

# The Kokkos Lectures

Module 4: Hierarchical Parallelism

July 28, 2026

## Online Resources:

- ▶ <https://github.com/kokkos>:
  - ▶ Primary Kokkos GitHub Organization
- ▶ <https://kokkos.org/kokkos-core-wiki/videolectures.html>
  - ▶ Slides, recording and Q&A for the Lectures
- ▶ <https://kokkos.org/kokkos-core-wiki>:
  - ▶ Programming guide and API reference documentation
- ▶ <https://kokkosteam.slack.com>:
  - ▶ Slack channel for Kokkos.
  - ▶ Please join: fastest way to get your questions answered.
  - ▶ Can whitelist domains, or invite individual people.

- ▶ Module 1: Introduction, Building and Parallel Dispatch
- ▶ Module 2: Views and Spaces
- ▶ Module 3: Data Structures + MultiDimensional Loops
- ▶ **Module 4: Hierarchical Parallelism**
- ▶ Module 5: Tasking, Streams and SIMD
- ▶ Module 6: Internode: MPI and PGAS
- ▶ Module 7: Tools: Profiling, Tuning and Debugging
- ▶ Module 8: Kernels: Sparse and Dense Linear Algebra
- ▶ Module 9: Fortran inter-op

## 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:**

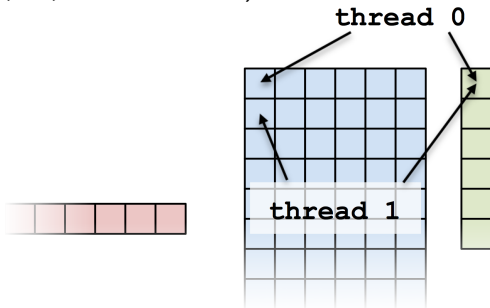
- ▶ Similarities and differences between outer and inner levels of parallelism
- ▶ Thread teams (league of teams of threads)
- ▶ Performance improvement with well-coordinated teams

## (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);

```



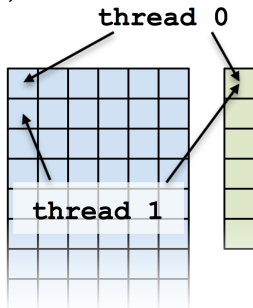
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```

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



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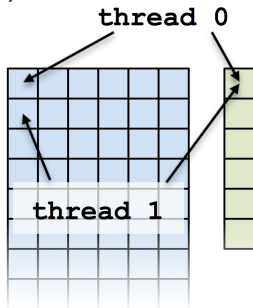
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```

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

**Solutions?**



## (Flat parallel) Kernel:

```

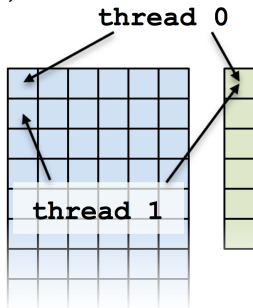
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```

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

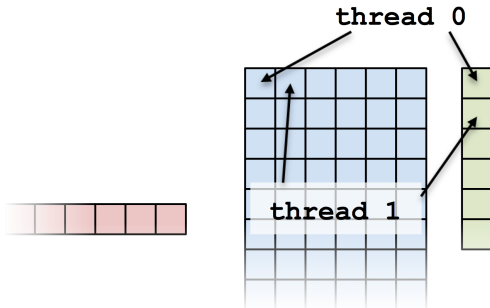
### Solutions?

- ▶ Atomics
- ▶ Thread teams



## Atoms kernel:

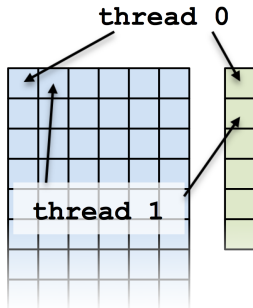
```
Kokkos::parallel_for("yAx", N*M,  
  KOKKOS_LAMBDA (const size_t index) {  
    const int row = extractRow(index);  
    const int col = extractCol(index);  
    atomic_add(&result, y(row) * A(row,col) * x(col));  
  });
```



## 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



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);
}
```

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

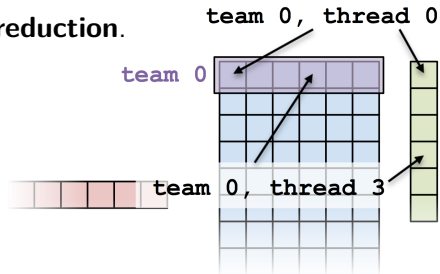
A collection of threads which are guaranteed to be executing **concurrently** and **can synchronize**.

## 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**.



## 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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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);
```

