

Kokkos Tutorial

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

Using your own \${HOME}

- ▶ Git
- ▶ GCC 4.8.4 (or newer) *OR* Intel 15 (or newer) *OR* Clang 3.5.2 (or newer)
- ▶ CUDA nvcc 9.0 (or newer) *AND* NVIDIA compute capability 3.0 (or newer)
- ▶ git clone <https://github.com/kokkos/kokkos>
into \${HOME}/Kokkos/kokkos
- ▶ git clone <https://github.com/kokkos/kokkos-tutorials>
into \${HOME}/Kokkos/kokkos-tutorials

Slides are in

\${HOME}/Kokkos/kokkos-tutorials/Intro-Full/Slides

Exercises are in

\${HOME}/Kokkos/kokkos-tutorials/Intro-Full/Exercises

Exercises' makefiles look for \${HOME}/Kokkos/kokkos

Online Resources:

- ▶ <https://github.com/kokkos>: Primary Kokkos GitHub Organization
- ▶ https://github.com/kokkos/kokkos-tutorials/blob/master/Intro-Full/Slides/KokkosTutorial_ORNL20.pdf: These slides.
- ▶ <https://github.com/kokkos/kokkos/wiki>: Wiki including API reference
- ▶ <https://github.com/kokkos/kokkos-tutorials/issues/28>: Instructions to get cloud instance with GPU
- ▶ <https://kokkosteam.slack.com>: Slack channel for Kokkos

Kokkos' basic capabilities:

- ▶ Simple 1D data parallel computational patterns
- ▶ Deciding where code is run and where data is placed
- ▶ Managing data access patterns for performance portability

Kokkos' advanced capabilities:

- ▶ Thread safety, thread scalability, and atomic operations
- ▶ Hierarchical patterns for maximizing parallelism

Kokkos' advanced capabilities not covered today:

- ▶ Multidimensional data parallelism
- ▶ Dynamic directed acyclic graph of tasks pattern
- ▶ Numerous *plugin* points for extensibility

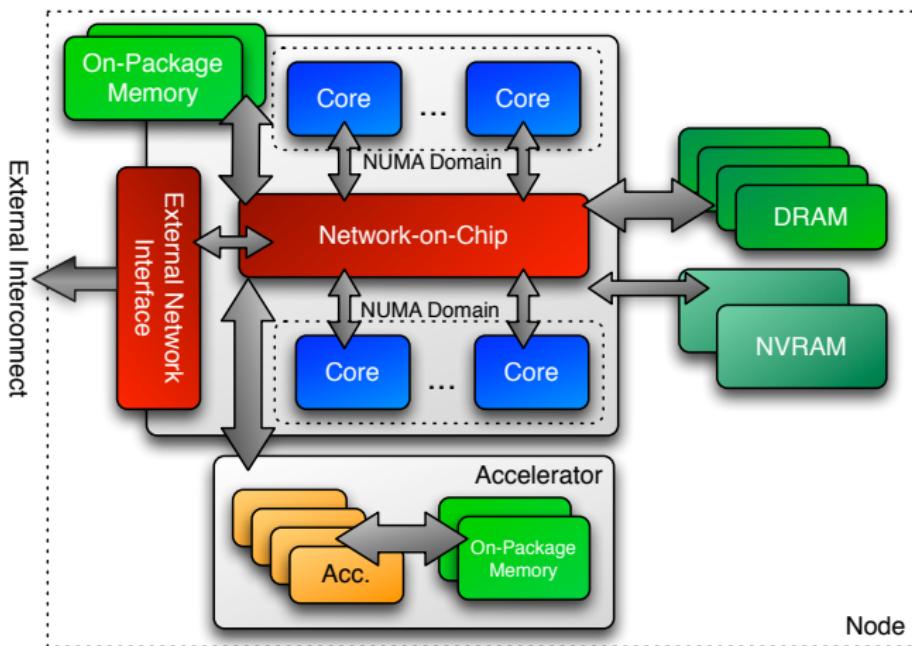
- ▶ Kokkos enables **Single Source Performance Portable Codes**
- ▶ **Simple things stay simple** - it is not much more complicated than OpenMP
- ▶ **Advanced performance optimizing capabilities** easier to use with Kokkos than e.g. CUDA
- ▶ Kokkos provides data abstractions critical for performance portability not available in OpenMP or OpenACC
Controlling data access patterns is key for obtaining performance

Assume you are here because:

- ▶ Want to use **all** HPC node architectures; including GPUs
- ▶ Are familiar with **C++**
- ▶ Want GPU programming to be **easier**
- ▶ Would like **portability**, as long as it doesn't hurt performance

Helpful for understanding nuances:

- ▶ Are familiar with **data parallelism**
- ▶ Are familiar with **OpenMP**
- ▶ Are familiar with **GPU architecture** and **CUDA**

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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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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#pragma omp parallel for
for (element = 0; element < numElements; ++element) {
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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 PHI *and* NVIDIA GPU *and* AMD GPU *and* ...

Option 1: OpenMP 4.5

```
#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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        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?

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

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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, GPUs, 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

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for (atomIndex = 0; atomIndex < numberAtoms; ++atomIndex) {  
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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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- ▶ 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.

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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 int64_t index) const {...}  
}
```

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struct Functor {  
    void operator()(const int64_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 int64_t atomIndex) const {  
        atomForces[atomIndex] = calculateForce(...data...);  
    }  
    ...  
}
```

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for (atomIndex = 0; atomIndex < numberAtoms; ++atomIndex) {  
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struct AtomForceFunctor {  
    ...  
    void operator()(const int64_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;  
    AtomForceFunctor(/* args */) {...}  
    void operator()(const int64_t atomIndex) const {  
        _atomForces[atomIndex] = calculateForce(_atomData);  
    }  
};
```

Putting it all together: the complete functor:

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struct AtomForceFunctor {  
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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);  
}
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Putting it all together: the complete functor:

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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(ForceType atomForces, AtomDataType data) :  
        _atomForces(atomForces), _atomData(data) {}  
  
    void operator()(const int64_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 tedious \Rightarrow C++11 Lambdas are concise

```
atomForces already exists
data already exists
Kokkos::parallel_for(numberOfAtoms ,
    [=] (const int64_t atomIndex) {
        atomForces[atomIndex] = calculateForce(data);
    }
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A lambda is not *magic*, it is the compiler **auto-generating** a **functor** for you.

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Warning: Lambda capture and C++ containers

For portability to GPU a lambda must capture by value [=].

Don't capture containers (e.g., std::vector) by value because it will copy the container's entire contents.

How does this compare to OpenMP?

Serial

```
for (int64_t i = 0; i < N; ++i) {  
    /* loop body */  
}
```

OpenMP

```
#pragma omp parallel for  
for (int64_t i = 0; i < N; ++i) {  
    /* loop body */  
}
```

Kokkos

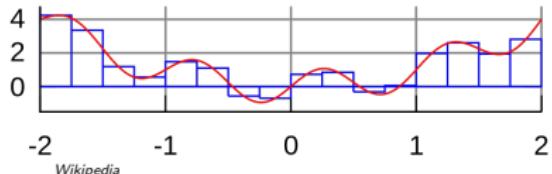
```
parallel_for(N, [=] (const int64_t i) {  
    /* loop body */  
});
```

Important concept

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

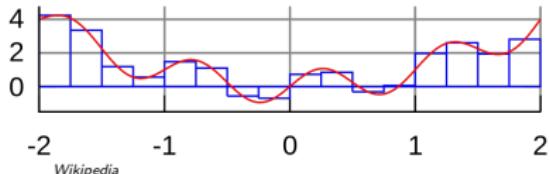
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$$y = \int_{\text{lower}}^{\text{upper}} \text{function}(x) dx$$



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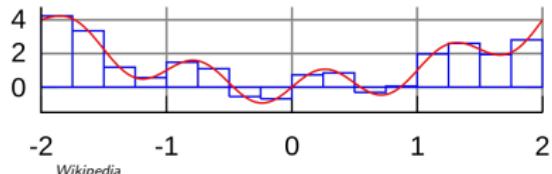
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```
double totalIntegral = 0;
for (int64_t i = 0; i < number_of_intervals; ++i) {
    const double x =
        lower + (i / number_of_intervals) * (upper - lower);
    const double this_intervals_contribution = function(x);
    totalIntegral += this_intervals_contribution;
}
totalIntegral *= dx;
```

Riemann-sum-style numerical integration:

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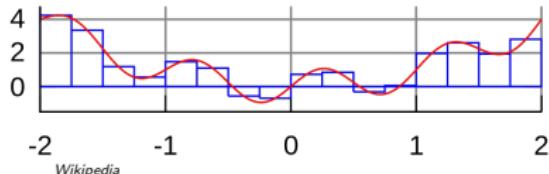


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How do we **parallelize** it? *Correctly?*

Riemann-sum-style numerical integration:

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



Pattern?

```
double totalIntegral = 0;
for (int64_t i = 0; i < number_of_intervals; ++i) {
    const double x =
        lower + (i / number_of_intervals) * (upper - lower);
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    totalIntegral += this_intervals_contribution;
}
totalIntegral *= dx;
```

Policy?

Body?

How do we **parallelize** it? *Correctly?*

An (incorrect) attempt:

```
double totalIntegral = 0;
Kokkos::parallel_for(numberOfIntervals,
    [=] (const int64_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 int64_t index) {
    const double x =
        lower + (index/numberOfIntervals) * (upper - lower);
    *totalIntegralPointer += function(x);
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});
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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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 (int64_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 (int64_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 (int64_t i = 0; i < numberOfIntervals; ++i) {  
    totalIntegral += function(...);  
}
```

```
double totalIntegral = 0;  
parallel_reduce(numberOfIntervals,  
 [=] (const int64_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 managed by Kokkos; it is not the final reduced value.

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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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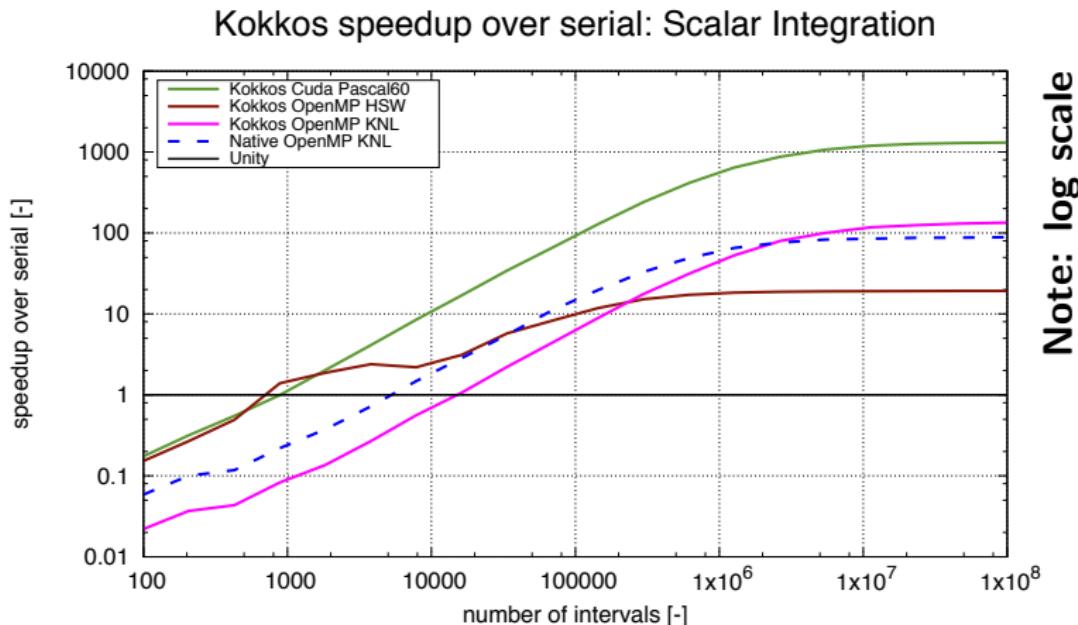
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- ▶ α = dispatch overhead
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- ▶ P = available concurrency

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

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



Always name your kernels!

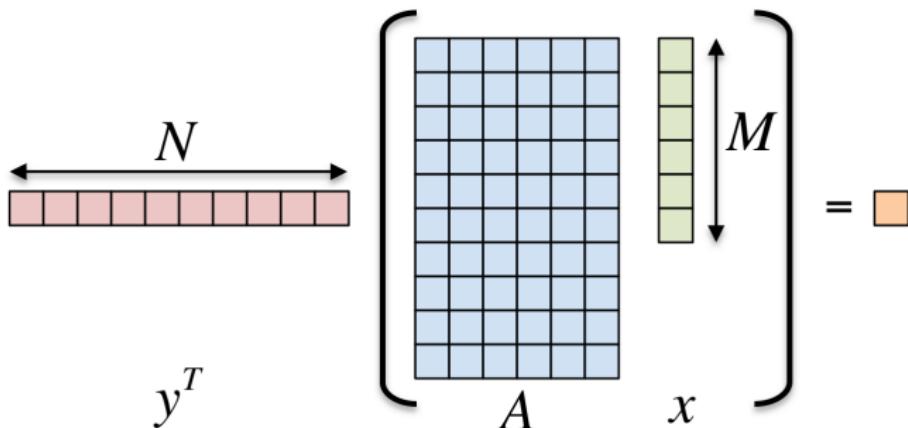
Giving unique names to each kernel is immensely helpful for debugging and profiling. You will regret it if you don't!

- ▶ Non-nested parallel patterns can take an optional string argument.
- ▶ The label doesn't need to be unique, but it is helpful.
- ▶ Anything convertible to "const std::string"
- ▶ Used by profiling and debugging tools (see Profiling Tutorial)

Example:

```
double totalIntegral = 0;
parallel_reduce("Reduction",numberOfIntervals,
 [=] (const int64_t i, double & valueToUpdate) {
    valueToUpdate += function(...);
},
 totalIntegral);
```

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

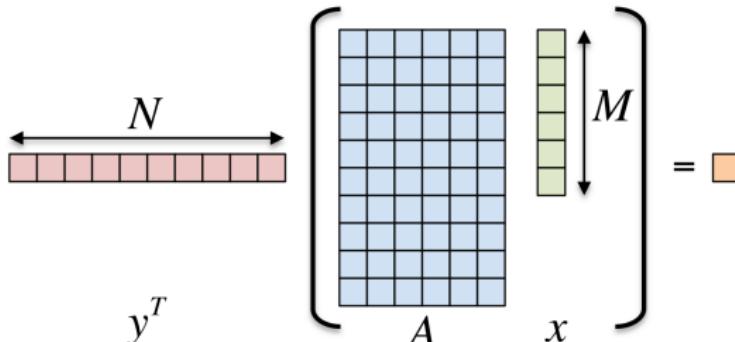
The **first step** in using Kokkos is to include, initialize, and finalize:

```
#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: [Intro-Full/Exercises/01/Begin/](#)
- ▶ 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

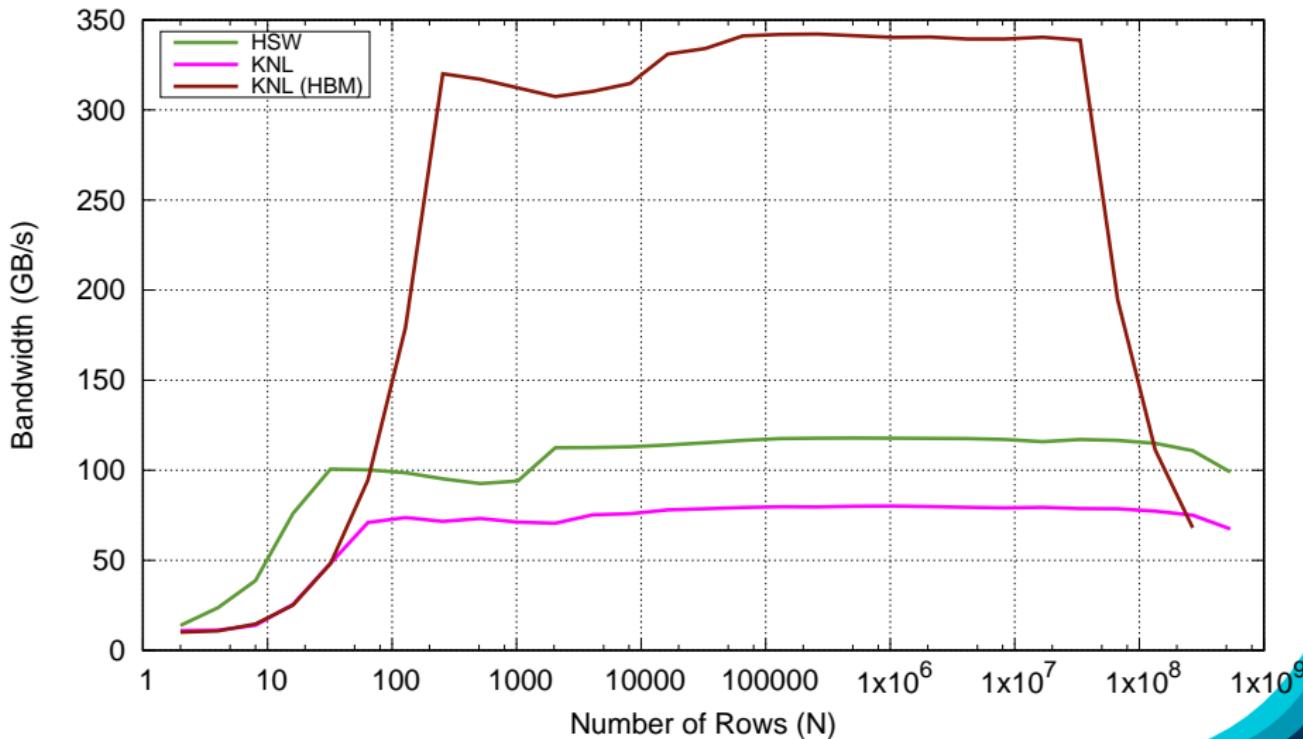
```
# gcc using OpenMP (default) and Serial back-ends,  
# (optional) change non-default arch with KOKKOS_ARCH  
make -j KOKKOS_DEVICES=OpenMP,Serial KOKKOS_ARCH=...
```

Running on CPU with OpenMP back-end

```
# Set OpenMP affinity  
export OMP_NUM_THREADS=8  
export OMP_PROC_BIND=spread OMP_PLACES=threads  
# 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 problem size with cline arg $-S s$
- ▶ Vary number of rows with cline arg $-N n$
- ▶ Num rows = 2^n , num cols = 2^m , total size = $2^s == 2^{n+m}$

$\langle y, Ax \rangle$ Exercise 01, Fixed Size

- ▶ Customizing `parallel_reduce` data type and reduction operator
 - e.g., minimum, maximum, ...
- ▶ `parallel_scan` pattern for exclusive and inclusive prefix sum
- ▶ Using *tag dispatch* interface to allow non-trivial functors to have multiple “`operator()`” functions.
 - very useful in large, complex applications

- ▶ **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.

Lambda

```
double * x = new double[N]; // also y
parallel_for("DAXPY",N, [=] (const int64_t i) {
    y[i] = a * x[i] + y[i];
});
```

Functor

```
struct Functor {
    double *_x, *_y, a;
    void operator()(const int64_t i) {
        _y[i] = _a * _x[i] + _y[i];
    }
};
```

Example: running daxpy on the GPU:

Lambda

```
double * x = new double[N]; // also y
parallel_for("DAXPY",N, [=] (const int64_t i) {
    y[i] = a * x[i] + y[i];
});
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Functor

```
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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double * x = new double[N]; // also y
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});
```

Functor

```
struct Functor {
    double *_x, *_y, a;
    void operator()(const int64_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("DAXPY", N, [=] (const int64_t i) {
    // Views x and y are captured by value (copy)
    y(i) = a * x(i) + y(i);
});
```

View abstraction

- ▶ A *lightweight* C++ class with a pointer to array data and a little meta-data,
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... populate x, y...

parallel_for("DAXPY", N, [=] (const int64_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 in your functors.

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.
- ▶ Access elements via "(...)" operator.

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- ▶ **Sizes of dimensions** set at compile-time or runtime.
e.g., 2x20, 50x50, etc.
- ▶ Access elements via "(...)" operator.

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
//Access
data(i,j,k) = 5.3;
```

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

What gets printed?

View life cycle:

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print a(0,2)
```

What gets printed?
3.0

View Properties:

- ▶ Accessing a View's sizes is done via its `extent(dim)` function.
Static extents can *additionally* be accessed via
`static_extent(dim)`.
- ▶ You can retrieve a raw pointer via its `data()` function.
- ▶ The label can be accessed via `label()`.

Example:

```
View<double*[5]> a("A",N0);
assert(a.extent(0)==N0);
assert(a.extent(1)==N0);
static_assert(a.static_extent(1)==5);
assert(a.data() != nullptr);
assert(std::string("A").compare(a.label())==0);
```

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

- ▶ Location: Intro-Full/Exercises/02/Begin/
- ▶ 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      # GPU - note UVM in Makefile
# 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; *covered later.*

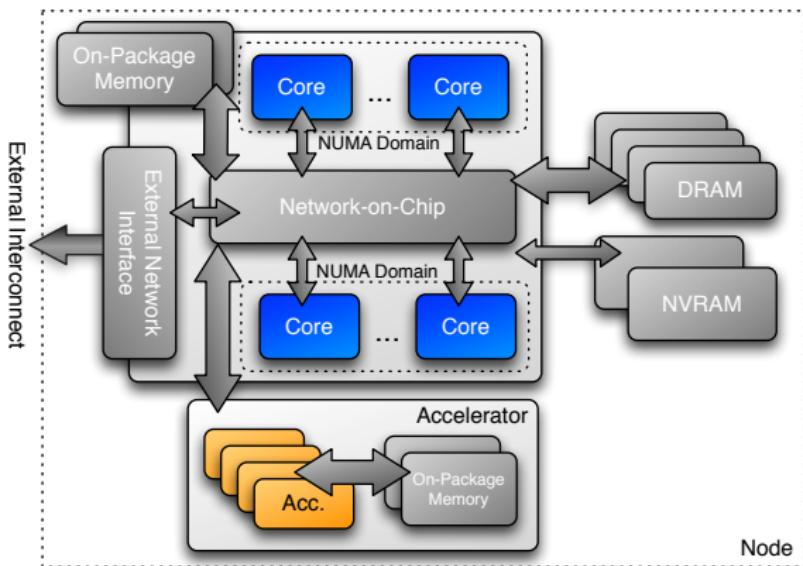
Execution and Memory Spaces

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.

Execution Space

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



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

Host

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

Kokkos::parallel_for("MyKernel", numberOfWorkers,
                     [=] (const int64_t workerIndex) {
    const double y = ...;
    // do something interesting
}
);
```

Parallel

Host

```
MPI_Reduce(...);  
FILE * file = fopen(...);  
runANormalFunction(...data...);  
  
Kokkos::parallel_for("MyKernel", numberOfWorkers,  
                     [=] (const int64_t workerIndex) {  
                         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...);  
  
Parallel Kokkos::parallel_for("MyKernel", numberOfWorkers,  
                           [=] (const int64_t workerIndex) {  
                               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**

```
Host MPI_Reduce(...);  
FILE * file = fopen(...);  
runANormalFunction(...data...);  
  
Parallel Kokkos::parallel_for("MyKernel", numberOfWorkers,  
                           [=] (const int64_t workerIndex) {  
                               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("Label",
    RangePolicy< ExecutionSpace >(0,numberOfIntervals),
    [=] (const int64_t i) {
        /* ... body ... */
    });
}
```

Default

```
parallel_for("Label",
    numberOfIntervals, // == RangePolicy<>(0,numberOfIntervals)
    [=] (const int64_t i) {
        /* ... body ... */
    });
}
```

Custom

```
parallel_for("Label",
    RangePolicy< ExecutionSpace >(0,numberOfIntervals),
    [=] (const int64_t i) {
        /* ... body ... */
    });
}
```

Default

```
parallel_for("Label",
    numberOfIntervals, // == RangePolicy<>(0,numberOfIntervals)
    [=] (const int64_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 int64_t s) const { ... }
    KOKKOS_INLINE_FUNCTION
    void operator()(const int64_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:

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struct ParallelFunctor {
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}
// Where kokkos defines:
#define KOKKOS_INLINE_FUNCTION inline /* #if CPU-only */
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```

Lambda annotation with KOKKOS_LAMBDA macro (requires CUDA 8.0)

```
Kokkos::parallel_for("Label", numberOflterations,
    KOKKOS_LAMBDA (const int64_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 (int64_t i = 0; i < size; ++i) {
    data(i) = ...read from file...
}

double sum = 0;
Kokkos::parallel_reduce("Label",
    RangePolicy<SomeExampleExecutionSpace>(0, size),
    KOKKOS_LAMBDA (const int64_t index, double & valueToUpdate) {
        valueToUpdate += data(index);
    },
    sum);
```

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

Memory space motivating example: summing an array

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    sum);
```

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

Memory space motivating example: summing an array

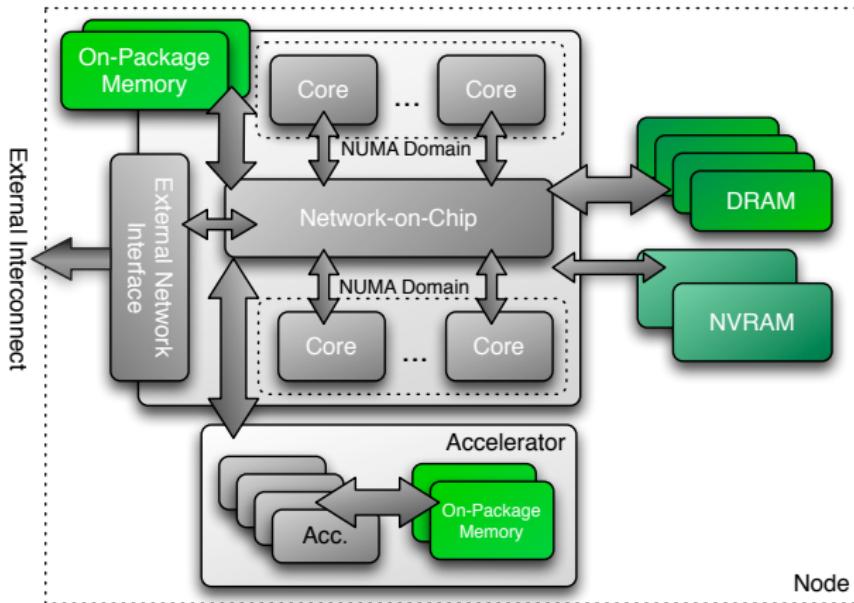
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    },
    sum);
```

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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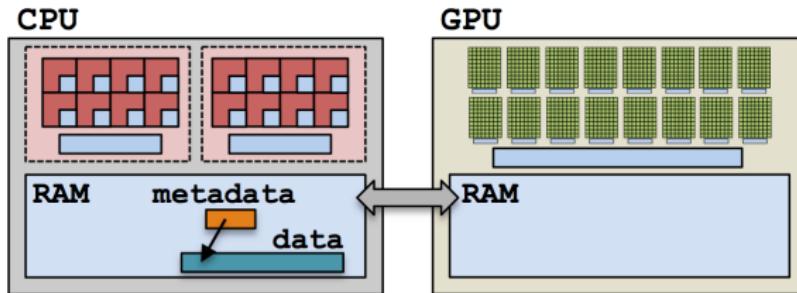
Important concept: Memory spaces

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

- ▶ `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**.

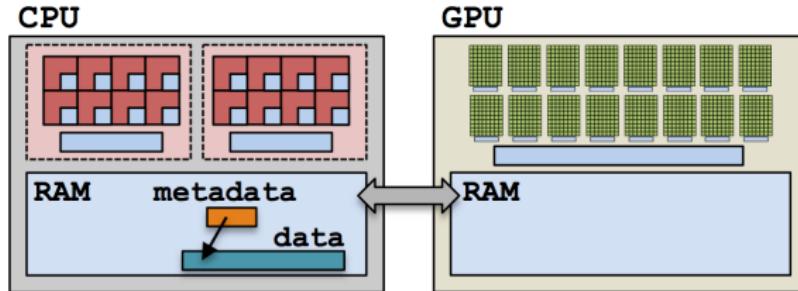
Example: HostSpace

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



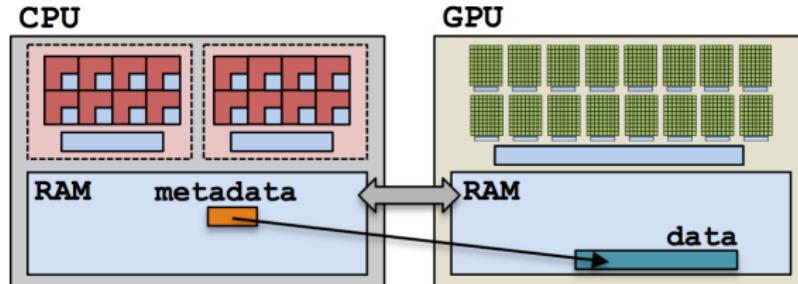
Example: HostSpace

```
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.

