Kokkos Tutorial

Sandia National Laboratories; November 5, 2017

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SAND2017-13419 PE

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 7.5 (or newer) *AND* NVIDIA compute capability 3.0 (or newer)
- clone github.com/kokkos/kokkos into ${HOME}/kokkos
- clone github.com/kokkos/kokkos-tutorials into ${HOME}/kokkos-tutorials

  Exercises are in ${HOME}/`kokkos-tutorials/Intro-Full/SNL2017`

  Exercises' makefiles look for ${HOME}/kokkos

Kokkos' basic capabilities:

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

Kokkos' advanced capabilities:

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

Kokkos' advanced capabilities not covered today:

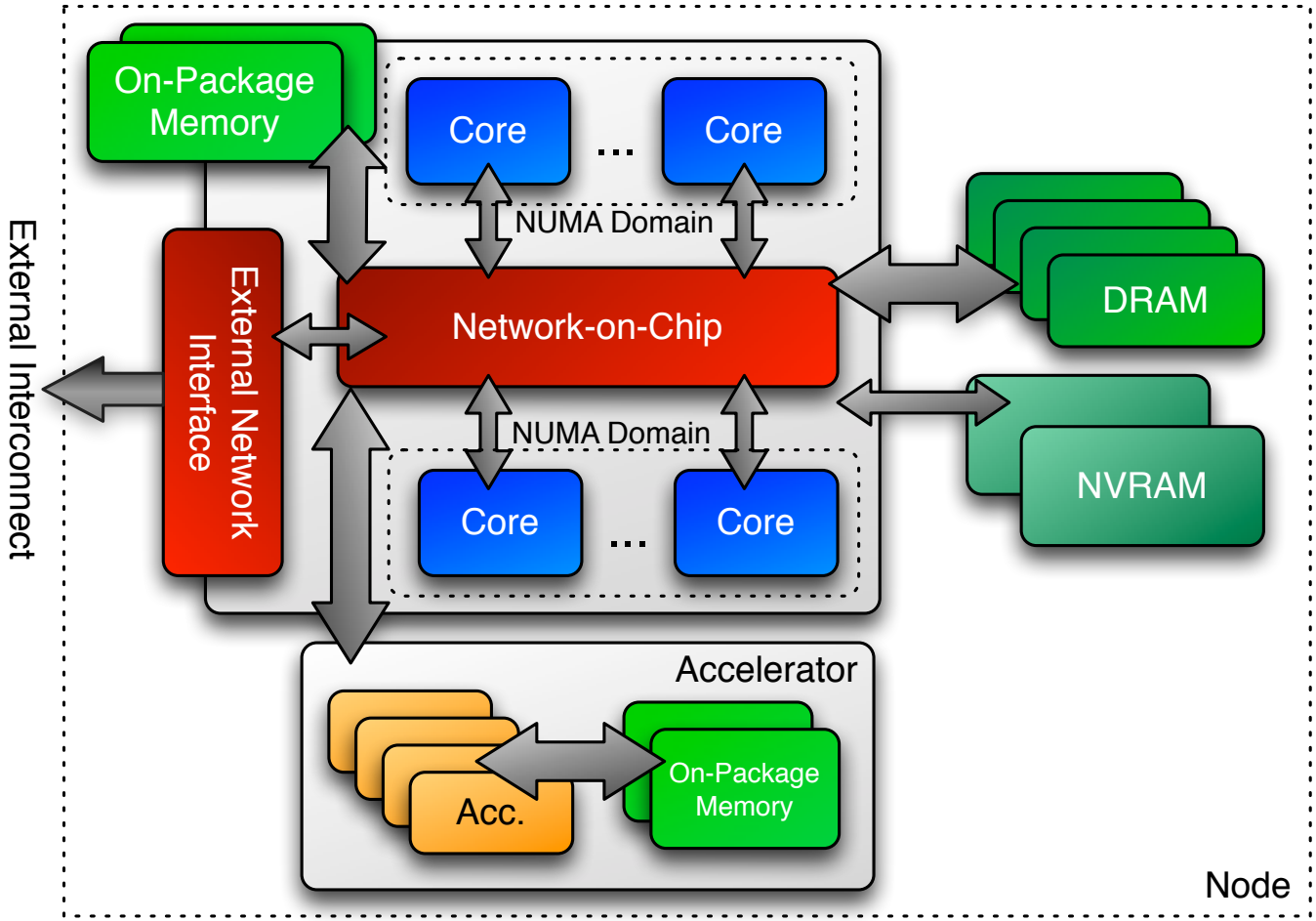
- Multidimensional data parallelism
- Dynamic directed acyclic graph of tasks pattern
- Numerous *pluggin* points for extensibility

- 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.

Assume you are here because:

- Want to use **all** HPC node architectures; including GPUs
- Are familiar with **C++**
- Are familiar with **data parallelism**
- A little familiar with **OpenMP**
- A little familiar with **NVIDIA GPU architecture**
  Spoiler alert: memory access patterns are important
- Want GPU programming to be **easier**
- Would like **portability**, as long as it doesn't hurt performance

Target machine:



Important Point

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

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

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

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Goal: write **one implementation** which:

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

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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 Policy

```
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

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

$\Rightarrow$ The **pattern** and **policy** drive the computational **body**.

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

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

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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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```

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

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

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

Option 1: OpenMP 4.0

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

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    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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if it is supported on the target architecture.

But what about performance?

Performance depends upon the computation's **memory access pattern**.

Problem: memory access pattern

```
#pragma something, opencl, etc.
for (element = 0; element < numElements; ++element) {
  total = 0;
  for (qp = 0; qp < numQPs; ++qp) {
    for (i = 0; i < vectorSize; ++i) {
      total +=
        left[element * numQPs * vectorSize +
             qp * vectorSize + i] *
        right[element * numQPs * vectorSize +
              qp * vectorSize + i];
    }
  }
  elementValues[element] = total;
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    }
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Memory access pattern problem: CPU data layout reduces GPU performance by more than 10X.

Important Point

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

How does Kokkos address performance portability?

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

- is a C++ **library**, not a new language or language extension.
- supports **clear, concise, thread-scalable** parallel patterns.
- lets you write algorithms once and run on **many architectures**
  e.g. multi-core CPU, NVidia GPU, 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 < numberOfAtoms; ++atomIndex) {
  atomForces[atomIndex] = calculateForce(...data...);
}
```

Kokkos maps **work** to cores

Data parallel patterns and work

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for (atomIndex = 0; atomIndex < numberOfAtoms; ++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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- each iteration of a computational body is a **unit of work**.
- an **iteration index** identifies a particular unit of work.
- an **iteration range** identifies a total amount of work.

Important concept: Work mapping

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

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

Warning: concurrency and order

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

How is data passed to computational bodies?

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

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

How is data passed to computational bodies?

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

How does the body access the data?

Important concept

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

Putting it all together: the complete functor:

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

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```

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

Serial

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

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

Functor

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

The complete picture (using functors):

1. Defining the functor (operator+data):

```
struct AtomForceFunctor {
  ForceType _atomForces;
  AtomDataType _atomData;

  AtomForceFunctor(atomForces, data) :
    _atomForces(atomForces) _atomData(data) {}

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

2. **Executing** in parallel with Kokkos pattern:

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

Functors are tedious ⇒ **C++11 Lambdas** are concise

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

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

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

Warning: Lambda capture and C++ containers

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

OpenMP

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

Kokkos

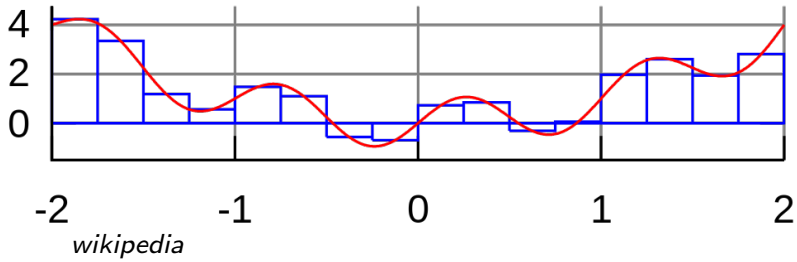
```
parallel_for(N, [=] (const size_t i) {
  /* loop body */
});
```

Important concept

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

Riemann-sum-style numerical integration:

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



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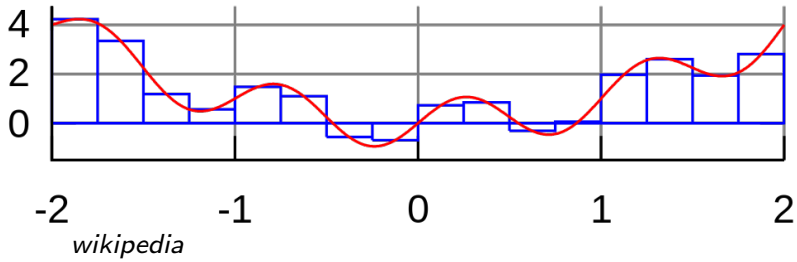


```
double totalIntegral = 0;
for (size_t i = 0; i < numberOfIntervals; ++i) {
  const double x =
    lower + (i/numberOfIntervals) * (upper - lower);
  const double thisIntervalsContribution = function(x);
  totalIntegral += thisIntervalsContribution;
}
totalIntegral *= dx;
```

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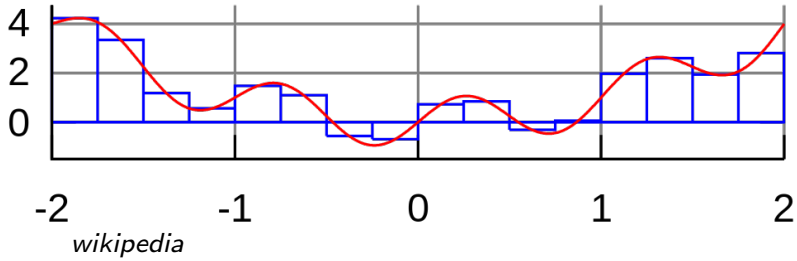


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How do we **parallelize** it? *Correctly?*

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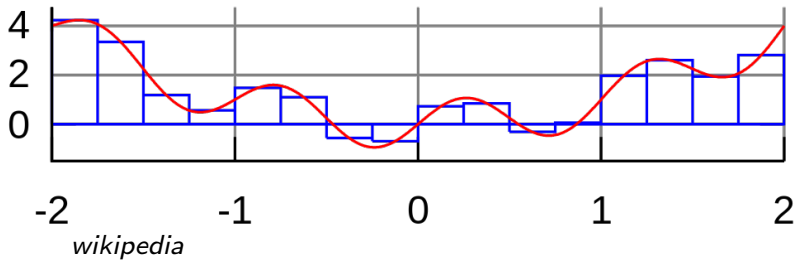

Pattern?

Policy?

Body?

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

An (incorrect) attempt:

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

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

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

```
double totalIntegral = 0;
double * totalIntegralPointer = &totalIntegral;
Kokkos::parallel_for(numberOfIntervals,
  [=] (const size_t index) {
    const double x =
      lower + (index/numberOfIntervals) * (upper - lower);
    *totalIntegralPointer += function(x);},
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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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How would we do this with **OpenMP**?

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

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for (size_t i = 0; i < N; ++i) {
  finalReducedValue += ...
}
```

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

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

Example: Scalar integration

OpenMP

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

Kokkos

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

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

Warning: Parallelism is NOT free

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

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

- $\alpha =$ dispatch overhead
- $\beta =$ time for a unit of work
- $N =$ number of units of work
- $P =$ available concurrency

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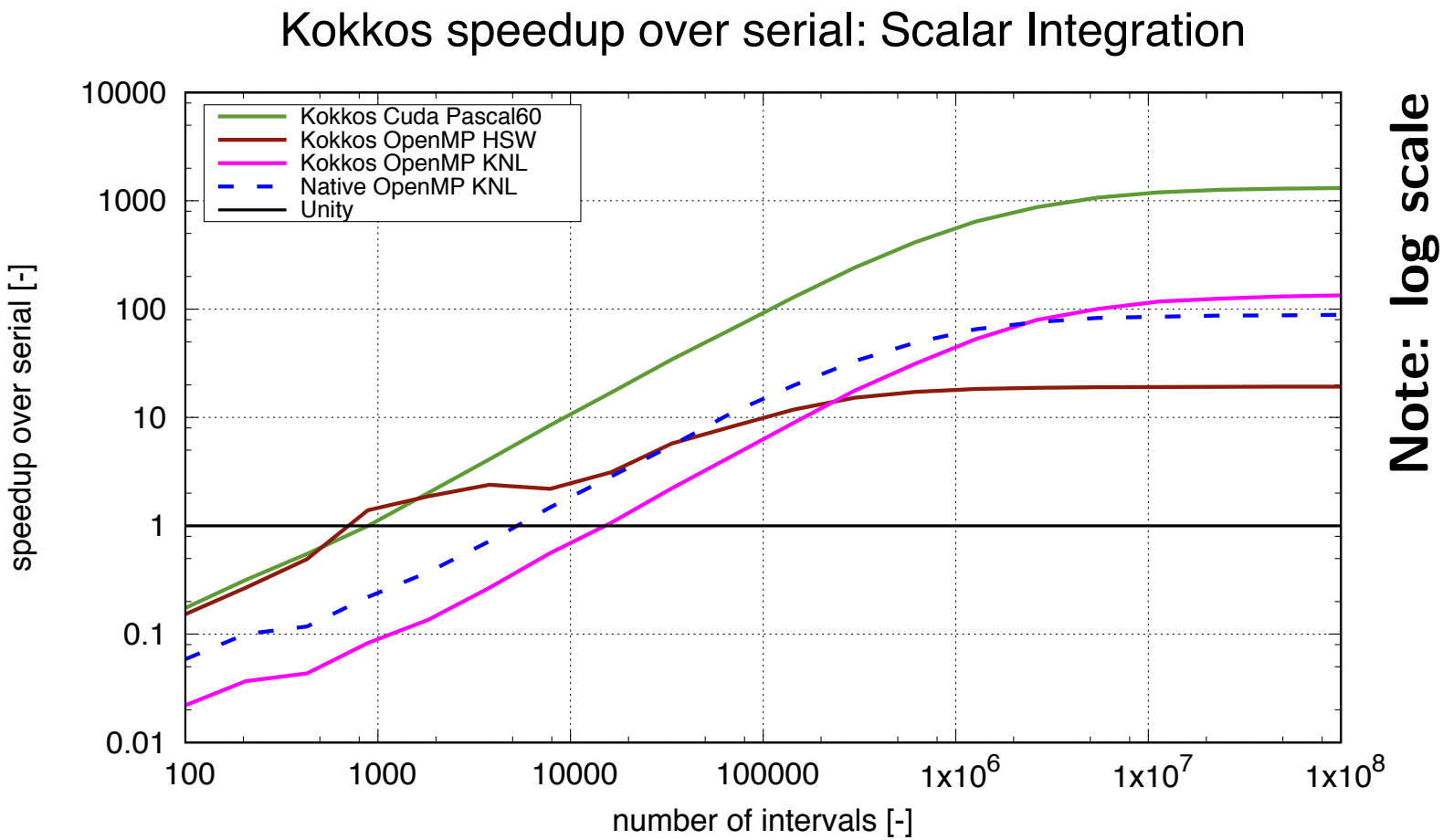
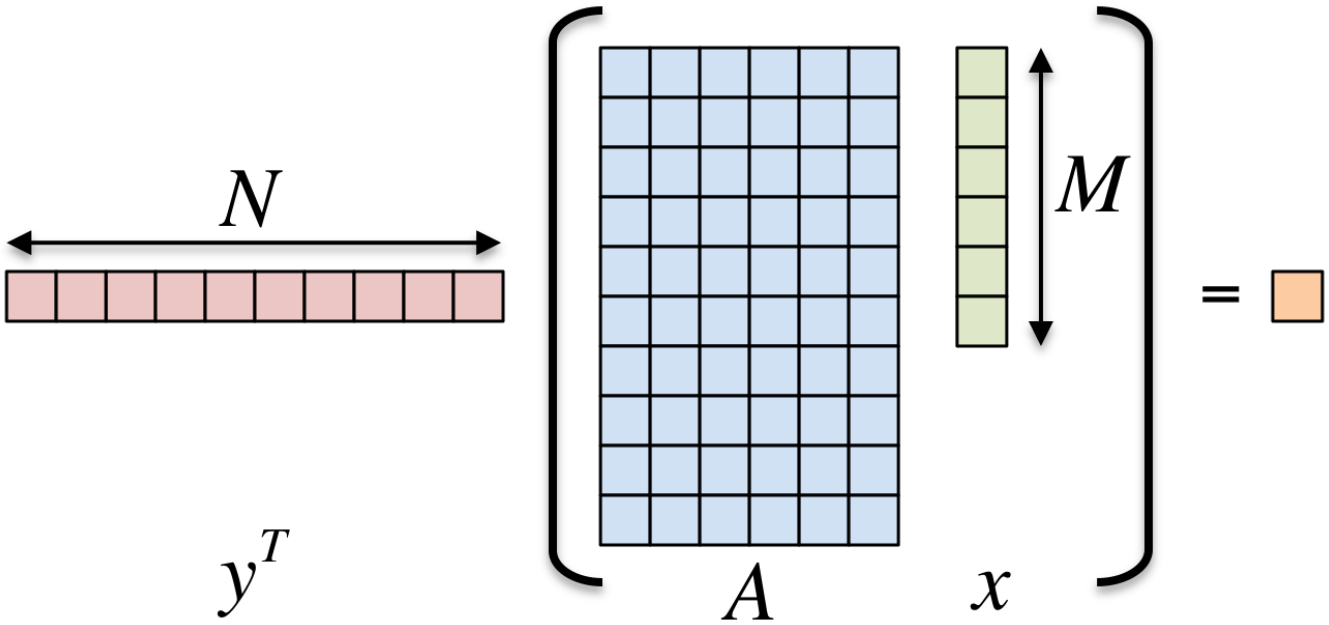
Speedup $= P \div \left(1 + \frac{\alpha * P}{\beta * N}\right)$