## Important point

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

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

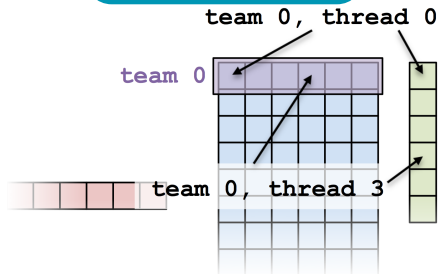
void operator()(const member_type & teamMember) {
    // How many teams are there?
    const unsigned int league_size = teamMember.league_size();

    // 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();

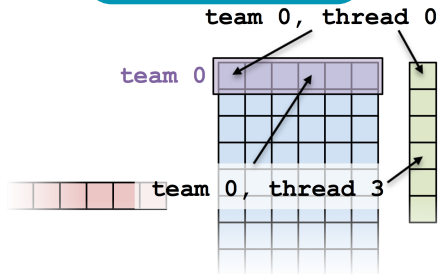
    // Which thread am I on this team?
    const unsigned int team_rank = teamMember.team_rank();

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



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));
}
```



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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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}
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If this were a parallel execution,  
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**Key idea:** this *is* a parallel execution.

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**Key idea:** this *is* a parallel execution.

⇒ **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) {  
        update += y(row) * thisRowsSum;  
    }  
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```

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            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.

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:**

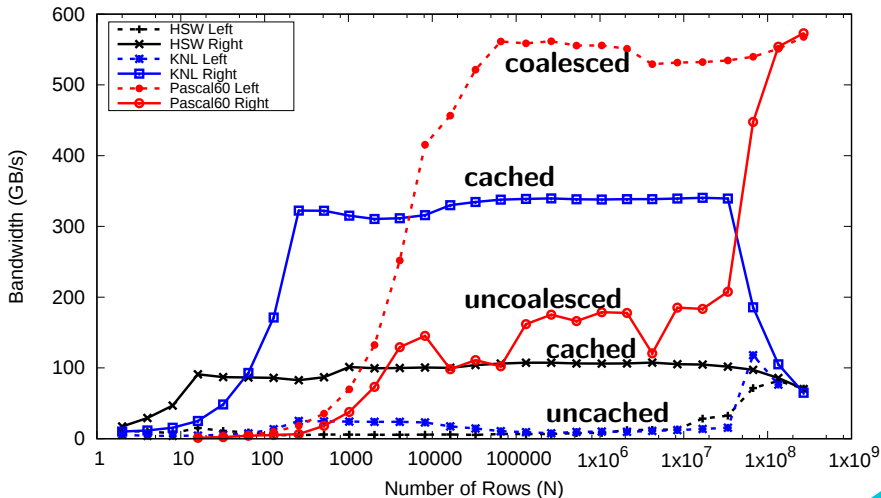
- ▶ Location: Exercises/team\_policy/
- ▶ Replace `RangePolicy<Space>` with `TeamPolicy<Space>`
- ▶ Use `AUTO` for `team_size`
- ▶ Make the inner loop a `parallel_reduce` with `TeamThreadRange` policy
- ▶ Experiment with the combinations of `Layout`, `Space`, `N` to view performance
- ▶ Hint: what should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

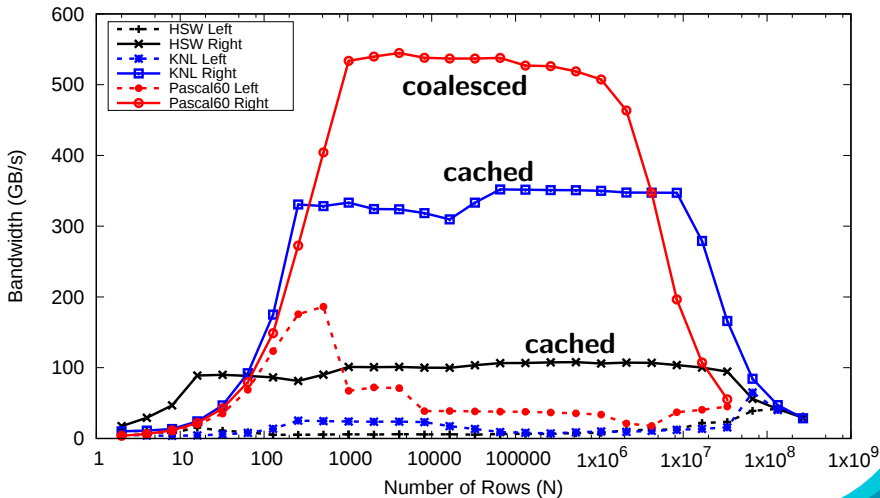
## <y|Ax> Exercise 04 (Layout) Fixed Size

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



## &lt;y|Ax&gt; Exercise 05 (Layout/Teams) Fixed Size

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



## 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);
```

