

Kokkos Tutorial

H. Carter Edwards ¹, Christian R. Trott ¹, Jeff Amelang ²

¹Sandia National Laboratories

²Google

Supercomputing'16, November 13, 2016

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

SAND2016-8015 C

SOFTWARE FOR LAB

Remote Desktop Software:

- ▶ Download NoMachine now for best performance from www.nomachine.com/download
- ▶ Alternatively you may use a VNC client or the provided browser-based VNC option

SSH Access Software (optional):

- ▶ PuTTy for Windows can be downloaded from www.putty.org
- ▶ Alternatively you may use a provided browser-based SSH option

CONNECTION INSTRUCTIONS

- ▶ Navigate to nvlabs.qwiklab.com
- ▶ Login or create a new account
- ▶ Select the **Instructor-Led Hands-on Labs** Class
- ▶ Find the lab called **Kokkos**, ..., select it, click Select, and finally click Start
- ▶ After a short wait, lab instance Connection information will be shown
- ▶ Please ask Lab Assistants for help!

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Knowledge of C++: class constructors, member variables, member functions, member operators, template arguments

Using NVIDIA's NVLABS

- ▶ Kokkos pre installed in \${HOME}/kokkos
- ▶ Exercises pre installed in \${HOME}/SC2016

Using your own \${HOME}

- ▶ Git
- ▶ GCC 4.8.4 (or newer) OR Intel 14 (or newer) OR Clang 3.5.2 (or newer)
- ▶ CUDA nvcc 7.5 (or newer) AND NVIDIA compute capability 3.0 (or newer)
- ▶ clone github.com/kokkos/kokkos into \${HOME}/kokkos
- ▶ clone github.com/kokkos/kokkos-tutorials/SC2016 into \${HOME}/SC2016
 - makefiles look for \${HOME}/kokkos*

Understand Kokkos Programming Model Abstractions

- ▶ What, how and why of *performance portability*
- ▶ Productivity and hope for future-proofing

Part One:

- ▶ Simple data parallel computations
- ▶ Deciding where code is run and where data is placed

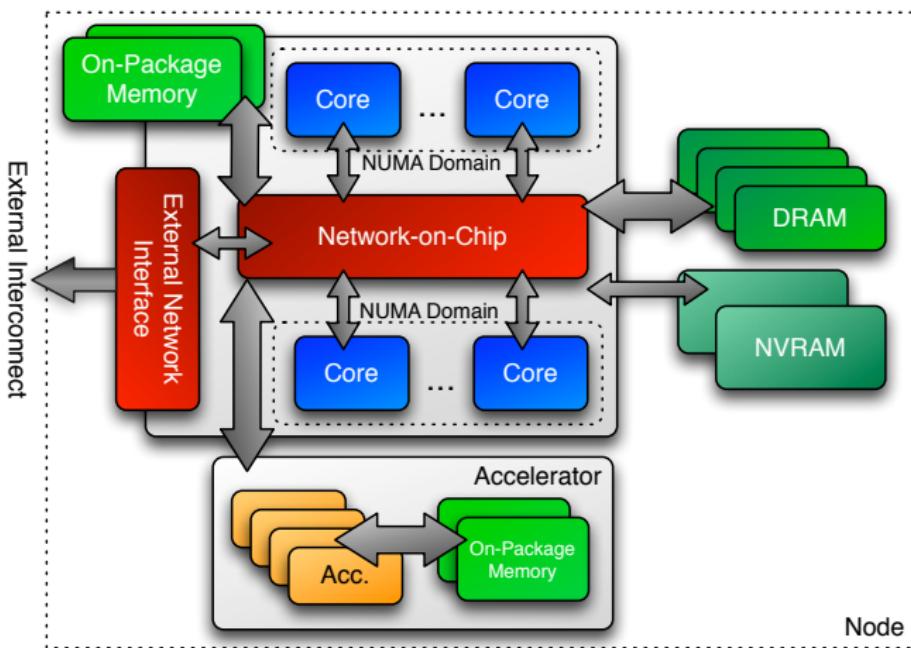
Part Two:

- ▶ Managing data access patterns for performance portability
- ▶ Thread safety and *thread scalability*
- ▶ Thread-teams for maximizing parallelism

- ▶ High performance computers are increasingly **heterogenous**
MPI-only is no longer sufficient.
- ▶ For **portability**: OpenMP, OpenACC, ... or Kokkos.
- ▶ Only Kokkos obtains performant memory access patterns via
architecture-aware arrays and work mapping.
*i.e., not just portable, *performance portable*.*
- ▶ With Kokkos, **simple things stay simple** (parallel-for, etc.).
*i.e., it's *no more difficult* than OpenMP.*
- ▶ **Advanced performance-optimizing patterns are simpler**
with Kokkos than with native versions.
*i.e., you're *not missing out* on advanced features.*

Target audience:

- ▶ **Wants** to use GPUs (and perhaps other accelerators)
- ▶ Is familiar with **data parallelism**
- ▶ **Has taken** “cuda programming 101”
- ▶ Familiar with **NVIDIA GPU architecture** at a *high* level
 - Aware that **coalesced** memory access is important
- ▶ Some familiarity with **OpenMP**
- ▶ Wants CUDA to be **easier**
- ▶ Would like **portability**, if it doesn't hurt performance

Target machine:

Important Point

There's a difference between *portability* and *performance portability*.

Example: implementations may target particular architectures and may not be *thread scalable*.

(e.g., locks on CPU won't scale to 100,000 threads on GPU)

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Goal: write **one implementation** which:

- ▶ compiles and **runs on multiple architectures**,
- ▶ obtains **performant memory access patterns** across architectures,
- ▶ can leverage **architecture-specific features** where possible.

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Example: implementations may target particular architectures and may not be *thread scalable*.

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Goal: write **one implementation** which:

- ▶ compiles and **runs on multiple architectures**,
- ▶ obtains **performant memory access patterns** across architectures,
- ▶ can leverage **architecture-specific features** where possible.

Kokkos: performance portability across manycore architectures.

Concepts for threaded data parallelism

Learning objectives:

- ▶ Terminology of pattern, policy, and body.
- ▶ The data layout problem.

```
for (element = 0; element < numElements; ++element) {  
    total = 0;  
    for (qp = 0; qp < numQPs; ++qp) {  
        total += dot(left[element][qp], right[element][qp]);  
    }  
    elementValues[element] = total;  
}
```

Pattern

```
for (element = 0; element < numElements; ++element) {  
    total = 0;  
    for (qp = 0; qp < numQPs; ++qp) {  
        total += dot(left[element][qp], right[element][qp]);  
    }  
    elementValues[element] = total;  
}
```

Body**Policy**

Terminology:

- ▶ **Pattern:** structure of the computations
for, reduction, scan, task-graph, ...
 - ▶ **Execution Policy:** how computations are executed
static scheduling, dynamic scheduling, thread teams, ...
 - ▶ **Computational Body:** code which performs each unit of work; e.g., the loop body
- ⇒ The **pattern** and **policy** drive the computational **body**.

What if we want to **thread** the loop?

```
for (element = 0; element < numElements; ++element) {  
    total = 0;  
    for (qp = 0; qp < numQPs; ++qp) {  
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What if we want to **thread** the loop?

```
#pragma omp parallel for
for (element = 0; element < numElements; ++element) {
    total = 0;
    for (qp = 0; qp < numQPs; ++qp) {
        total += dot(left[element][qp], right[element][qp]);
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}
```

(Change the *execution policy* from “serial” to “parallel.”)

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    }
    elementValues[element] = total;
}
```

(Change the *execution policy* from “serial” to “parallel.”)

OpenMP is simple for parallelizing loops on multi-core CPUs,
but what if we then want to do this on **other architectures?**

Intel MIC *and* NVIDIA GPU *and* AMD Fusion *and* ...

Option 1: OpenMP 4.0

```
#pragma omp target data map(...)
#pragma omp teams num_teams(...) num_threads(...) private(...)
#pragma omp distribute
for (element = 0; element < numElements; ++element) {
    total = 0
#pragma omp parallel for
    for (qp = 0; qp < numQPs; ++qp)
        total += dot(left[element][qp], right[element][qp]);
    elementValues[element] = total;
}
```

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    for (qp = 0; qp < numQPs; ++qp)
        total += dot(left[element][qp], right[element][qp]);
    elementValues[element] = total;
}
```

Option 2: OpenACC

```
#pragma acc parallel copy(...) num_gangs(...) vector_length(...)
#pragma acc loop gang vector
for (element = 0; element < numElements; ++element) {
    total = 0;
    for (qp = 0; qp < numQPs; ++qp)
        total += dot(left[element][qp], right[element][qp]);
    elementValues[element] = total;
}
```

A standard thread parallel programming model
may give you portable parallel execution
if it is supported on the target architecture.

But what about performance?

A standard thread parallel programming model
may give you portable parallel execution
if it is supported on the target architecture.

But what about performance?

Performance depends upon the computation's
memory access pattern.

Problem: memory access pattern

```
#pragma something, opencl, etc.
for (element = 0; element < numElements; ++element) {
    total = 0;
    for (qp = 0; qp < numQPs; ++qp) {
        for (i = 0; i < vectorSize; ++i) {
            total +=
                left[element * numQPs * vectorSize +
                      qp * vectorSize + i] *
                right[element * numQPs * vectorSize +
                      qp * vectorSize + i];
        }
    }
    elementValues[element] = total;
}
```

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Memory access pattern problem: CPU data layout reduces GPU performance by more than 10X.

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    }
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```

Memory access pattern problem: CPU data layout reduces GPU performance by more than 10X.

Important Point

For performance, the memory access pattern *must* depend on the architecture.

How does Kokkos address performance portability?

Kokkos is a *productive, portable, performant*, shared-memory programming model.

- ▶ is a C++ **library**, not a new language or language extension.
- ▶ supports **clear, concise, thread-scalable** parallel patterns.
- ▶ lets you write algorithms once and run on **many architectures**
e.g. multi-core CPU, Nvidia GPGPU, Xeon Phi, ...
- ▶ **minimizes** the amount of architecture-specific
implementation details users must know.
- ▶ *solves the data layout problem* by using multi-dimensional arrays with architecture-dependent **layouts**

Data parallel patterns

Learning objectives:

- ▶ How computational bodies are passed to the Kokkos runtime.
- ▶ How work is mapped to cores.
- ▶ The difference between `parallel_for` and `parallel_reduce`.
- ▶ Start parallelizing a simple example.

Data parallel patterns and work

```
for (atomIndex = 0; atomIndex < numberAtoms; ++atomIndex) {  
    atomForces[atomIndex] = calculateForce(...data...);  
}
```

Kokkos maps **work** to cores

Data parallel patterns and work

```
for (atomIndex = 0; atomIndex < numberAtoms; ++atomIndex) {  
    atomForces[atomIndex] = calculateForce(...data...);  
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```

Kokkos maps **work** to cores

- ▶ each iteration of a computational body is a **unit of work**.
- ▶ an **iteration index** identifies a particular unit of work.
- ▶ an **iteration range** identifies a total amount of work.

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- ▶ each iteration of a computational body is a **unit of work**.
- ▶ an **iteration index** identifies a particular unit of work.
- ▶ an **iteration range** identifies a total amount of work.

Important concept: Work mapping

You give an **iteration range** and **computational body** (kernel) to Kokkos, Kokkos maps iteration indices to cores and then runs the computational body on those cores.

How are computational bodies given to Kokkos?

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As **functors** or *function objects*, a common pattern in C++.

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As **functors** or *function objects*, a common pattern in C++.

Quick review, a **functor** is a function with data. Example:

```
struct ParallelFunctor {
    ...
    void operator()( a work assignment ) const {
        /* ... computational body ... */
        ...
    };
};
```

How is work assigned to functor operators?

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A total amount of work items is given to a Kokkos pattern,

```
ParallelFunctor functor;  
Kokkos::parallel_for(numberOfIterations, functor);
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and work items are assigned to functors one-by-one:

```
struct Functor {  
    void operator()(const size_t index) const {...}  
}
```

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```

and work items are assigned to functors one-by-one:

```
struct Functor {  
    void operator()(const size_t index) const {...}  
}
```

Warning: concurrency and order

Concurrency and ordering of parallel iterations is *not* guaranteed by the Kokkos runtime.

How is data passed to computational bodies?

```
for (atomIndex = 0; atomIndex < numberAtoms; ++atomIndex) {  
    atomForces[atomIndex] = calculateForce(...data...);  
}  
  
struct AtomForceFunctor {  
    ...  
    void operator()(const size_t atomIndex) const {  
        atomForces[atomIndex] = calculateForce(...data...);  
    }  
    ...  
}
```

How is data passed to computational bodies?

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for (atomIndex = 0; atomIndex < numberOfAtoms; ++atomIndex) {  
    atomForces[atomIndex] = calculateForce(...data...);  
}  
  
struct AtomForceFunctor {  
    ...  
    void operator()(const size_t atomIndex) const {  
        atomForces[atomIndex] = calculateForce(...data...);  
    }  
    ...  
}
```

How does the body access the data?

Important concept

A parallel functor body must have access to all the data it needs through the functor's **data members**.

Putting it all together: the complete functor:

```
struct AtomForceFunctor {
    ForceType _atomForces;
    AtomDataType _atomData;
    void operator()(const size_t atomIndex) const {
        _atomForces[atomIndex] = calculateForce(_atomData);
    }
}
```

Putting it all together: the complete functor:

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    void operator()(const size_t atomIndex) const {  
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    }  
}
```

Q/ How would we **reproduce serial execution** with this functor?

Serial

```
for (atomIndex = 0; atomIndex < numberAtoms; ++atomIndex){  
    atomForces[atomIndex] = calculateForce(data);  
}
```

Putting it all together: the complete functor:

```
struct AtomForceFunctor {  
    ForceType _atomForces;  
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    }  
}
```

Q/ How would we **reproduce serial execution** with this functor?

Serial

```
for (atomIndex = 0; atomIndex < numberAtoms; ++atomIndex){  
    atomForces[atomIndex] = calculateForce(data);  
}
```

Functor

```
AtomForceFunctor functor(atomForces, data);  
for (atomIndex = 0; atomIndex < numberAtoms; ++atomIndex){  
    functor(atomIndex);  
}
```

The complete picture (using functors):

1. Defining the functor (operator+data):

```
struct AtomForceFunctor {  
    ForceType _atomForces;  
    AtomDataType _atomData;  
  
    AtomForceFunctor(atomForces, data) :  
        _atomForces(atomForces) _atomData(data) {}  
  
    void operator()(const size_t atomIndex) const {  
        _atomForces[atomIndex] = calculateForce(_atomData);  
    }  
}
```

2. Executing in parallel with Kokkos pattern:

```
AtomForceFunctor functor(atomForces, data);  
Kokkos::parallel_for(numberOfAtoms, functor);
```

Functors are verbose ⇒ C++11 Lambdas are concise

```
atomForces already exists
data already exists
Kokkos::parallel_for(numberOfAtoms ,
    [=] (const size_t atomIndex) {
        atomForces[atomIndex] = calculateForce(data);
    }
);
```

Functors are verbose ⇒ C++11 Lambdas are concise

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A lambda is not *magic*, it is the compiler **auto-generating** a **functor** for you.

Functors are verbose ⇒ C++11 Lambdas are concise

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A lambda is not *magic*, it is the compiler **auto-generating** a **functor** for you.

Warning: Lambda capture and C++ containers

For portability (e.g., to GPU) a lambda must capture by value [=]. Don't capture containers (e.g., std::vector) by value because this copies the container's entire contents.

How does this compare to OpenMP?

Serial

```
for (size_t i = 0; i < N; ++i) {  
    /* loop body */  
}
```

OpenMP

```
#pragma omp parallel for  
for (size_t i = 0; i < N; ++i) {  
    /* loop body */  
}
```

Kokkos

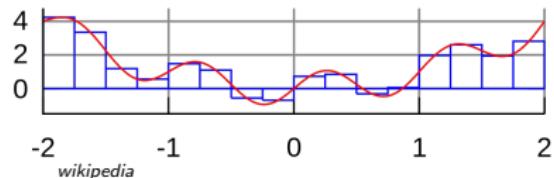
```
parallel_for(N, [=] (const size_t i) {  
    /* loop body */  
});
```

Important concept

Simple Kokkos usage is **no more conceptually difficult** than OpenMP, the annotations just go in different places.

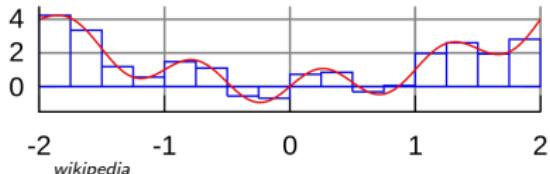
Riemann-sum-style numerical integration:

$$y = \int_{\text{lower}}^{\text{upper}} \text{function}(x) dx$$



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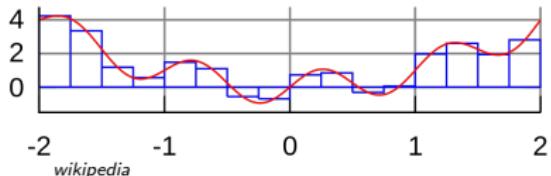
$$y = \int_{\text{lower}}^{\text{upper}} \text{function}(x) dx$$



```
double totalIntegral = 0;
for (size_t i = 0; i < number0fIntervals; ++i) {
    const double x =
        lower + (i/number0fIntervals) * (upper - lower);
    const double thisIntervalsContribution = function(x);
    totalIntegral += thisIntervalsContribution;
}
totalIntegral *= dx;
```

Riemann-sum-style numerical integration:

$$y = \int_{\text{lower}}^{\text{upper}} \text{function}(x) dx$$

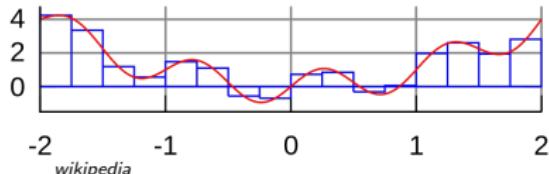


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How would we **parallelize** it?

Riemann-sum-style numerical integration:

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Pattern?