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



Exercise: Inner product $< y, A * x >$



Details:

- y is Nx1, A is NxM, x is Mx1
- We'll use this exercise throughout the tutorial

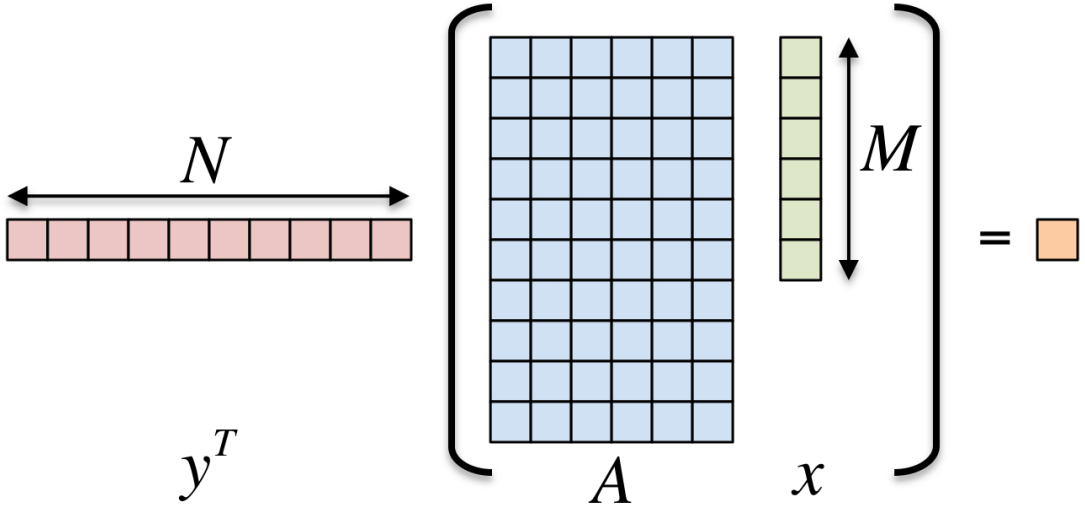
The **first step** in using Kokkos is to include, initialize, and finalize:

```
#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 $< y, A * x >$



Details:

- Location: `SNL2017/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

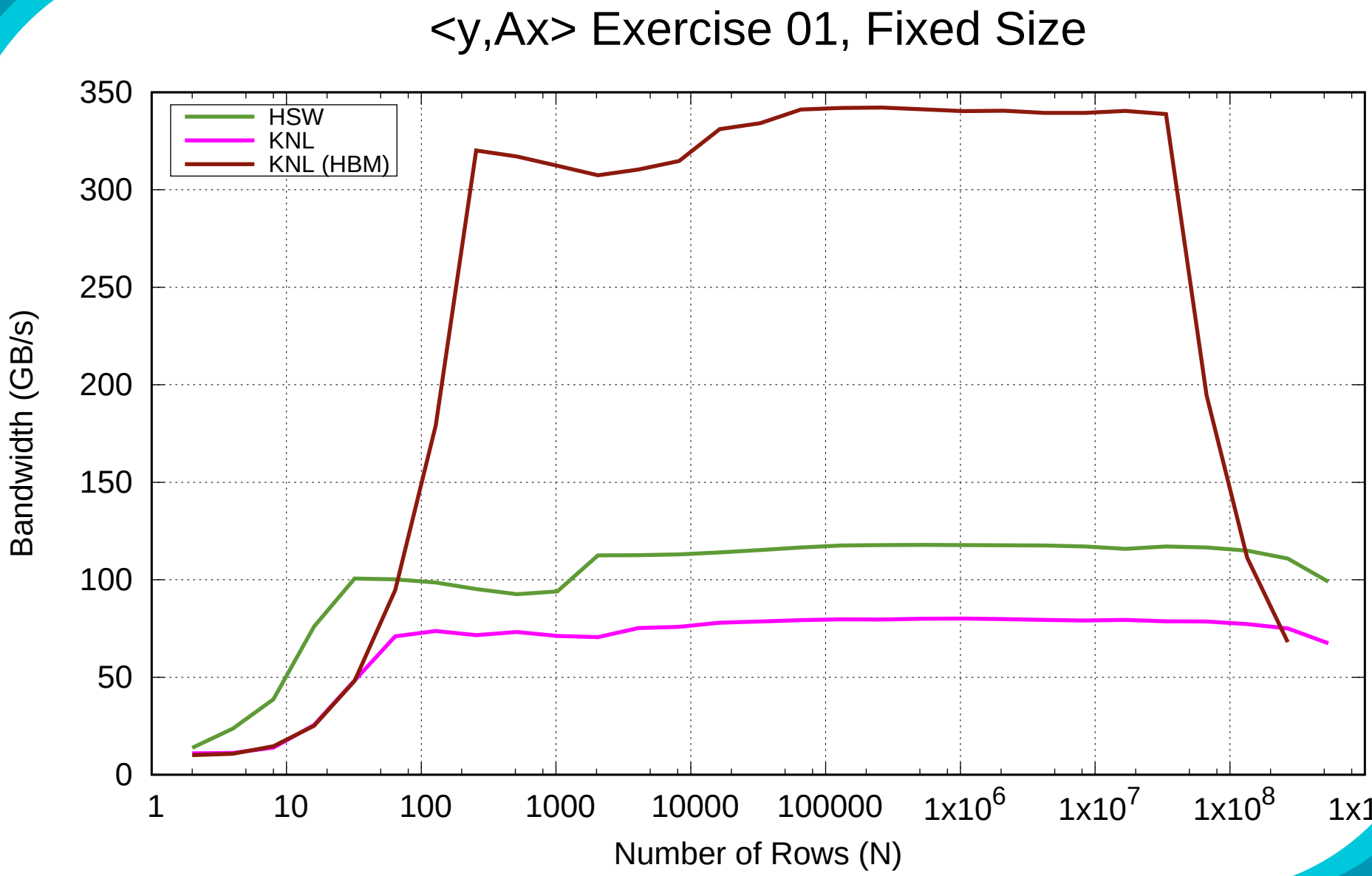
```
# gcc using OpenMP (default) and Serial back-ends
make -j [KOKKOS_DEVICES=OpenMP,Serial]
```

Running on CPU with OpenMP back-end

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

Things to try:

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


<y,Ax> Exercise 01, Fixed Size
HSW
KNL
KNL (HBM)
Bandwidth (GB/s)
0
50
100
150
200
250
300
350
1
10
100
1000
10000
100000
1x10^6
1x10^7
1x10^8
1x10^9
Number of Rows (N)

- 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.

Example: running `daxpy` on the GPU:

Lambda

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

Functor

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

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Problem: `x` and `y` reside in CPU memory.

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

Problem: `x` and `y` reside in CPU memory.

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

$\Rightarrow$ **Views**

View abstraction

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

High-level example of Views for daxpy using lambda:

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

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

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  });
```

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.

View overview:

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- **Sizes of dimensions** set at compile-time or runtime.
  e.g., 2x20, 50x50, etc.

Example:

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

Note: runtime-sized dimensions must come first.

View life cycle:

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

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Example:

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

What gets printed?

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```

What gets printed?

