The Kokkos Lectures

Module 4: Hierarchical Parallelism

June 17, 2024

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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://kokkos.github.io/kokkos-core-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.

- 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

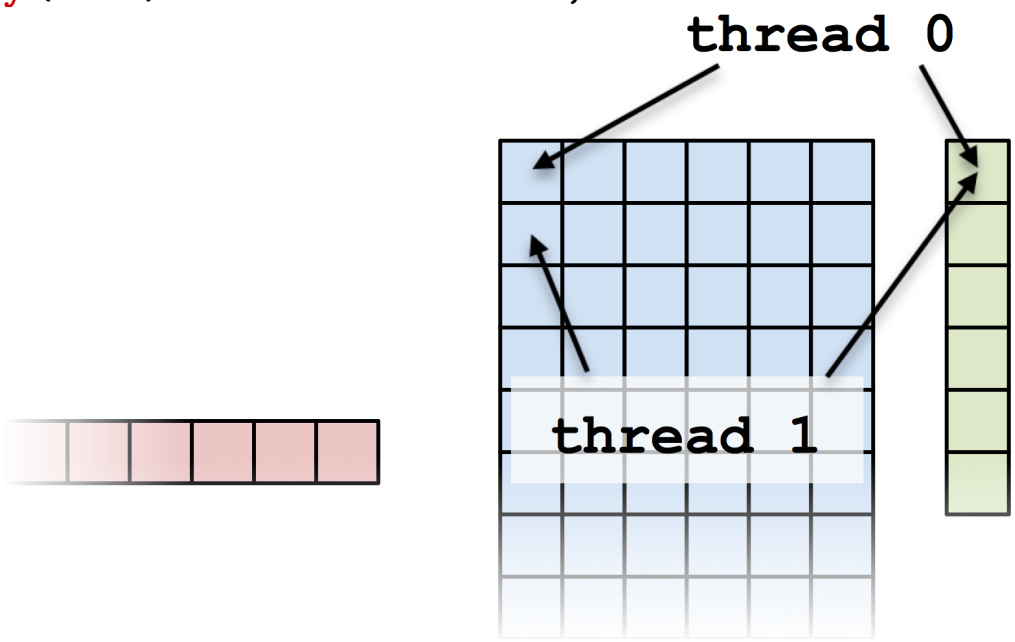
Finding and exploiting more parallelism in your computations.

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

(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);
```



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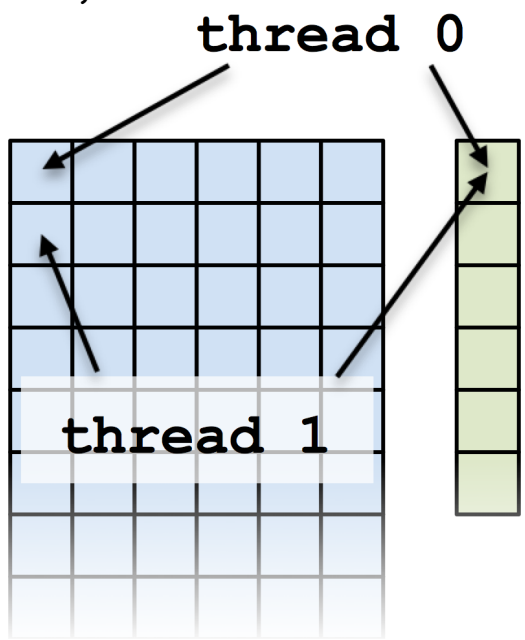
```

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



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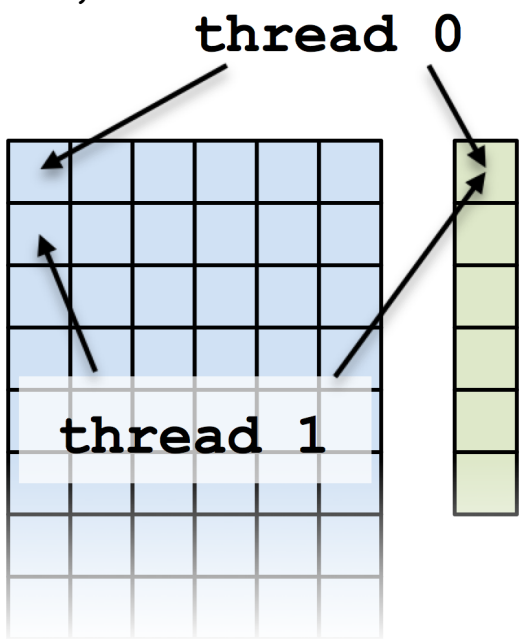

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Solutions?

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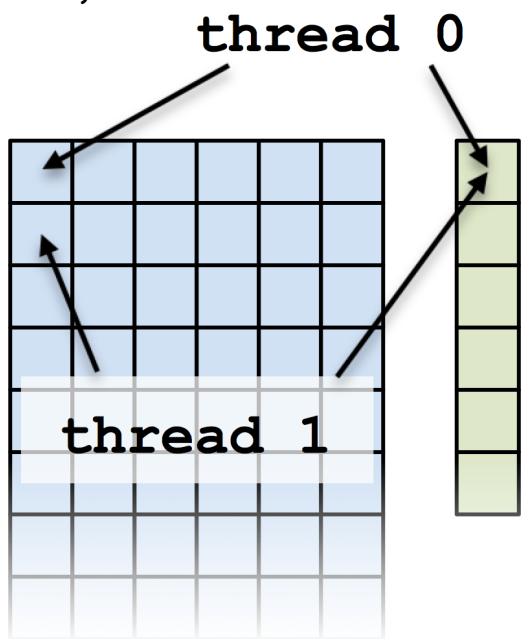


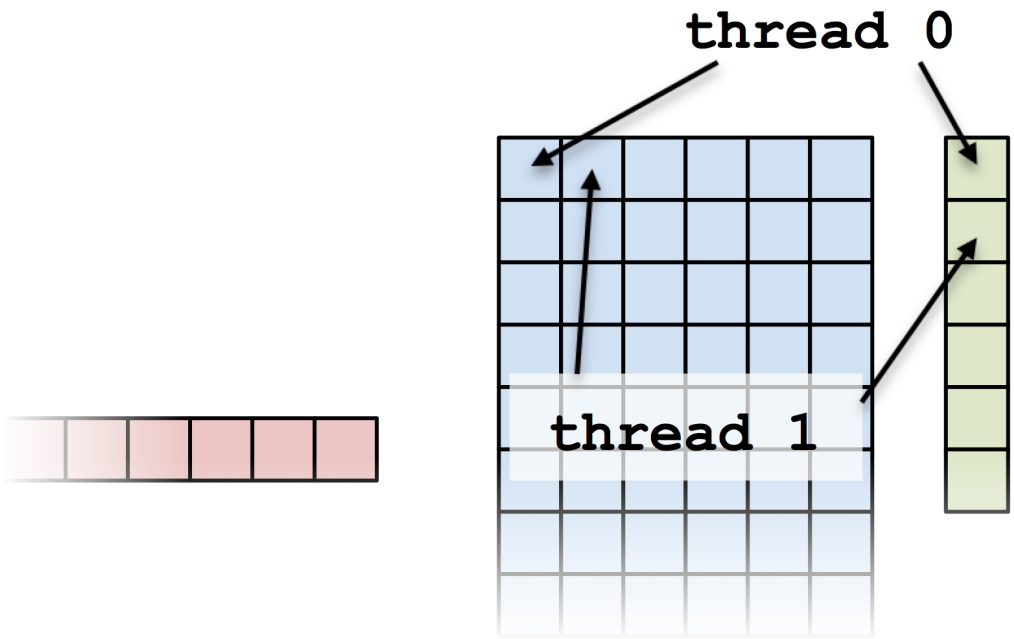
Problem: What if we don't have enough rows to saturate the GPU?