```
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for (size_t i = 0; i < number0fIntervals; ++i) {
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    const double thisIntervalsContribution = function(x);
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}
totalIntegral *= dx;
```

Policy?

Body?

How would we **parallelize** it?

An (incorrect) attempt:

```
double totalIntegral = 0;
Kokkos::parallel_for(numberOfIntervals,
    [=] (const size_t index) {
        const double x =
            lower + (index/numberOfIntervals) * (upper - lower);
        totalIntegral += function(x);},
    );
totalIntegral *= dx;
```

First problem: compiler error; cannot increment `totalIntegral`
(lambda captures by value and are treated as const!)

An (incorrect) solution to the (incorrect) attempt:

```
double totalIntegral = 0;
double * totalIntegralPointer = &totalIntegral;
Kokkos::parallel_for(numberOfIntervals,
 [=] (const size_t index) {
    const double x =
        lower + (index/numberOfIntervals) * (upper - lower);
    *totalIntegralPointer += function(x); ,
);
totalIntegral *= dx;
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    const double x =
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    *totalIntegralPointer += function(x);
});
totalIntegral *= dx;
```

Second problem: race condition

step	thread 0	thread 1
0	load	
1	increment	load
2	write	increment
3		write

Root problem: we're using the **wrong pattern**, *for* instead of *reduction*

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Important concept: Reduction

Reductions combine the results contributed by parallel work.

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Important concept: Reduction

Reductions combine the results contributed by parallel work.

How would we do this with **OpenMP**?

```
double finalReducedValue = 0;  
#pragma omp parallel for reduction(+:finalReducedValue)  
for (size_t i = 0; i < N; ++i) {  
    finalReducedValue += ...  
}
```

Root problem: we're using the **wrong pattern**, for instead of *reduction*

Important concept: Reduction

Reductions combine the results contributed by parallel work.

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```
double finalReducedValue = 0;
#pragma omp parallel for reduction(+:finalReducedValue)
for (size_t i = 0; i < N; ++i) {
    finalReducedValue += ...
}
```

How will we do this with **Kokkos**?

```
double finalReducedValue = 0;
parallel_reduce(N, functor, finalReducedValue);
```

```
double totalIntegral = 0;
#pragma omp parallel for reduction(+:totalIntegral)
for (size_t i = 0; i < number0fIntervals; ++i) {
    totalIntegral += function(...);
}
```

```
double totalIntegral = 0;
parallel_reduce(number0fIntervals,
 [=] (const size_t i, double & valueToUpdate) {
    valueToUpdate += function(...);
},
 totalIntegral);
```

- ▶ The operator takes **two arguments**: a work index and a value to update.
- ▶ The second argument is a **thread-private value** that is made and used by Kokkos; it is not the final reduced value.

Warning: Parallelism is NOT free

Dispatching (launching) parallel work has non-negligible cost.

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Simplistic data-parallel performance model: $\text{Time} = \alpha + \frac{\beta * N}{P}$

- ▶ α = dispatch overhead
- ▶ β = time for a unit of work
- ▶ N = number of units of work
- ▶ P = available concurrency

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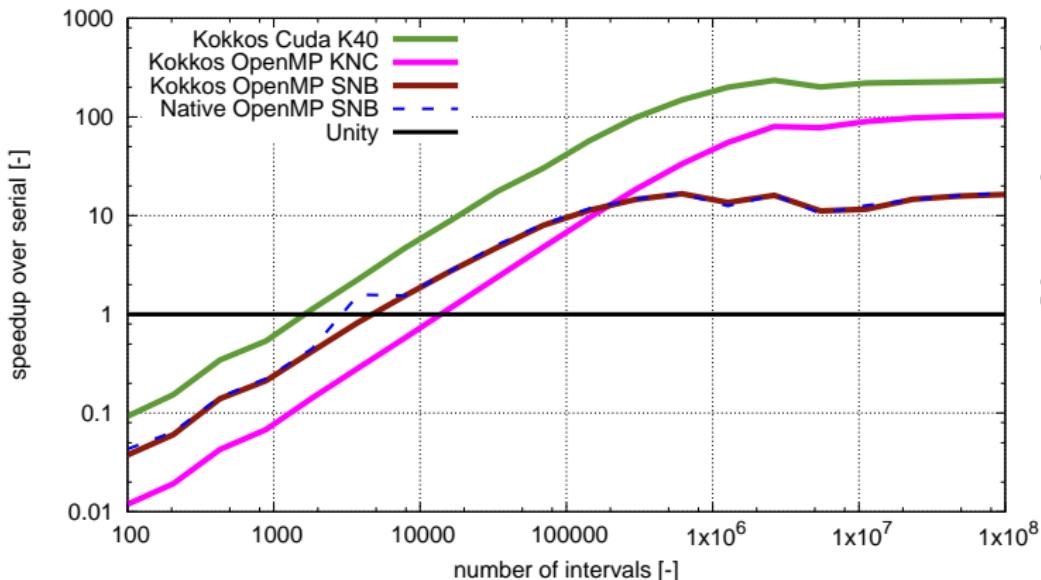
- ▶ α = dispatch overhead
- ▶ β = time for a unit of work
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- ▶ P = available concurrency

$$\text{Speedup} = P \div \left(1 + \frac{\alpha * P}{\beta * N}\right)$$

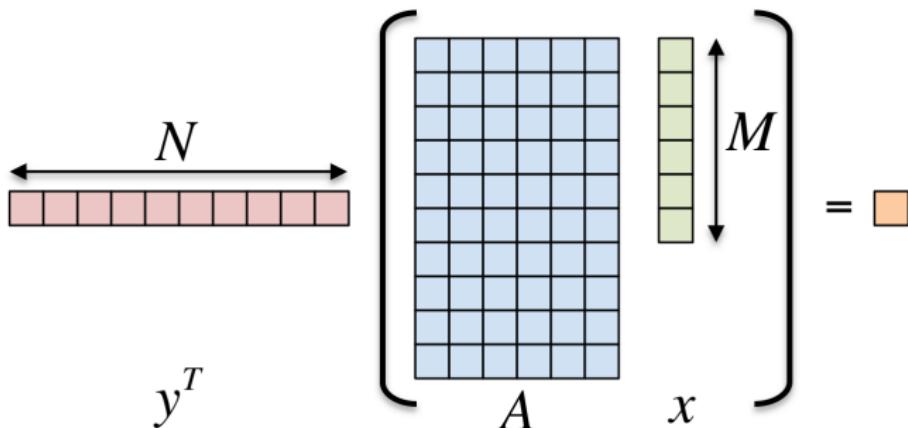
- ▶ Should have $\alpha * P \ll \beta * N$
- ▶ All runtimes strive to minimize launch overhead α
- ▶ Find more parallelism to increase N
- ▶ Merge (fuse) parallel operations to increase β

Results: illustrates simple speedup model $= P \div \left(1 + \frac{\alpha * P}{\beta * N}\right)$

Kokkos speedup over serial: Scalar Integration



Exercise: Inner product $\langle y, A * x \rangle$



Details:

- ▶ y is $N \times 1$, A is $N \times M$, x is $M \times 1$
- ▶ We'll use this exercise throughout the tutorial

Exercise #1: include, initialize, finalize Kokkos

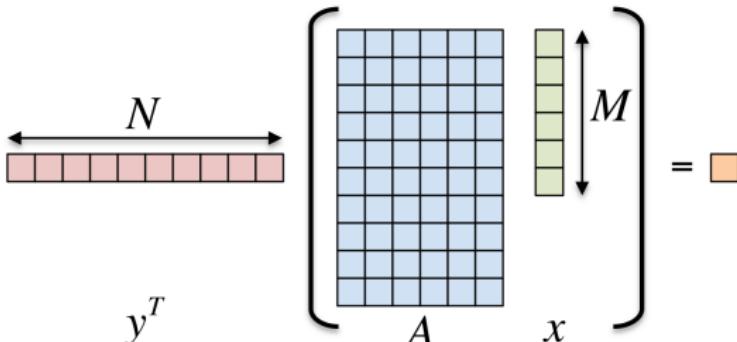
The **first step** in using Kokkos is to include, initialize, and finalize:

```
#include <Kokkos_Core.hpp>
int main(int argc, char** argv) {
    /* ... do any necessary setup (e.g., initialize MPI) ... */
    Kokkos::initialize(argc, argv);
    /* ... do computations ... */
    Kokkos::finalize();
    return 0;
}
```

(Optional) Command-line arguments:

--kokkos-threads=INT	total number of threads (or threads within NUMA region)
--kokkos-numa=INT	number of NUMA regions
--kokkos-device=INT	device (GPU) ID to use

Exercise: Inner product $\langle y, A * x \rangle$



Details:

$$y^T$$

- ▶ Location: `~/SC2016/Exercises/01/`
- ▶ Look for comments labeled with “EXERCISE”
- ▶ Need to include, initialize, and finalize Kokkos library
- ▶ Parallelize loops with `parallel_for` or `parallel_reduce`
- ▶ Use lambdas instead of functors for computational bodies.
- ▶ For now, this will only use the CPU.

Compiling for CPU

```
cd ~/SC2016/Exercises/01/Begin  
# gcc using OpenMP (default) and Serial back-ends  
make -j [KOKKOS_DEVICES=OpenMP,Serial]
```

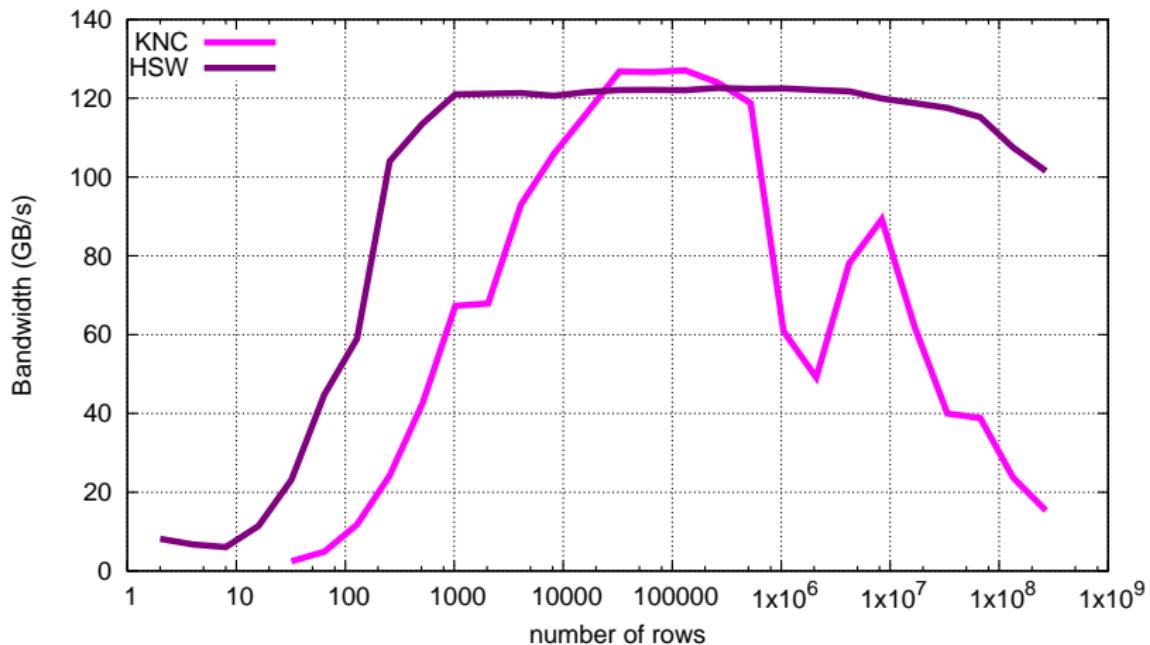
Running on CPU with OpenMP back-end

```
# Set OpenMP affinity  
export OMP_NUM_THREADS=8  
export GOMP_CPU_AFFINITY=0-8  
# Print example command line options:  
.01_Exercise.host -h  
# Run with defaults on CPU  
.01_Exercise.host  
# Run larger problem  
.01_Exercise.host -S 26
```

Things to try:

- ▶ Vary number of threads
- ▶ Vary problem size
- ▶ Vary number of rows (-N ...)

<y,Ax> Exercise01, fixed problem size



- ▶ Customized reduction type and operator
- ▶ Exclusive and inclusive **prefix scan** with the parallel_scan pattern.
- ▶ Using *tag dispatch* interface to allow non-trivial functors to have multiple “operator()” functions.
- ▶ **NEW:** Directed acyclic graph (DAG) of tasks pattern.
- ▶ **Concurrently** executing parallel kernels on CPU and GPU (experimental).
- ▶ Hierarchical parallelism with **team policies**, covered later.

- ▶ **Simple** usage is similar to OpenMP, advanced features are also straightforward
- ▶ Three common **data-parallel patterns** are parallel_for, parallel_reduce, and parallel_scan.
- ▶ A parallel computation is characterized by its **pattern**, **policy**, and **body**.
- ▶ User provides **computational bodies** as functors or lambdas which handle a single work item.

Views

Learning objectives:

- ▶ Motivation behind the View abstraction.
- ▶ Key View concepts and template parameters.
- ▶ The View life cycle.

Example: running daxpy on the GPU:

Lambda

```
double * x = new double[N]; // also y
parallel_for(N, [=] (const size_t i) {
    y[i] = a * x[i] + y[i];
});
```

Functor

```
struct Functor {
    double *_x, *_y, a;
    void operator()(const size_t i) {
        _y[i] = _a * _x[i] + _y[i];
    }
};
```

Example: running daxpy on the GPU:

Lambda

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Functor

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struct Functor {
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    }
};
```

Problem: x and y reside in CPU memory.

Example: running daxpy on the GPU:

Lambda

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parallel_for(N, [=] (const size_t i) {
    y[i] = a * x[i] + y[i];
});
```

Functor

```
struct Functor {
    double *_x, *_y, a;
    void operator()(const size_t i) {
        _y[i] = _a * _x[i] + _y[i];
    }
};
```

Problem: x and y reside in CPU memory.

Solution: We need a way of storing data (multidimensional arrays) which can be communicated to an accelerator (GPU).

⇒ Views

View abstraction

- ▶ A *lightweight* C++ class with a pointer to array data and a little meta-data,
- ▶ that is *templated* on the data type (and other things).

High-level example of Views for daxpy using lambda:

```
View<double*, ...> x(...), y(...);
... populate x, y...

parallel_for(N, [=] (const size_t i) {
    // Views x and y are captured by value (copy)
    y(i) = a * x(i) + y(i);
});
```

View abstraction

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... populate x, y...

parallel_for(N, [=] (const size_t i) {
    // Views x and y are captured by value (copy)
    y(i) = a * x(i) + y(i);
});
```

Important point

Views are **like pointers**, so copy them when passing.

View overview:

- ▶ **Multi-dimensional array** of 0 or more dimensions
scalar (0), vector (1), matrix (2), etc.
- ▶ **Number of dimensions (rank)** is fixed at compile-time.
- ▶ Arrays are **rectangular**, not ragged.
- ▶ **Sizes of dimensions** set at compile-time or runtime.
e.g., 2x20, 50x50, etc.

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- ▶ Arrays are **rectangular**, not ragged.
- ▶ **Sizes of dimensions** set at compile-time or runtime.
e.g., 2x20, 50x50, etc.

Example:

```
View<double***> data("label", N0, N1, N2); 3 run, 0 compile
View<double**[N2]> data("label", N0, N1);    2 run, 1 compile
View<double*[N1][N2]> data("label", N0);    1 run, 2 compile
View<double[N0][N1][N2]> data("label");      0 run, 3 compile
```

Note: runtime-sized dimensions must come first.

View life cycle:

- ▶ Allocations only happen when *explicitly* specified.
i.e., there are **no hidden allocations**.
- ▶ Copy construction and assignment are **shallow** (like pointers).
so, you pass Views by value, *not* by reference
- ▶ Reference counting is used for **automatic deallocation**.
- ▶ They behave like `shared_ptr`

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- ▶ They behave like `shared_ptr`

Example:

```
View<double*> a("a", N0), b("b", N0);
a = b;
View<double*> c(b);
a(0) = 1;
b(0) = 2;
c(0) = 3;
print a(0)
```

What gets printed?

View life cycle:

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i.e., there are **no hidden allocations**.
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c(0) = 3;
print a(0)
```

What gets printed?
3.0

Exercise #2: Inner Product, Flat Parallelism on the CPU, with Views

- ▶ Location: ~/SC2016/Exercises/02/
- ▶ Assignment: Change data storage from arrays to Views.
- ▶ Compile and run on CPU, and then on GPU with UVM

```
make -j KOKKOS_DEVICES=OpenMP    # CPU-only using OpenMP
make -j KOKKOS_DEVICES=Cuda \
      KOKKOS_CUDA_OPTIONS=force_uvm,enable_lambda
# Run exercise
./02_Exercise.host -S 26
./02_Exercise.cuda -S 26
# Note the warnings, set appropriate environment variables
```

- ▶ Vary problem size: **-S #**
- ▶ Vary number of rows: **-N #**
- ▶ Vary repeats: **-nrepeat #**
- ▶ Compare performance of CPU vs GPU

- ▶ **Memory space** in which view's data resides; *covered next.*
- ▶ **deep_copy** view's data; *covered later.*
Note: Kokkos *never* hides a deep_copy of data.
- ▶ **Layout** of multidimensional array; *covered later.*
- ▶ **Memory traits**; *covered later.*
- ▶ **Subview**: Generating a view that is a “slice” of other multidimensional array view; *will not be covered today.*

Execution and Memory Spaces

Learning objectives:

- ▶ Heterogeneous nodes and the **space** abstractions.
- ▶ How to control where parallel bodies are run, **execution space**.
- ▶ How to control where view data resides, **memory space**.
- ▶ How to avoid illegal memory accesses and manage data movement.
- ▶ The need for Kokkos::initialize and finalize.
- ▶ Where to use Kokkos annotation macros for portability.