3.0

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

- Location: `SNL2017/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 \
  KOKKOS_CUDA_OPTIONS=force_uvm,enable_lambda
# Run exercise
./02_Exercise.host -S 26
./02_Exercise.cuda -S 26
# Note the warnings, set appropriate environment variables
```

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

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

Execution and Memory Spaces

Learning objectives:

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

Thought experiment: Consider this code:

section 1
```
MPI_Reduce(...);
FILE * file = fopen(...);
runANormalFunction(...data...);
```
section 2
```
Kokkos::parallel_for(numberOfSomethings,
                     [=] (const size_t somethingIndex) {
                       const double y = ...;
                       // do something interesting
                     }
                     );
```

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Kokkos::parallel_for(numberOfSomethings,
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- Where will section 1 be run? CPU? GPU?
- Where will section 2 be run? CPU? GPU?
- How do I **control** where code is executed?

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                     }
                     );
```
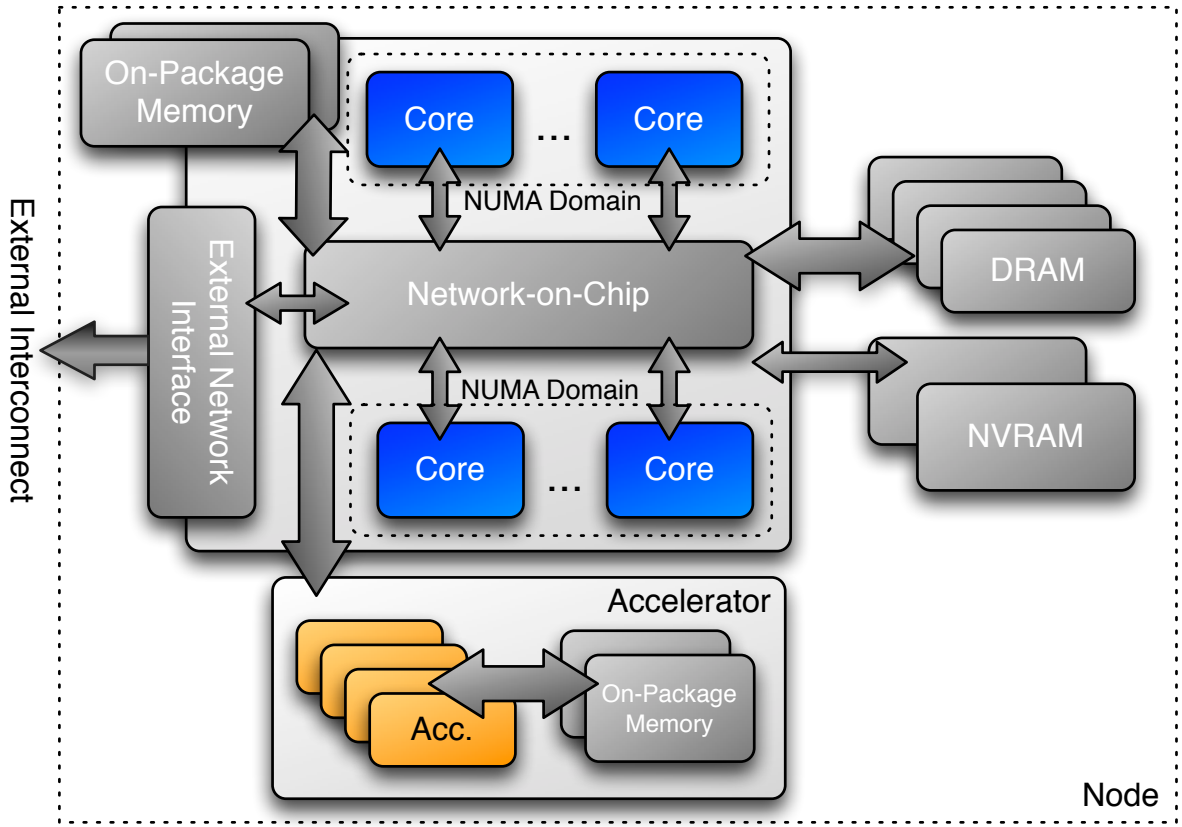

- Where will section 1 be run? CPU? GPU?
- Where will section 2 be run? CPU? GPU?
- How do I **control** where code is executed?

$\Rightarrow$ **Execution spaces**

Execution Space

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



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

Execution spaces (2)

Host

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

Parallel

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

Host

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

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

- Where will Host code be run? CPU? GPU?

  $\Rightarrow$ Always in the **host process**

Host

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

Parallel

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

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

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```
MPI_Reduce(...);
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runANormalFunction(...data...);
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```
Kokkos::parallel_for(numberOfSomethings,
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                       // do something interesting
                     }
                     );
```

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

Changing the parallel execution space:

Custom

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

Default

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

Changing the parallel execution space:

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Default

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    /* ... body ... */
  });
```

Requirements for enabling execution spaces:

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

Kokkos function and lambda portability annotation macros:

Function annotation with `KOKKOS_INLINE_FUNCTION` macro

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

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```

Lambda annotation with `KOKKOS_LAMBDA` macro (requires CUDA 8.0)

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

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

Memory space motivating example: summing an array

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

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

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

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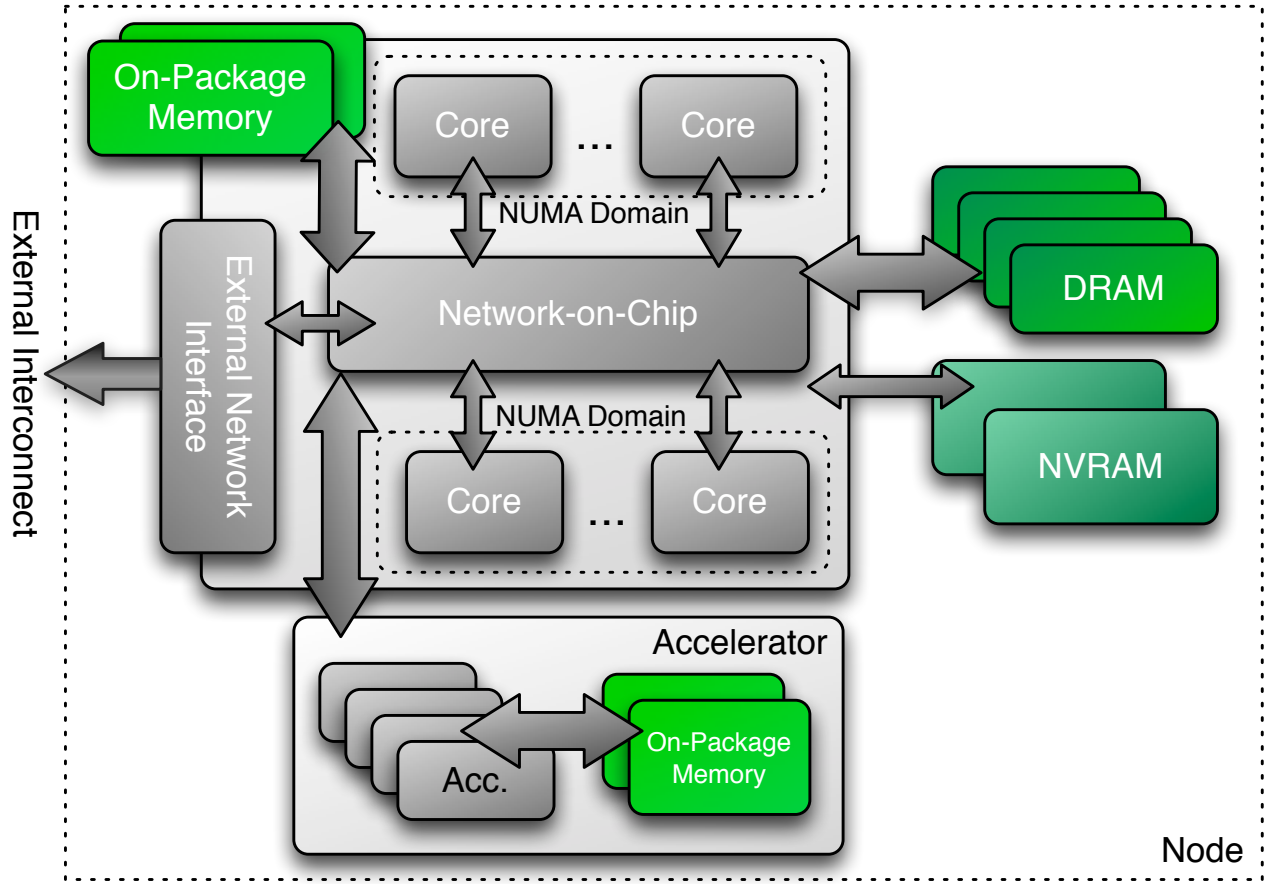
Question: Where is the data stored? GPU memory? CPU memory? Both?