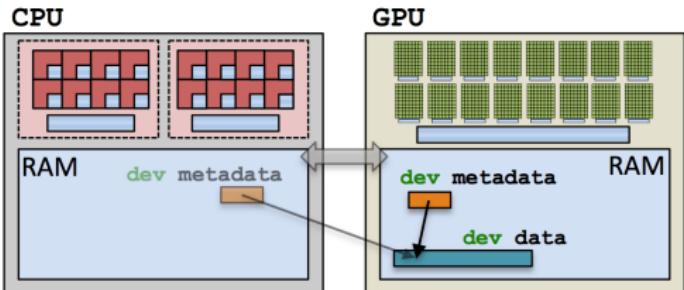
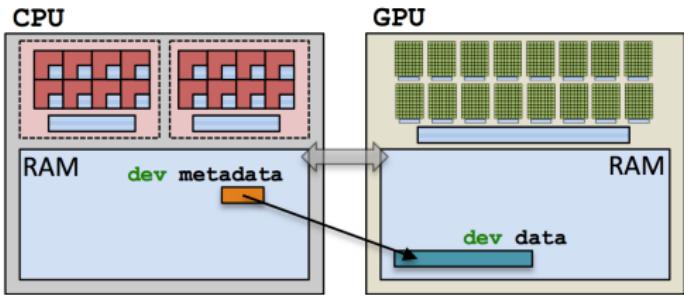
```
#define KL KOKKOS_LAMBDA
View<int*, Cuda> dev(...);
parallel_for("Label", N,
    KL (int i) {
        dev(i) = ...;
    });
}
```

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

Example: one view

```
#define KL KOKKOS_LAMBDA
View<int*, Cuda> dev;
parallel_for("Label", N,
    KL (int i) {
        dev(i) = ...;
    });

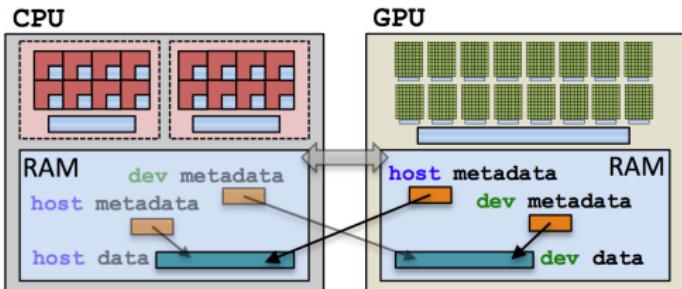
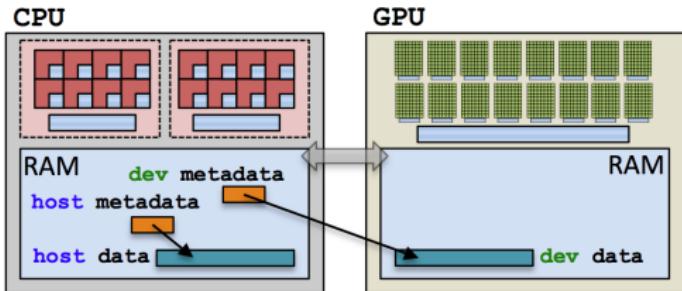
```



Example: two views

```
#define KL KOKKOS_LAMBDA
View<int*, Cuda> dev;
View<int*, Host> host;
parallel_for("Label", N,
    KL (int i) {
        dev(i) = ...;
        host(i) = ...;
    });

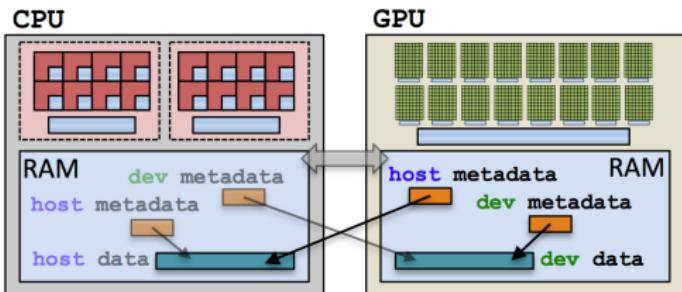
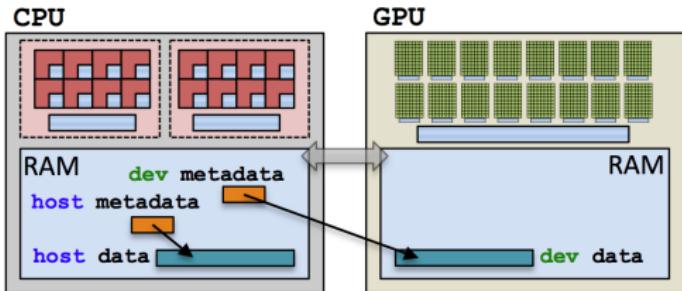
```



Example: two views

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View<int*, Cuda> dev;
View<int*, Host> host;
parallel_for("Label", N,
    KL (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 (int64_t i = 0; i < size; ++i) {
    array(i) = ...read from file...
}

double sum = 0;
Kokkos::parallel_reduce( "Label",
RangePolicy< Cuda>(0, size),
KOKKOS_LAMBDA (const int64_t index, double & valueToUpdate) {
    valueToUpdate += array(index);
},
sum);
```

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Kokkos::parallel_reduce( "Label",
    RangePolicy< Cuda>(0, size),
    KOKKOS_LAMBDA (const int64_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 (int64_t i = 0; i < size; ++i) {
    array(i) = ...read from file...
}

double sum = 0;
Kokkos::parallel_reduce("Label",
    RangePolicy< Cuda>(0, size),
    KOKKOS_LAMBDA (const int64_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 (int64_t i = 0; i < size; ++i) {
    array(i) = ...read from file...
}

double sum = 0;
Kokkos::parallel_reduce("Label",
    RangePolicy< Cuda>(0, size),
    KOKKOS_LAMBDA (const int64_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 (int64_t i = 0; i < size; ++i) {
    array(i) = ...read from file...
}

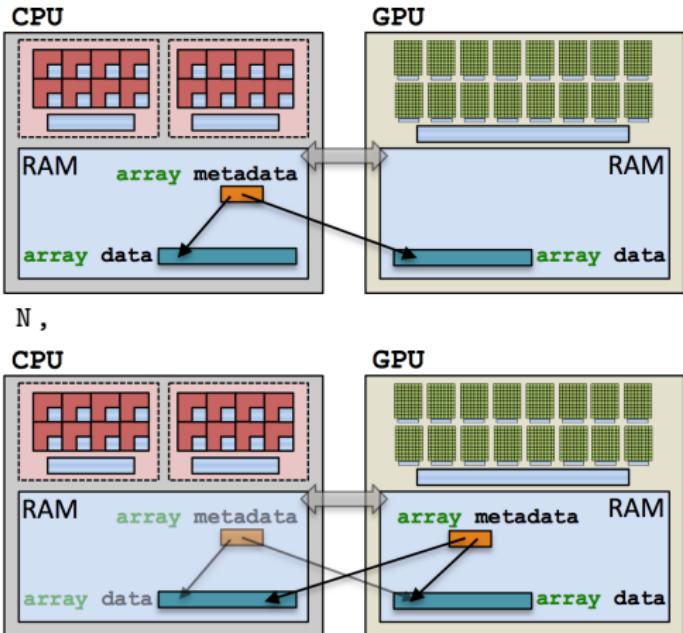
double sum = 0;
Kokkos::parallel_reduce("Label",
    RangePolicy< Cuda>(0, size),
    KOKKOS_LAMBDA (const int64_t index, double & valueToUpdate) {
        valueToUpdate += array(index);           illegal access
    },
    sum);
```

What's the solution?

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

CudaUVMSpace

```
#define KL KOKKOS_LAMBDA
View<double*, CudaUVMSpace> array
array = ...from file...
double sum = 0;
parallel_reduce("Label", N,
    KL (int i,
        double & d) {
    d += array(i);
},
sum);
```



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

Important concept: Mirrors

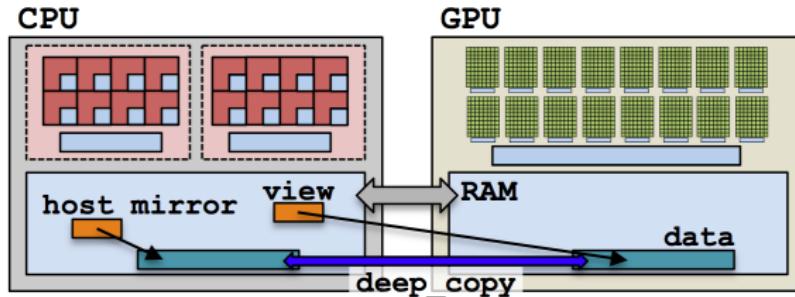
Mirrors are views of equivalent arrays residing in possibly different memory spaces.

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;  
ViewType view(...);
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```

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```
ViewType::HostMirror hostView =  
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ViewType::HostMirror hostView =  
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4. Deep copy `hostView`'s array to `view`'s array.

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

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

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typedef Kokkos::View<double*, Space> ViewType;  
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4. **Deep copy** `hostView`'s array to `view`'s array.

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

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

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

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

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ViewType view(...);
```

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```
Kokkos::parallel_for("Label",  
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: Intro-Full/Exercises/03/Begin/
- ▶ 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.
- ▶ **Heterogeneous nodes** have one or more memory spaces.
- ▶ **Mirroring** is used for performant access to views in host and device memory.
- ▶ Heterogeneous 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.

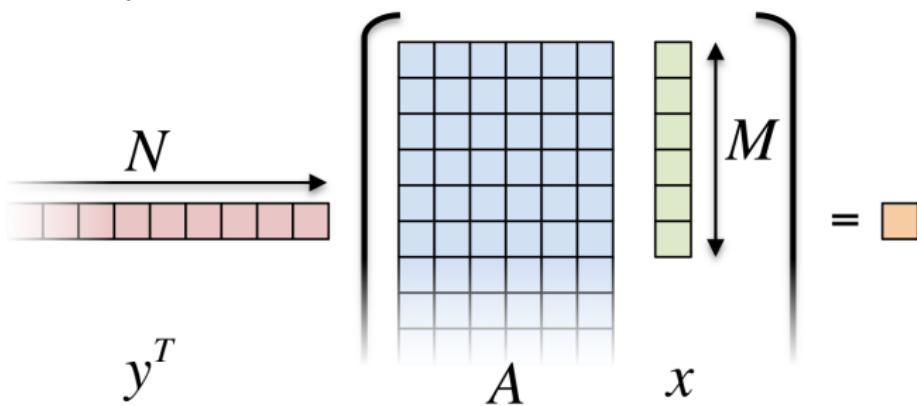
Managing memory access patterns for performance portability

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.

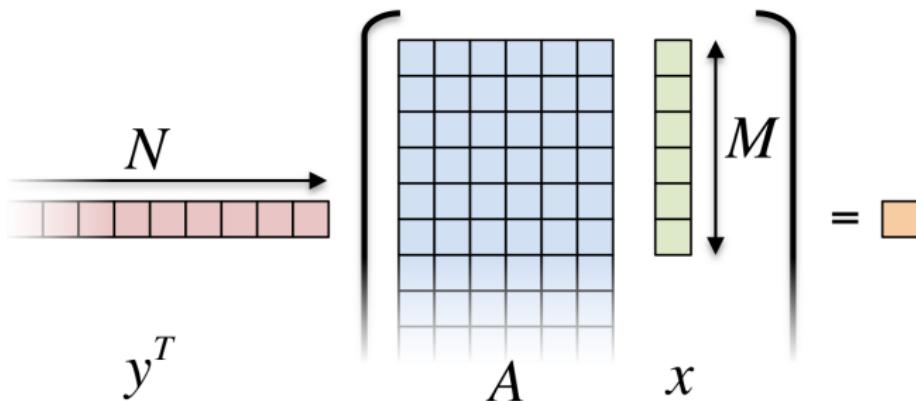
Example: inner product (0)

```
Kokkos::parallel_reduce("Label",
    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)

```
Kokkos::parallel_reduce("Label",
    RangePolicy<ExecutionSpace>(0, N),
    KOKKOS_LAMBDA (const size_t row, double & valueToUpdate) {
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```

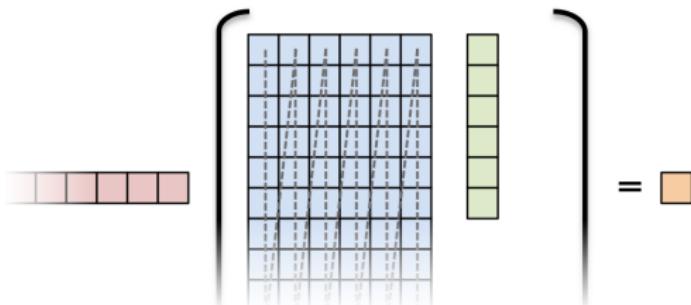


Driving question: How should A be laid out in memory?

Layout is the mapping of multi-index to memory:

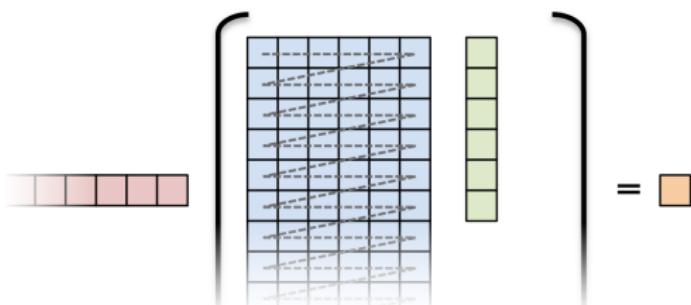
LayoutLeft

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.