Thought experiment: Consider this code:

```
MPI_Reduce(...);
FILE * file = fopen(...);
runANormalFunction(...data...);

Kokkos::parallel_for(numberOfSomethings,
                     [=] (const size_t somethingIndex) {
    const double y = ...;
    // do something interesting
}
);
```

section 1

section 2

Thought experiment: Consider this code:

```
MPI_Reduce(...);
FILE * file = fopen(...);
runANormalFunction(...data...);

Kokkos::parallel_for(numberOfSomethings,
                     [=] (const size_t somethingIndex) {
    const double y = ...;
    // do something interesting
});

```

section 2

- ▶ Where will **section 1** be run? CPU? GPU?
- ▶ Where will **section 2** be run? CPU? GPU?
- ▶ How do I **control** where code is executed?

Thought experiment: Consider this code:

```
MPI_Reduce(...);
FILE * file = fopen(...);
runANormalFunction(...data...);

Kokkos::parallel_for(numberOfSomethings,
                     [=] (const size_t somethingIndex) {
    const double y = ...;
    // do something interesting
});

```

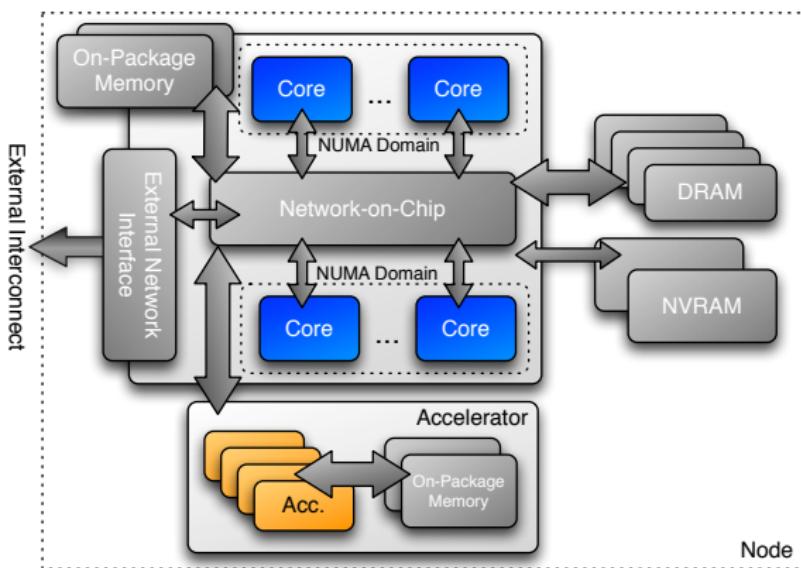
section 2

- ▶ Where will **section 1** be run? CPU? GPU?
- ▶ Where will **section 2** be run? CPU? GPU?
- ▶ How do I **control** where code is executed?

⇒ **Execution spaces**

Execution Space

a homogeneous set of cores and an execution mechanism
(i.e., “place to run code”)



Execution spaces: Serial, Threads, OpenMP, Cuda, ...

Host

```
MPI_Reduce(...);
FILE * file = fopen(...);
runANormalFunction(...data...);

Kokkos::parallel_for(numberOfSomethings,
                     [=] (const size_t somethingIndex) {
    const double y = ...;
    // do something interesting
}
);
```

Parallel

Host

```
MPI_Reduce(...);
FILE * file = fopen(...);
runANormalFunction(...data...);

Kokkos::parallel_for(numberOfSomethings,
                     [=] (const size_t somethingIndex) {
    const double y = ...;
    // do something interesting
}
);
```

Parallel

- ▶ Where will **Host** code be run? CPU? GPU?
⇒ Always in the **host process**

Host

```
MPI_Reduce(...);
FILE * file = fopen(...);
runANormalFunction(...data...);

Kokkos::parallel_for(numberOfSomethings,
                     [=] (const size_t somethingIndex) {
    const double y = ...;
    // do something interesting
}
);
```

Parallel

- ▶ Where will **Host** code be run? CPU? GPU?
⇒ Always in the **host process**
- ▶ Where will **Parallel** code be run? CPU? GPU?
⇒ The **default execution space**

```
Host MPI_Reduce(...);  
FILE * file = fopen(...);  
runANormalFunction(...data...);  
  
Parallel Kokkos::parallel_for(numberOfSomethings,  
                           [=] (const size_t somethingIndex) {  
                               const double y = ...;  
                               // do something interesting  
                           }  
                           );
```

- ▶ Where will **Host** code be run? CPU? GPU?
 ⇒ Always in the **host process**
- ▶ Where will **Parallel** code be run? CPU? GPU?
 ⇒ The **default execution space**
- ▶ How do I **control** where the **Parallel** body is executed?
 Changing the default execution space (*at compilation*),
 or specifying an execution space in the **policy**.

Changing the parallel execution space:

Custom

```
parallel_for(
    RangePolicy< ExecutionSpace >(0,numberOfIntervals),
    [=] (const size_t i) {
        /* ... body ... */
    });
}
```

Default

```
parallel_for(
    numberOfIntervals, // == RangePolicy<>(0,numberOfIntervals)
    [=] (const size_t i) {
        /* ... body ... */
    });
}
```

Custom

```
parallel_for<  
    RangePolicy< ExecutionSpace >(0,numberOfIntervals),  
    [=] (const size_t i) {  
        /* ... body ... */  
    };
```

Default

```
parallel_for(  
    numberOfIntervals, // == RangePolicy<>(0,numberOfIntervals)  
    [=] (const size_t i) {  
        /* ... body ... */  
    };
```

Requirements for enabling execution spaces:

- ▶ Kokkos must be **compiled** with the execution spaces enabled.
- ▶ Execution spaces must be **initialized** (and **finalized**).
- ▶ **Functions** must be marked with a **macro** for non-CPU spaces.
- ▶ **Lambdas** must be marked with a **macro** for non-CPU spaces.

Kokkos function and lambda portability annotation macros:

Function annotation with KOKKOS_INLINE_FUNCTION macro

```
struct ParallelFunctor {
    KOKKOS_INLINE_FUNCTION
    double helperFunction(const size_t s) const {...}
    KOKKOS_INLINE_FUNCTION
    void operator()(const size_t index) const {
        helperFunction(index);
    }
}
// Where kokkos defines:
#define KOKKOS_INLINE_FUNCTION inline /* #if CPU-only */
#define KOKKOS_INLINE_FUNCTION inline __device__ __host__ /* #if CPU+Cuda */
```

Kokkos function and lambda portability annotation macros:

Function annotation with KOKKOS_INLINE_FUNCTION macro

```
struct ParallelFunctor {
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}
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```

Lambda annotation with KOKKOS_LAMBDA macro (requires CUDA 7.5)

```
Kokkos::parallel_for(numberOfIterations,
    KOKKOS_LAMBDA (const size_t index) {...});

// Where kokkos defines:
#define KOKKOS_LAMBDA [=] /* #if CPU-only */
#define KOKKOS_LAMBDA [=] __device__ __host__ /* #if CPU+Cuda */
```

Memory space motivating example: summing an array

```
View<double*> data("data", size);
for (size_t i = 0; i < size; ++i) {
    data(i) = ...read from file...
}

double sum = 0;
Kokkos::parallel_reduce(
    RangePolicy<SomeExampleExecutionSpace>(0, size),
    KOKKOS_LAMBDA (const size_t index, double & valueToUpdate) {
        valueToUpdate += data(index);
    },
    sum);
```

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Question: Where is the data stored? GPU memory? CPU memory? Both?

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```

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Memory space motivating example: summing an array

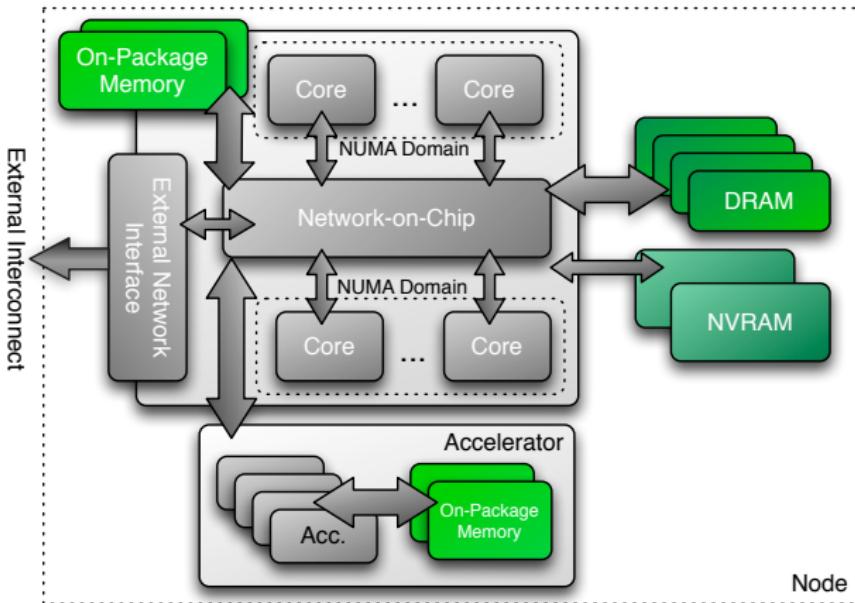
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    },
    sum);
```

Question: Where is the data stored? GPU memory? CPU memory? Both?

⇒ **Memory Spaces**

Memory space:
explicitly-manageable memory resource
(i.e., “place to put data”)



Important concept: Memory spaces

Every view stores its data in a **memory space** set at compile time.

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- ▶ `View<double***, MemorySpace> data(...);`

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- ▶ `View<double***, MemorySpace> data(...);`
- ▶ Available **memory spaces**:
`HostSpace, CudaSpace, CudaUVMSpace, ... more`

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Every view stores its data in a **memory space** set at compile time.

- ▶ `View<double***, MemorySpace> data(...);`
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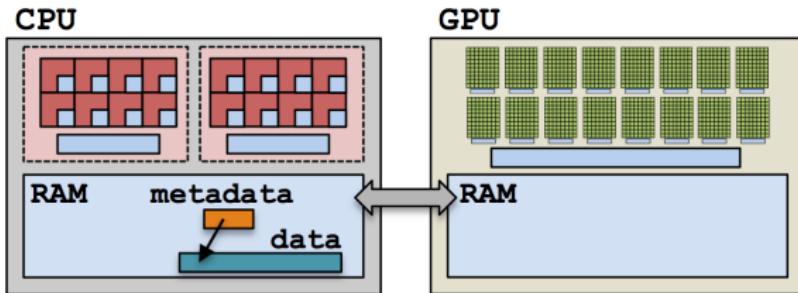
Important concept: Memory spaces

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- ▶ `View<double***, MemorySpace> data(...);`
- ▶ Available **memory spaces**:
 HostSpace, CudaSpace, CudaUVMSpace, ... more
- ▶ Each **execution space** has a default memory space, which is used if **Space** provided is actually an execution space
- ▶ If no Space is provided, the view's data resides in the **default memory space of the default execution space**.

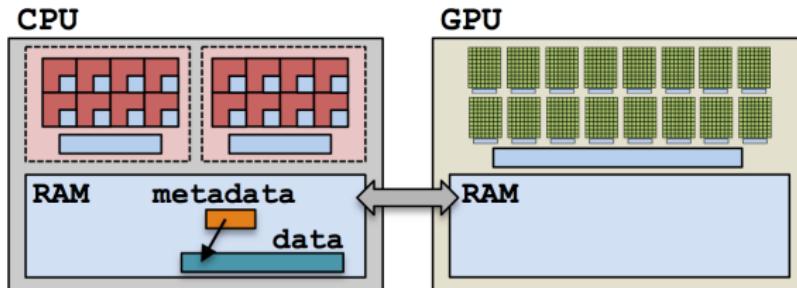
Example: HostSpace

```
View<double**, HostSpace> hostView(...constructor arguments...);
```



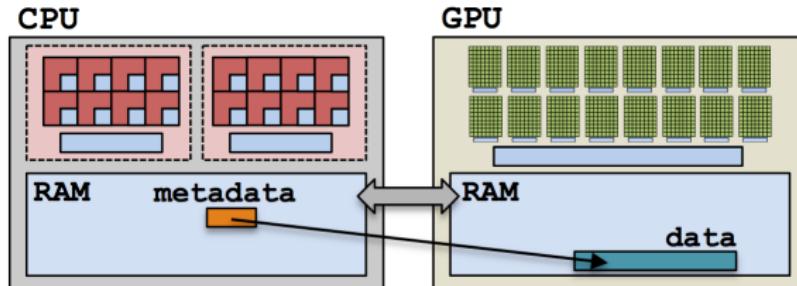
Example: HostSpace

```
View<double**, HostSpace> hostView(...constructor arguments...);
```



Example: CudaSpace

```
View<double**, CudaSpace> view(...constructor arguments...);
```



Anatomy of a kernel launch:

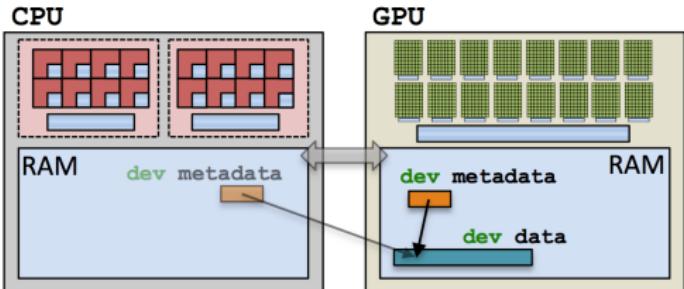
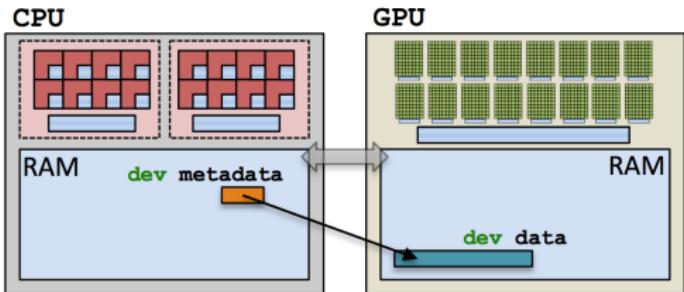
1. User declares views, allocating.
2. User instantiates a functor with views.
3. User launches parallel_something:
 - ▶ Functor is copied to the device.
 - ▶ Kernel is run.
 - ▶ Copy of functor on the device is released.

```
View<int*, Cuda> dev(...  
parallel_for(N,  
 [=] (int i) {  
     dev(i) = ...;  
});
```

Note: **no deep copies** of array data are performed;
views are like pointers.