$\Rightarrow$ **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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- Available **memory spaces**:

  `HostSpace, CudaSpace, CudaUVMSpace, ...` more

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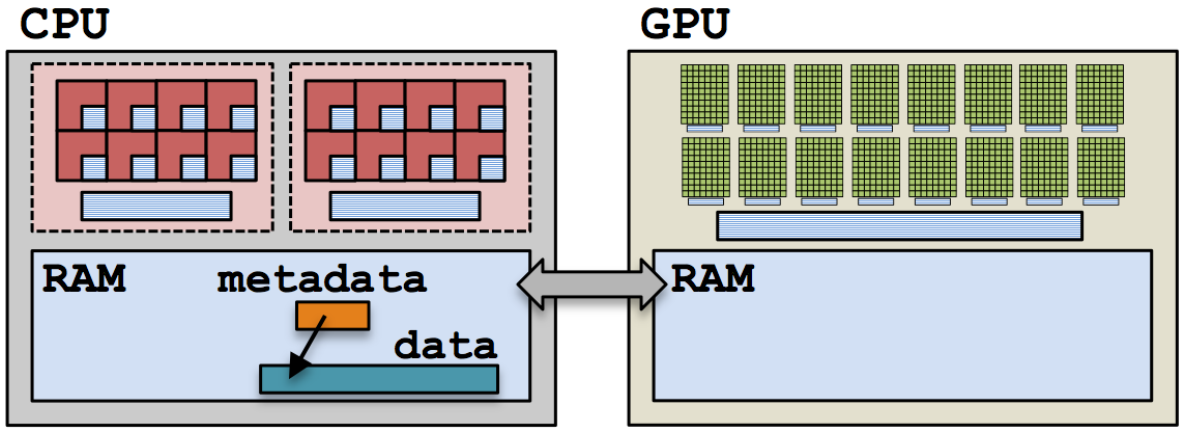
- `View<double***,`*Memory***Space**`> data(...);`
- Available **memory spaces**:

  `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...);
```



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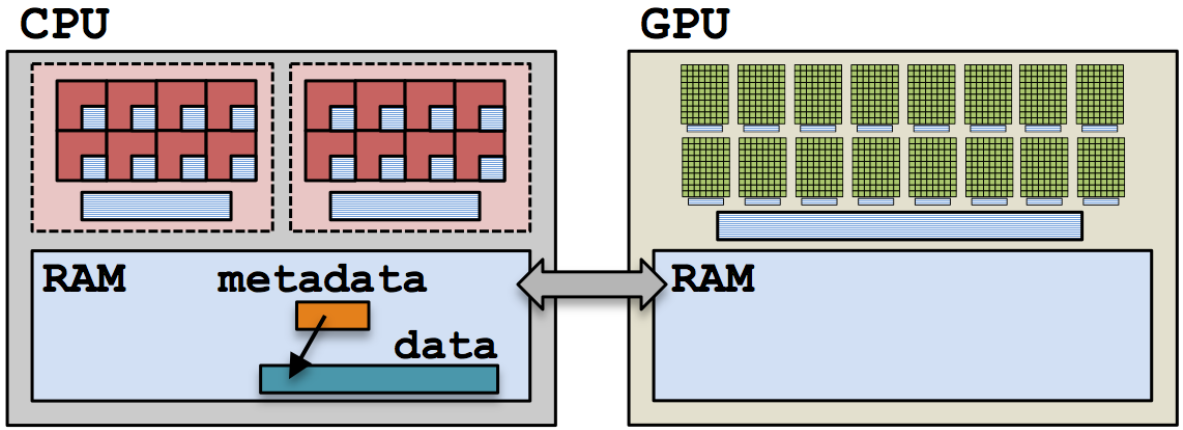
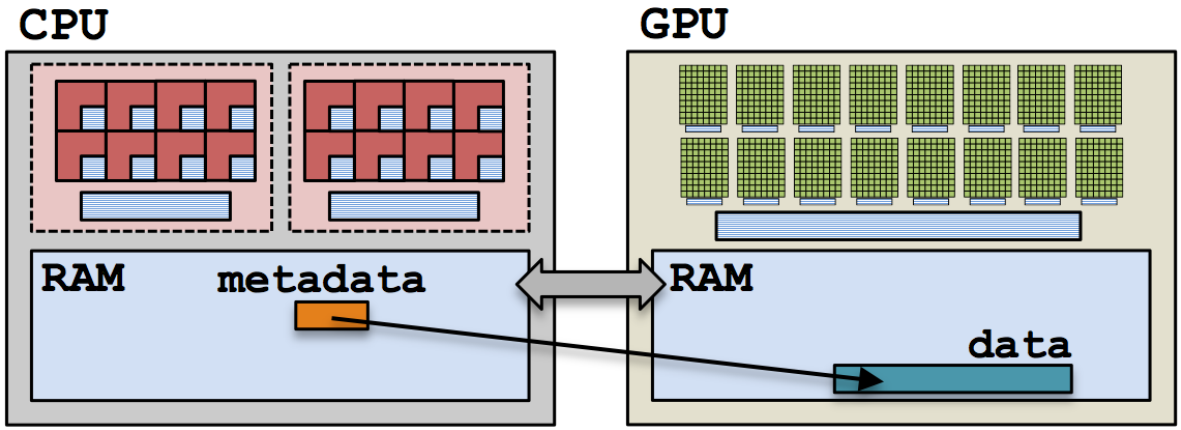


Example: CudaSpace

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



Anatomy of a kernel launch:

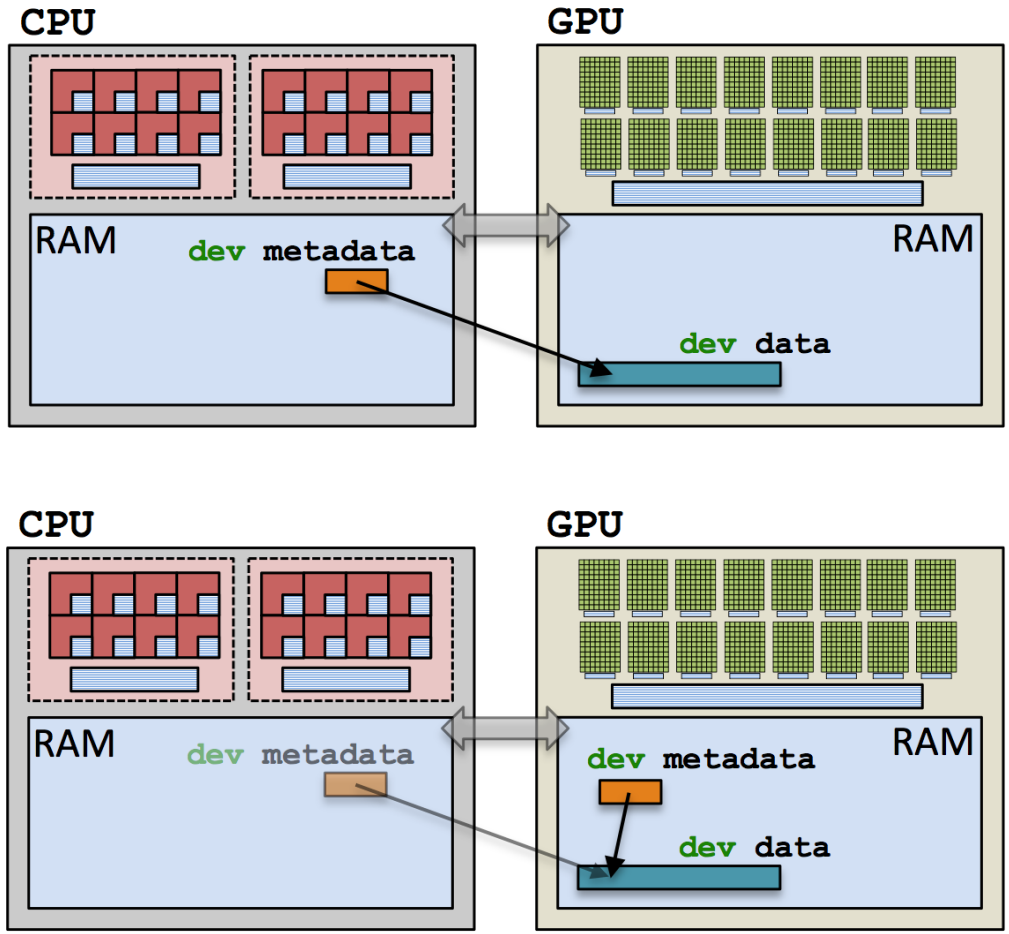
1. User declares views, allocating.
2. User instantiates a functor with views.