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

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

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

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        }
        partialSum += thisThreadsSum;
    }, totalSum);
```

`totalSum = numberOfTeams * team_size * 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) {
    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);
```

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parallel_reduce("Sum", TeamPolicy<>(numberOfTeams, team_size),
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        [=] (const int index, int& thisTeamsPartialSum) {
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        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:**

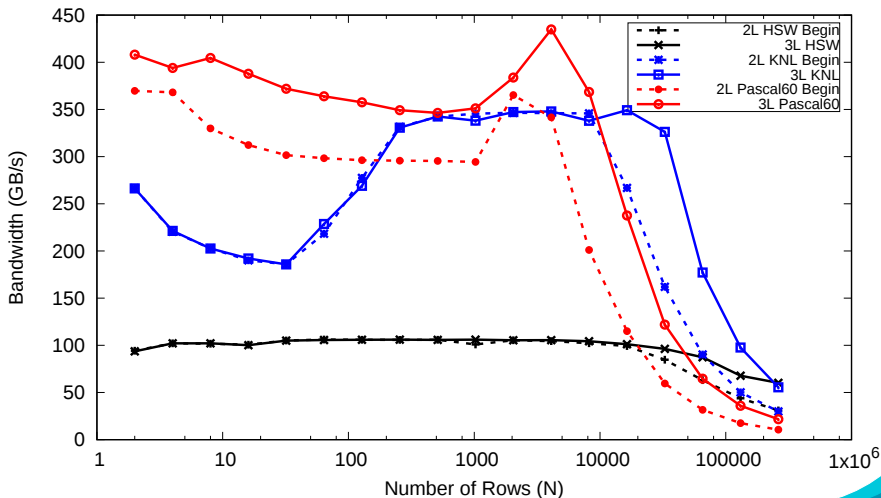
- ▶ Location: Exercises/team\_vector\_loop/
- ▶ Use the `single` policy instead of checking team rank
- ▶ Parallelize all three loop levels.

**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

## &lt;y|Ax&gt; 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.

### Team or Thread private memory

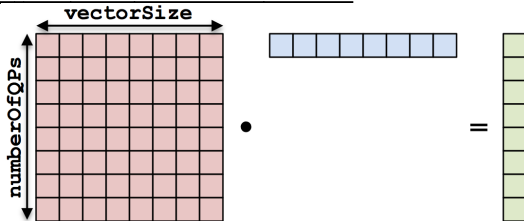
- ▶ Typically used for per work-item temporary storage.
- ▶ Advantage over pre-allocated memory is aggregate size scales with number of threads, not number of work-items.

### Manually Managed Cache

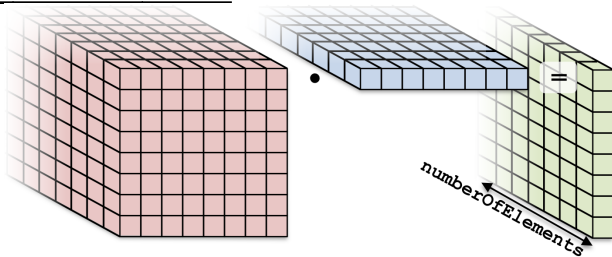
- ▶ Explicitly cache frequently used data.
- ▶ Exposes hardware specific on-core scratch space (e.g. NVIDIA GPU Shared Memory).