Solutions?

- Atomics
- Thread teams

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));
  });
```



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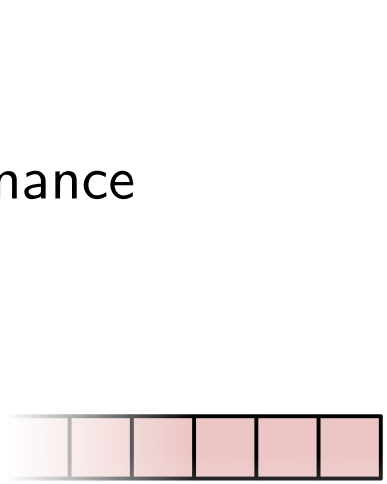
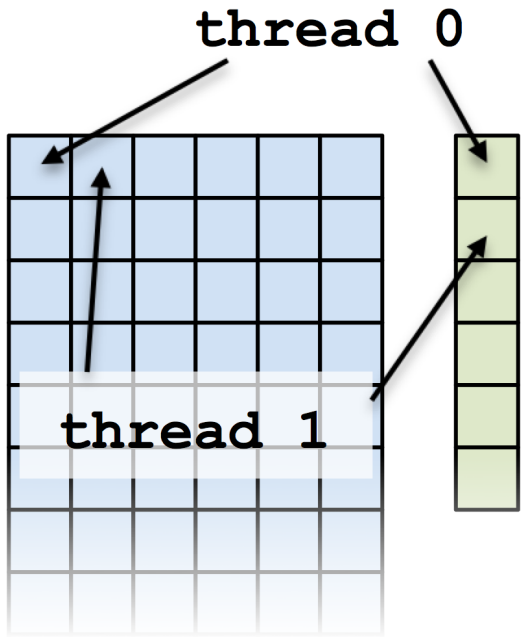
Problem: Poor performance





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**.

Important concept: Thread team

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

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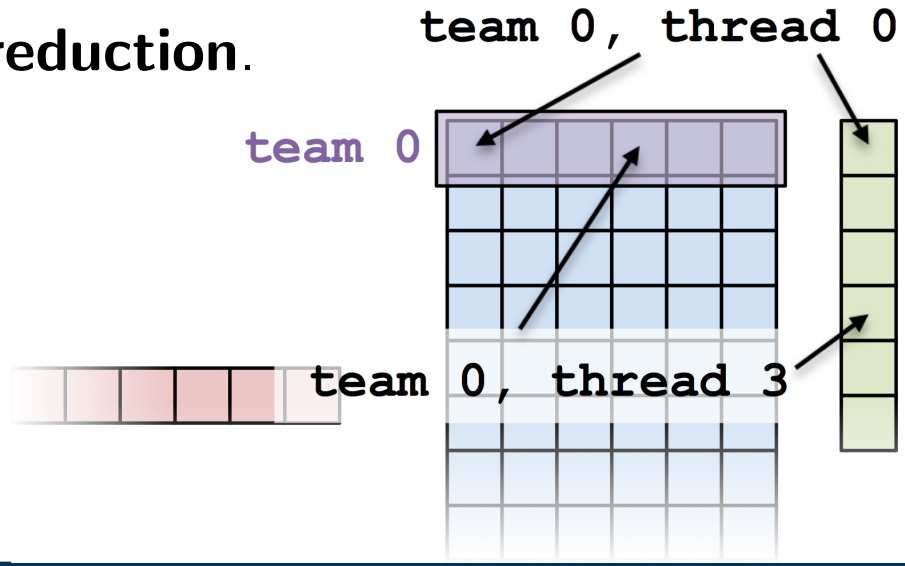
A collection of threads which are guaranteed to be executing **concurrently** and **can synchronize**.

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**.



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);
```

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);
```

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

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```
// 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);
```

Important point

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

```
using member_type = typename TeamPolicy<ExecSpace>::member_type;

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

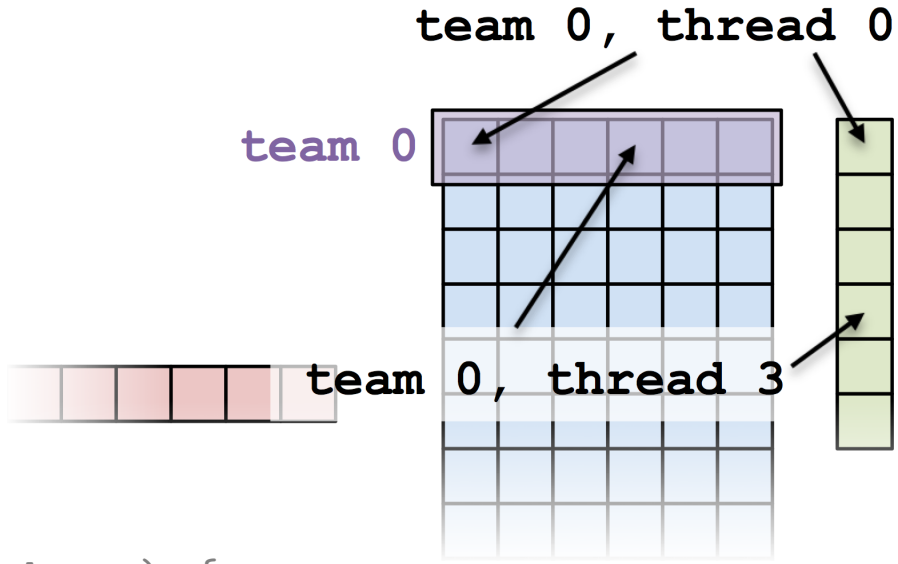
  // Which team am I on?
  const unsigned int league_rank = teamMember.league_rank();

  // 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();
}
```