3. User launches `parallel_something`:
   - Functor is copied to the device.
   - Kernel is run.
   - Copy of functor on the device is released.

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

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

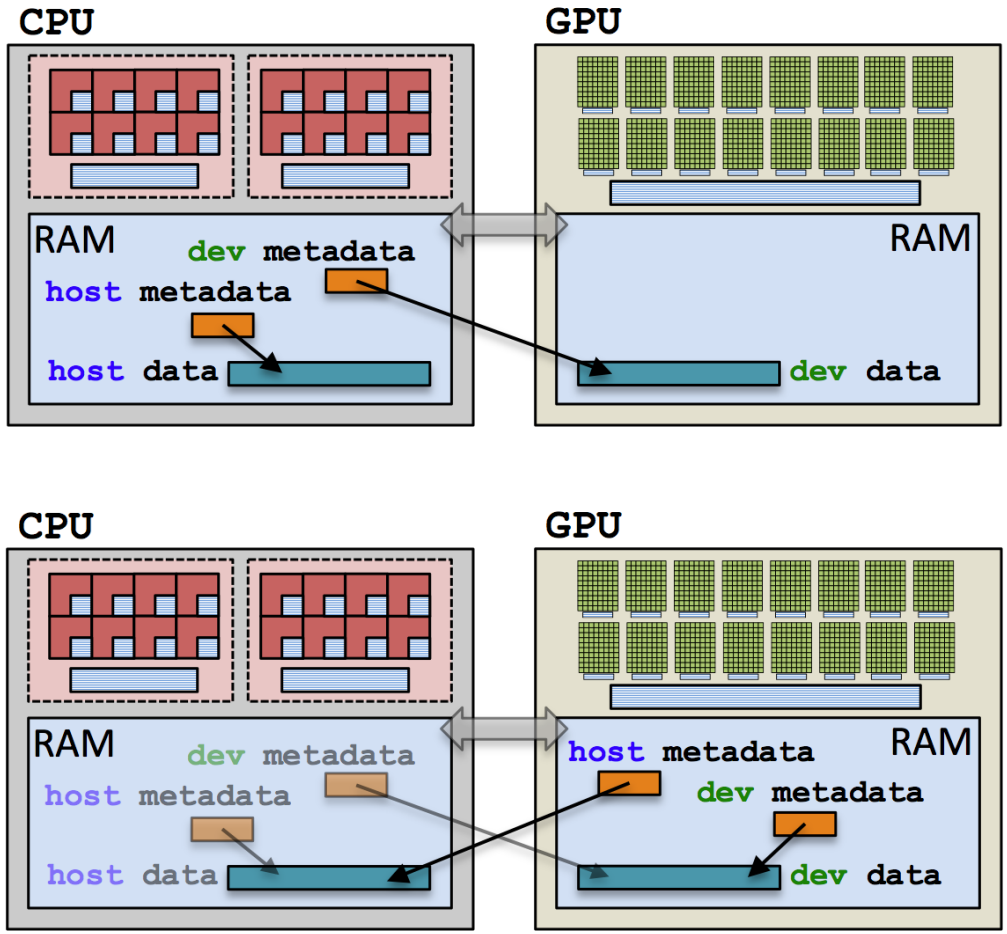
Example: one view

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



Example: two views

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



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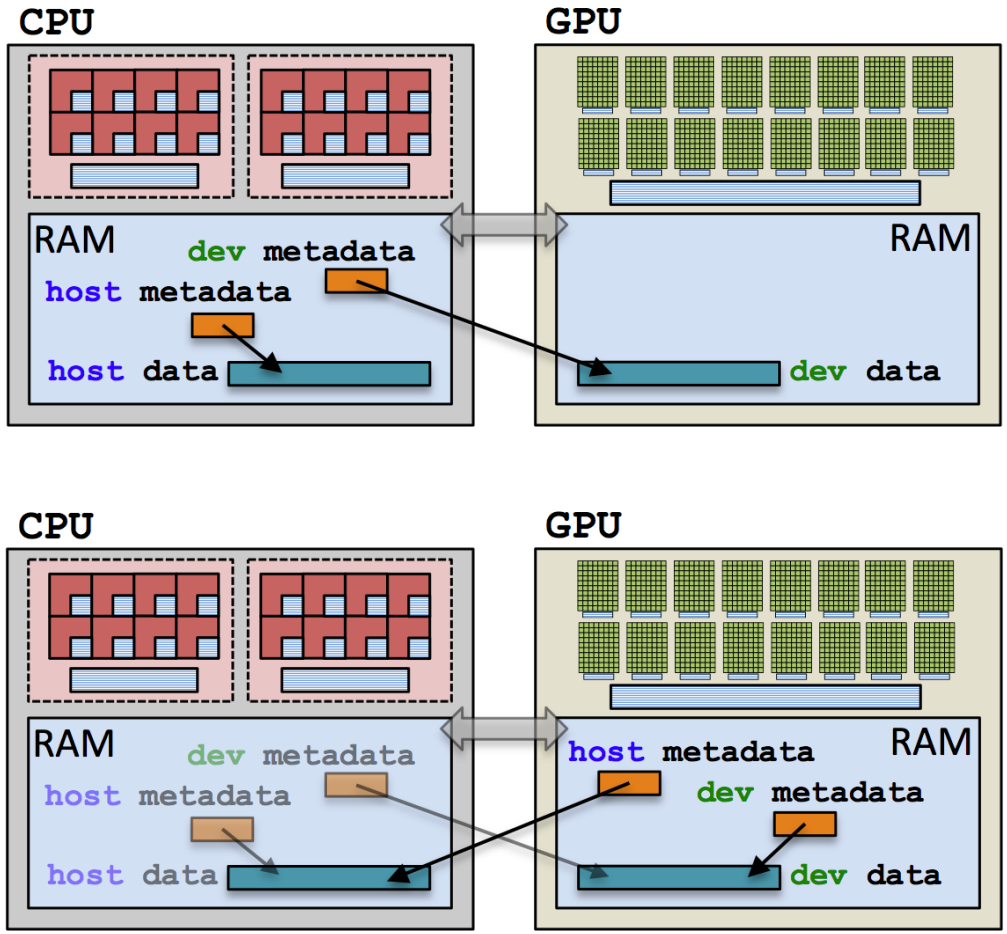

Example (redux): summing an array with the GPU

(failed) Attempt 1: `View` lives in `CudaSpace`

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

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

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  },
  sum);
```