```
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:

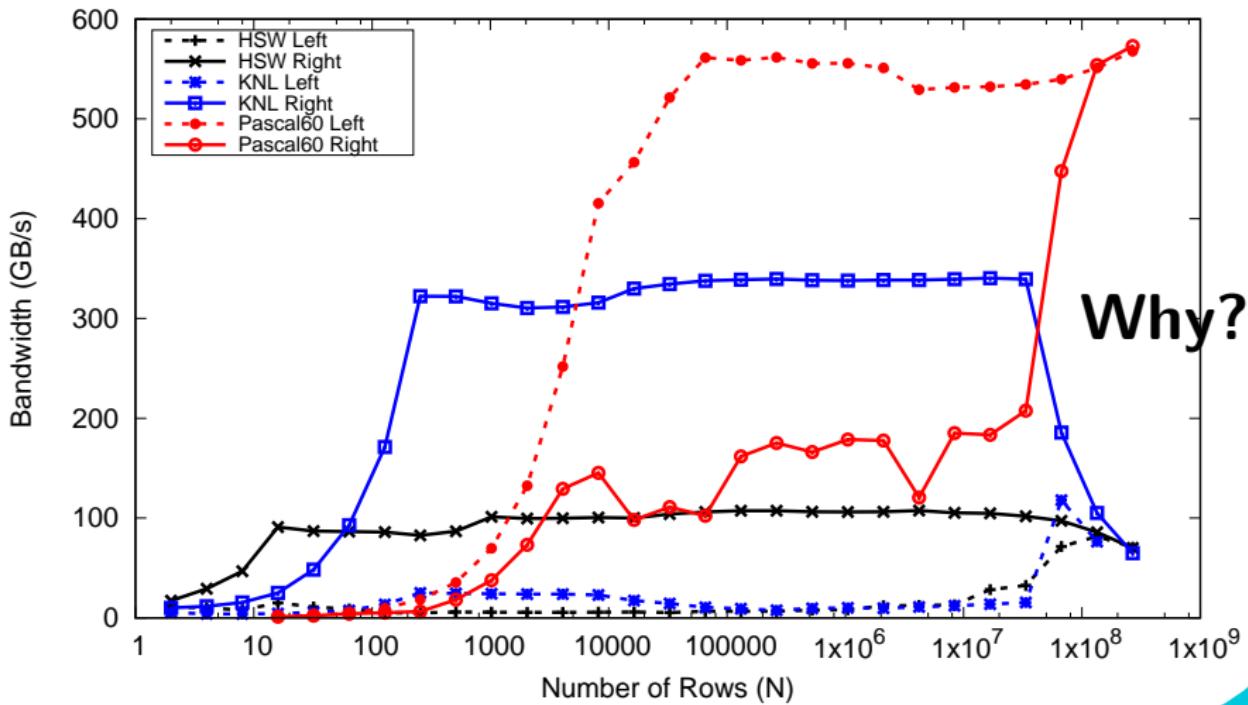
- ▶ Location: Intro-Full/Exercises/04/Begin/
- ▶ Replace ‘‘N’’ in parallel dispatch with RangePolicy<ExecSpace>
- ▶ Add MemSpace to all Views and Layout to A
- ▶ Experiment with the combinations of ExecSpace, Layout to view performance

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.

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

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



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:

```
operator()(const size_t index, double & valueToUpdate) {  
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- ▶ **CPU** threads are independent.
i.e., threads may execute at any rate.

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- ▶ **CPU** threads are independent.
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- ▶ **GPU** threads benefit (NVIDIA Volta) or must synchronize (AMD) in groups.
i.e., threads in groups can/must execute instructions together.

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

Thread independence:

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    const double d = _data(index);  
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}
```

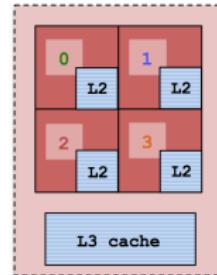
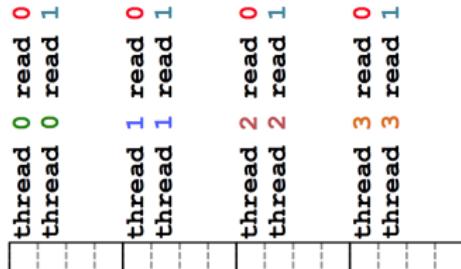
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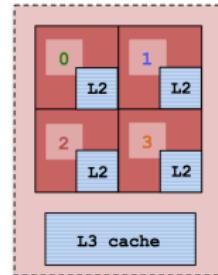
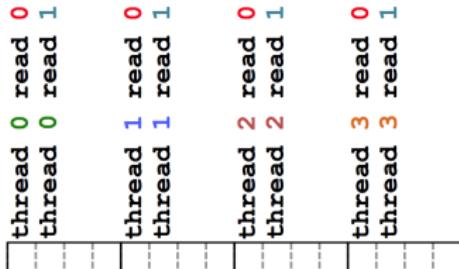
In particular, all threads in a group (*warp* or *wavefront*) must finished their loads before *any* thread can move on.

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

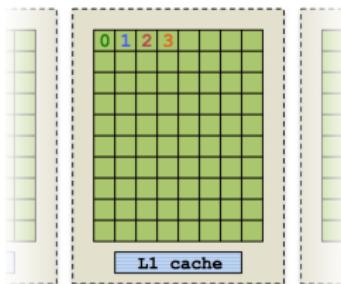
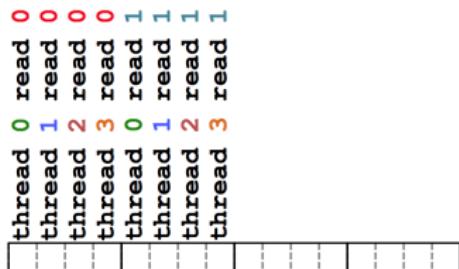
CPUs: few (independent) cores with separate caches:



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.

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

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

Warning

Uncoalesced access on GPUs and non-cached loads on CPUs
greatly reduces performance (can be $\downarrow 10X$)

Consider the array summation example:

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

double sum = 0;
Kokkos::parallel_reduce("Label",
    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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Given P threads, **which indices** do we want thread 0 to handle?

Contiguous:

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

CPU

Strided:

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);  
    valueToUpdate += d;  
}
```

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

Iterating for the execution space:

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

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("Label", ... ,
    KOKKOS_LAMBDA (const size_t workIndex) {
    ...
        view(..., ... , workIndex ) = ...;
        view(... , workIndex, ... ) = ...;
        view(workIndex, ... , ... ) = ...;
    });
...
}
```

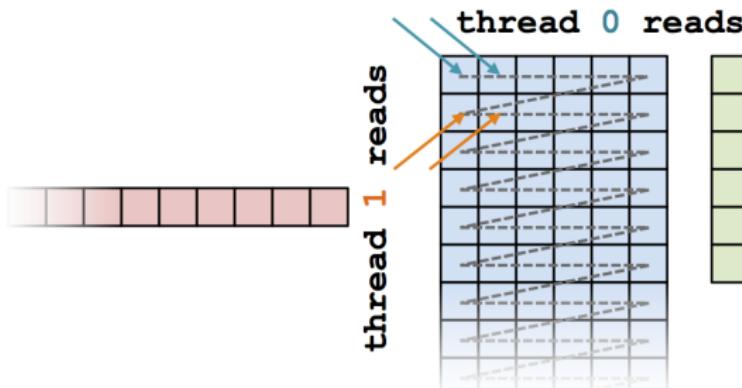
Important point

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

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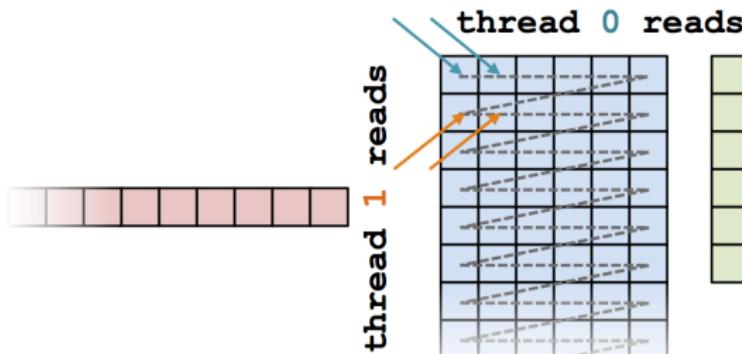
Analysis: row-major (LayoutRight)



Important point

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

Analysis: row-major (LayoutRight)

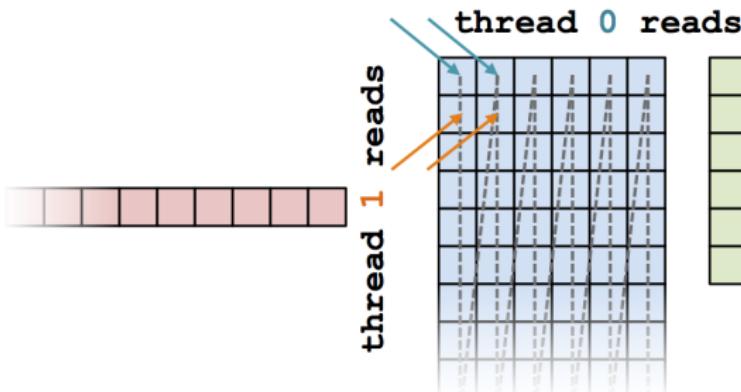


- ▶ **HostSpace:** cached (good)
- ▶ **CudaSpace:** uncoalesced (bad)

Important point

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

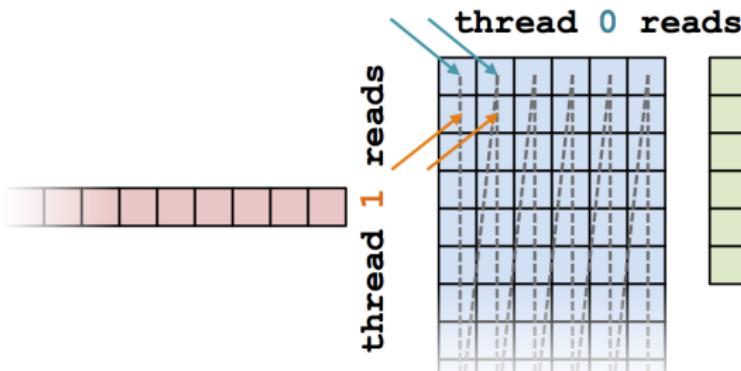
Analysis: column-major (LayoutLeft)



Important point

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

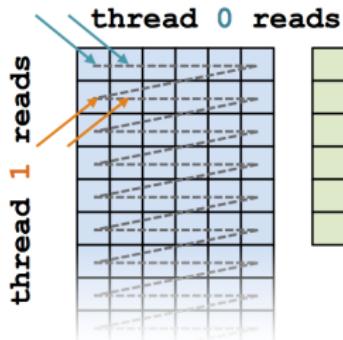
Analysis: column-major (LayoutLeft)



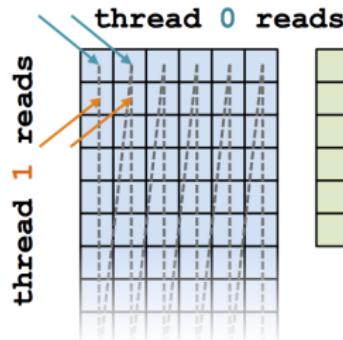
- ▶ **HostSpace:** uncached (**bad**)
- ▶ **CudaSpace:** coalesced (**good**)

Analysis: Kokkos architecture-dependent

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



(a) OpenMP

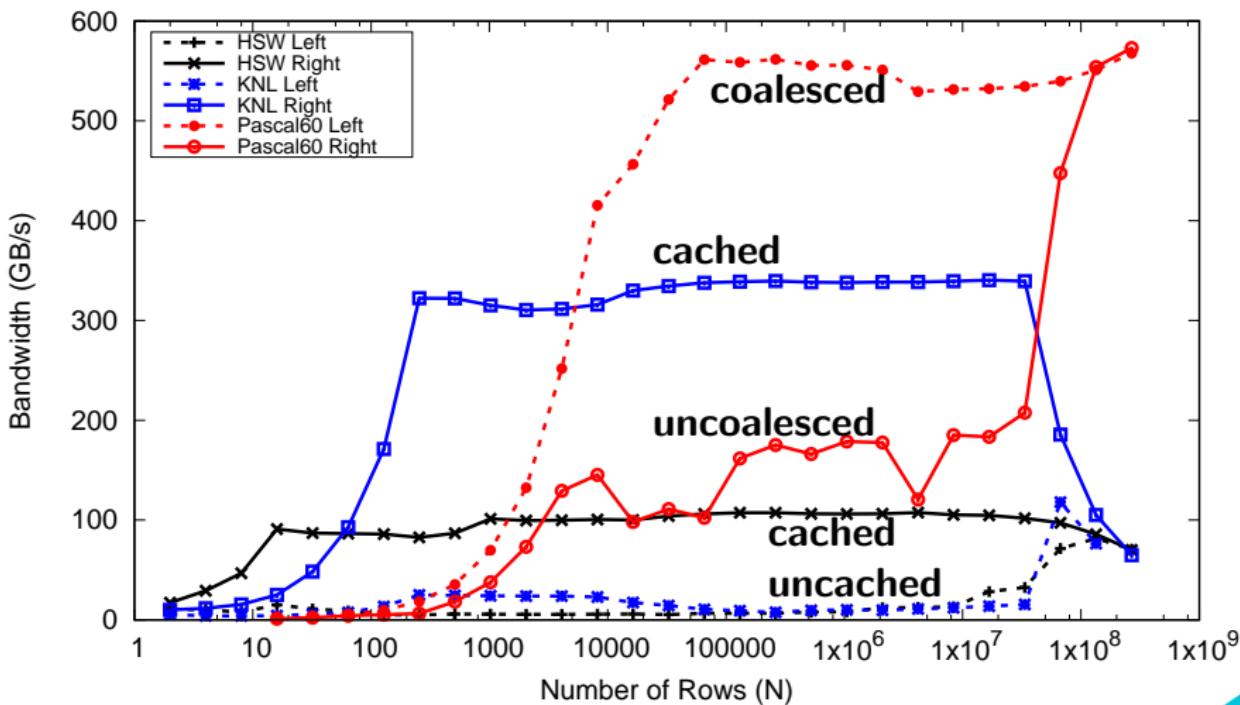


(b) Cuda

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

$\langle y | Ax \rangle$ Exercise 04 (Layout) Fixed Size

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

DualView

Learning objectives:

- ▶ Motivation and Value Added.
- ▶ Usage.
- ▶ Exercises.

Motivation and Value-added

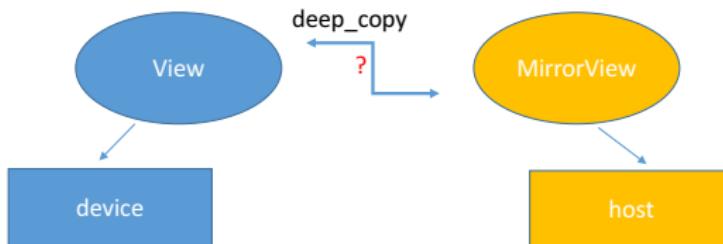
- ▶ DualView was designed to help transition codes to Kokkos.

Motivation and Value-added

- ▶ DualView was designed to help transition codes to Kokkos.
- ▶ DualView simplifies the task of managing data movement between memory spaces, e.g., host and device.