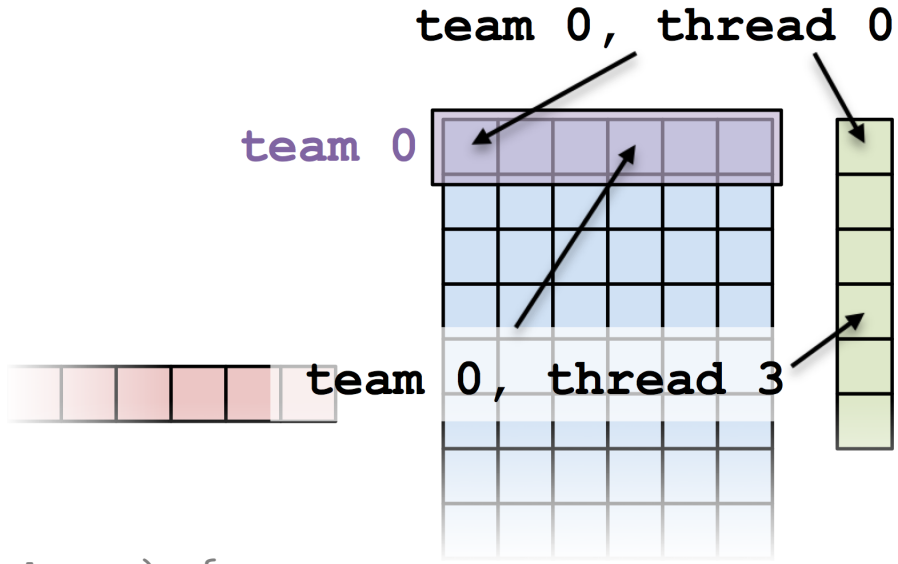
TeamThreadRange (0)



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)



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}
```

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

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));
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  }
}
```

- 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;
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If this were a parallel execution,

we'd use `Kokkos::parallel_reduce`.

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Key idea: this *is* a parallel execution.

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$\Rightarrow$ **Nested parallel patterns**

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) {
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  }
}
```

- 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.

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

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

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Intel Xeon Phi:

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

Details:

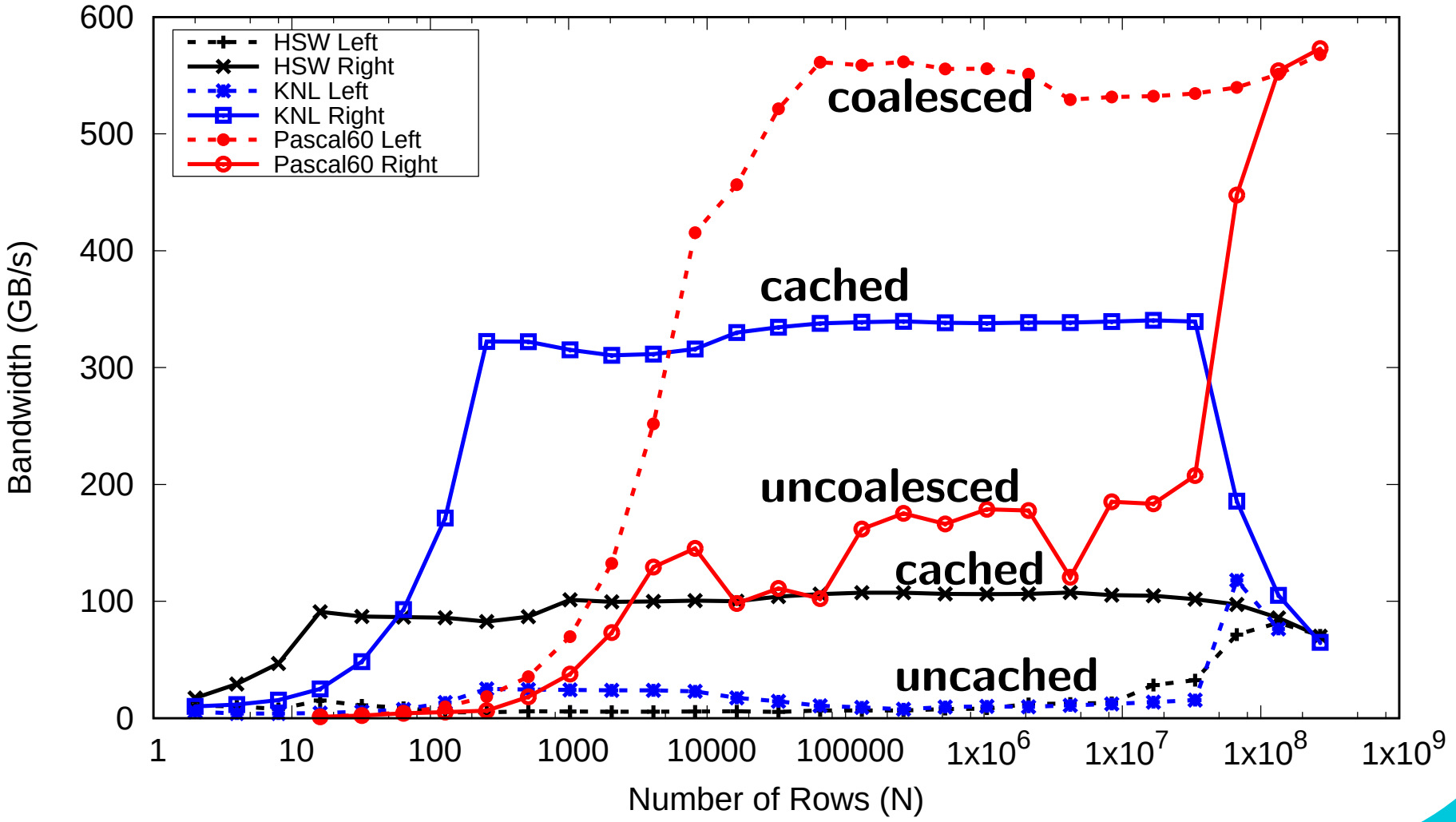
- Location: `Exercises/team_policy/`
- Replace `RangePolicy<Space>` with `TeamPolicy<Space>`
- Use `AUTO` for `team_size`
- Make the inner loop a `parallel_reduce` with `TeamThreadRange` policy
- Experiment with the combinations of `Layout`, `Space`, `N` to view performance
- Hint: what should the layout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

<y|Ax> Exercise 04 (Layout) Fixed Size

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



<y|Ax> Exercise 05 (Layout/Teams) Fixed Size

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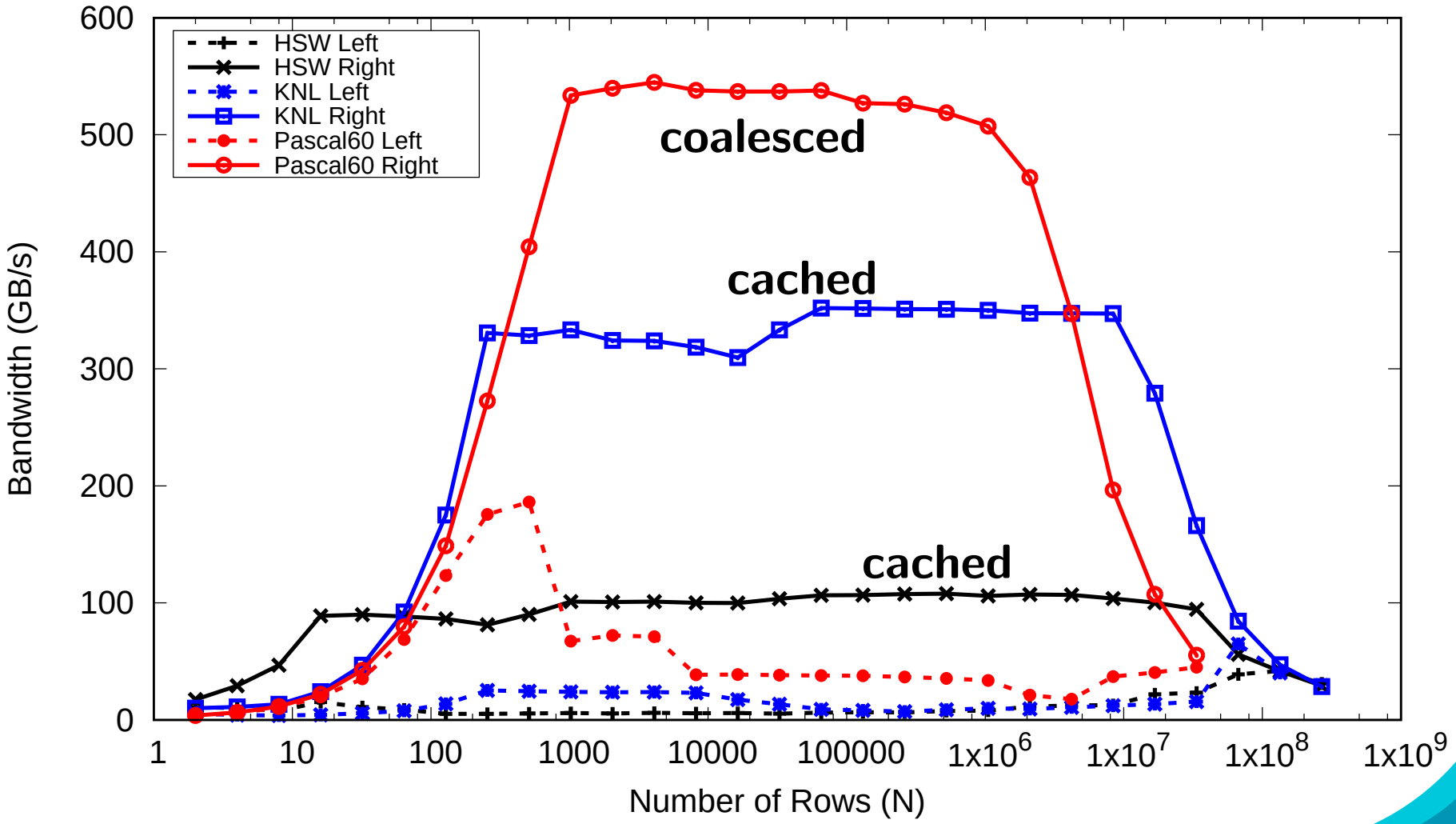

Exposing Vector Level Parallelism

- 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 */
  }[, ...]);
```