**Now: Discuss Manually Managed Cache Usecase.**

## One slice of contractDataFieldScalar:

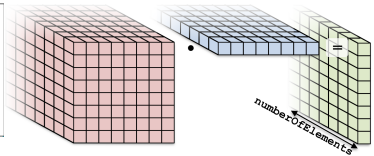


```
for (qp = 0; qp < numberOfQPs; ++qp) {  
    total = 0;  
    for (i = 0; i < vectorSize; ++i) {  
        total += A(qp, i) * B(i);  
    }  
    result(qp) = total;  
}
```

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;  
    }  
}
```

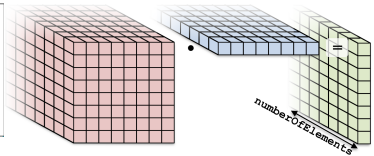
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    }  
    result(element, qp) = total;  
  }  
}
```



### Parallelization approaches:

- ▶ Each thread handles an element.  
Threads: numberOfElements

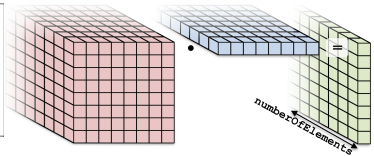
```
for (element = 0; element < numberOfElements; ++element) {  
  for (qp = 0; qp < numberOfQPs; ++qp) {  
    total = 0;  
    for (i = 0; i < vectorSize; ++i) {  
      total += A(element, qp, i) * B(element, i);  
    }  
    result(element, qp) = total;  
  }  
}
```



### Parallelization approaches:

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

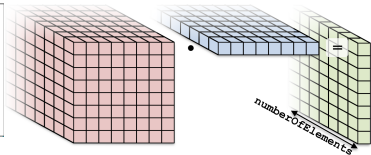
```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
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}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



### 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.*

```
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.

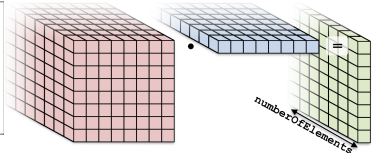
Threads: numberOfElements \* numberOfQPs

- ▶ Each thread handles an i.

Threads: numElements \* numQPs \* vectorSize

*Requires a parallel\_reduce.*

```
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;
  }
}
```



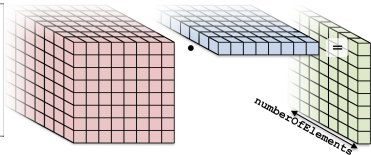
## Flat kernel: Each thread handles a quadrature point

```
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;
  }
}

```



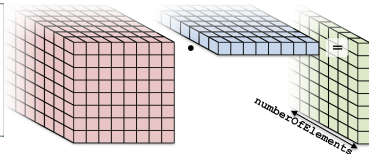
## Teams kernel: Each team handles an element

```

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;
    });
}

```

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

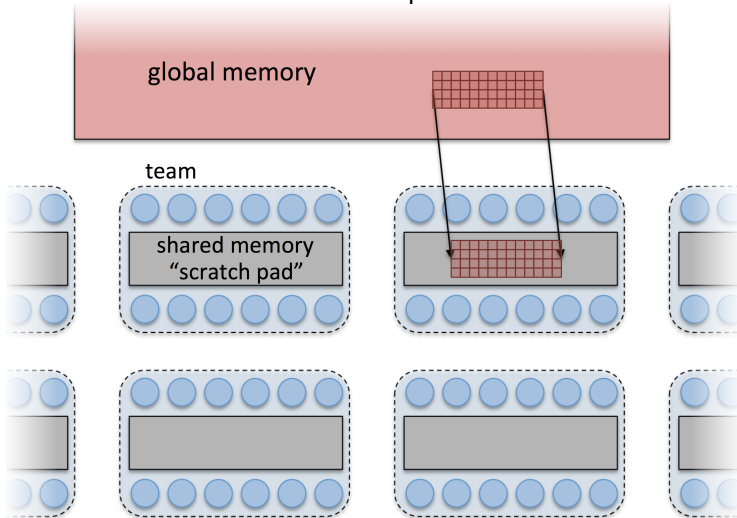


## Teams kernel: Each team handles an element

```
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)

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  $N \times W$ .
- ▶ **With scratch memory:** Kokkos pre-allocates space for each Team or Thread of size  $T \times W$ .
- ▶ `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:

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- ▶ 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);

});
```

