);
parallel_for("L", N, KOKKOS_LAMBDA(int i) {
  int id = token.acquire();
  RandomGen gen = pool(id);
  ...
  token.release(id);
});
```

UniqueToken is a pool of IDs

- User acquires an ID and releases it again.

```
UniqueToken<ExecutionSpace> token;
int number_of_uniqe_ids = token.size();
RandomGenPool pool(number_of_unique_ids,seed);
parallel_for("L", N, KOKKOS_LAMBDA(int i) {
  int id = token.acquire();
  RandomGen gen = pool(id);
  ...
  token.release(id);
});
```

- Do not acquire more than one token in an iteration.
- You must release the token again.
- By default the range of ids is 0 to `ExecSpace().concurrency()`.

Unique Token - Global vs. Instance Scope

Sometimes you need a Global UniqueToken

- Submitting concurrent kernels to CUDA streams (Module 5)
- Shared resource in a multi-threaded environment like Legion

Unique Token - Global vs. Instance Scope

Sometimes you need a Global UniqueToken

- Submitting concurrent kernels to CUDA streams (Module 5)
- Shared resource in a multi-threaded environment like Legion

UniqueToken is Scoped

UniqueToken has a Scope template parameter which by default is 'Instance' but can be 'Global'.

Unique Token - Global vs. Instance Scope

Sometimes you need a Global UniqueToken

- Submitting concurrent kernels to CUDA streams (Module 5)
- Shared resource in a multi-threaded environment like Legion

UniqueToken is Scoped

UniqueToken has a Scope template parameter which by default is 'Instance' but can be 'Global'.

```
void foo() {
  UniqueToken<ExecSpace,UniqueTokenScope::Global> token_foo;
  parallel_for("L", RangePolicy<ExecSpace>(stream1,0,N)
     , functor_a(token_foo));
}
void bar() {
  UniqueToken<ExecSpace,UniqueTokenScope::Global> token_bar;
  parallel_for("L", RangePolicy<ExecSpace>(stream2,0,N)
     , functor_b(token_bar));
}
```

Unique Token - Global vs. Instance Scope

Sometimes you need a Global UniqueToken

- Submitting concurrent kernels to CUDA streams (Module 5)
- Shared resource in a multi-threaded environment like Legion

UniqueToken is Scoped

UniqueToken has a Scope template parameter which by default is 'Instance' but can be 'Global'.

```
void foo() {
  UniqueToken<ExecSpace,UniqueTokenScope::Global> token_foo;
  parallel_for("L", RangePolicy<ExecSpace>(stream1,0,N)
    , functor_a(token_foo));
}
void bar() {
  UniqueToken<ExecSpace,UniqueTokenScope::Global> token_bar;
  parallel_for("L", RangePolicy<ExecSpace>(stream2,0,N)
    , functor_b(token_bar));
}
```

token_foo and token_bar will provide non-conflicting ids.

UniqueToken can also be used for Per-Team resources

There are less teams active than threads. How to get an ID?

Unique Token - Per Team

UniqueToken can also be used for Per-Team resources

There are less teams active than threads. How to get an ID?

Sized UniqueToken

UniqueToken supports custom ranges of ids via constructing sized tokens.

UniqueToken can also be used for Per-Team resources

There are less teams active than threads. How to get an ID?

Sized UniqueToken

UniqueToken supports custom ranges of ids via constructing sized tokens.

Acquiring a per-team unique id requires three steps:

- Compute the range via `concurrency` and `team_size`.
- Create a sized `UniqueToken`.
  - For performance reason make it a bit larger than necessary.
- Acquire and broadcast a token in a `single` pattern.

Unique Token - Per Team

```
// Figure out the team size
int team_size = ...;
// How many teams are actually in-flight
int num_active_teams = ExecSpace().concurrency()/team_size;
// Create the token
UniqueToken<ExecSpace> token(num_active_teams * 1.2);

parallel_for("L", TeamPolicy<ExecSpace>(N,team_size),
  KOKKOS_LAMBDA(const team_t& team) {
    int id;
    // Acquire an id and broadcast it with a single thread
    single(PerTeam(team),[&](int &lid) {
      lid = token.acquire();
    },id);
    ...
    // Release the id again (likely you want a barrier first!)
    single(PerTeam(team),[&]() {
      token.release(id);
    });
```

Exercise UniqueToken

- Location: `Exercises/unique_token/Begin/`
- Assignment: Convert scatter_add_loop to use `UniqueToken`, removing #ifdef's
- Compile and run on both CPU and GPU

```
make -j KOKKOS_DEVICES=OpenMP  # CPU-only using OpenMP
make -j KOKKOS_DEVICES=Cuda    # GPU - note UVM in Makefile
# Run exercise
./uniquetoken.host
./uniquetoken.cuda
# Note the warnings, set appropriate environment variables
```

- Compare performance on CPU of the three variants
- Compare performance on GPU of the two variants
- Vary problem size: first and second optional argument

- **UniqueToken** provides a thread safe portable way to divide thread or team specific resources
- **UniqueToken** can be sized, such that it returns only ids within a specific range.
- A **Global** scope UniqueToken can be acquired, allowing safe ids accross disjoint concurrent code sections.

Hierarchal Parallelism

- **Hierarchical work** can be parallelized via hierarchical parallelism.
- Hierarchical parallelism is leveraged using **thread teams** launched with a `TeamPolicy`.
- Team "worksets" are processed by a team in nested `parallel_for` (or `reduce` or `scan`) calls with a `TeamThreadRange` and `ThreadVectorRange` policy.
- Execution can be restricted to a subset of the team with the `single` pattern using either a `PerTeam` or `PerThread` policy.
- Teams can be used to **reduce contention** for global resources even in "flat" algorithms.

Scratch Space

- **Scratch Memory** can be use with the `TeamPolicy` to provide thread or team **private** memory.
- Usecase: per work-item temporary storage or manual caching.
- Scratch memory exposes on-chip user managed caches (e.g. on NVIDIA GPUs)
- The size must be determined before launching a kernel.
- Two levels are available: large/slow and small/fast.

Unique Token

- **UniqueToken** give a thread safe portable way to divide thread specific resources
- **UniqueToken** can be sized to restrict ids to a range.
- A **Global** UniqueToken is available.

Task Parallelism:

- Basic interface for fine-grained tasking in Kokkos
- How to express dynamic dependency structures in Kokkos

Streams: Concurrent Execution Spaces

- How to use Streams within Kokkos Execution spaces

SIMD: Portable vector intrinsic types

- How to use SIMD types to improve vectorization
- Alternative to ThreadVector loops and outer loop vectorization

Don't Forget: Join our Slack Channel and drop into our office hours on Tuesday.

Updates at: kokkos.link/the-lectures-updates

Recordings/Slides: kokkos.link/the-lectures