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);
```

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```

`totalSum = numberOfThreads * 10`

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) {
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`totalSum = numberOfTeams * team_size * 10`

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    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;
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      int thisThreadsSum = 0;
      for (int i = 0; i < 10; ++i) {
        ++thisThreadsSum;
      }
      thisTeamsPartialSum += thisThreadsSum;
    }, thisTeamsSum);
    partialSum += thisTeamsSum;
}, totalSum);
```

`totalSum = numberOfTeams * team_size * team_size * 10`

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:

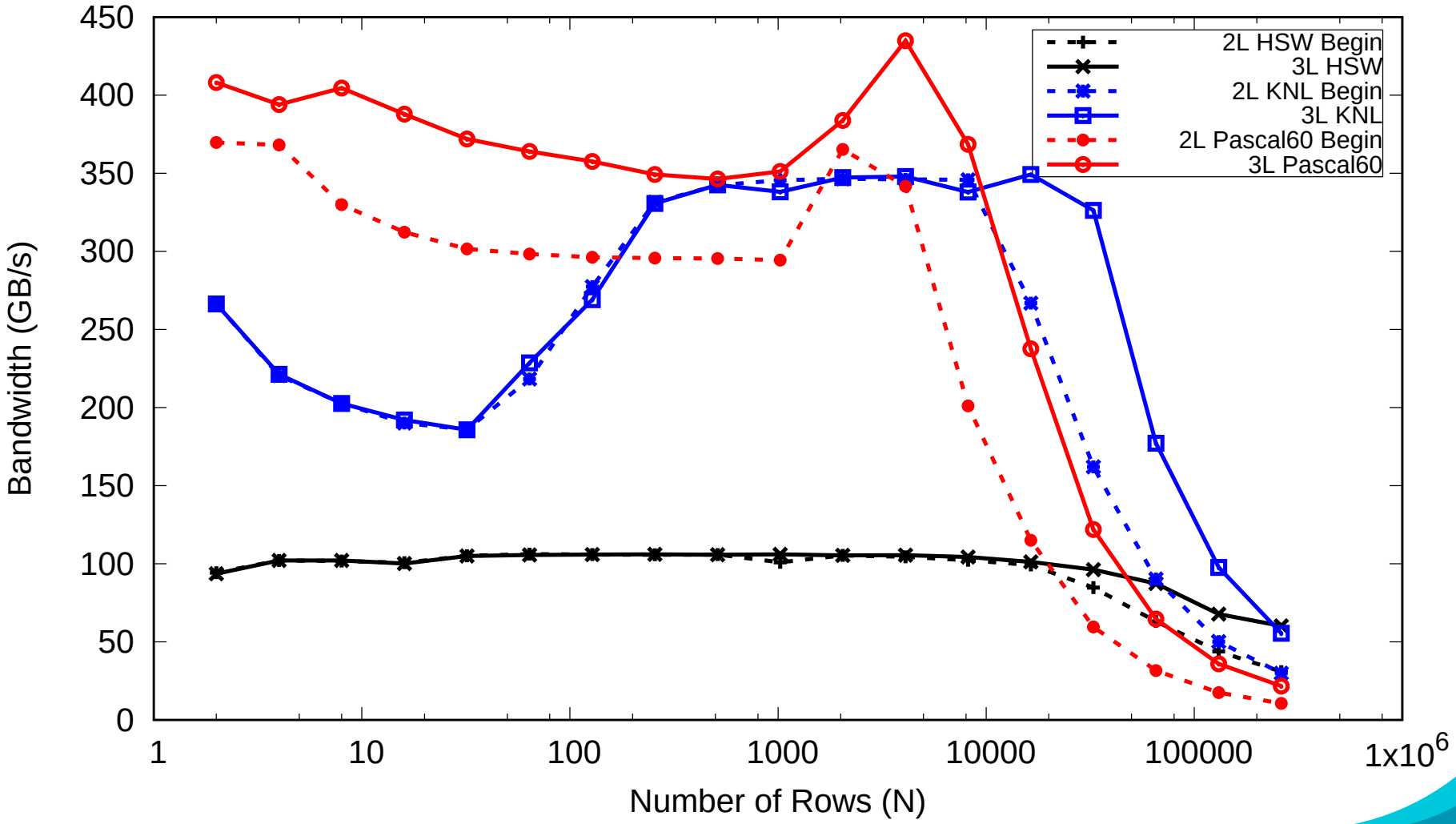
- Location: `Exercises/team_vector_loop/`
- Use the `single` policy instead of checking team rank
- Parallelize all three loop levels.