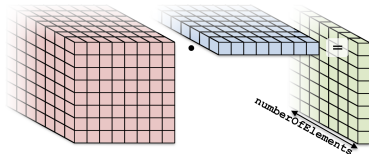
## Kernel outline for teams with scratch memory:

```

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;
        });
}

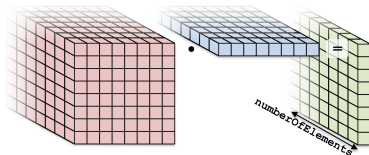
```



## 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);  
    }  
}
```



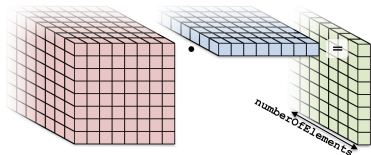
## How to populate the scratch memory?

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

```
if (teamMember.team_rank() == 0) {  
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    }  
}
```

- ▶ Each thread loads one entry?

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



## How to populate the scratch memory?

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

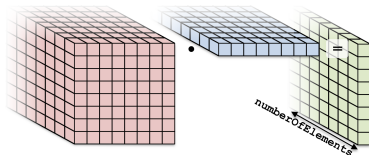
```
if (teamMember.team_rank() == 0) {
    for (int i = 0; i < vectorSize; ++i) {
        scratch(i) = B(element, i);
    }
}
```

- ▶ ~~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**

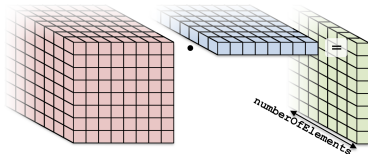
```
if (teamMember.team_rank() == 0) {
    for (int i = 0; i < vectorSize; ++i) {
        scratch(i) = B(element, i);
    }
}
```

- ▶ ~~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;  
        });  
}
```

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```
operator()(member_type teamMember) {
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    parallel_for(TeamThreadRange(teamMember, numberOfQPs),
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            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:

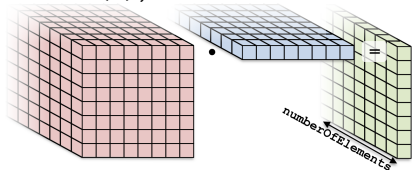
```

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:**

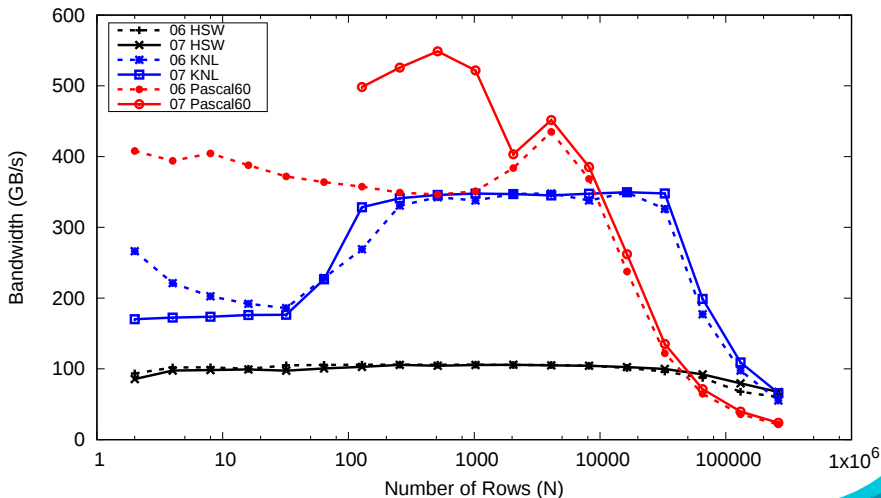
- ▶ Location: `Exercises/team_scratch_memory/`
- ▶ Create a scratch view
- ▶ Fill the scratch view in parallel using a `TeamVectorRange`

### **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:

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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 = 100000000
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

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int N = 100000000
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**How many generators do we need ( $K$ )?**

**How to get a unique one in the loop ( $gen\_id$ )?**

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    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??  
});
```

## Motivating Example

### OpenMP

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

## Motivating Example

### OpenMP

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    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.

⇒ **UniqueToken**

## UniqueToken is a pool of IDs

- ▶ User acquires an ID and releases it again.

```
UniqueToken<ExecutionSpace> token;  
int number_of_unique_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_unique_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()`.

## Sometimes you need a **Global UniqueToken**

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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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        , 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

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.

```
// 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

**Slack channel:** <https://kokkosteam.slack.com/>

## **Recordings/Slides:**

<https://kokkos.org/kokkos-core-wiki/videolectures.html>

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