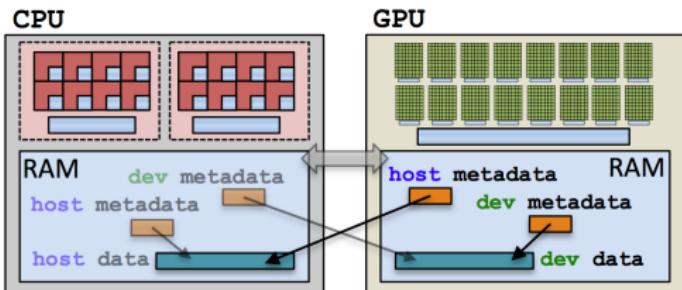
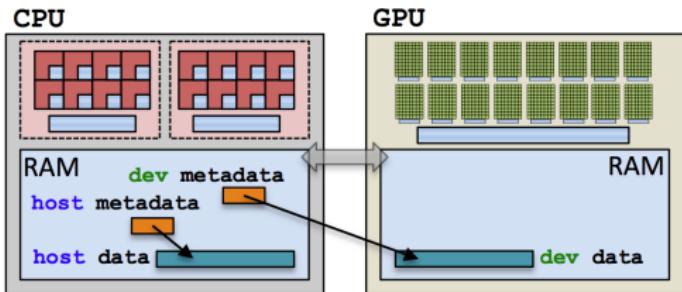
Example: one view

```
View<int*, Cuda> dev;
parallel_for(N,
 [=] (int i) {
    dev(i) = ...;
});
```



Example: two views

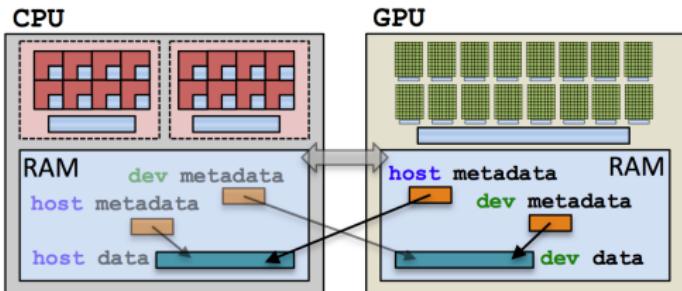
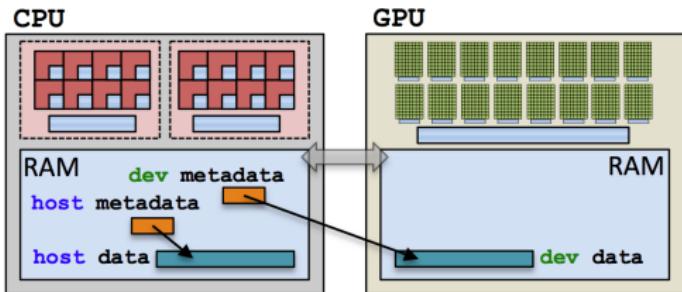
```
View<int*, Cuda> dev;
View<int*, Host> host;
parallel_for(N,
 [=] (int i) {
    dev(i) = ...;
    host(i) = ...;
});
```



Example: two views

```
View<int*, Cuda> dev;
View<int*, Host> host;
parallel_for(N,
    [=] (int i) {
        dev(i) = ...;
        host(i) = ...;
    });

```



Example (redux): summing an array with the GPU

(failed) Attempt 1: View lives in CudaSpace

```
View<double*, CudaSpace> array("array", size);
for (size_t i = 0; i < size; ++i) {
    array(i) = ...read from file...
}

double sum = 0;
Kokkos::parallel_reduce(
    RangePolicy< Cuda>(0, size),
    KOKKOS_LAMBDA (const size_t index, double & valueToUpdate) {
        valueToUpdate += array(index);
    },
    sum);
```

Example (redux): summing an array with the GPU

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    KOKKOS_LAMBDA (const size_t index, double & valueToUpdate) {
        valueToUpdate += array(index);
    },
    sum);
```

Example (redux): summing an array with the GPU

(failed) Attempt 2: View lives in HostSpace

```
View<double*, HostSpace> array("array", size);
for (size_t i = 0; i < size; ++i) {
    array(i) = ...read from file...
}

double sum = 0;
Kokkos::parallel_reduce(
    RangePolicy< Cuda>(0, size),
    KOKKOS_LAMBDA (const size_t index, double & valueToUpdate) {
        valueToUpdate += array(index);
    },
    sum);
```

Example (redux): summing an array with the GPU

(failed) Attempt 2: View lives in HostSpace

```
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for (size_t i = 0; i < size; ++i) {
    array(i) = ...read from file...
}

double sum = 0;
Kokkos::parallel_reduce(
    RangePolicy< Cuda>(0, size),
    KOKKOS_LAMBDA (const size_t index, double & valueToUpdate) {
        valueToUpdate += array(index);           illegal access
    },
    sum);
```

Example (redux): summing an array with the GPU

(failed) Attempt 2: View lives in HostSpace

```
View<double*, HostSpace> array("array", size);
for (size_t i = 0; i < size; ++i) {
    array(i) = ...read from file...
}

double sum = 0;
Kokkos::parallel_reduce(
    RangePolicy< Cuda>(0, size),
    KOKKOS_LAMBDA (const size_t index, double & valueToUpdate) {
        valueToUpdate += array(index);           illegal access
    },
    sum);
```

What's the solution?

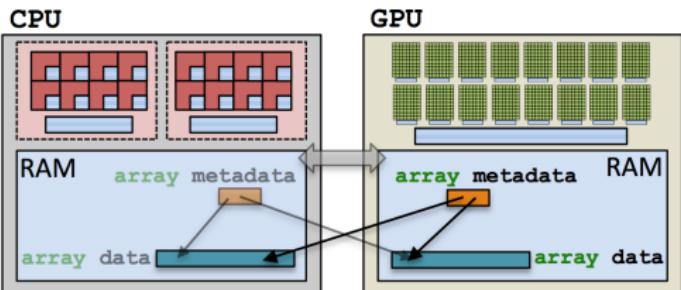
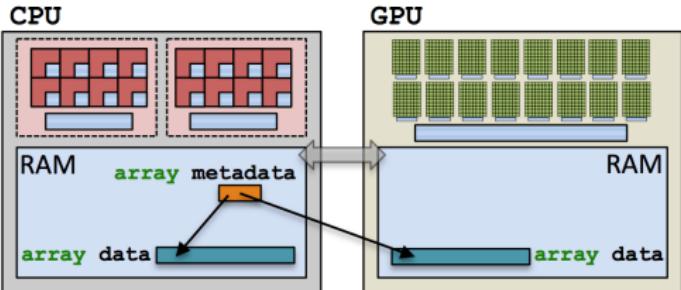
- ▶ CudaUVMSpace
- ▶ CudaHostPinnedSpace (skipping)
- ▶ Mirroring

CudaUVMSpace

```

View<double*,
    CudaUVMSpace> array
array = ...from file...
double sum = 0;
parallel_reduce(N,
[=] (int i,
      double & d) {
    d += array(i);
},
sum);

```



Cuda runtime automatically handles data movement,
at a **performance hit**.

Important concept: Mirrors

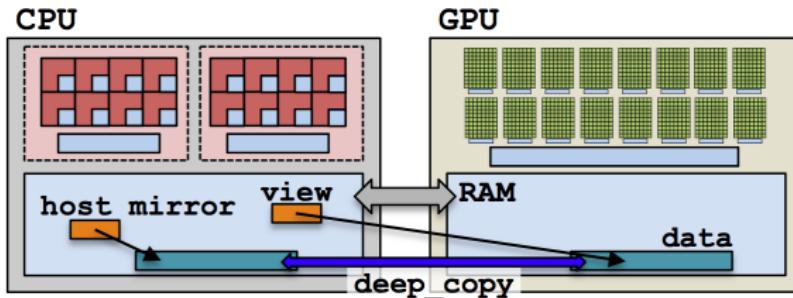
Mirrors are views of equivalent arrays residing in possibly different memory spaces.

Important concept: Mirrors

Mirrors are views of equivalent arrays residing in possibly different memory spaces.

Mirroring schematic

```
typedef Kokkos::View<double**, Space> ViewType;  
ViewType view(...);  
ViewType::HostMirror hostView =  
Kokkos::create_mirror_view(view);
```



1. Create a `view`'s array in some memory space.

```
typedef Kokkos::View<double*, Space> ViewType;  
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```
ViewType::HostMirror hostView =  
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```

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4. Deep copy `hostView`'s array to `view`'s array.

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Kokkos::deep_copy(view, hostView);
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```
Kokkos::deep_copy(view, hostView);
```

5. **Launch** a kernel processing the `view`'s array.

```
Kokkos::parallel_for(  
RangePolicy<Space>(0, size),  
KOKKOS_LAMBDA (...) { use and change view });
```

1. **Create** a `view`'s array in some memory space.

```
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Kokkos::parallel_for(  
RangePolicy<Space>(0, size),  
KOKKOS_LAMBDA (...) { use and change view });
```

6. If needed, **deep copy** the `view`'s updated array back to the `hostView`'s array to write file, etc.

```
Kokkos::deep_copy(hostView, view);
```

What if the View is in HostSpace too? Does it make a copy?

```
typedef Kokkos::View<double*, Space> ViewType;  
ViewType view("test", 10);  
ViewType::HostMirror hostView =  
Kokkos::create_mirror_view(view);
```

- ▶ `create_mirror_view` allocates data only if the host process cannot access `view`'s data, otherwise `hostView` references the same data.
- ▶ `create_mirror` **always** allocates data.
- ▶ Reminder: Kokkos *never* performs a **hidden deep copy**.

Details:

- ▶ Location: ~ /SC2016/Exercises/03/
- ▶ Add HostMirror Views and deep copy
- ▶ Make sure you use the correct view in initialization and Kernel

```
# Compile for CPU  
make -j KOKKOS_DEVICES=OpenMP  
# Compile for GPU (we do not need UVM anymore)  
make -j KOKKOS_DEVICES=Cuda  
# Run on GPU  
. /03_Exercise.cuda -S 26
```

Things to try:

- ▶ Vary problem size and number of rows (-S ...; -N ...)
- ▶ Change number of repeats (-nrepeat ...)
- ▶ Compare behavior of CPU vs GPU

- ▶ Data is stored in Views that are “pointers” to **multi-dimensional arrays** residing in **memory spaces**.
- ▶ Views **abstract away** platform-dependent allocation, (automatic) deallocation, and access.
- ▶ **Heterogenous nodes** have one or more memory spaces.
- ▶ **Mirroring** is used for performant access to views in host and device memory.
- ▶ Heterogenous nodes have one or more **execution spaces**.
- ▶ You **control where** parallel code is run by a template parameter on the execution policy, or by compile-time selection of the default execution space.

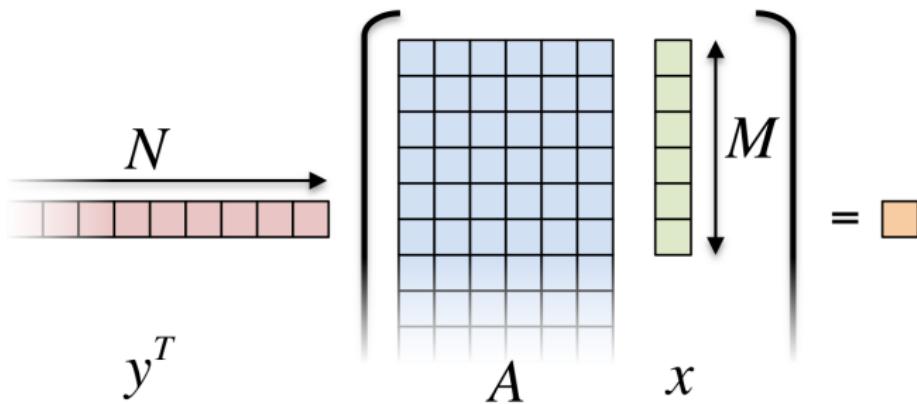
Managing memory access patterns for performance portability

Learning objectives:

- ▶ How the View's Layout parameter controls data layout.
- ▶ How memory access patterns result from Kokkos mapping parallel work indices **and** layout of multidimensional array data
- ▶ Why memory access patterns and layouts have such a performance impact (caching and coalescing).
- ▶ See a concrete example of the performance of various memory configurations.

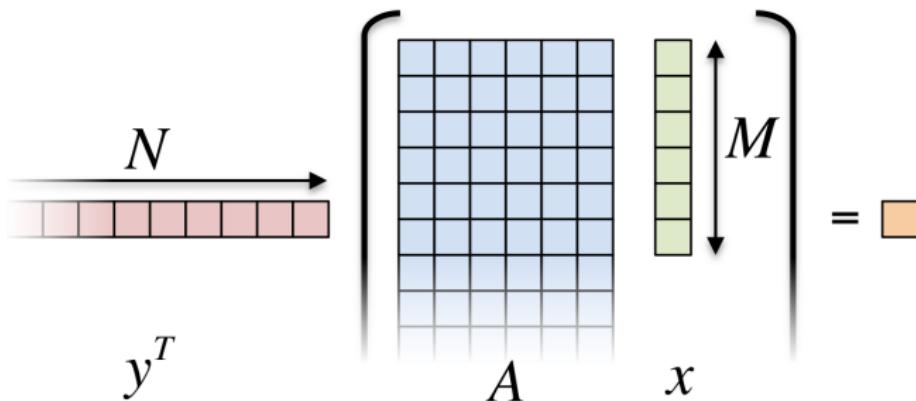
Example: inner product (0)

```
Kokkos::parallel_reduce(
    RangePolicy<ExecutionSpace>(0, N),
    KOKKOS_LAMBDA (const size_t row, double & valueToUpdate) {
        double thisRowSum = 0;
        for (size_t entry = 0; entry < M; ++entry) {
            thisRowSum += A(row, entry) * x(entry);
        }
        valueToUpdate += y(row) * thisRowSum;
    }, result);
```



Example: inner product (0)

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    RangePolicy<ExecutionSpace>(0, N),
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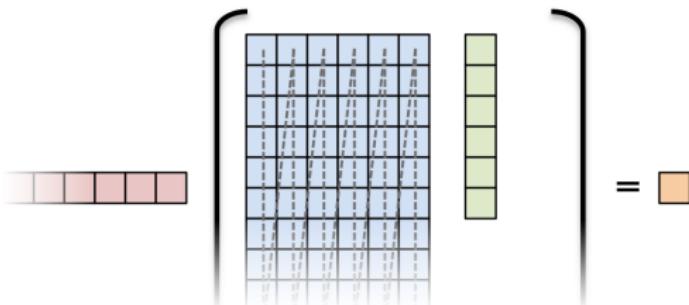


Driving question: How should A be laid out in memory?

Layout is the mapping of multi-index to memory:

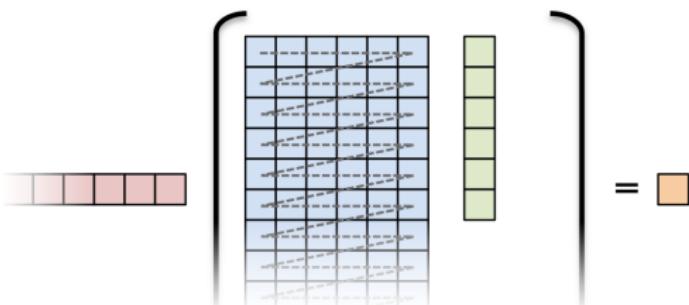
LayoutLeft

in 2D, “column-major”



LayoutRight

in 2D, “row-major”



Important concept: Layout

Every View has a multidimensional array Layout set at compile-time.

```
View<double***, Layout, Space> name(...);
```

Important concept: Layout

Every View has a multidimensional array Layout set at compile-time.

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View<double***, Layout, Space> name(...);
```

- ▶ Most-common layouts are LayoutLeft and LayoutRight.
 - LayoutLeft: left-most index is stride 1.
 - LayoutRight: right-most index is stride 1.
- ▶ If no layout specified, default for that memory space is used.
 - LayoutLeft for CudaSpace, LayoutRight for HostSpace.
- ▶ Layouts are extensible: ~50 lines
- ▶ Advanced layouts: LayoutStride, LayoutTiled, ...

Details:

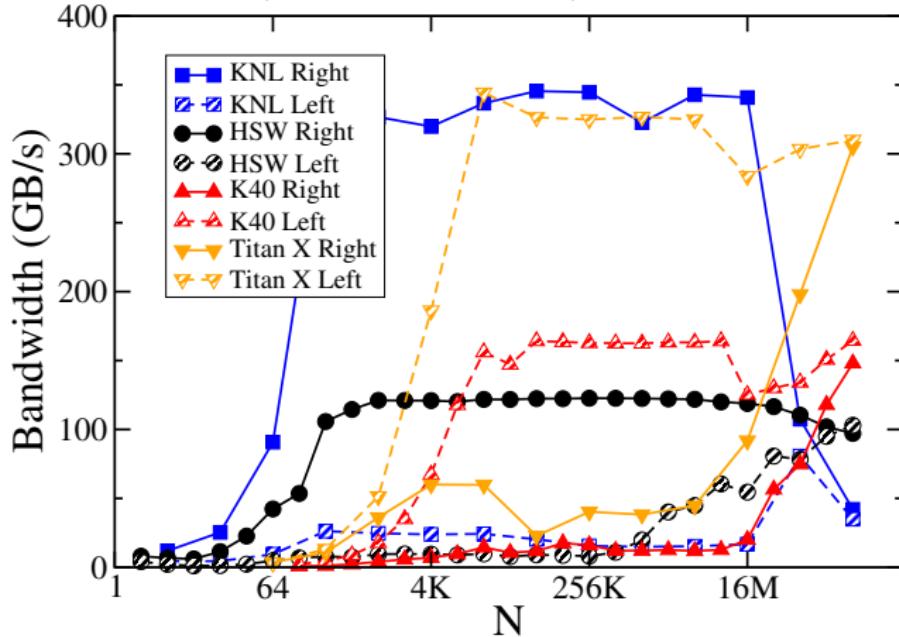
- ▶ Location: ~/SC2016/Exercises/04/
- ▶ Replace ‘‘N’’ in parallel dispatch with RangePolicy<ExecSpace>
- ▶ Add MemSpace to all Views and Layout to A
- ▶ Experiment with the combinations of ExecSpace, Layout to view performance

Things to try:

- ▶ Vary problem size and number of rows (-S ...; -N ...)
- ▶ Change number of repeats (-nrepeat ...)
- ▶ Compare behavior of CPU vs GPU
- ▶ Compare using UVM vs not using UVM on GPUs
- ▶ Check what happens if MemSpace and ExecSpace do not match.

<ylAx> Exercise 04 (Layout)

KNL: Xeon Phi 68c; HSW: Dual Xeon Haswell 2x16c; K40: Nvidia K40 / Titan X Pascal GPU



Why?

Thread independence:

```
operator()(const size_t index, double & valueToUpdate) {  
    const double d = _data(index);  
    valueToUpdate += d;  
}
```

Question: once a thread reads d, does it need to wait?

Thread independence:

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i.e., threads may execute at any rate.

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- ▶ **GPU** threads are synchronized in groups (of 32).
i.e., threads in groups must execute instructions together.

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In particular, all threads in a group (*warp*) must finished their loads before *any* thread can move on.