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



- **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

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).

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.

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- Typically used for per work-item temporary storage.
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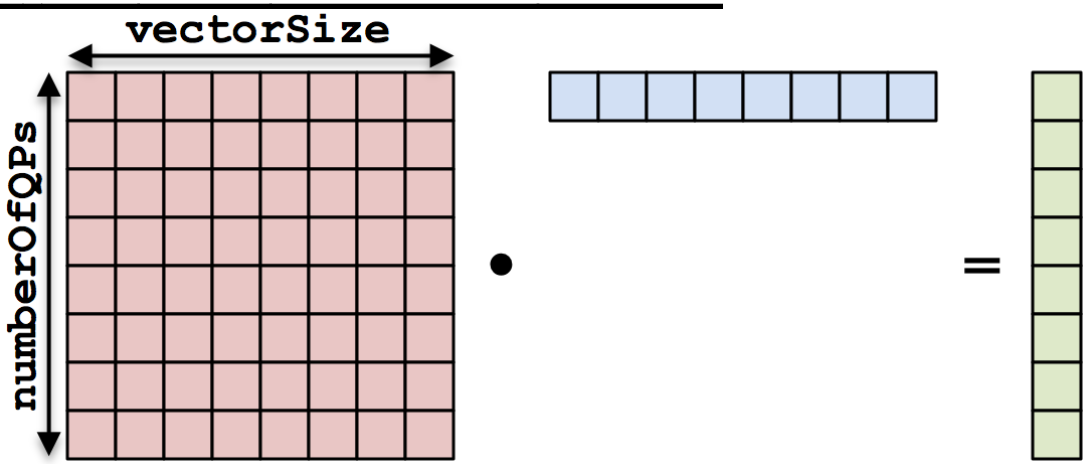
Manually Managed Cache

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

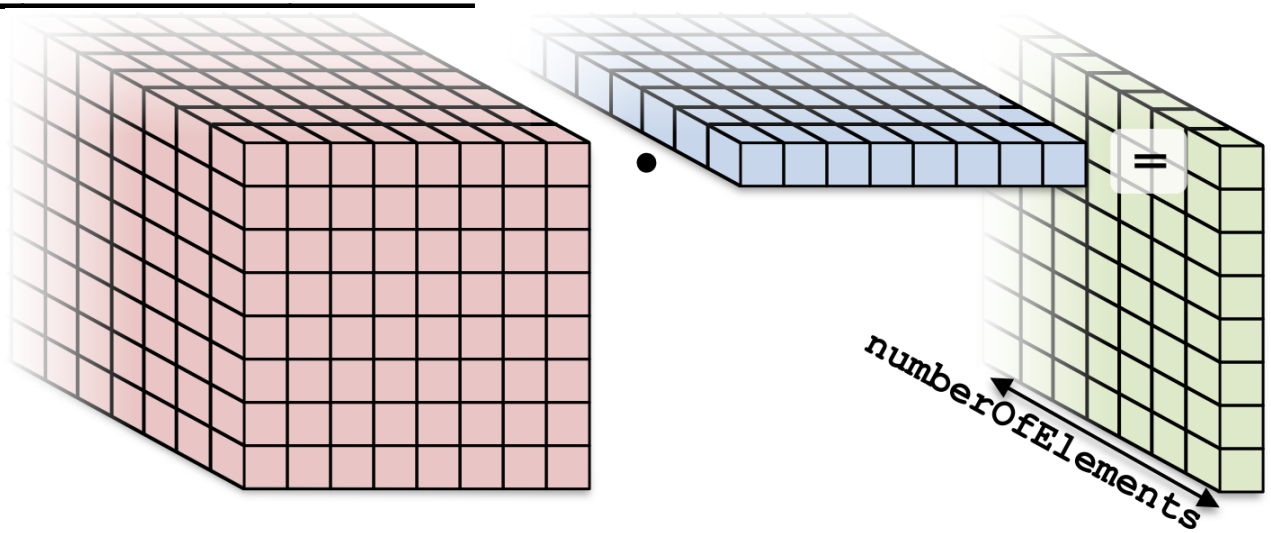
Now: Discuss Manually Managed Cache Usecase.

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;
}
```

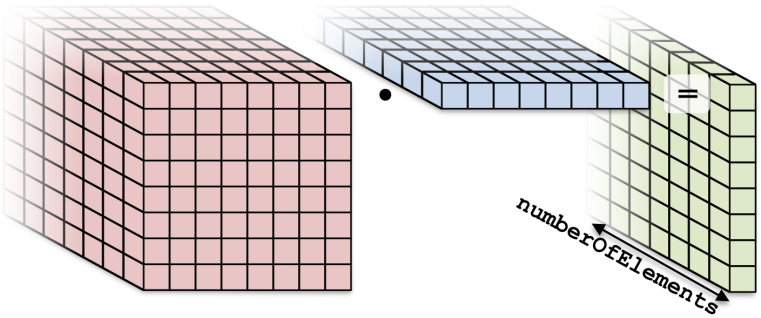
contractDataFieldScalar:




```
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;
  }
}
```



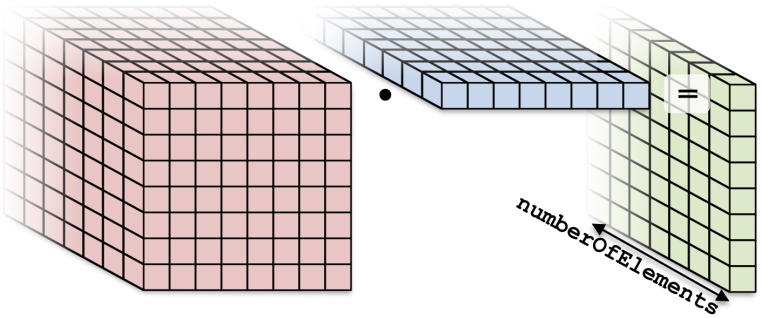
Parallelization approaches:

- Each thread handles an `element`.

  Threads: `numberOfElements`

Example: contractDataFieldScalar (3)

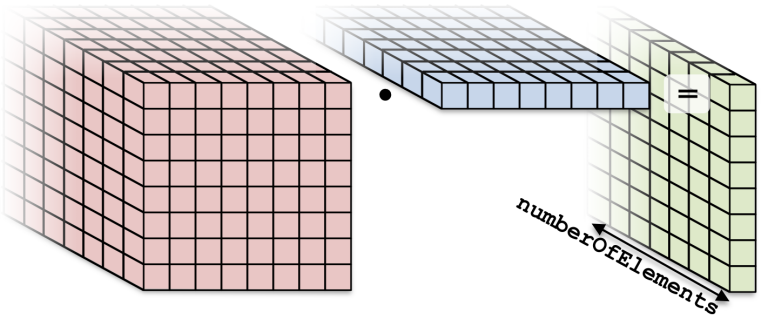
```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```



Parallelization approaches:

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

```
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;
  }
}
```

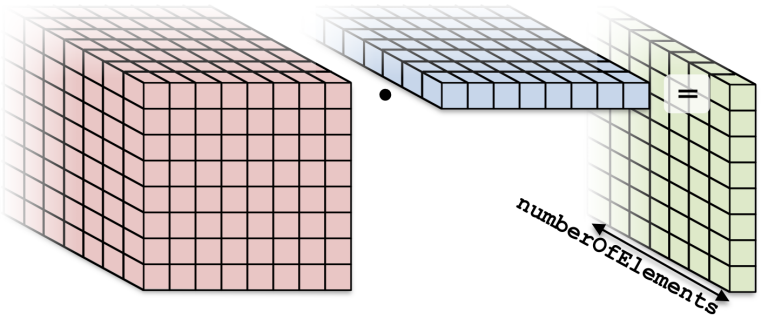


Parallelization approaches:

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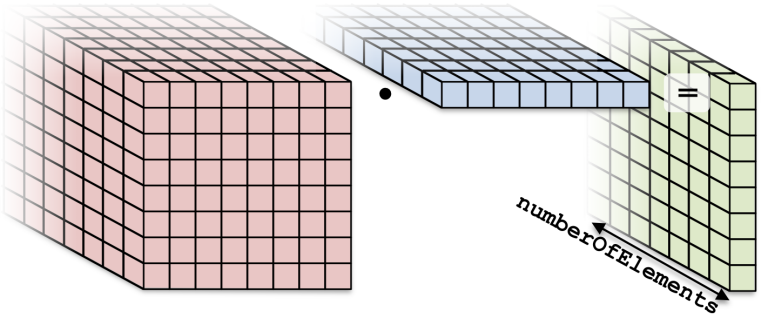
- Each thread handles a `qp`.
  Threads: `numberOfElements * numberOfQPs`
- Each thread handles an `i`.
  Threads: `numElements * numQPs * vectorSize`
  Requires a `parallel_reduce`.

Example: contractDataFieldScalar (4)

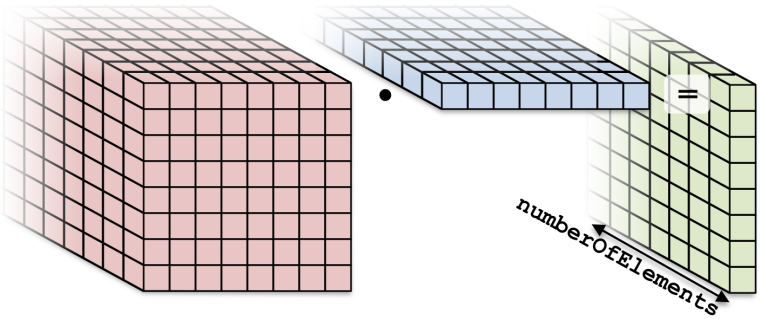
```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```



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;
}
```

```
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;
  }
}
```