Motivation and Value-added

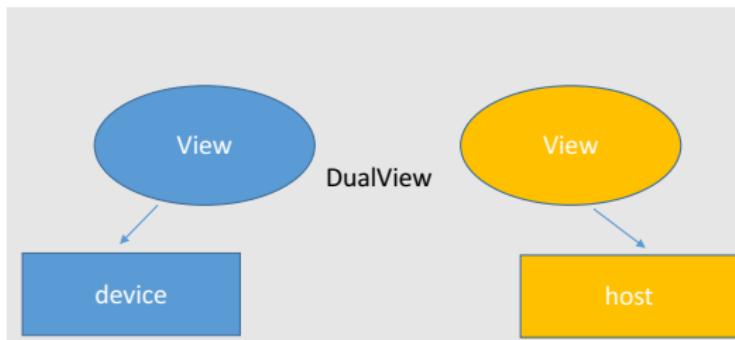
- ▶ DualView was designed to help transition codes to Kokkos.
- ▶ DualView simplifies the task of managing data movement between memory spaces, e.g., host and device.
- ▶ When converting a typical app to use Kokkos, there is usually no holistic view of such data transfers.



Without DualView, could use MirrorViews, but

- ▶ deep copies are expensive, use sparingly
- ▶ do I need a deep copy here?
- ▶ where is the most recent data?
- ▶ is data on the host or device stale?
- ▶ was code modified upstream? is data here now stale, but not in previous version?

DualView bundles two views, a Host View and a Device View



There is no automatic tracking of data freshness:

- ▶ you must tell Kokkos when data has been modified on a memory space.
- ▶ If you mark data as modified when you modify it, then Kokkos will know if it needs to move data

DualView bundles two views, a Host View and a Device View

- ▶ Data members for the two views

```
DualView::t_host h_view  
DualView::t_dev d_view
```

- ▶ Retrieve data members

```
t_host view_host();  
t_dev view_device();
```

- ▶ Mark data as modified

```
void modify_host();  
void modify_device();
```

DualView bundles two views, a Host View and a Device View

- ▶ Sync data in a direction if not in sync

```
void sync_host();  
void sync_device();
```

- ▶ Check sync status

```
void need_sync_host();  
void need_sync_device();
```

DualView has templated functions for generic use in templated code

- ▶ Retrieve data members

```
template<class Space>
auto view();
```

- ▶ Mark data as modified

```
template<class Space>
void modify();
```

- ▶ Sync data in a direction if not in sync

```
template<class Space>
void sync();
```

- ▶ Check sync status

```
template<class Space>
void need_sync();
```

Details:

- ▶ Location: Intro-Full/Exercises/dualview/Begin/
- ▶ Modify or create a new compute_enthalpy function in dual_view_exercise.cpp to:
 - ▶ 1. Take (dual)views as arguments
 - ▶ 2. Call **modify()** and/or **sync()** when appropriate for the dual views
 - ▶ 3. Runs the kernel on host or device execution spaces

```
# 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
./dualview.cuda -S 26
```

Tightly Nested Loops with MDRangePolicy

Learning objectives:

- ▶ Demonstrate usage of the MDRangePolicy with tightly nested loops.
- ▶ Syntax - Required and optional settings
- ▶ Code demo and example

Motivating example: Consider the nested for loops:

```
for ( int i = 0; i < Ni; ++i )
for ( int j = 0; j < Nj; ++j )
for ( int k = 0; k < Nk; ++k )
    some_init_fcn(i, j, k);
```

Based on Kokkos lessons thus far, you might parallelize this as

```
Kokkos::parallel_for(Ni,
                      KOKKOS_LAMBDA (const i) {
                          for ( int j = 0; j < Nj; ++j )
                              for ( int k = 0; k < Nk; ++k )
                                  some_init_fcn(i, j, k);
                      }
                  );
```

- ▶ This only parallelizes along one dimension, leaving potential parallelism unexploited.
- ▶ What if Ni is too small to amortize the cost of constructing a parallel region, but $Ni * Nj * Nk$ makes it worthwhile?

Solution: Use an MDRangePolicy

```
for ( int i = 0; i < Ni; ++i )
for ( int j = 0; j < Nj; ++j )
for ( int k = 0; k < Nk; ++k )
    some_init_fcn(i, j, k);
```

Instead, use the MDRangePolicy with the parallel for

```
Kokkos::parallel_for(Kokkos::MDRangePolicy<Kokkos::Rank<3>>
                      ({0,0,0}, {Ni,Nj,Nk}),
                      KOKKOS_LAMBDA (int i, int j, int k) {
                          some_init_fcn(i, j, k);
                      }
                  );
```

Required Template Parameters to MDRangePolicy

Kokkos :: Rank< N, IterateOuter , IterateInner >

- ▶ **N: (Required)** the rank of the index space (limited from 2 to 6)
- ▶ **IterateOuter (Optional)** iteration pattern between tiles
 - ▶ **Options:** IterateLeft, IterateRight, IterateDefault
- ▶ **IterateInner (Optional)** iteration pattern within tiles
 - ▶ **Options:** IterateLeft, IterateRight, IterateDefault

Optional Template Parameters

ExecutionSpace

- ▶ **Options:** Serial, OpenMP, Threads, Cuda

Schedule < Options >

- ▶ **Options:** Static, Dynamic

IndexType < Options >

- ▶ **Options:** int, long, etc

WorkTag

- ▶ **Options:** SomeClass

```
MDRangePolicy< Rank<2,OP,IP>, OpenMP, Schedule<Static>,
                IndexType<int> > mdrpolicy;
```

Policy Arguments

BeginList

- ▶ **Initializer List or Kokkos::Array (Required):** rank arguments for starts of index space
 - ▶ **Example** Rank 2: {b0,b1}

EndList

- ▶ **Initializer List or Kokkos::Array (Required):** rank arguments for ends of index space
 - ▶ **Example** Rank 2: {e0,e1}

TileDimList

- ▶ **Initializer List or Kokkos::Array (Optional):** rank arguments for dimension of tiles
 - ▶ **Example** Rank 2: {t0,t1}

```
mdrpolicy( {b0 , b1} , {e0 , e1} , {t0 , t1} );
```

Details:

- ▶ Location: Intro-Full/Exercises/mdrange/Begin/
- ▶ This begins with the Solution of 02
- ▶ Initialize the device Views x and y directly on the device using a parallel for and RangePolicy
- ▶ Initialize the device View matrix A directly on the device using a parallel for and MDRangePolicy

```
# 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
./mdrange_exercise.cuda -S 26
```

Things to try:

- ▶ Name the kernels - pass a string as the first argument of the parallel pattern
- ▶ Try changing the iteration patterns for the tiles in the MDRangePolicy, notice differences in performance

Subviews: Taking 'slices' of Views

Learning objectives:

- ▶ Introduce Kokkos::subview - basic capabilities and syntax
- ▶ Suggested usage and practices

Subview description:

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 - ▶ Same syntax as a View - access data using (multi-)index entries
 - ▶ The 'slice' and original View point to the same data - no extra memory allocation or copying
- ▶ Can be constructed on host or within a kernel (no allocation of memory occurs)
- ▶ Similar capability as provided by Matlab, Fortran, Python, etc. using 'colon' notation

Introductory Usage Demo:

Begin with a View:

```
Kokkos::View< double*** > v("v", N0, N1, N2);
```

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Say we want a 2-dimensional slice at an index i_0 in the first dimension - that is, in Matlab/Fortran/Python notation:

```
slicei0 = v(i0, :, :);
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```

Say we want a 2-dimensional slice at an index i_0 in the first dimension - that is, in Matlab/Fortran/Python notation:

```
slicei0 = v(i0, :, :);
```

This can be accomplished in Kokkos using a subview as follows:

```
auto slicei0 =
    Kokkos::subview(v, i0, Kokkos::ALL, Kokkos::ALL);

auto slicei0 =
    Kokkos::subview(v, i0, std::make_pair(0,v.extent(1)),
                    std::make_pair(0,v.extent(2)));
// extent(N) returns the size of dimension N of the View
```

Syntax:

```
Kokkos::subview( Kokkos::View<...> view ,  
                  arg0 ,  
                  ... )
```

- ▶ **view:** First argument to the subview is the view of which a slice will be taken
- ▶ **argN:** Slice info for rank N - provide same number of arguments as rank
- ▶ **Options for argN:**
 - ▶ **index:** integral type single value
 - ▶ **partial-range:** std::pair or Kokkos::pair of integral types to provide sub-range of a rank's range [0,N)
 - ▶ **full-range:** use Kokkos::ALL rather than providing the full range as a pair

Suggested usage:

- ▶ Use 'auto' to determine the return type of a subview
- ▶ A subview can help with encapsulation - e.g. can pass into functions expecting a lower-dimensional View
- ▶ Use Kokkos::pair for partial ranges if subview created within a kernel
- ▶ Avoid usage if very few data accesses will be made to the subview
 - ▶ Construction of subview costs 20-40 operations

Details:

- ▶ Location: Intro-Full/Exercises/subview/Begin/
- ▶ This begins with the Solution of 04
- ▶ In the parallel reduce kernel, create a subview for row j of view A
- ▶ Use this subview when computing $A(j,:)*x(:)$ rather than the matrix A

```
# 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
./subview_exercise.cuda -S 26
```

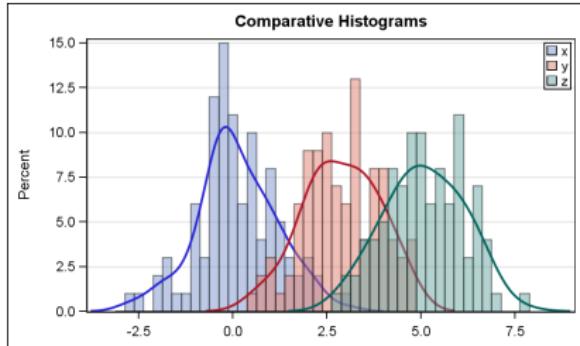
Thread safety and atomic operations

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);  
});
```

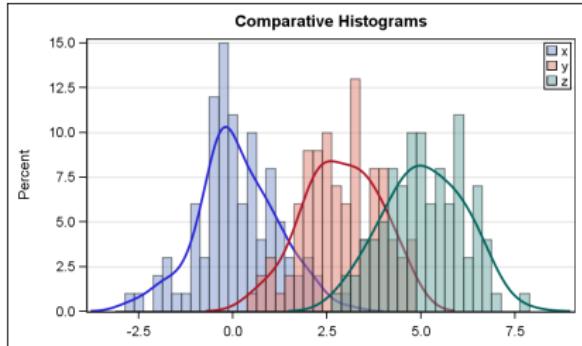


<http://www.farmaceuticas.com.br/tag/graficos/>

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    const Something value = ...;  
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Problem: Multiple threads may try to write to the same location.



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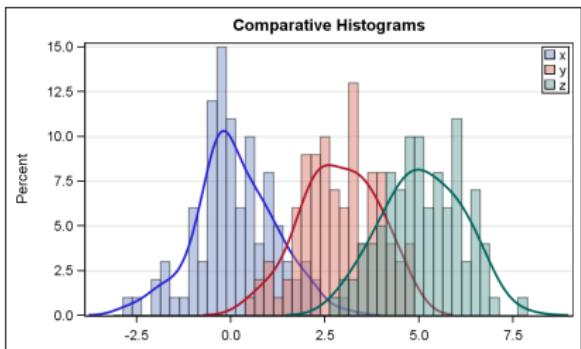
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    const Something value = ...;  
    const size_t bucketIndex = computeBucketIndex(value);  
    ++_histogram(bucketIndex);  
});
```

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

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

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

Atomics: the portable and thread-scalable solution

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

- ▶ Atomics are the **only scalable** solution to thread safety.
- ▶ Locks are **not portable**.

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 are the **only scalable** solution to thread safety.
- ▶ Locks are **not portable**.
- ▶ Data replication is **not thread scalable**.

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);
```