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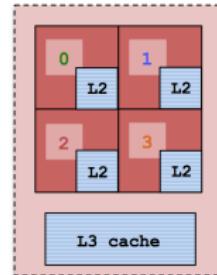
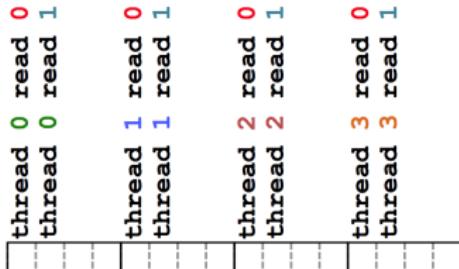
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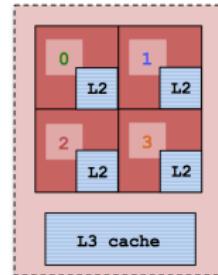
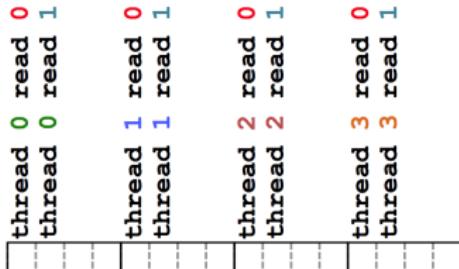
In particular, all threads in a group (*warp*) must finished their loads before *any* thread can move on.

So, **how many cache lines** must be fetched before threads can move on?

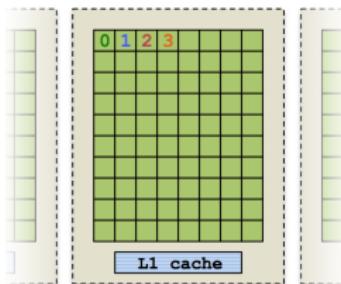
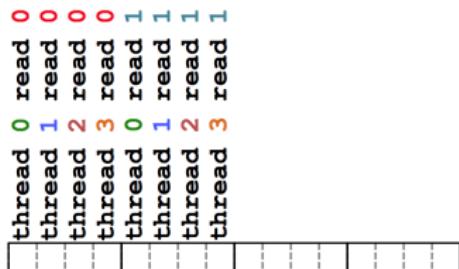
CPUs: few (independent) cores with separate caches:



CPUs: few (independent) cores with separate caches:



GPUs: many (synchronized) cores with a shared cache:



Important point

For performance, accesses to views in HostSpace must be **cached**, while access to views in CudaSpace must be **coalesced**.

Caching: if thread t's current access is at position i,
thread t's next access should be at position i+1.

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Warning

Uncoalesced access in CudaSpace *greatly* reduces performance
(more than 10X)

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Warning

Uncoalesced access in CudaSpace *greatly* reduces performance
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Note: uncoalesced *read-only, random* access in CudaSpace is okay
through Kokkos const RandomAccess views (more later).

Consider the array summation example:

```
View<double*, Space> data("data", size);
... populate data...

double sum = 0;
Kokkos::parallel_reduce(
    RangePolicy< Space>(0, size),
    KOKKOS_LAMBDA (const size_t index, double & valueToUpdate) {
        valueToUpdate += data(index);
    },
    sum);
```

Question: is this cached (for OpenMP) and coalesced (for Cuda)?

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Given P threads, **which indices** do we want thread 0 to handle?

Contiguous:

0, 1, 2, ..., N/P

Strided:

0, N/P, 2*N/P, ...

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CPU

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0, N/P, 2*N/P, ...

GPU

Why?

Iterating for the execution space:

```
operator()(const size_t index, double & valueToUpdate) {  
    const double d = _data(index);  
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}
```

As users we don't control how indices are mapped to threads, so how do we achieve good memory access?

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As users we don't control how indices are mapped to threads, so how do we achieve good memory access?

Important point

Kokkos maps indices to cores in **contiguous chunks** on CPU execution spaces, and **strided** for Cuda.

Rule of Thumb

Kokkos index mapping and default layouts provide efficient access if **iteration indices** correspond to the **first index** of array.

Example:

```
View<double***, ...> view(...);
...
Kokkos::parallel_for( ... ,
    KOKKOS_LAMBDA (const size_t workIndex) {
        ...
        view(..., ... , workIndex ) = ...;
        view(... , workIndex, ... ) = ...;
        view(workIndex, ... , ... ) = ...;
    });
...

```

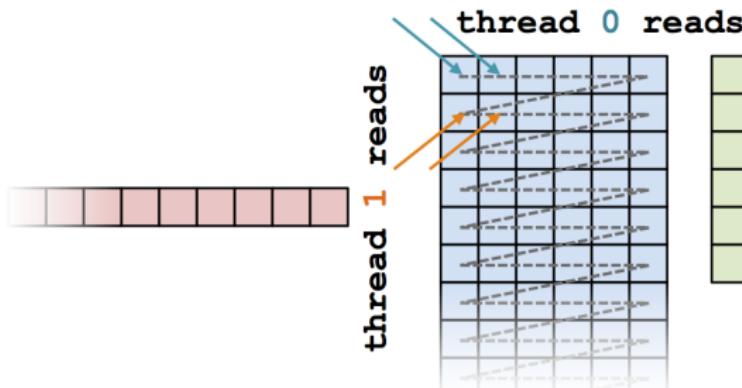
Important point

Performant memory access is achieved by Kokkos mapping parallel work indices **and** multidimensional array layout *optimally for the architecture*.

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Analysis: row-major (LayoutRight)



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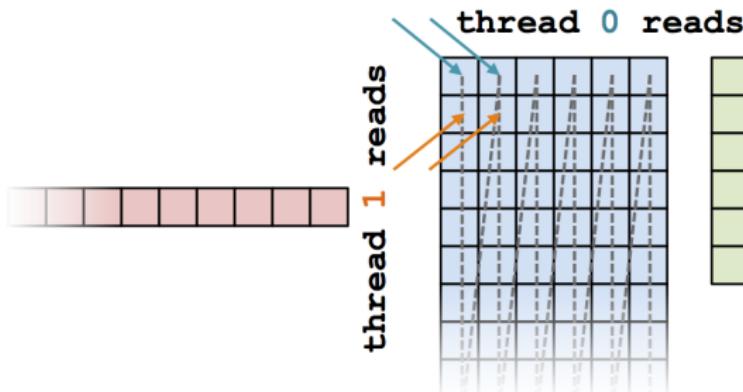


- ▶ **HostSpace:** cached (good)
- ▶ **CudaSpace:** uncoalesced (bad)

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Performant memory access is achieved by Kokkos mapping parallel work indices **and** multidimensional array layout *optimally for the architecture*.

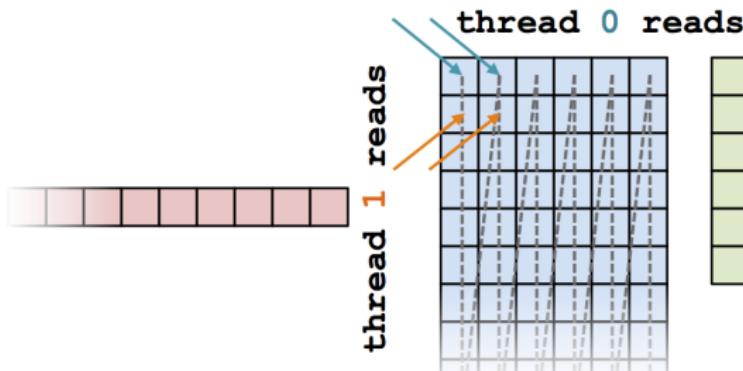
Analysis: column-major (LayoutLeft)



Important point

Performant memory access is achieved by Kokkos mapping parallel work indices **and** multidimensional array layout *optimally for the architecture*.

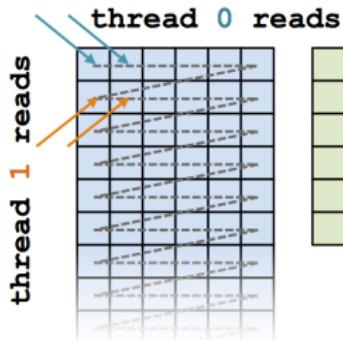
Analysis: column-major (LayoutLeft)



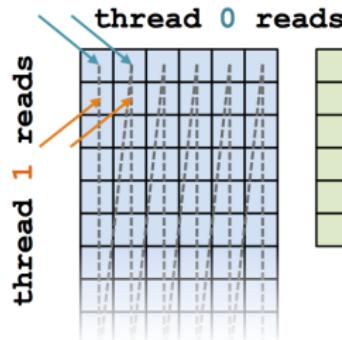
- ▶ **HostSpace:** uncached (**bad**)
- ▶ **CudaSpace:** coalesced (**good**)

Analysis: Kokkos architecture-dependent

```
View<double**, ExecutionSpace> A(N, M);
parallel_for(RangePolicy< ExecutionSpace>(0, N),
... thisRowSum += A(j, i) * x(i);
```



(a) OpenMP

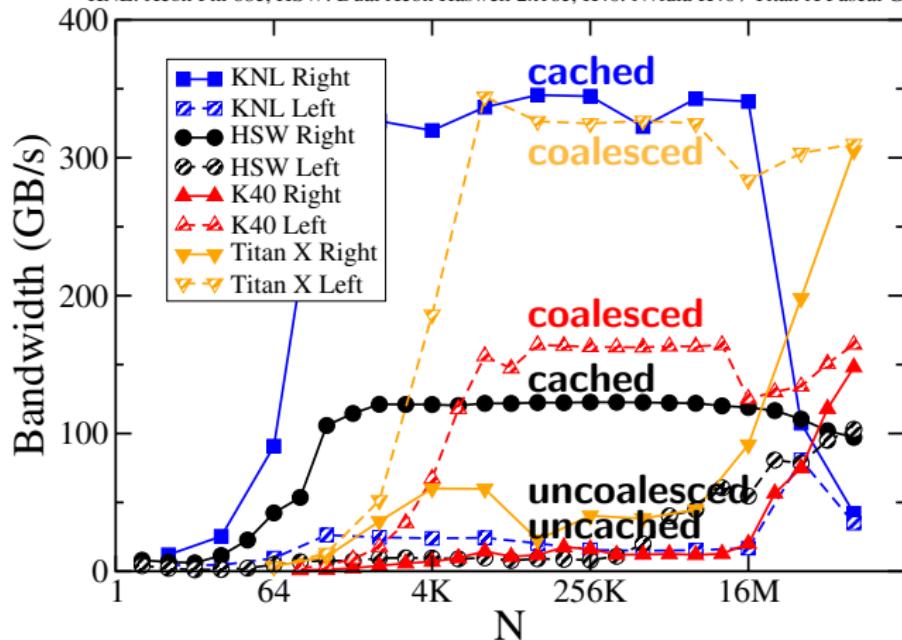


(b) Cuda

- ▶ **HostSpace**: cached (good)
- ▶ **CudaSpace**: coalesced (good)

<ylAx> Exercise 04 (Layout)

KNL: Xeon Phi 68c; HSW: Dual Xeon Haswell 2x16c; K40: Nvidia K40 / Titan X Pascal GPU



- ▶ Every View has a Layout set at compile-time through a **template parameter**.
- ▶ LayoutRight and LayoutLeft are **most common**.
- ▶ Views in HostSpace default to LayoutRight and Views in CudaSpace default to LayoutLeft.
- ▶ Layouts are **extensible** and **flexible**.
- ▶ For performance, memory access patterns must result in **caching** on a CPU and **coalescing** on a GPU.
- ▶ Kokkos maps parallel work indices *and* multidimensional array layout for **performance portable memory access patterns**.
- ▶ There is **nothing in** OpenMP, OpenACC, or OpenCL to manage layouts.
⇒ You'll need multiple versions of code or pay the performance penalty.

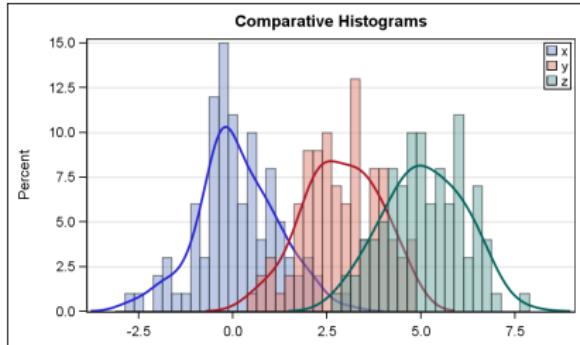
Thread safety and atomic operations

Learning objectives:

- ▶ Understand that coordination techniques for low-count CPU threading are not scalable.
- ▶ Understand how atomics can parallelize the **scatter-add** pattern.
- ▶ Gain **performance intuition** for atomics on the CPU and GPU, for different data types and contention rates.

Histogram kernel:

```
parallel_for(N, KOKKOS_LAMBDA(const size_t index) {  
    const Something value = ...;  
    const size_t bucketIndex = computeBucketIndex(value);  
    ++_histogram(bucketIndex);  
});
```

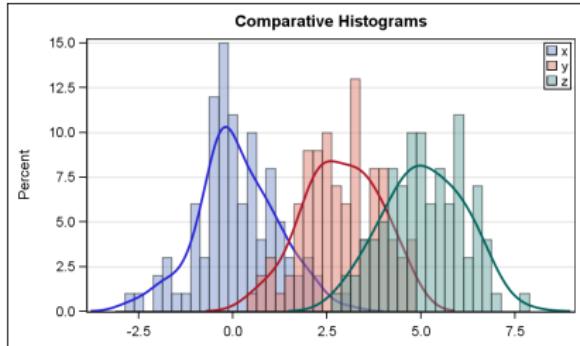


<http://www.farmaceuticas.com.br/tag/graficos/>

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Problem: Multiple threads may try to write to the same location.



<http://www.farmaceuticas.com.br/tag/graficos/>

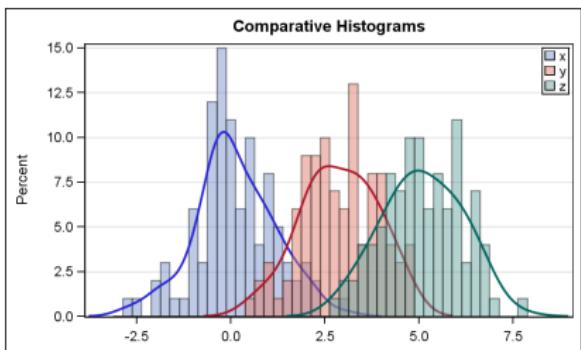
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```

Problem: Multiple threads may try to write to the same location.

Solution strategies:

- ▶ Locks: not feasible on GPU
- ▶ Thread-private copies:
not thread-scalable
- ▶ Atomics



<http://www.farmaceuticas.com.br/tag/graficos/>

Atomics: the portable and thread-scalable solution

```
parallel_for(N, KOKKOS_LAMBDA(const size_t index) {  
    const Something value = ...;  
    const int bucketIndex = computeBucketIndex(value);  
    Kokkos::atomic_add(&_histogram(bucketIndex), 1);  
});
```

Atomics: the portable and thread-scalable solution

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- ▶ Atomics are the **only scalable** solution to thread safety.

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});
```

- ▶ Atomics are the **only scalable** solution to thread safety.
- ▶ Locks or data replication are **strongly discouraged**.

How expensive are atomics?

Thought experiment: scalar integration

```
operator()(const unsigned int intervalIndex,
           double & valueToUpdate) const {
    double contribution = function(...);
    valueToUpdate += contribution;
}
```

How expensive are atomics?

Thought experiment: scalar integration

```
operator()(const unsigned int intervalIndex,
           double & valueToUpdate) const {
    double contribution = function(...);
    valueToUpdate += contribution;
}
```

Idea: what if we instead do this with parallel_for and atomics?

```
operator()(const unsigned int intervalIndex) const {
    const double contribution = function(...);
    Kokkos::atomic_add(&globalSum, contribution);
}
```

How much of a performance penalty is incurred?

Two costs: (independent) work and coordination.

```
parallel_reduce(numberOfIntervals,  
    KOKKOS_LAMBDA (const unsigned int intervalIndex,  
                    double & valueToUpdate) {  
    valueToUpdate += function(...);  
}, totalIntegral);
```

Two costs: (independent) work and coordination.