Example (redux): summing an array with the GPU

(failed) Attempt 2: `View` lives in `HostSpace`

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

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

Example (redux): summing an array with the GPU

(failed) Attempt 2: View lives in HostSpace

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

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

Example (redux): summing an array with the GPU

(failed) Attempt 2: `View` lives in `HostSpace`

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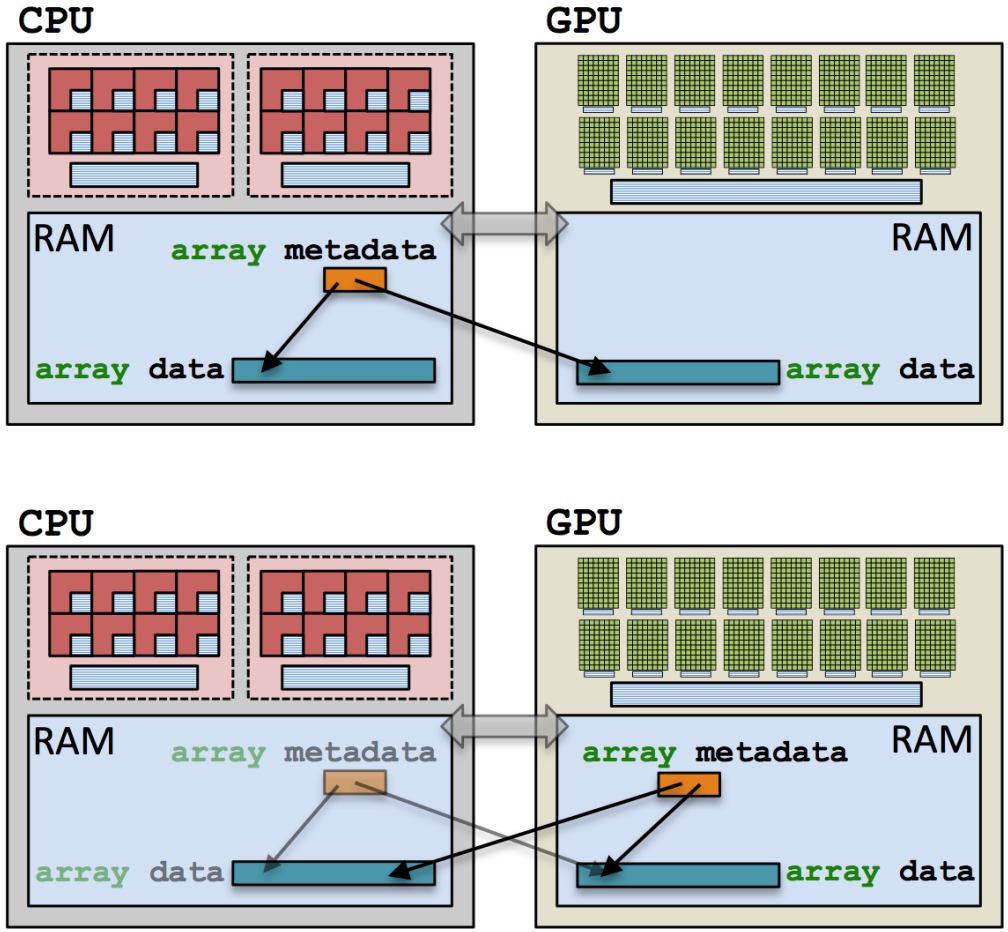
    valueToUpdate += array(index);          illegal access
  },
  sum);
```

What's the solution?

- CudaUVMSpace
- CudaHostPinnedSpace (skipping)
- Mirroring

CudaUVMSpace

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



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

Important concept: Mirrors

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

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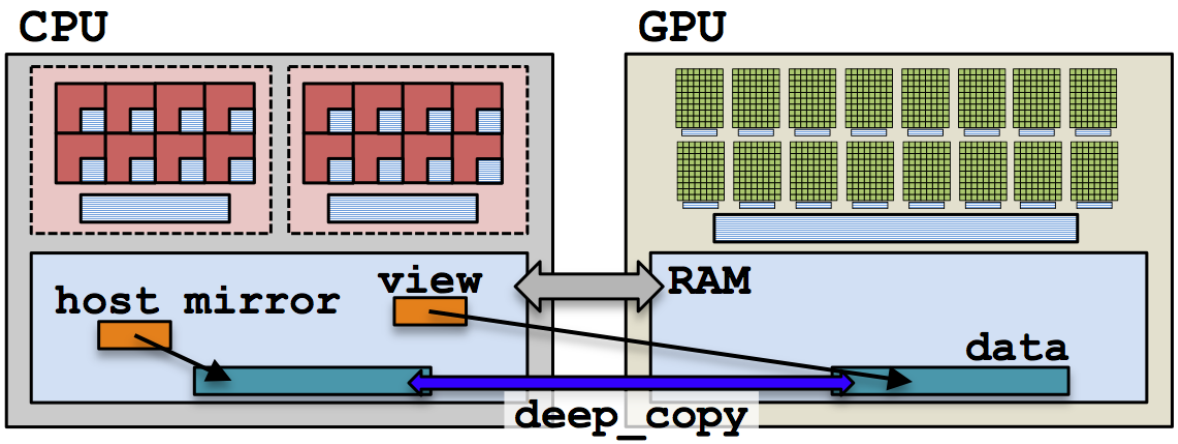
Mirroring schematic

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



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

```
Kokkos::deep_copy(view, hostView);
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5. **Launch** a kernel processing the `view`'s array.

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

Exercise #3: Flat Parallelism on the GPU, Views and Host Mirrors

Details:

- Location: `SNL2017/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.
- **Heterogenous nodes** have one or more memory spaces.
- **Mirroring** is used for performant access to views in host and device memory.
- Heterogenous nodes have one or more **execution spaces**.
- You **control where** parallel code is run by a template parameter on the execution policy, or by compile-time selection of the default execution space.

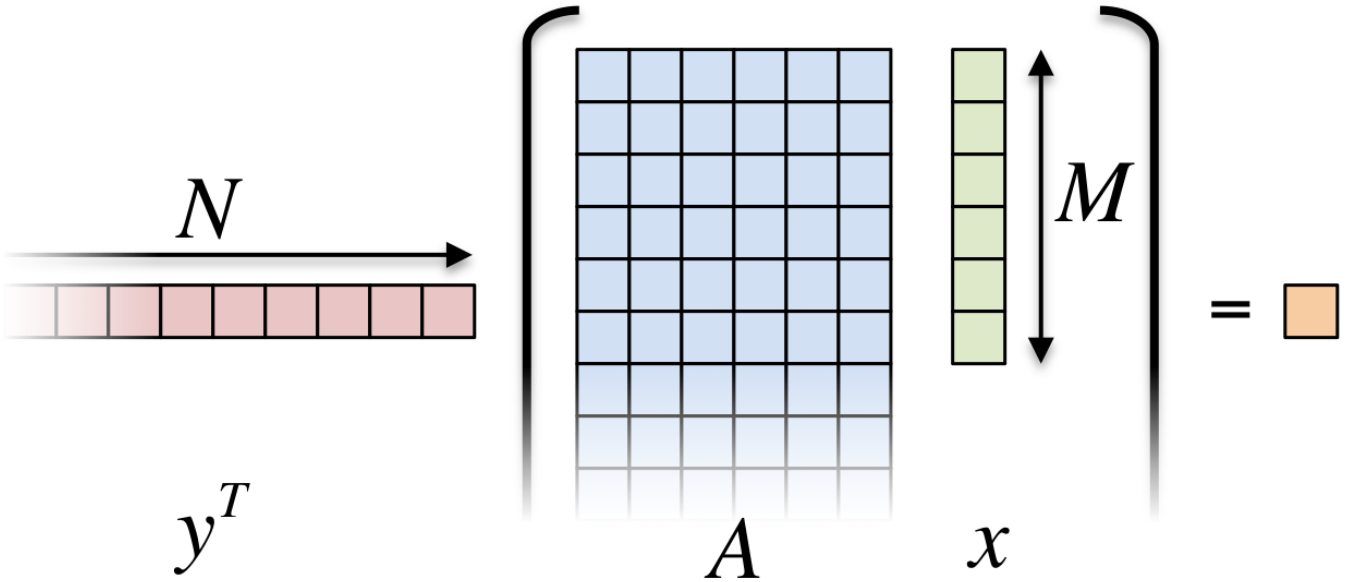
Managing memory access patterns for performance portability

Learning objectives:

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

Example: inner product (0)

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



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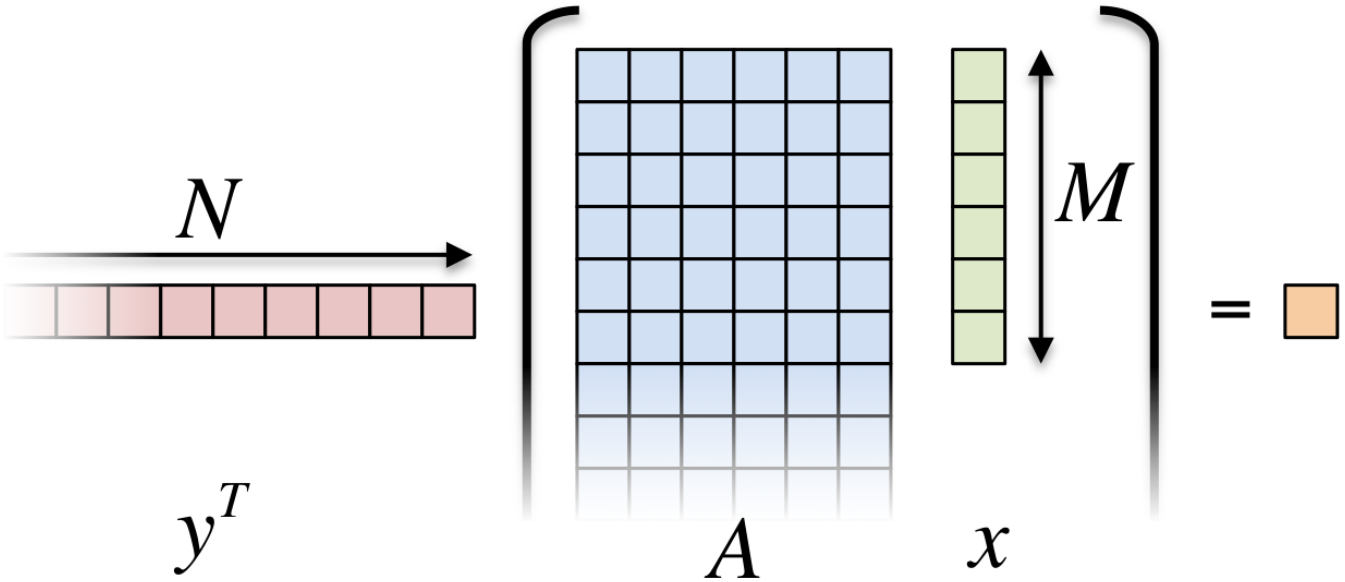
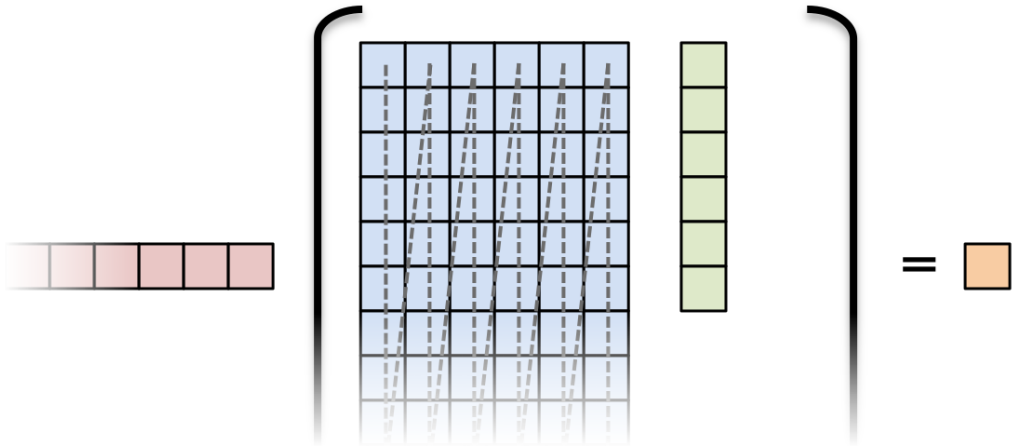


Driving question: How should `A` be laid out in memory?