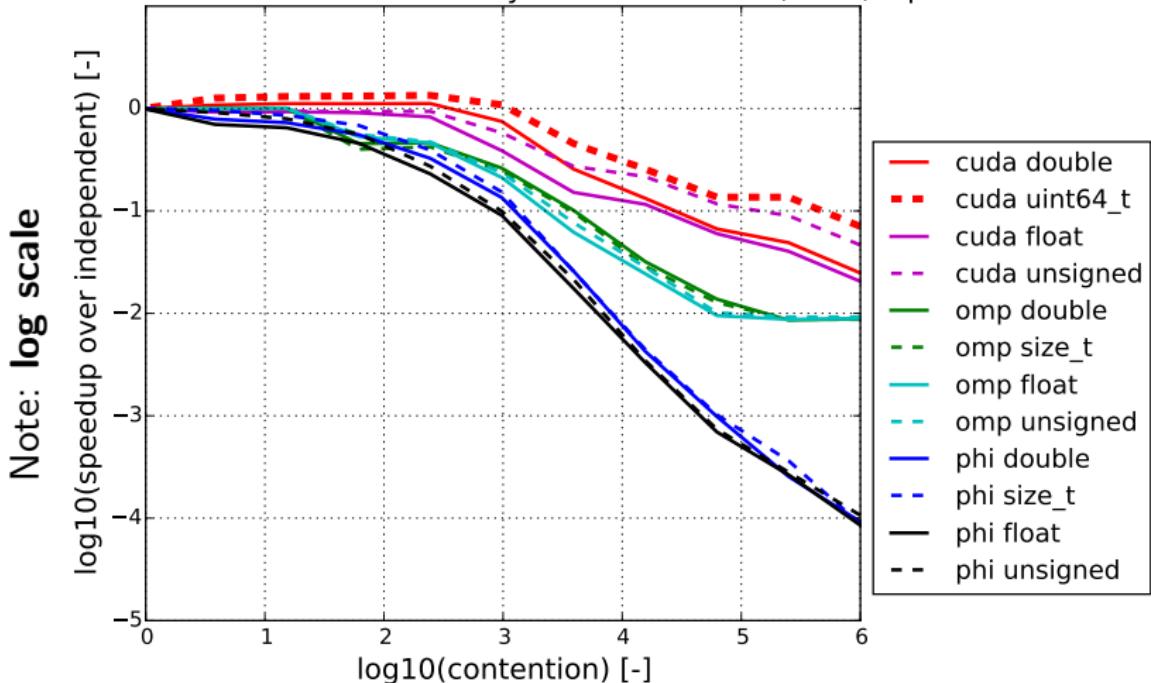
Experimental setup

```
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**)

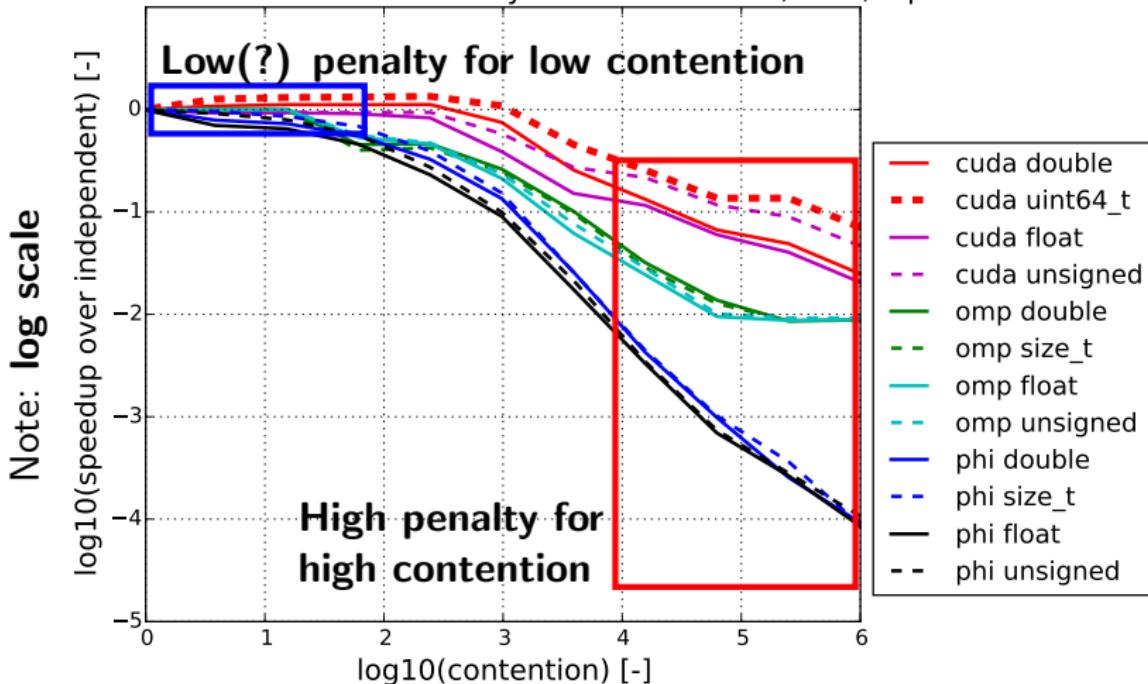
Atomics performance: 1 million adds, **no** work per kernel

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



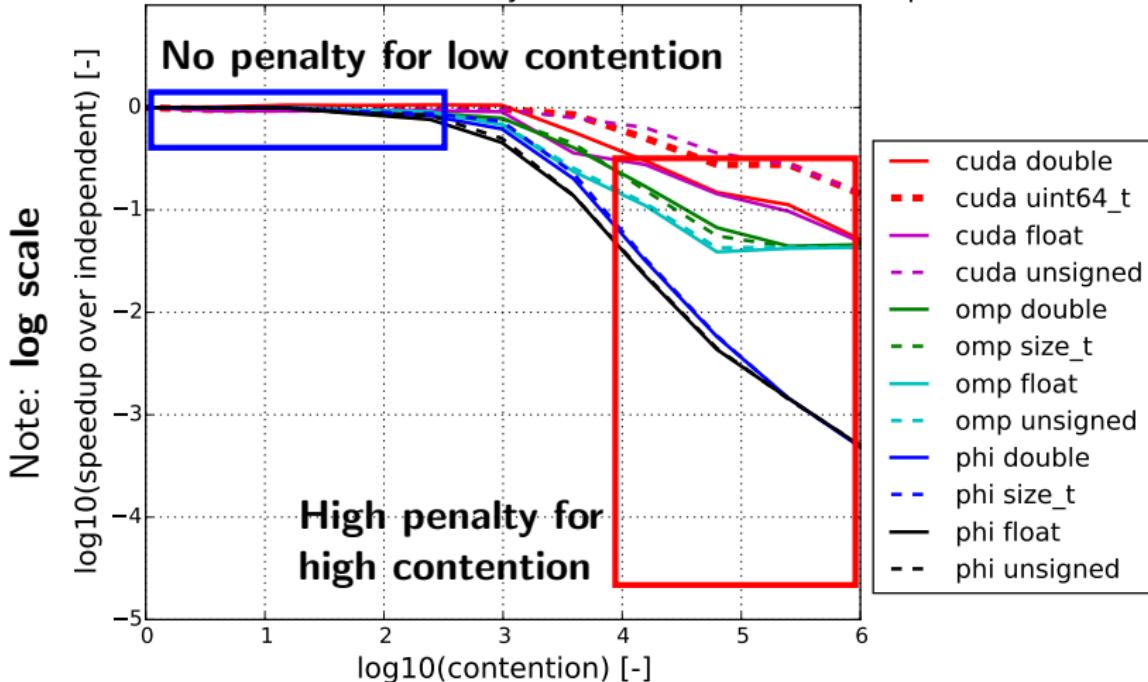
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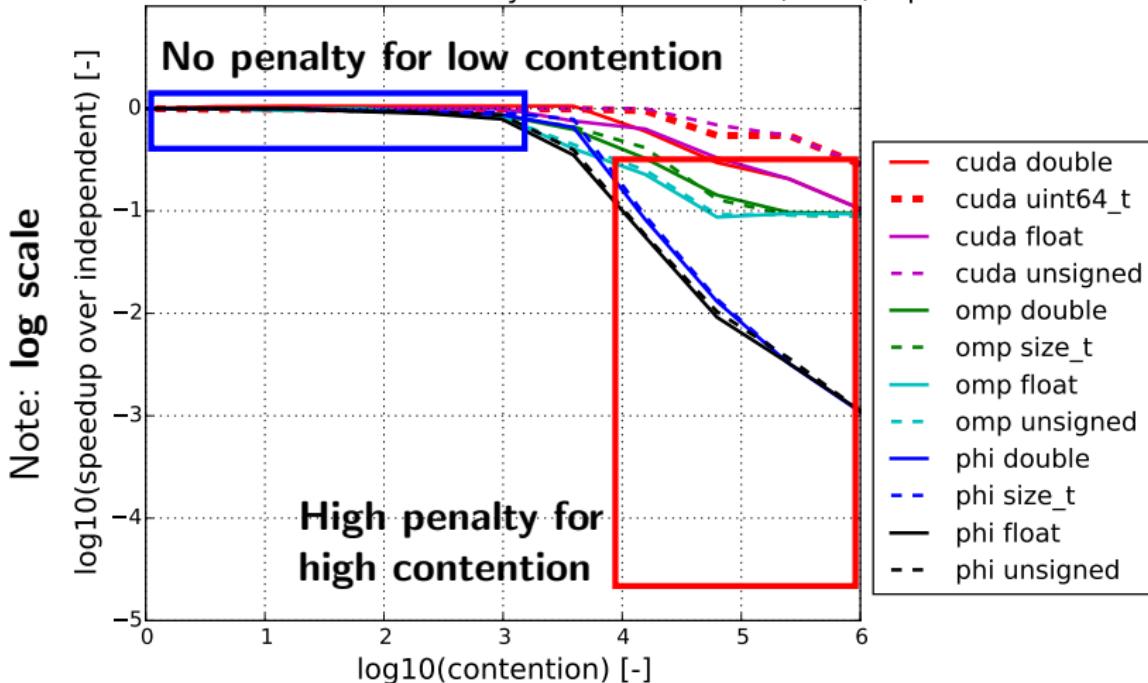
Atomics performance: 1 million adds, **some** work per kernel

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(...);
```

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

```
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      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);
```

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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(...);
```

Histogram generation is an example of the **Scatter Contribute** pattern.

- ▶ Like a reduction but with many results.
- ▶ Number of results scales with number of inputs.
- ▶ Each results gets contributions from a small number of inputs/iterations.
- ▶ Uses an inputs-to-results map not inverse.

Examples:

- ▶ Particles contributing to neighbors forces.
- ▶ Cells contributing forces to nodes.
- ▶ Computing histograms.
- ▶ Computing a density grid from point source contributions.

There are two useful algorithms::

- ▶ **Atomics:** thread-scalable but depends on atomic performance.
- ▶ **Data Replication:** every thread owns a copy of the output, not thread-scalable but good for low (≤ 16) threads count architectures.

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Important Capability: ScatterView

ScatterView can transparently switch between **Atomic** and **Data Replication** based scatter algorithms.

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- ▶ **Atomics:** thread-scalable but depends on atomic performance.
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Important Capability: ScatterView

ScatterView can transparently switch between **Atomic** and **Data Replication** based scatter algorithms.

- ▶ Abstracts over scatter contribute algorithms.
- ▶ Compile time choice with backend-specific defaults.
- ▶ Only limited number of operations are supported.
- ▶ Part of Kokkos Containers.

Example:

```
// Begin with a normal View
Kokkos::View<double*> results("results",N);
// Create a scatter view wrapping the original view
Kokkos::ScatterView<double*> scatter(results);
// Reset contributions if necessary
scatter.reset();
// Start parallel operation
Kokkos::parallel_for("ScatterAlg", M,
    KOKKOS_LAMBDA(int i) {
    // Get the accessor - e.g. the thread specific copy
    // or an atomic view of the data.
    auto scatter.access();

    for(int j=0; j<num_neighs(i); j++) {
        // Get the destination index
        int neigh = neighbors(i,j);
        // Add the contribution
        access(neigh) += contribution(i,neigh);
    }
});
// Combine the results - no op if ScatterView was using atomics in
Kokkos::Experimental::contribute(results,scatter);
```

- ▶ Location: Intro-Full/Exercises/scatter_view/Begin/
- ▶ Assignment: Convert scatter_view_loop to use ScatterView.
- ▶ Compile and run on both CPU and GPU

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

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

- ▶ 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

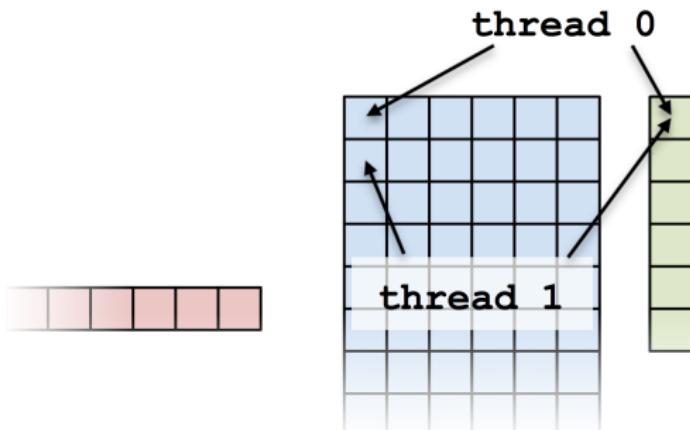
Finding and exploiting more parallelism in your computations.

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:

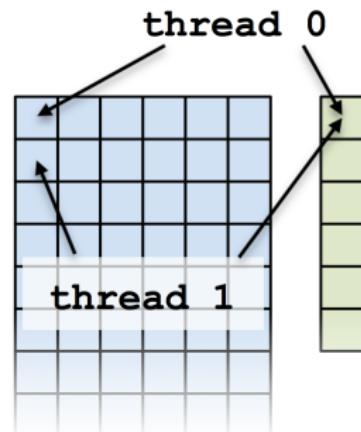
```
Kokkos::parallel_reduce("yAx",N,
    KOKKOS_LAMBDA (const int row, double & valueToUpdate) {
        double thisRowsSum = 0;
        for (int col = 0; col < M; ++col) {
            thisRowsSum += A(row,col) * x(col);
        }
        valueToUpdate += y(row) * thisRowsSum;
    }, result);
```



(Flat parallel) Kernel:

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    }, result);
```

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

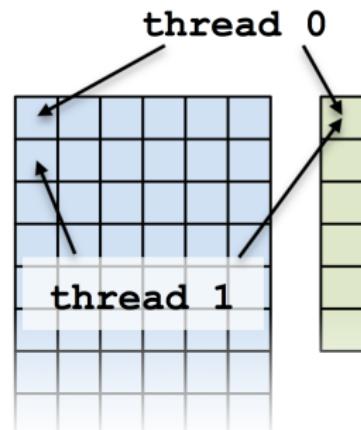


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Solutions?



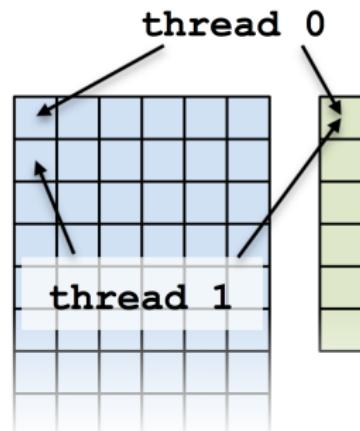
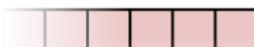
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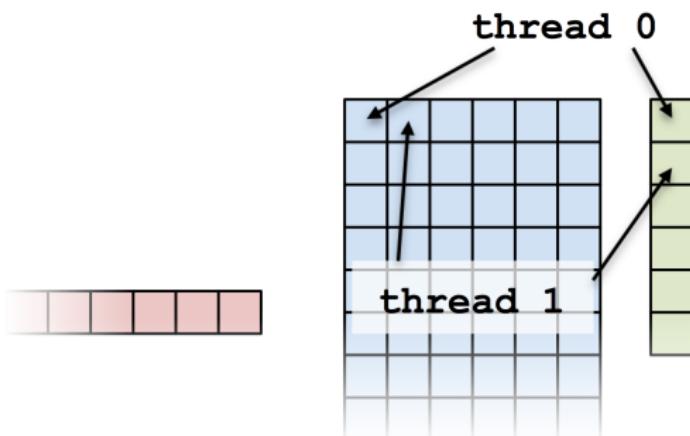
Solutions?