```
parallel_reduce(numberOfIntervals,
    KOKKOS_LAMBDA (const unsigned int intervalIndex,
                    double & valueToUpdate) {
        valueToUpdate += function(...);
    }, totalIntegral);
```

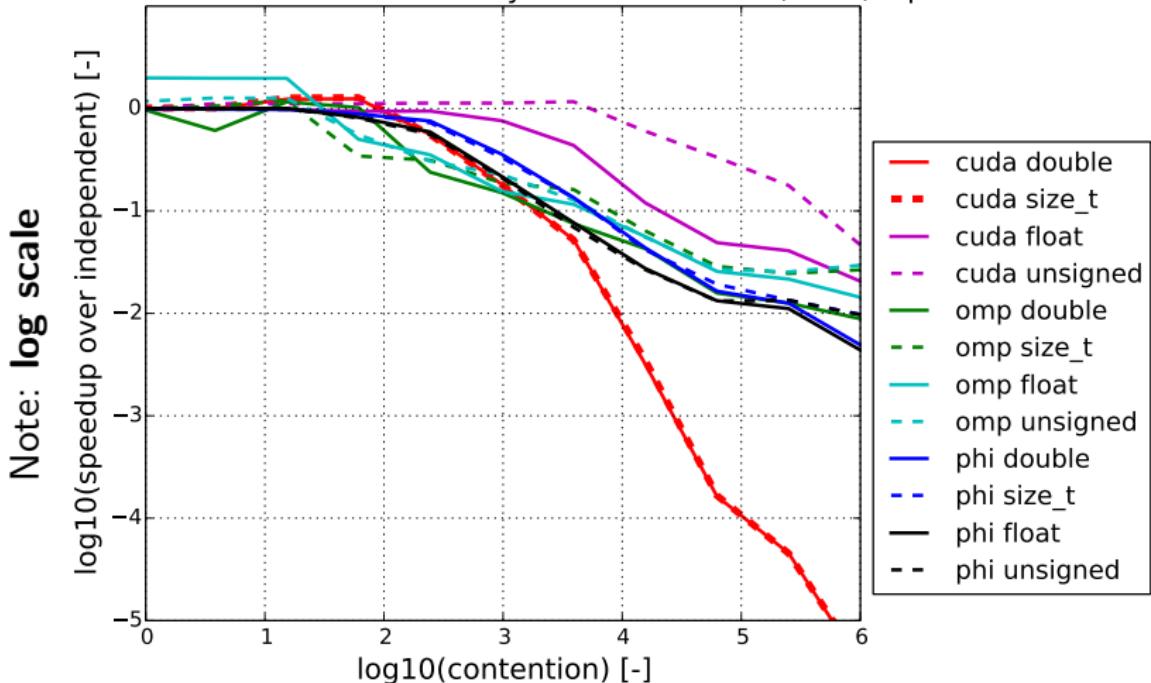
Experimental setup

```
operator()(const unsigned int index) const {
    Kokkos::atomic_add(&globalSums[index % atomicStride], 1);
}
```

- ▶ This is the most extreme case: **all coordination** and **no work**.
- ▶ Contention is captured by the `atomicStride`.
 - `atomicStride → 1` ⇒ Scalar integration (**bad**)
 - `atomicStride → large` ⇒ Independent (**good**)

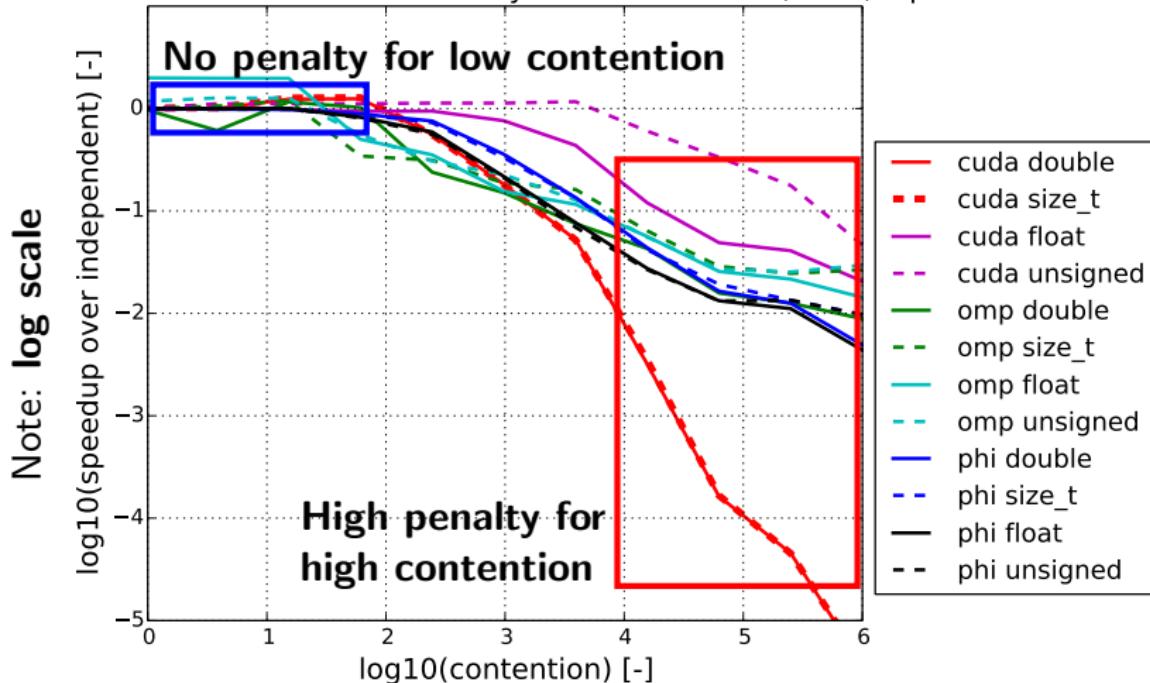
Atomics performance: 1 million adds, **no** work per kernel

Slowdown from atomics: Summary for 1 million adds, mod, 0 pows



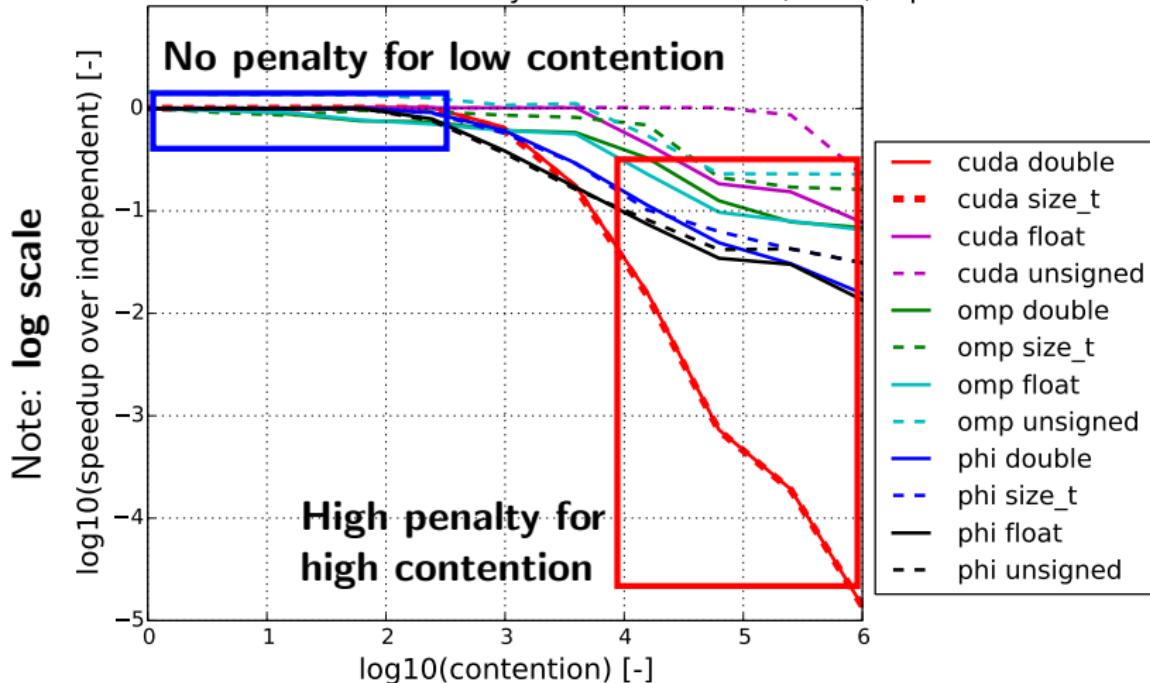
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Slowdown from atomics: Summary for 1 million adds, mod, 0 pows



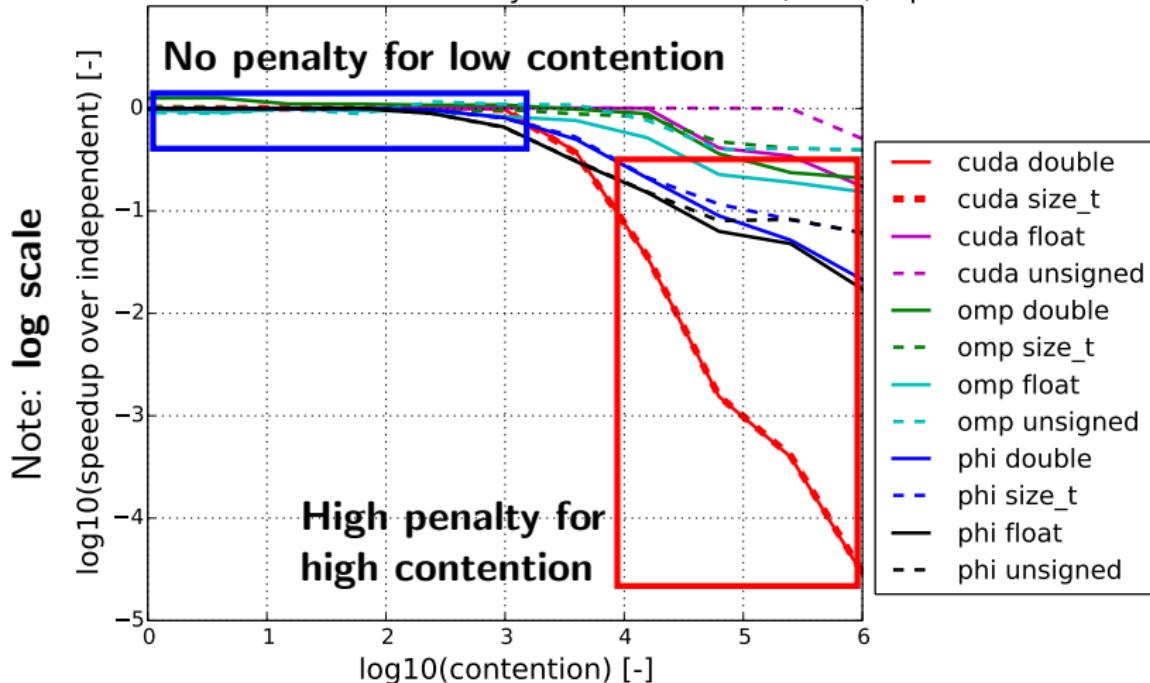
Atomics performance: 1 million adds, **some** work per kernel

Slowdown from atomics: Summary for 1 million adds, mod, 2 pows



Atomics performance: 1 million adds, lots of work per kernel

Slowdown from atomics: Summary for 1 million adds, mod, 5 pows



Atomics on arbitrary types:

- ▶ Atomic operations work if the corresponding operator exists, i.e., `atomic_add` works on any data type with “+”.
- ▶ Atomic exchange works on any data type.

```
// Assign *dest to val, return former value of *dest
template<typename T>
T atomic_exchange(T * dest, T val);
// If *dest == comp then assign *dest to val
// Return true if succeeds.
template<typename T>
bool atomic_compare_exchange_strong(T * dest, T comp, T val);
```

Slight detour: View memory traits:

- ▶ Beyond a Layout and Space, Views can have memory traits.
- ▶ Memory traits either provide **convenience** or allow for certain **hardware-specific optimizations** to be performed.

Example: If all accesses to a View will be atomic, use the Atomic memory trait:

```
View<double**, Layout, Space,  
      MemoryTraits<Atomic>> forces(...);
```

Slight detour: View memory traits:

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Example: If all accesses to a View will be atomic, use the Atomic memory trait:

```
View<double**, Layout, Space,  
      MemoryTraits<Atomic>> forces(...);
```

Many memory traits exist or are experimental, including Read, Write, ReadWrite, ReadOnce (non-temporal), Contiguous, and RandomAccess.

Example: RandomAccess memory trait:

On **GPUs**, there is a special pathway for fast **read-only, random** access, originally designed for textures.

Example: RandomAccess memory trait:

On **GPUs**, there is a special pathway for fast **read-only, random** access, originally designed for textures.

How to access texture memory via **CUDA**:

```
cudaResourceDesc resDesc;
memset(&resDesc, 0, sizeof(resDesc));
resDesc.resType = cudaResourceTypeLinear;
resDesc.res.linear.devPtr = buffer;
resDesc.res.linear.desc.f = cudaChannelFormatKindFloat;
resDesc.res.linear.desc.x = 32; // bits per channel
resDesc.res.linear.sizeInBytes = N*sizeof(float);

cudaTextureDesc texDesc;
memset(&texDesc, 0, sizeof(texDesc));
texDesc.readMode = cudaReadModeElementType;

cudaTextureObject_t tex=0;
cudaCreateTextureObject(&tex, &resDesc, &texDesc, NULL);
```

Example: RandomAccess memory trait:

On **GPUs**, there is a special pathway for fast **read-only, random** access, originally designed for textures.

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resDesc.res.linear.sizeInBytes = N*sizeof(float);

cudaTextureDesc texDesc;
memset(&texDesc, 0, sizeof(texDesc));
texDesc.readMode = cudaReadModeElementType;

cudaTextureObject_t tex=0;
cudaCreateTextureObject(&tex, &resDesc, &texDesc, NULL);
```

How to access texture memory via **Kokkos**:

```
View< const double***, Layout, Space,
      MemoryTraits<RandomAccess> > name(...);
```

- ▶ Atomics are the only thread-scalable solution to thread safety.
 - ▶ Locks or data replication are **not portable or scalable**
- ▶ Atomic performance **depends on ratio** of independent work and atomic operations.
 - ▶ With more work, there is a lower performance penalty, because of increased opportunity to interleave work and atomic.
- ▶ The Atomic **memory trait** can be used to make all accesses to a view atomic.
- ▶ The cost of atomics can be negligible:
 - ▶ **CPU** ideal: contiguous access, integer types
 - ▶ **GPU** ideal: scattered access, 32-bit types
- ▶ Many programs with the **scatter-add** pattern can be thread-scalably parallelized using atomics without much modification.

Hierarchical parallelism

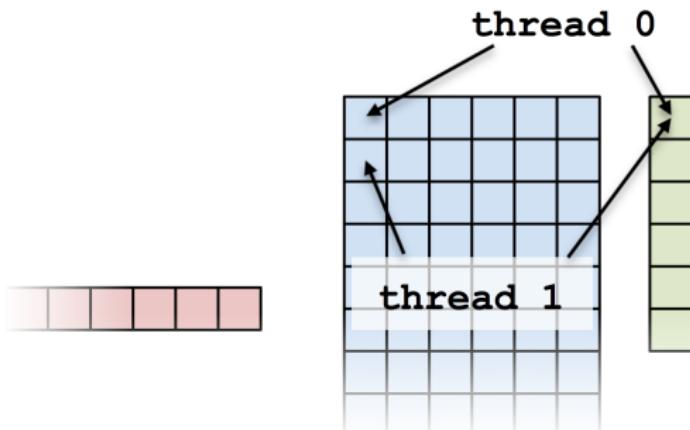
Finding and exploiting more parallelism in your computations.

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:

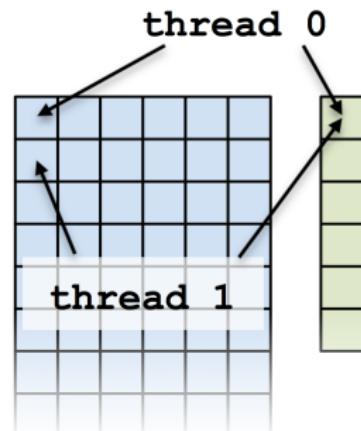
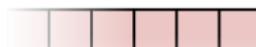
```
Kokkos::parallel_reduce(N,
    KOKKOS_LAMBDA (const int row, double & valueToUpdate) {
        double thisRowsSum = 0;
        for (int col = 0; col < M; ++col) {
            thisRowsSum += A(row,col) * x(col);
        }
        valueToUpdate += y(row) * thisRowsSum;
    }, result);
```



(Flat parallel) Kernel:

```
Kokkos::parallel_reduce(N,
    KOKKOS_LAMBDA (const int row, double & valueToUpdate) {
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    }, result);
```

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

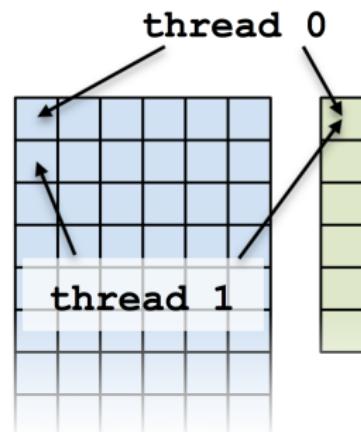


(Flat parallel) Kernel:

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Kokkos::parallel_reduce(N,
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    }, result);
```

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

Solutions?



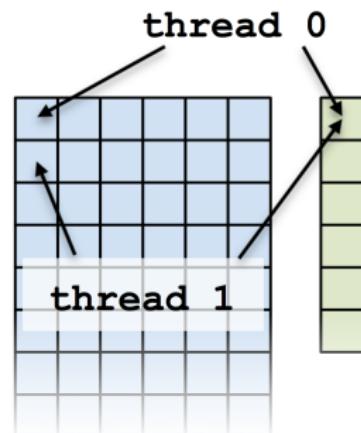
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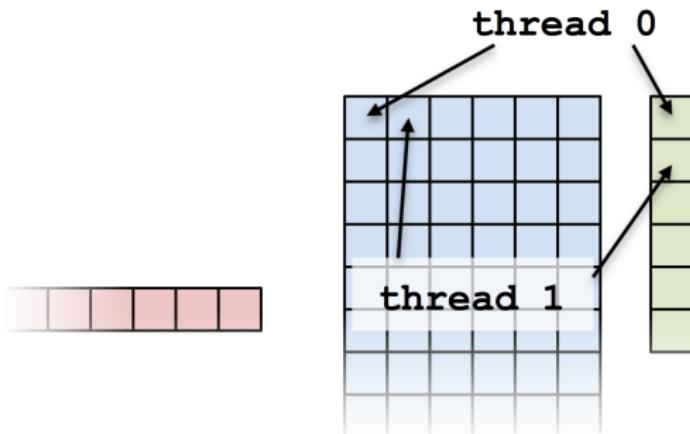
Solutions?

- ▶ Atomics
- ▶ Thread teams



Atomics kernel:

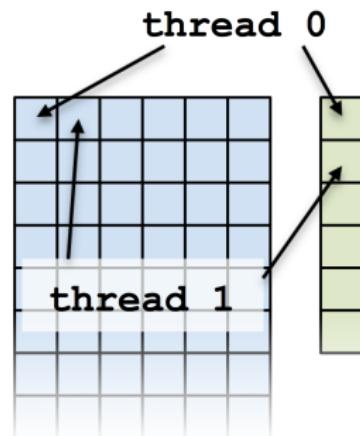
```
Kokkos::parallel_for(N,
    KOKKOS_LAMBDA (const size_t index) {
        const int row = extractRow(index);
        const int col = extractCol(index);
        atomic_add(&result, A(row,col) * x(col));
    });
}
```



Atomics kernel:

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

Problem: Poor performance



Doing each individual row with atomics is like doing scalar integration with atomics.

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

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

Doing each individual row with atomics is like doing scalar integration with atomics.

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

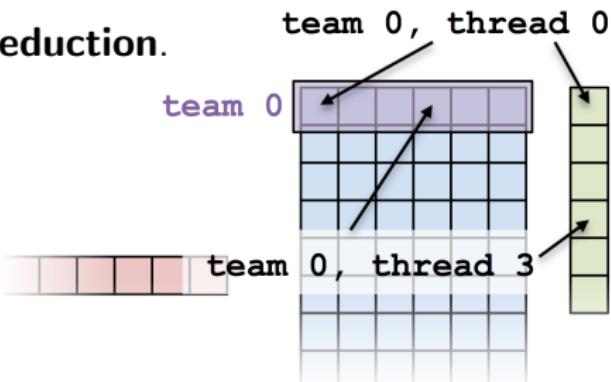
A collection of threads which are guaranteed to be executing **concurrently** and **can synchronize**.

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 of M threads.
2. Each thread performs **one** entry in the row.
3. The threads within **teams perform a reduction**.
4. The thread teams **perform a reduction**.



The final hierarchical parallel kernel:

```
parallel_reduce(
    team_policy(N, Kokkos::AUTO),
    KOKKOS_LAMBDA (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(
    RangePolicy<ExecutionSpace>(0,N), functor);
```

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(
    RangePolicy<ExecutionSpace>(0, N), functor);
```

“**Hierarchical** parallelism” uses TeamPolicy:

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

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

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) {
    // Which team am I on?
    const unsigned int leagueRank = teamMember.league_rank();
    // Which thread am I on this team?
    const unsigned int teamRank = teamMember.team_rank();
}
```

Important point

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

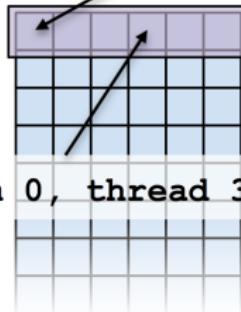
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    // Which team am I on?
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}
```

Warning

There may be more (or fewer) team members than pieces of your algorithm's work per team

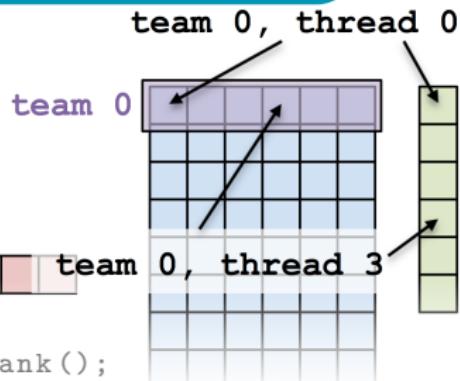
team 0, thread 0

team 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));  
}
```



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?
- ▶ `atomic_add` performs badly under high contention, how can team's member threads performantly cooperate for a nested reduction?

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

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

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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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}
```

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we'd use Kokkos::parallel_reduce.

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;
    }
}
```

TeamThreadRange:

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                    }, 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.
- ▶ Intra-team **reduction handled** by Kokkos.

Anatomy of nested parallelism:

```
parallel_outer(
    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`, `reduce`, or `scan`.
- ▶ 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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NVIDIA GPU:

- ▶ Special hardware available for coordination within a team.
- ▶ Within a team 32 threads (*warp*) execute “lock step.”
- ▶ Maximum team size: **1024**; Recommended team size: **256**

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- ▶ Special hardware available for coordination within a team.
- ▶ Within a team 32 threads (*warp*) execute “lock step.”
- ▶ Maximum team size: **1024**; Recommended team size: **256**

Intel Xeon Phi:

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

Details:

- ▶ Location: ~/SC2016/Exercises/05/
- ▶ 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?

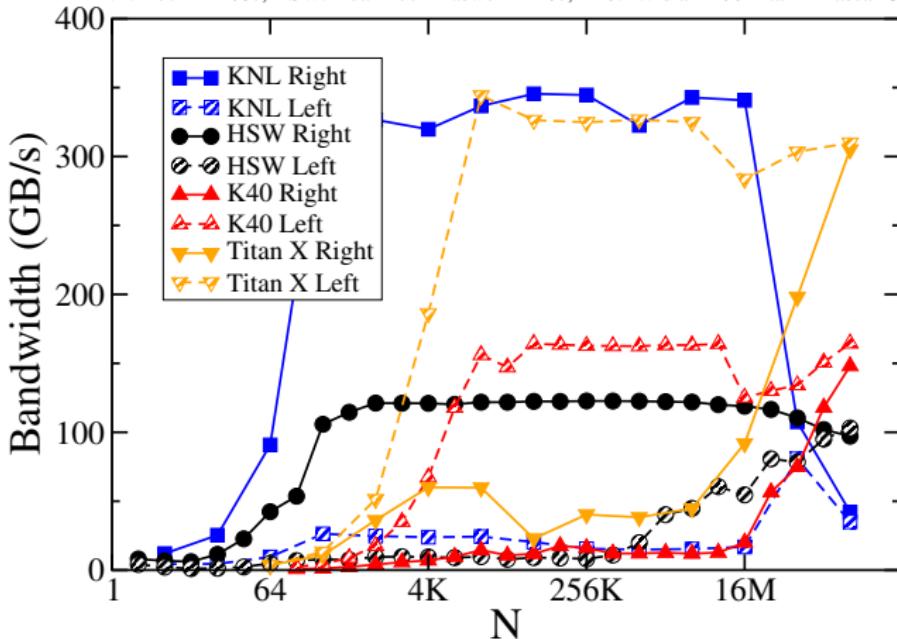
Things to try:

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

Reminder: Exercise 4 results (flat parallelism)

<ylAx> Exercise 04 (Layout)

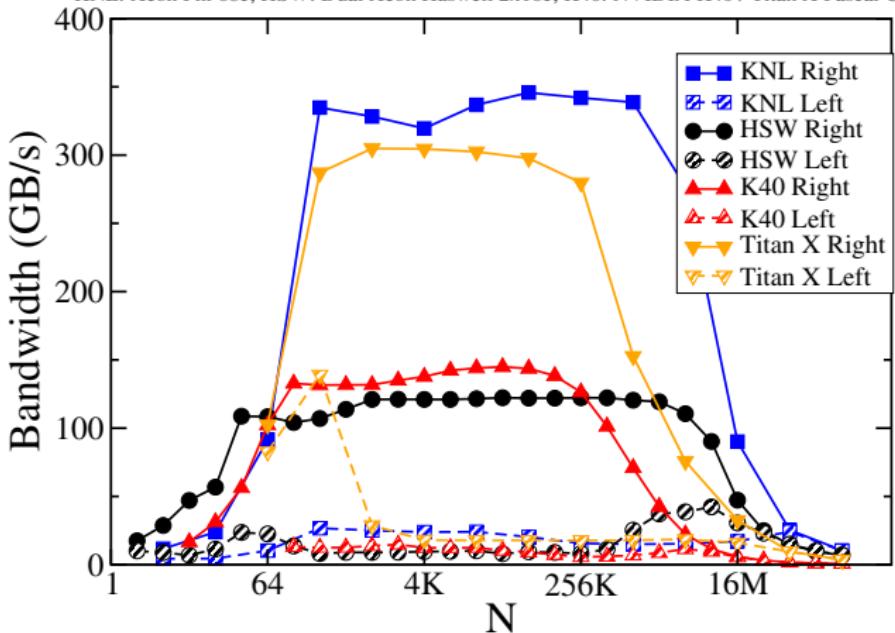
KNL: Xeon Phi 68c; HSW: Dual Xeon Haswell 2x16c; K40: Nvidia K40 / Titan X Pascal GPU



New: Exercise 5 results (hierarchical parallelism)

<ylAx> Exercise 05 (Layouts/Teams)

KNL: Xeon Phi 68c; HSW: Dual Xeon Haswell 2x16c; K40: NVIDIA K40 / Titan X Pascal 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.

Anatomy of nested parallelism:

```
parallel_outer(
    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 */
                    }[, ...]);
                /* end of outer body */
            }[, ...]);
    }
```

Question: What will the value of totalSum be?

```
int totalSum = 0;
parallel_reduce(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);
```

totalSum = numberOfThreads * 10

Question: What will the value of totalSum be?

```
int totalSum = 0;
parallel_reduce(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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        ++thisThreadsSum;
    }
    partialSum += thisThreadsSum;
}, totalSum);
```

```
totalSum = numberOfTeams * team_size * 10
```

Question: What will the value of totalSum be?

```
int totalSum = 0;
parallel_reduce(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);
```

Question: What will the value of totalSum be?

```
int totalSum = 0;
parallel_reduce(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

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:

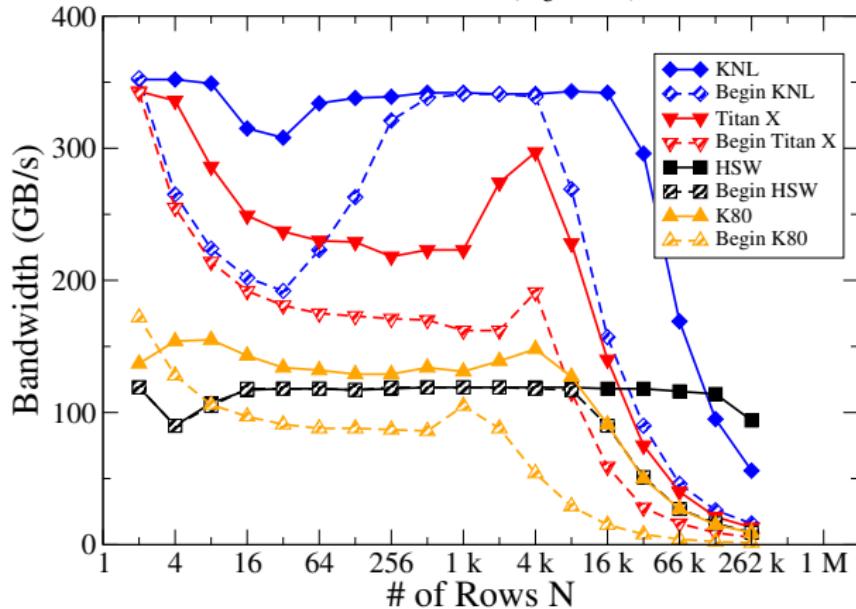
- ▶ Location: `~/SC2016/Exercises/06/`
- ▶ Use the `single` policy instead of checking team rank
- ▶ Parallelize all three loop levels.

Things to try:

- ▶ Vary problem size and number of rows (`-S ...; -N ...`)
- ▶ Compare behaviour with Exercise 5 for very non-square matrices
- ▶ Compare behavior of CPU vs GPU

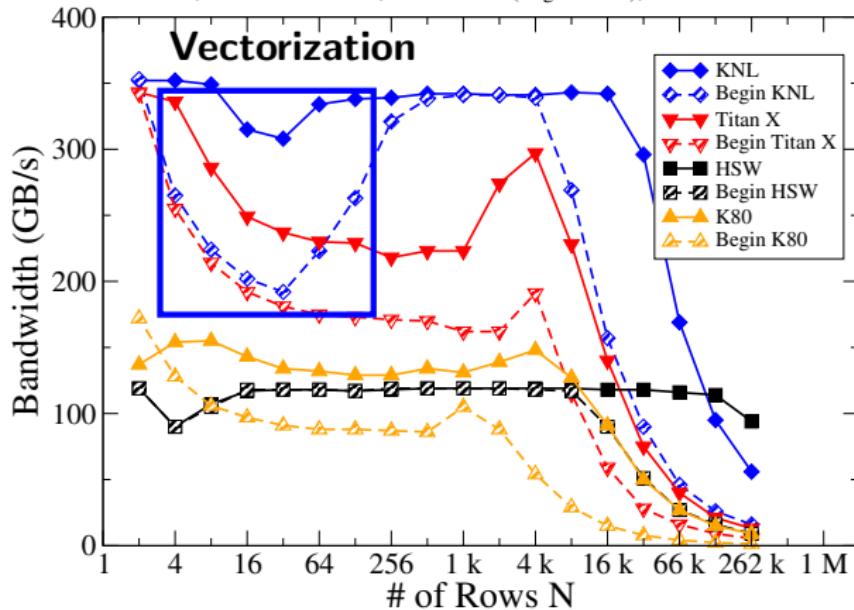
Exercise 06 (Three Level Parallelism)

Xeon Phi KNL 68c; Dual Haswell 2x16c; NVIDIA K80 (single device); NVIDIA GeForce Titan X Pascal



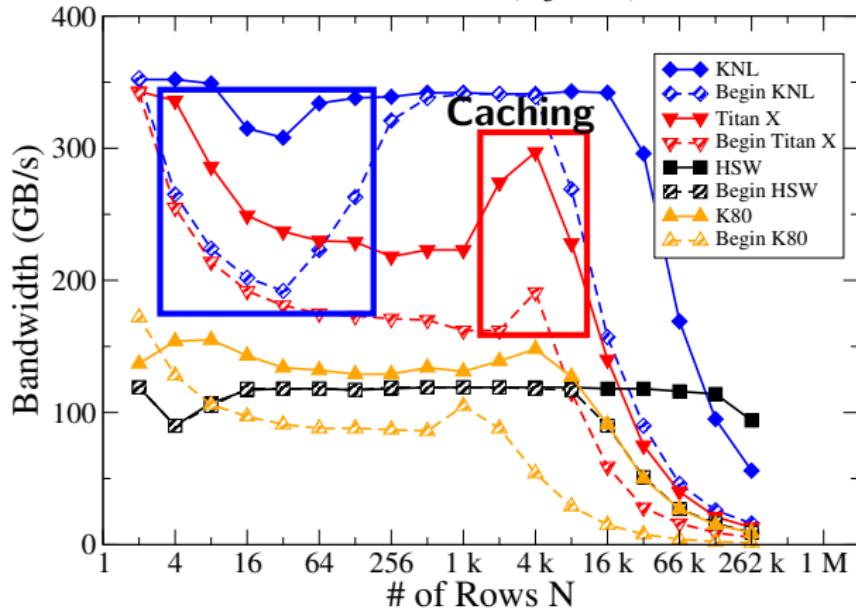
Exercise 06 (Three Level Parallelism)

Xeon Phi KNL 68c; Dual Haswell 2x16c; NVIDIA K80 (single device); NVIDIA GeForce Titan X Pascal



Exercise 06 (Three Level Parallelism)

Xeon Phi KNL 68c; Dual Haswell 2x16c; NVIDIA K80 (single device); NVIDIA GeForce Titan X Pascal



- ▶ **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 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.
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Team or Thread private memory

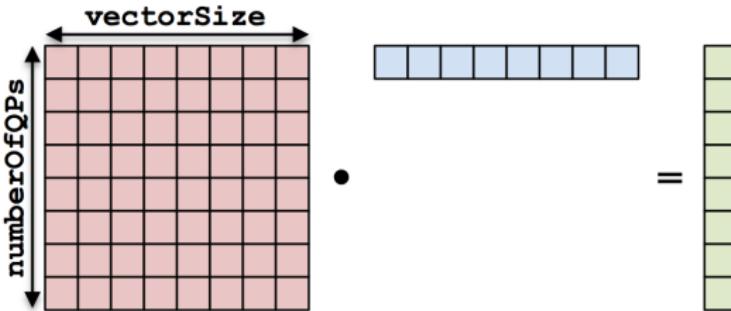
- ▶ Typically used for per work-item temporary storage.
- ▶ Advantage over pre allocated memory is aggregate size scales with number of threads, not number of work-items.

Manually Managed Cache

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- ▶ Exposes hardware specific on-core scratch space (e.g. NVIDIA GPU Shared Memory).

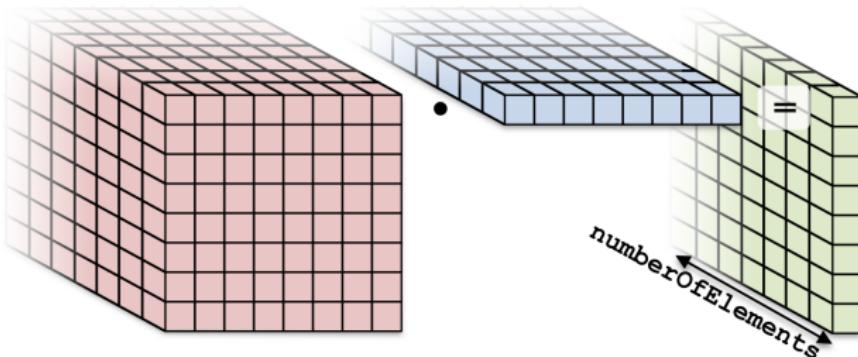
Now: Discuss Manually Managed Cache Use Case.

One slice of contractDataFieldScalar:



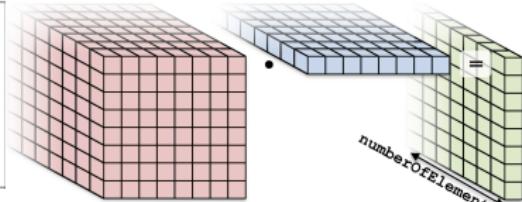
```
for (qp = 0; qp < numberOfQPs; ++qp) {  
    total = 0;  
    for (i = 0; i < vectorSize; ++i) {  
        total += A(qp, i) * B(i);  
    }  
    result(qp) = total;  
}
```

contractDataFieldScalar:



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

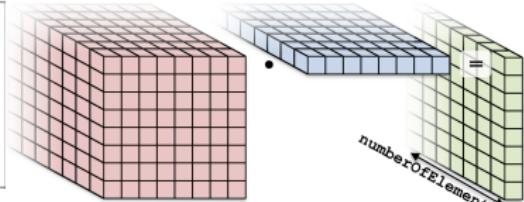
```
for (element = 0; element < numberElements; ++element) {  
    for (qp = 0; qp < numberQPs; ++qp) {  
        total = 0;  
        for (i = 0; i < vectorSize; ++i) {  
            total += A(element, qp, i) * B(element, i);  
        }  
        result(element, qp) = total;  
    }  
}
```



Parallelization approaches:

- ▶ Each thread handles an element.
Threads: numberElements

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



Parallelization approaches:

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Threads: numberElements

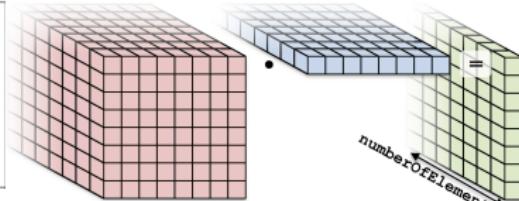
- ▶ Each thread handles a qp.

Threads: $\text{numberElements} * \text{numberQPs}$

```

for (element = 0; element < numberElements; ++element) {
    for (qp = 0; qp < numberQPs; ++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: numberElements

- ▶ Each thread handles a qp.