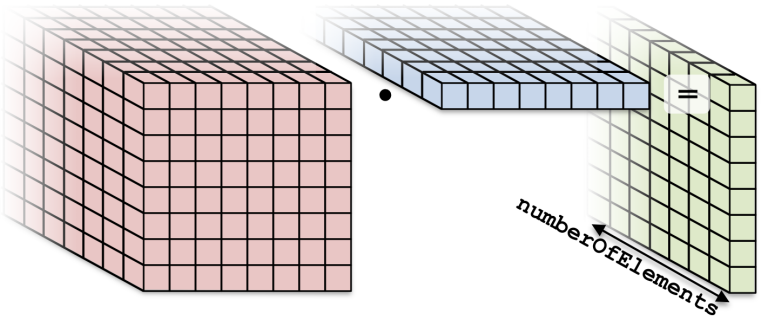


Teams kernel: Each team handles an element

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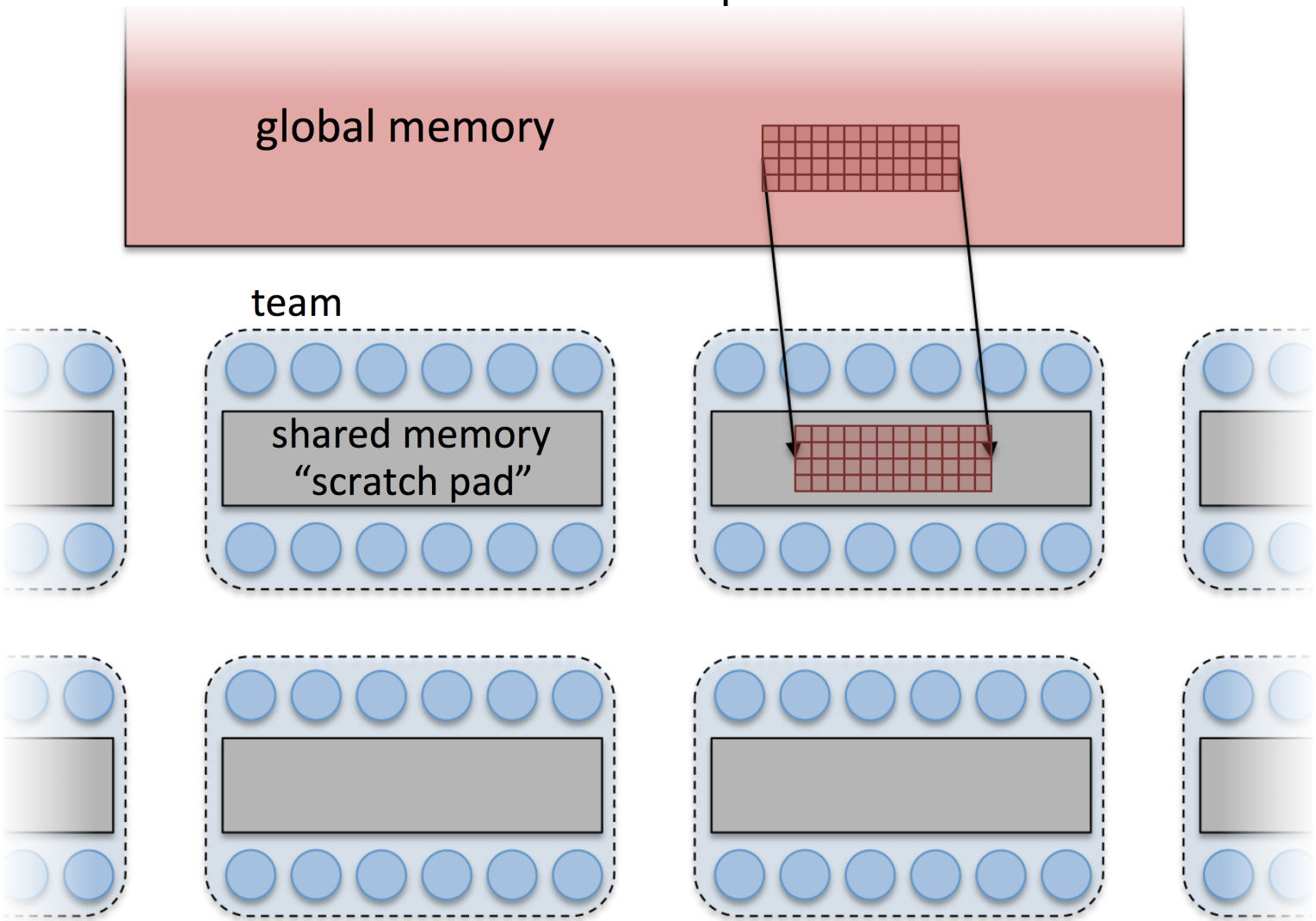
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * B(element, i);
      }
      result(element, qp) = total;
    });
}
```

No real advantage (yet)

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.

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- **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 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 for temporary per work-item storage:

- Scenario: Algorithm requires temporary workspace of size W.
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- **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.

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.

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);

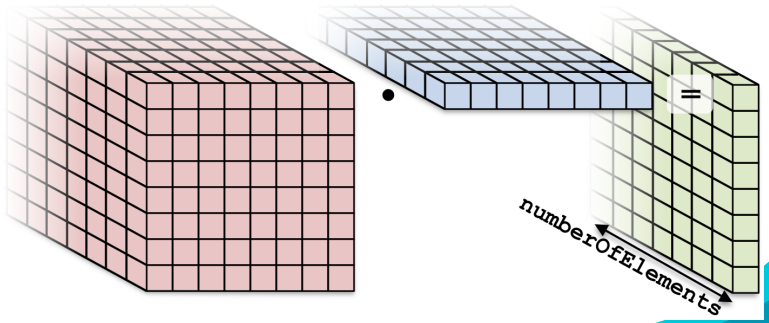
// Tell the policy how much scratch memory is needed
int level = 0;
parallel_for(policy.set_scratch_size(level, PerTeam(bytes)),
  KOKKOS_LAMBDA (const member_type& teamMember) {

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

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

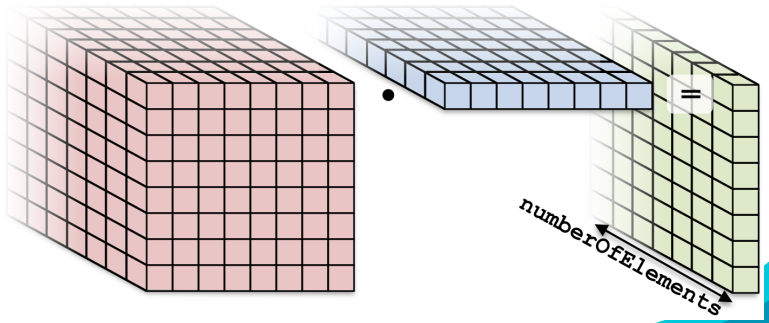
  parallel_for(
    TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        // total += A(element, qp, i) * B(element, i);
        total += A(element, qp, i) * scratch(i);
      }
      result(element, qp) = total;
    });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



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);
  }
}
```



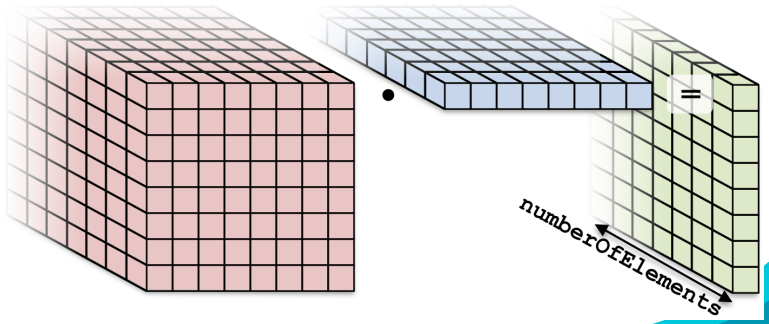
How to populate the scratch memory?

- ~~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);
```



How to populate the scratch memory?

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

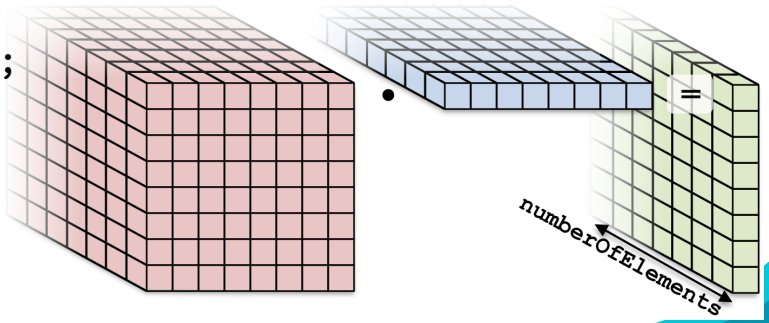
```
if (teamMember.team_rank() == 0) {
  for (int i = 0; i < vectorSize; ++i) {
    scratch(i) = B(element, i);
  }
}
```

- ~~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

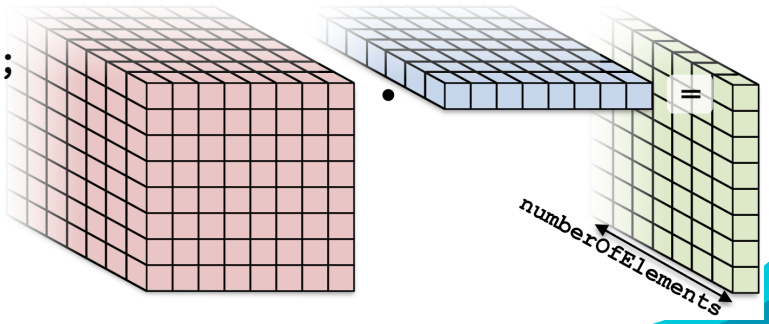
```
if (teamMember.team_rank() == 0) {
  for (int i = 0; i < vectorSize; ++i) {
    scratch(i) = B(element, i);
  }
}
```

- ~~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);
  });
```