- ▶ Atomics
- ▶ Thread teams



Atomics kernel:

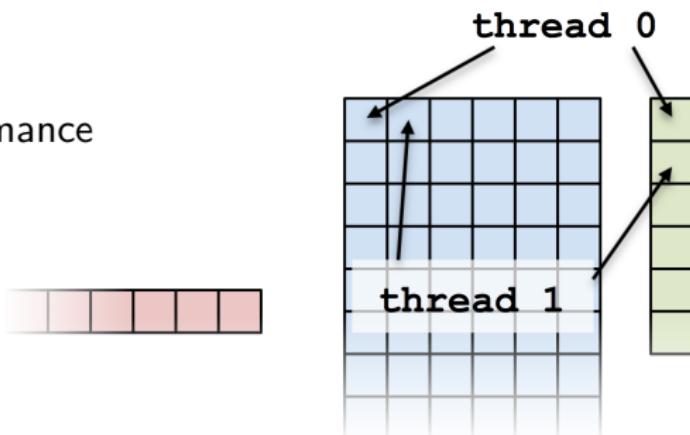
```
Kokkos::parallel_for("yAx", N,
    KOKKOS_LAMBDA (const size_t index) {
        const int row = extractRow(index);
        const int col = extractCol(index);
        atomic_add(&result, A(row,col) * x(col));
    });
}
```



Atomics kernel:

```
Kokkos::parallel_for("yAx", 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

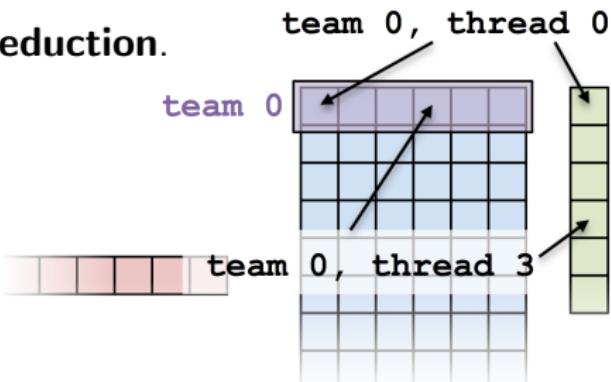
A collection of threads which are guaranteed to be executing **concurrently** and **can synchronize**.

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("yAx",
    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("Label",
    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("Label",
    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("Label",
    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

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

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typedef typename TeamPolicy<ExecSpace>::member_type member_type;

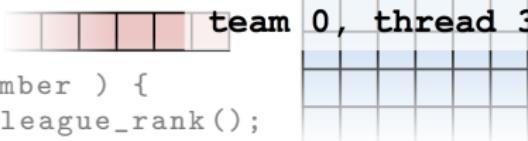
void operator()(const member_type & teamMember) {
    // Which team am I on?
    const unsigned int leagueRank = teamMember.league_rank();
    // Which thread am I on this team?
    const unsigned int teamRank = teamMember.team_rank();
}
```

Warning

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

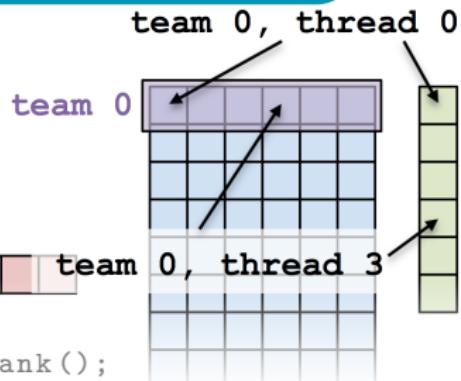
team 0, thread 0

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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    const int row = teamMember.league_rank();  
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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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}
```

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

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

Anatomy of nested parallelism:

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

- ▶ `parallel_outer` and `parallel_inner` may be any combination of `for`, `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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```
parallel_something(  
    TeamPolicy<ExecutionSpace>(numberOfTeams, Kokkos::AUTO),  
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GPUs

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

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128/256

Intel Xeon Phi:

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

Details:

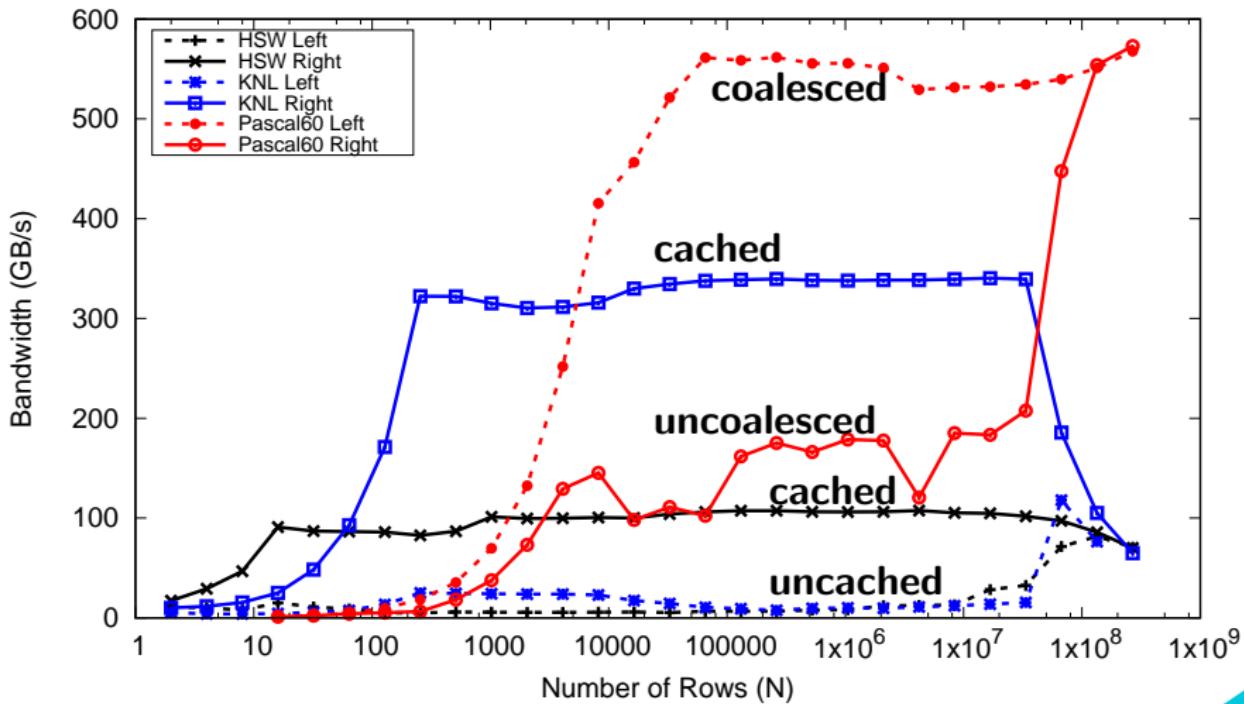
- ▶ Location: Intro-Full/Exercises/05/
- ▶ Replace RangePolicy<Space> with TeamPolicy<Space>
- ▶ Use AUTO for team_size
- ▶ Make the inner loop a parallel_reduce with TeamThreadRange policy
- ▶ Experiment with the combinations of Layout, Space, N to view performance
- ▶ Hint: what should the layout of A be?

Things to try:

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

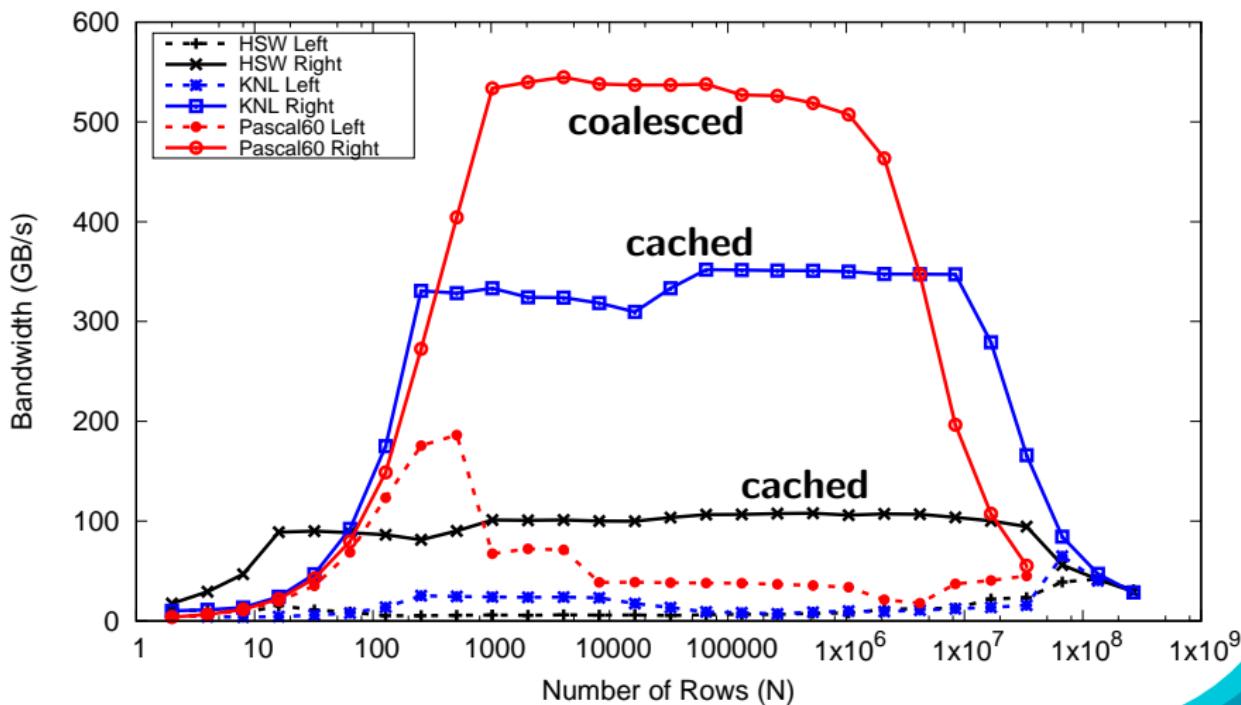
< y | Ax > Exercise 04 (Layout) Fixed Size

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



$\langle y | Ax \rangle$ Exercise 05 (Layout/Teams) Fixed Size

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



Exposing Vector Level Parallelism

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

Anatomy of nested parallelism:

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

Question: What will the value of totalSum be?

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

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

totalSum = numberOfThreads * 10

Question: What will the value of totalSum be?

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

totalSum = numberOfTeams * team_size * 10

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

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```
int totalSum = 0;
parallel_reduce("Sum", TeamPolicy<>(numberOfTeams, team_size),
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        [=] (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:

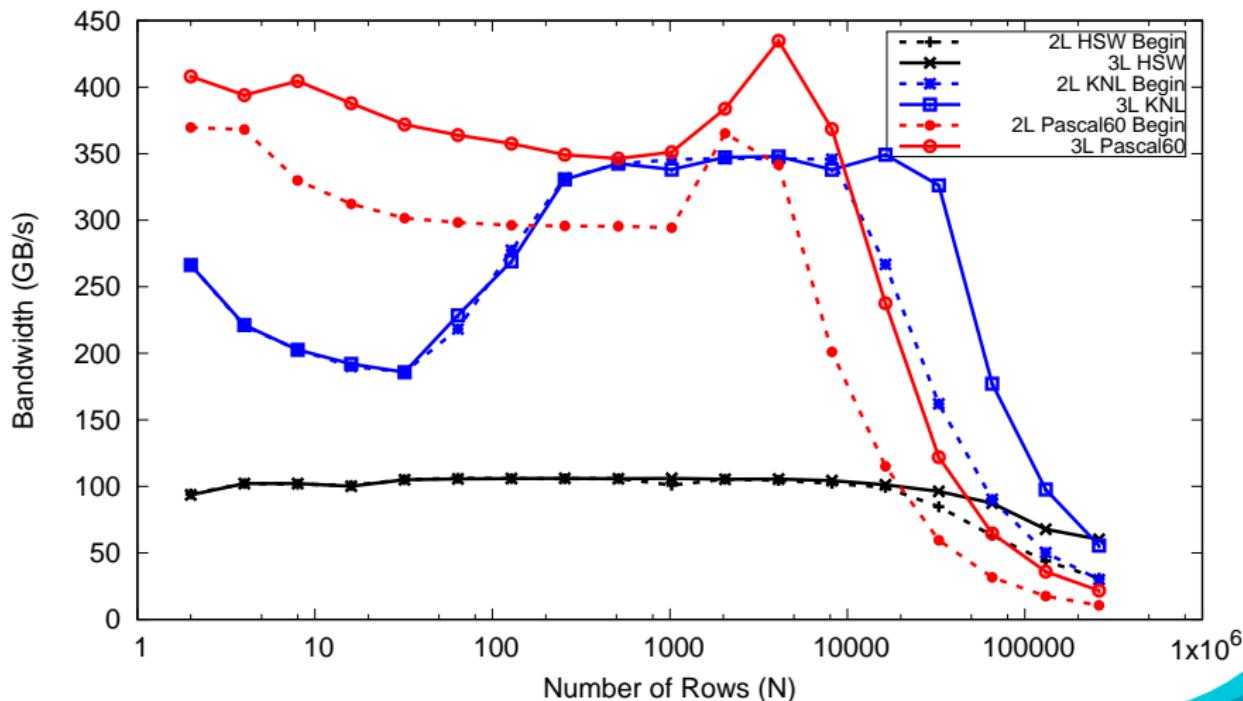
- ▶ Location: [Intro-Full/Exercises/06/](#)
- ▶ Use the single policy instead of checking team rank
- ▶ Parallelize all three loop levels.

Things to try:

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

$\langle y | Ax \rangle$ Exercise 06 (Three Level Parallelism) Fixed Size

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



- ▶ **Hierarchical work** can be parallelized via hierarchical parallelism.
- ▶ Hierarchical parallelism is leveraged using **thread teams** launched with a TeamPolicy.
- ▶ Team “worksets” are processed by a team in nested parallel_for (or reduce or scan) calls with a TeamThreadRange 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).

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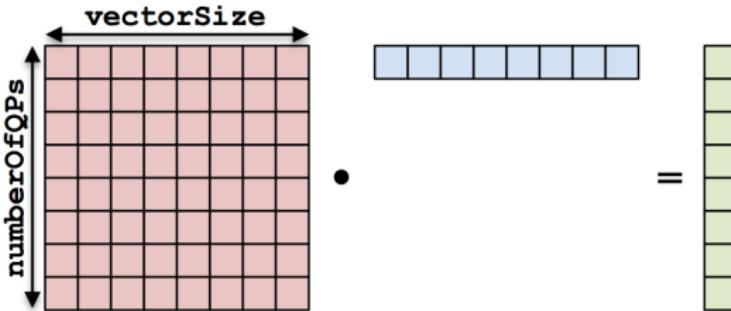
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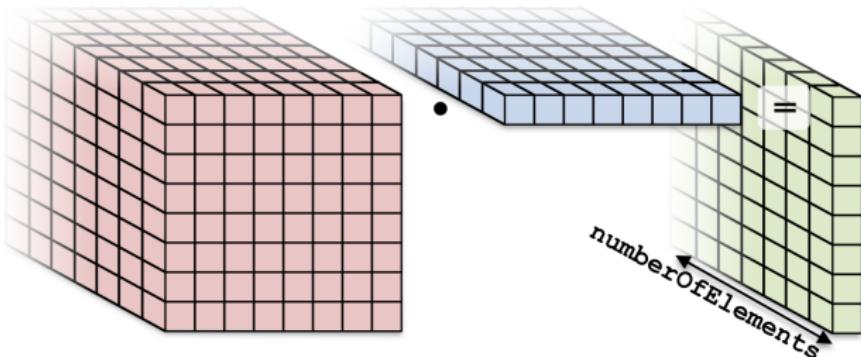
Now: Discuss Manually Managed Cache Usecase.

One slice of contractDataFieldScalar:



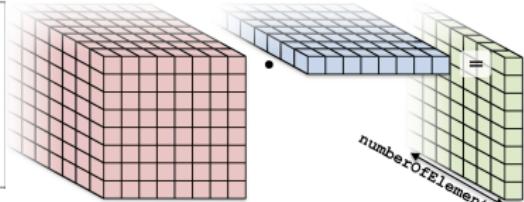
```
for (qp = 0; qp < numberOfQPs; ++qp) {  
    total = 0;  
    for (i = 0; i < vectorSize; ++i) {  
        total += A(qp, i) * B(i);  
    }  
    result(qp) = total;  
}
```

contractDataFieldScalar:



```
for (element = 0; element < 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;  
    }  
}
```

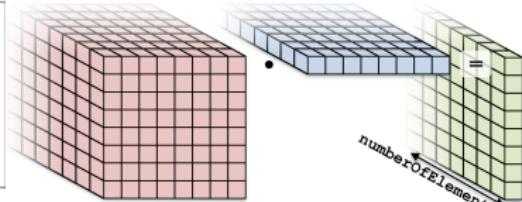
```
for (element = 0; element < numberElements; ++element) {  
    for (qp = 0; qp < numberQPs; ++qp) {  
        total = 0;  
        for (i = 0; i < vectorSize; ++i) {  
            total += A(element, qp, i) * B(element, i);  
        }  
        result(element, qp) = total;  
    }  
}
```



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

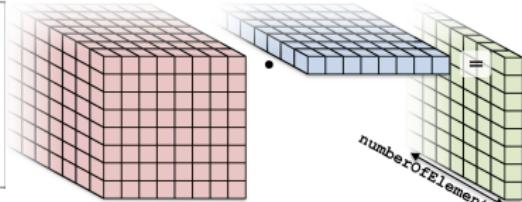
- ▶ Each thread handles a qp.

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;
    }
}

```



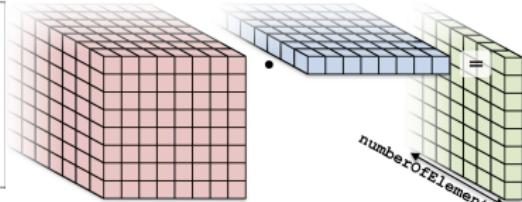
Parallelization approaches:

- ▶ Each thread handles an element.
Threads: numberElements
- ▶ Each thread handles a qp.
Threads: $\text{numberElements} * \text{numberQPs}$
- ▶ Each thread handles an i.
Threads: $\text{numElements} * \text{numQPs} * \text{vectorSize}$
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.

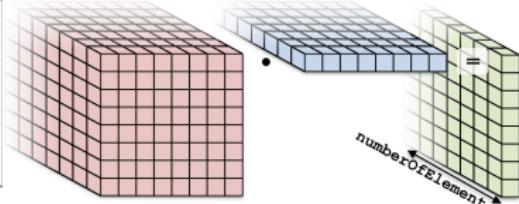
Threads: `numElements * numQPs * vectorSize`

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

```

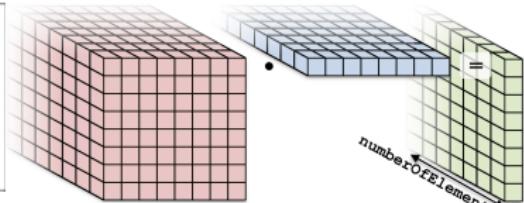
operator()(int index) {
    int element = extractElementFromIndex(index);
    int qp = extractQPFromIndex(index);
    double total = 0;
    for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
}

```

```

for (element = 0; element < 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

```

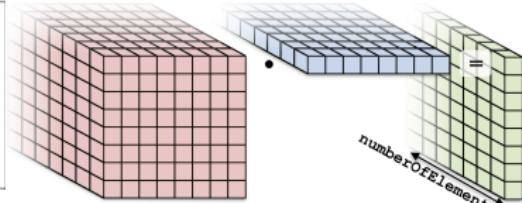
operator()(member_type teamMember) {
    int element = teamMember.league_rank();
    parallel_for(
        TeamThreadRange(teamMember, number_of_QPs),
        [=] (int qp) {
            double total = 0;
            for (int i = 0; i < vector_size; ++i) {
                total += A(element, qp, i) *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

```

```

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

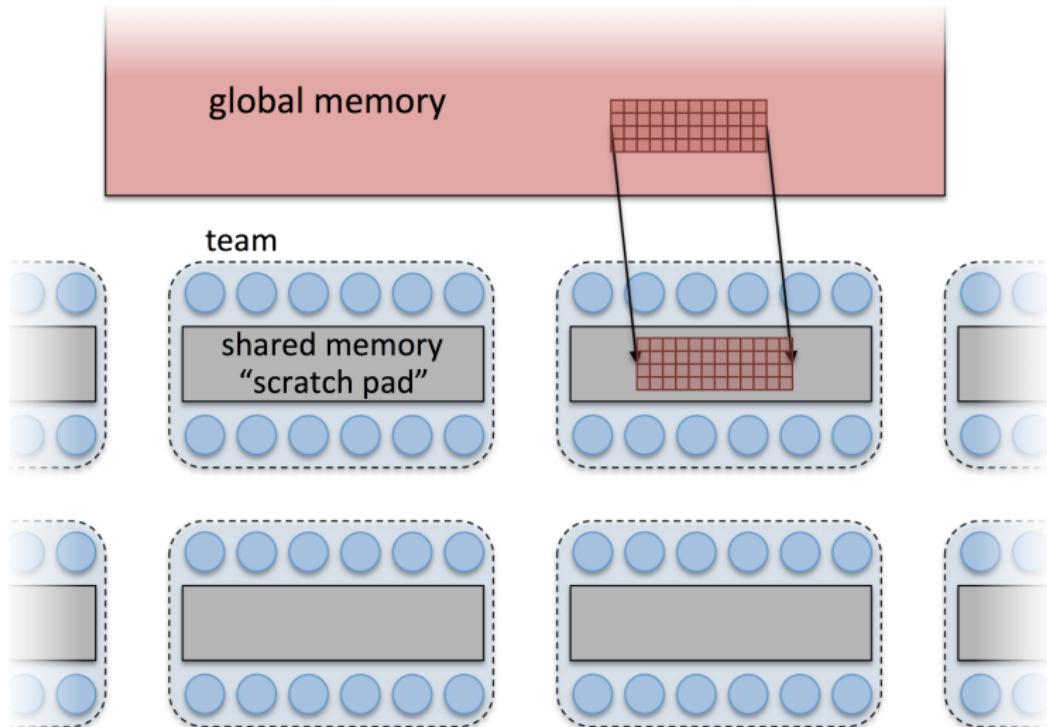
```

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.

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- ▶ PerThread and PerTeam scratch can be used concurrently.
- ▶ Level 0 and Level 1 scratch memory can be used concurrently.

Important concept

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

To use scratch memory, you need to:

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

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1. **Tell Kokkos how much** scratch memory you'll need.
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```
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) {

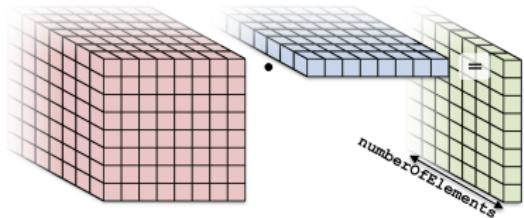
    // Create a view from the pre-existing scratch memory
    ScratchPadView scratch(teamMember.team_scratch(level),
                           vectorSize);
});
```

Kernel outline for teams with scratch memory:

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

    // TODO: load slice of B into scratch

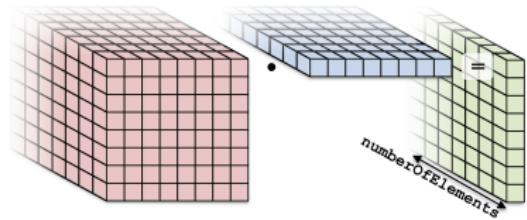
    parallel_for(
        TeamThreadRange(teamMember, number0fQPs),
        [=] (int qp) {
            double total = 0;
            for (int i = 0; i < vectorSize; ++i) {
                total += A(element, qp, i) * scratch(i);
            }
            result(element, qp) = total;
        });
}
```



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);  
    }  
}
```



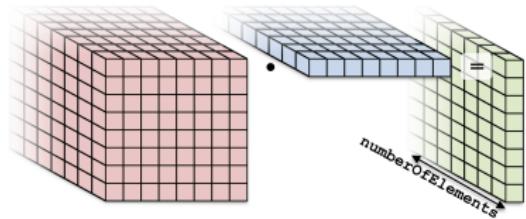
How to populate the scratch memory?

- ▶ ~~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);
    }
}
```

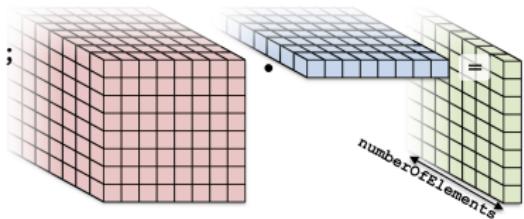
- ▶ ~~Each thread loads one entry?~~ **teamSize ≠ vectorSize**

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

- ▶ TeamThreadRange or ThreadVectorRange

```
parallel_for(
    ThreadVectorRange(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);
    }
}
```

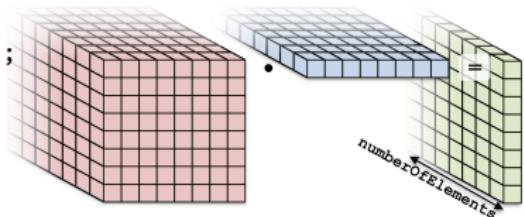
- ▶ ~~Each thread loads one entry?~~ **teamSize ≠ vectorSize**

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

- ▶ **TeamThreadRange or ThreadVectorRange**

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

```



(incomplete) Kernel for teams with scratch memory:

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

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

    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;
        });
}
```

(incomplete) Kernel for teams with scratch memory:

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

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

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

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

Kernel for teams with scratch memory:

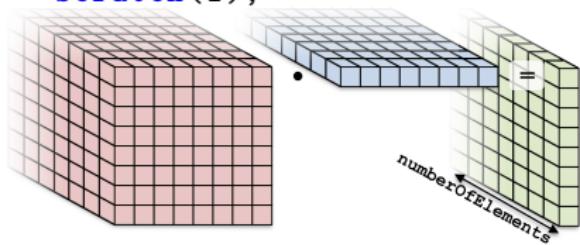
```

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

    parallel_for(ThreadVectorRange(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:

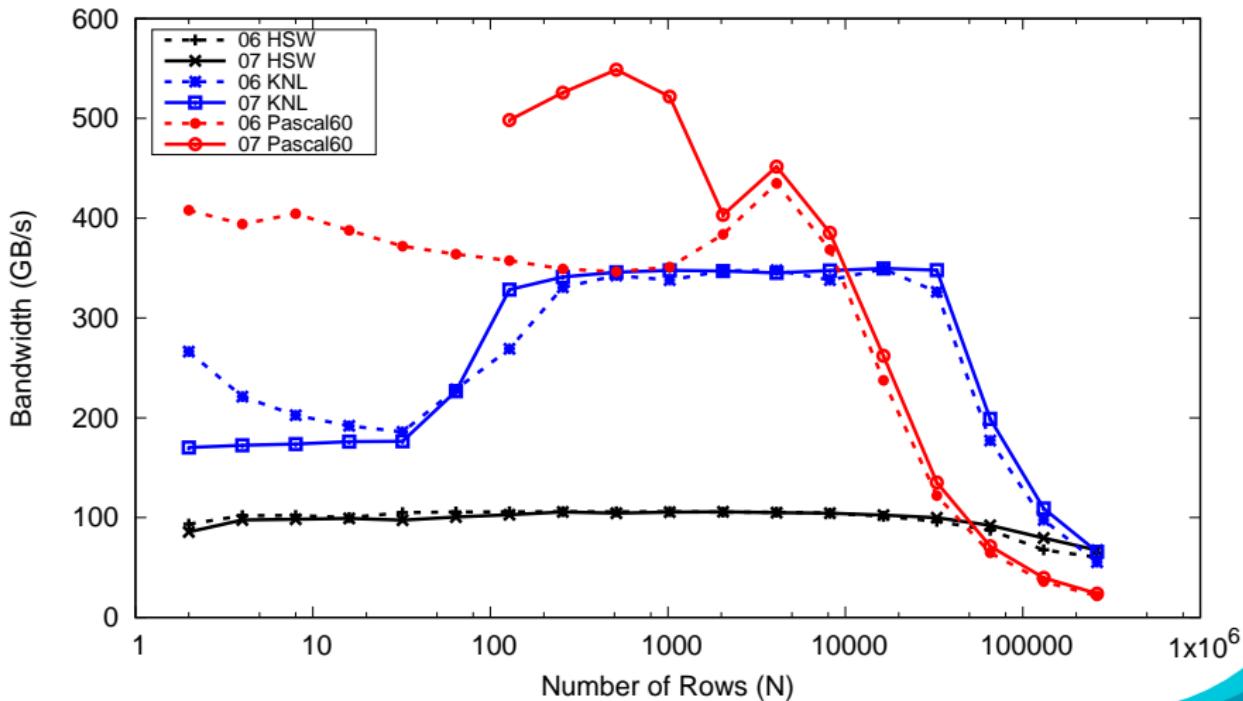
- ▶ Location: Intro-Full/Exercises/07/
- ▶ Create a scratch view
- ▶ Fill the scratch view in parallel using a TeamThreadRange or ThreadVectorRange

Things to try:

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

Exercise 07 (Scratch Memory) Fixed Size

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



Allocating scratch in different levels:

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

Allocating scratch in different levels:

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

Using PerThread, PerTeam or both:

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

Allocating scratch in different levels:

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

Using PerThread, PerTeam or both:

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

Using both levels of scratch:

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

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

- ▶ **Scratch Memory** can be 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.

Kokkos advanced capabilities NOT covered today

- ▶ Directed acyclic graph (DAG) of tasks pattern
 - ▶ Dynamic graph of heterogeneous tasks (maximum flexibility)
 - ▶ Static graph of homogeneous task (low overhead)
- ▶ Portable, thread scalable memory pool
- ▶ Plugging in customized multidimensional array data layout
 - e.g., arbitrarily strided, hierarchical tiling

- ▶ 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.*
 - ▶ *full day tutorial only*