Threads: numberElements * numberQPs

- ▶ Each thread handles an i.

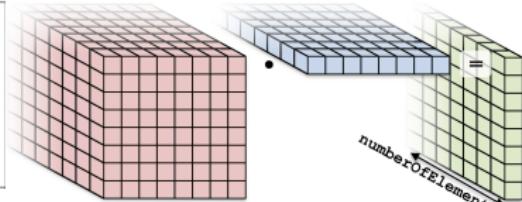
Threads: numElements * numQPs * vectorSize

Requires a parallel_reduce.

```

for (element = 0; element < numberElements; ++element) {
    for (qp = 0; qp < numQPs; ++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: numberElements

- ▶ Each thread handles a qp.

Threads: numberElements * numQPs

- ▶ Each thread handles an i.

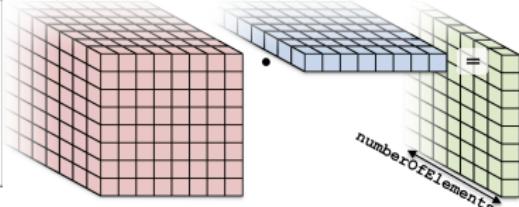
Threads: numElements * numQPs * vectorSize

Requires a parallel_reduce.

```

for (element = 0; element < numberElements; ++element) {
    for (qp = 0; qp < numberQPs; ++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

```

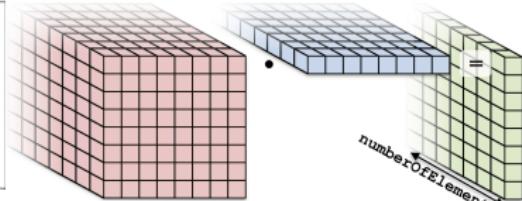
operator()(int index) {
    int element = extractElementFromIndex(index);
    int qp = extractQPFromIndex(index);
    double total = 0;
    for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
}

```

```

for (element = 0; element < numberOfElements; ++element) {
    for (qp = 0; qp < numberQPs; ++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

```

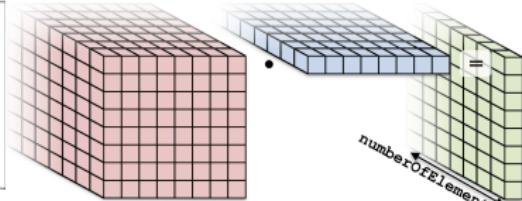
operator()(member_type teamMember) {
    int element = teamMember.league_rank();
    parallel_for(
        TeamThreadRange(teamMember, numberQPs),
        [=] (int qp) {
            double total = 0;
            for (int i = 0; i < vectorSize; ++i) {
                total += A(element, qp, i) * B(element,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

```

```

for (element = 0; element < number_of_elements; ++element) {
    for (qp = 0; qp < number_of_QPs; ++qp) {
        total = 0;
        for (i = 0; i < vector_size; ++i) {
            total += A(element, qp, i) * B(element, i);
        }
        result(element, qp) = total;
    }
}

```



Teams kernel: Each team handles an element

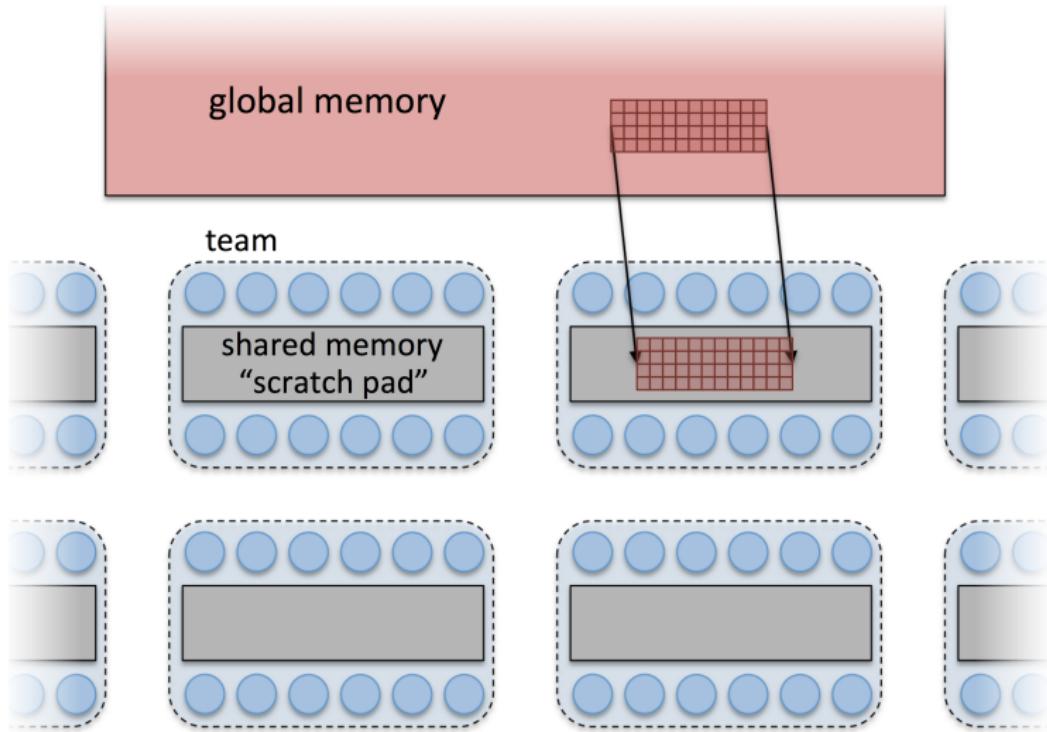
```

operator()(member_type teamMember) {
    int element = teamMember.league_rank();
    parallel_for(
        TeamThreadRange(teamMember, number_of_QPs),
        [=] (int qp) {
            double total = 0;
            for (int i = 0; i < vector_size; ++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:

- ▶ Scenario: Algorithm requires temporary workspace of size W .
- ▶ **Without scratch memory:** pre-allocate space for N work-items of size $N \times W$.
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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's 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
typedef View<double*, ExecutionSpace::scratch_memory_space
            , MemoryUnmanaged> ScratchPadView;
// 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(0),
                           vectorSize);
});
```

Kernel outline for teams with scratch memory:

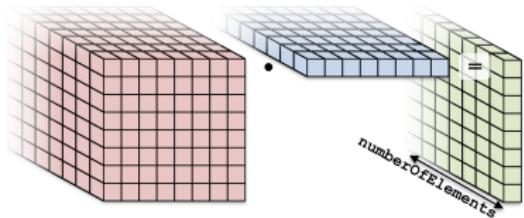
```

operator()(member_type teamMember) {
    ScratchPadView scratch(teamMember.team_scratch(0),
                           vectorSize);

    // TODO: load slice of B into scratch

    parallel_for(
        TeamThreadRange(teamMember, number0fQPs),
        [=] (int qp) {
            double total = 0;
            for (int i = 0; i < vectorSize; ++i) {
                total += A(element, qp, i) * scratch(i);
            }
            result(element, qp) = total;
        });
}

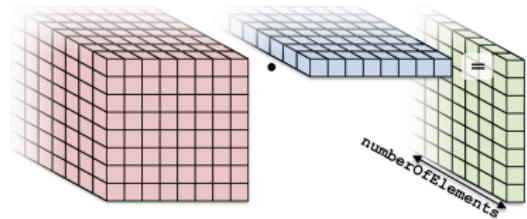
```



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);  
    }  
}
```



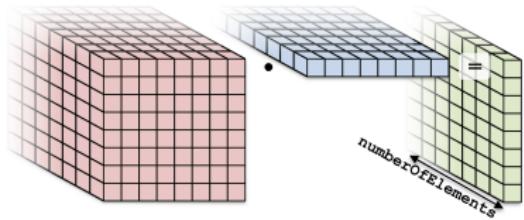
How to populate the scratch memory?

- ▶ ~~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);
    }
}
```

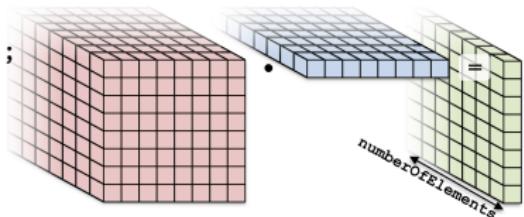
- ▶ ~~Each thread loads one entry?~~ **teamSize ≠ vectorSize**

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

- ▶ **TeamThreadRange**

```
parallel_for(
    TeamThreadRange(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);
    }
}
```

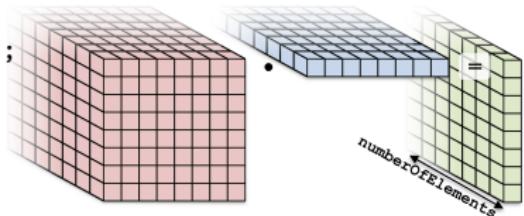
- ▶ ~~Each thread loads one entry?~~ **teamSize ≠ vectorSize**

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

- ▶ **TeamThreadRange**

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

```



(incomplete) Kernel for teams with scratch memory:

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

    parallel_for(TeamThreadRange(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) {
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    parallel_for(TeamThreadRange(teamMember, vectorSize),
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        });
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    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;
        });
}
```

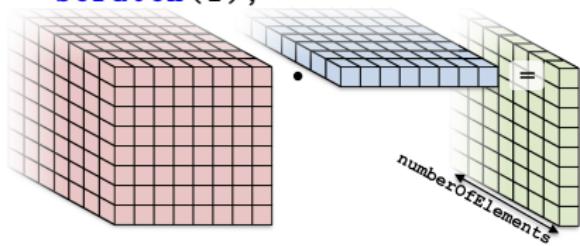
Problem: threads may start to use `scratch` before all threads are done loading.

Kernel for teams with scratch memory:

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

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

    parallel_for(TeamThreadRange(teamMember, number_of_QPs),
        [=] (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:

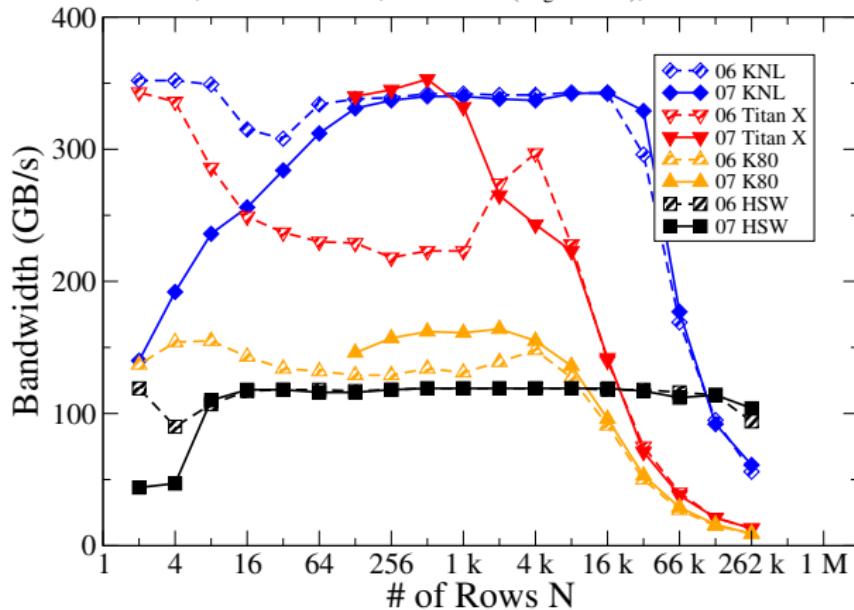
- ▶ Location: ~/SC2016/Exercises/07/
- ▶ Use the single policy instead of checking team rank
- ▶ Parallelize all three loop levels.

Things to try:

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

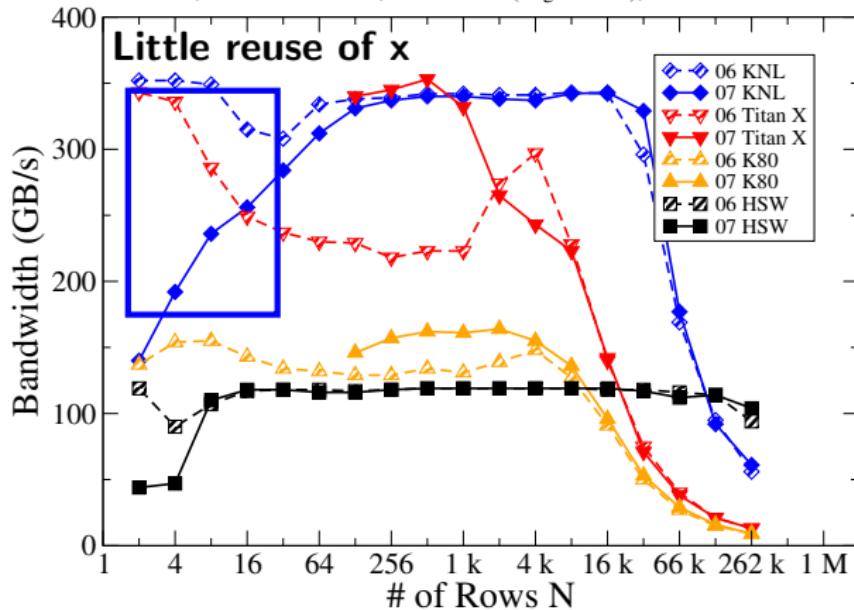
Exercise 07 (Scratch Memory)

Xeon Phi KNL 68c; Dual Haswell 2x16c; NVIDIA K80 (single device); NVIDIA GeForce Titan X Pascal



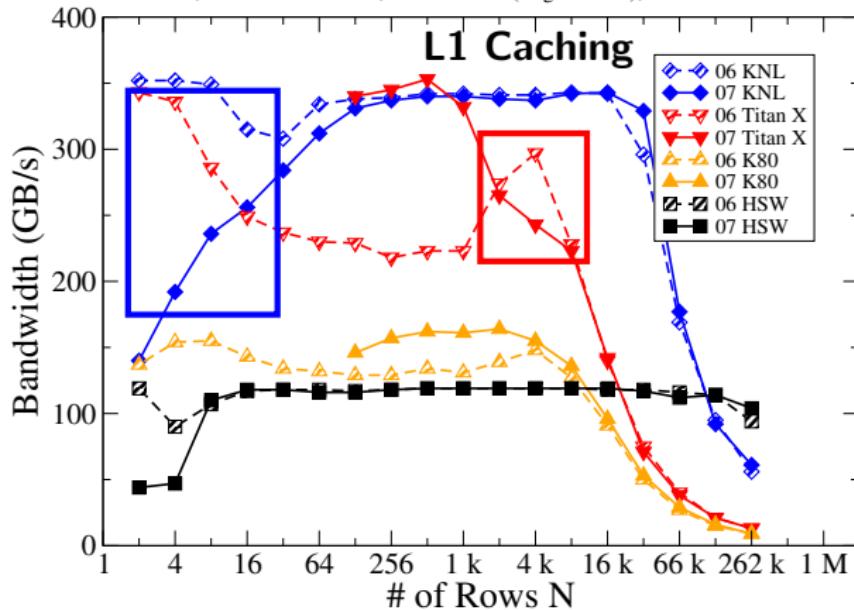
Exercise 07 (Scratch Memory)

Xeon Phi KNL 68c; Dual Haswell 2x16c; NVIDIA K80 (single device); NVIDIA GeForce Titan X Pascal



Exercise 07 (Scratch Memory)

Xeon Phi KNL 68c; Dual Haswell 2x16c; NVIDIA K80 (single device); NVIDIA GeForce Titan X Pascal



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 used with the TeamPolicy to provide thread or team **private** memory.
- ▶ Use case: 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.

- ▶ High performance computers are increasingly **heterogenous**
MPI-only is no longer sufficient.
- ▶ For **portability**: OpenMP, OpenACC, ... or Kokkos.
- ▶ Only Kokkos obtains performant memory access patterns via
architecture-aware arrays and work mapping.
*i.e., not just portable, *performance portable*.*
- ▶ With Kokkos, **simple things stay simple** (parallel-for, etc.).
*i.e., it's *no more difficult* than OpenMP.*
- ▶ **Advanced performance-optimizing patterns are simpler**
with Kokkos than with native versions.
*i.e., you're *not missing out* on advanced features.*