(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;
    });
}
```

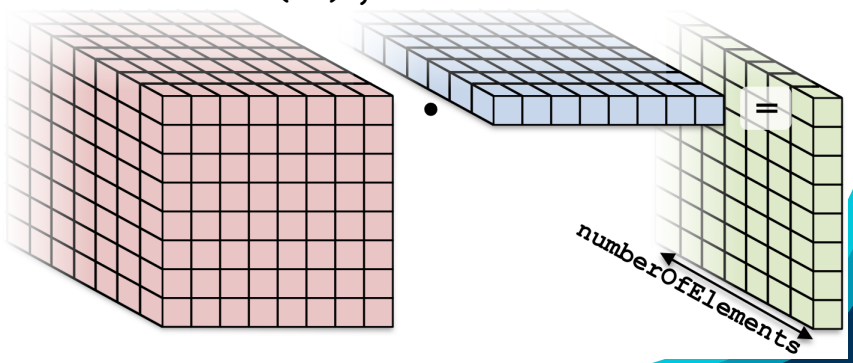
Problem: threads may start to use `scratch` before all threads are done loading.

Kernel for teams with scratch memory:

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

  parallel_for(TeamVectorRange(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;
    });
}
```



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

Details:

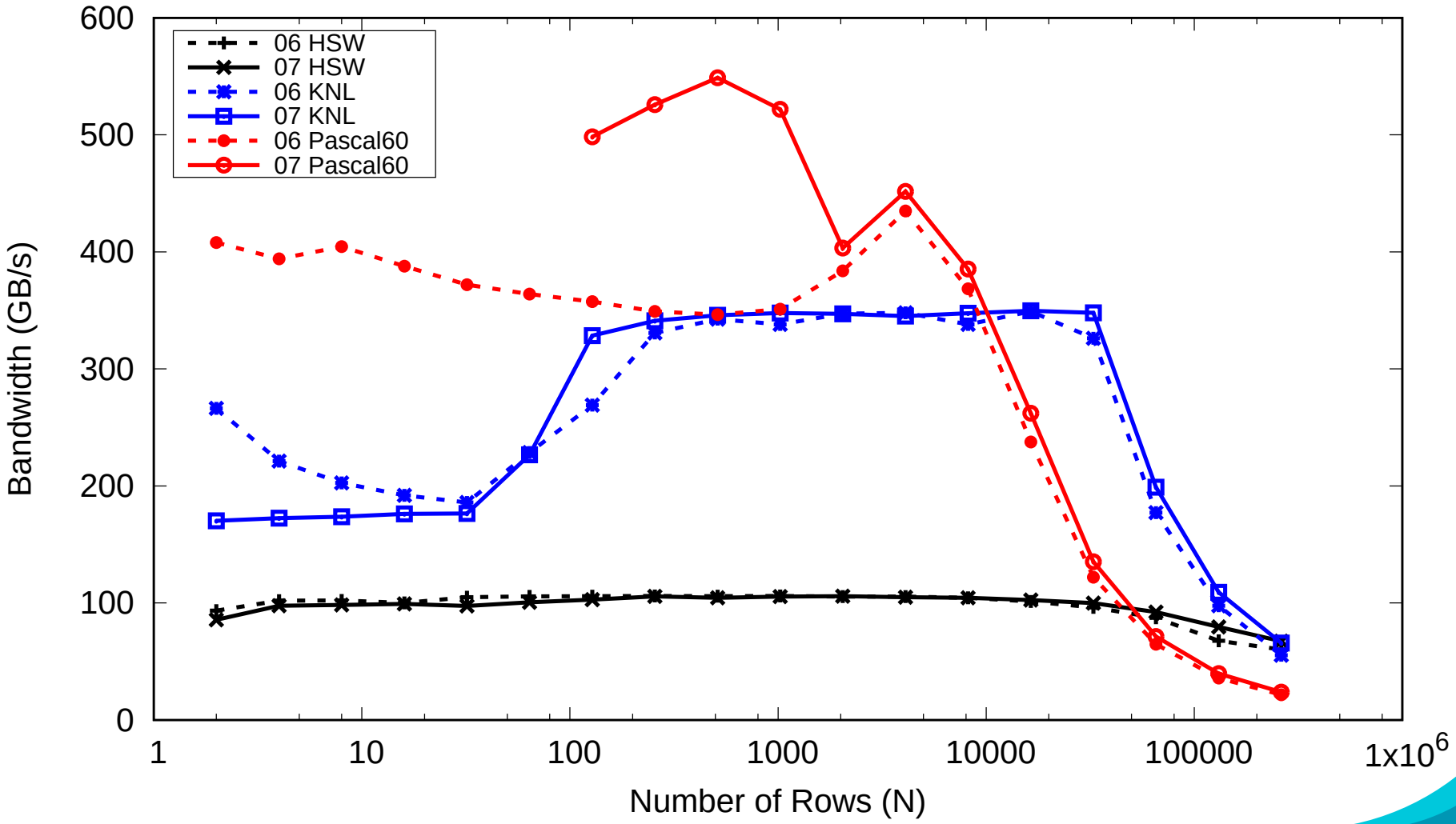
- Location: `Exercises/team_scratch_memory/`
- Create a scratch view
- Fill the scratch view in parallel using a TeamVectorRange

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



Allocating scratch in different levels:

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

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));
```

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.

- **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.

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 = ...
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```

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??
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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);
});
```

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  ...
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});
```

- 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()`.

Sometimes you need a Global UniqueToken

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

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```
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));
}
```

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}
```

`token_foo` and `token_bar` will provide non-conflicting ids.

UniqueToken can also be used for Per-Team resources

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Sized UniqueToken

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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);
    });
```

- 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 the Slack Channel and drop into our office hours on Monday.

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

Recordings/Slides: kokkos.link/the-lectures