Layout is the mapping of multi-index to memory:

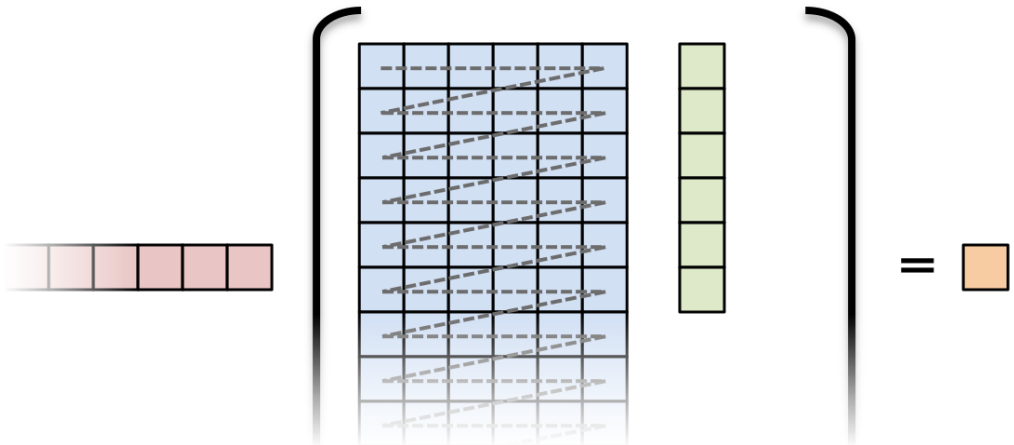
LayoutLeft

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(...);
```

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

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- 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:

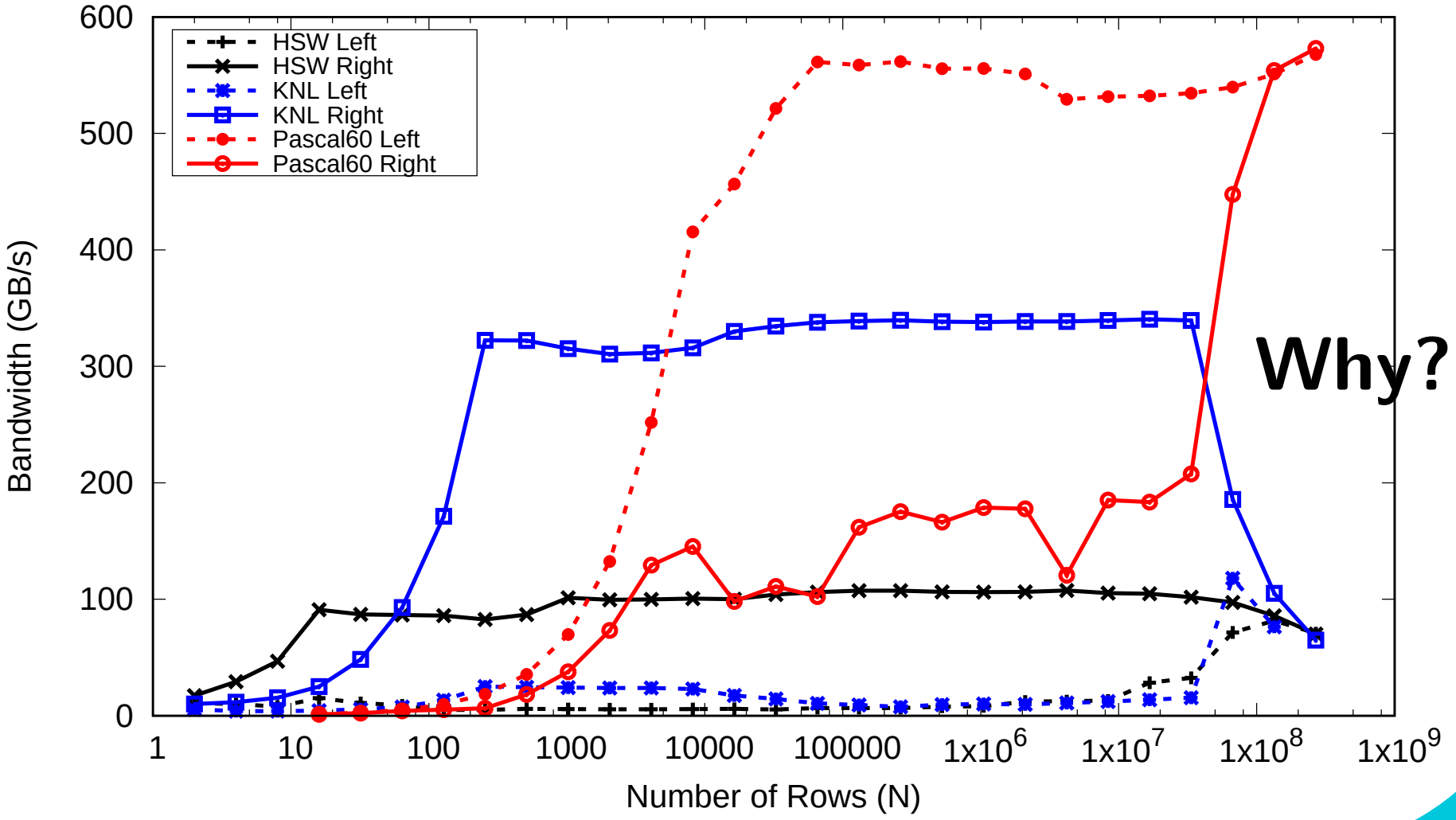
- Location: `SNL2017/Exercises/04/Begin/`
- Replace ``N'' in parallel dispatch with `RangePolicy<ExecSpace>`
- Add `MemSpace` to all `Views` and `Layout` to `A`
- Experiment with the combinations of `ExecSpace`, `Layout` to view performance

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.

<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:

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operator()(const size_t index, double & valueToUpdate) {
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- **GPU** threads are synchronized in groups (of 32).
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In particular, all threads in a group (*warp*) must finished their loads before *any* thread can move on.

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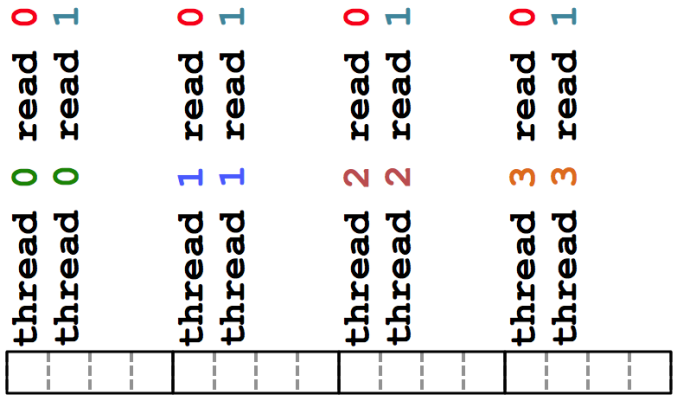
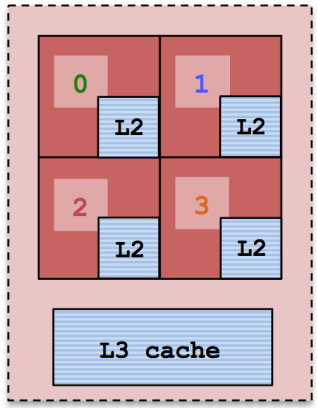
In particular, all threads in a group (*warp*) must finished their loads before *any* thread can move on.

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

CPUs: few (independent) cores with separate caches:





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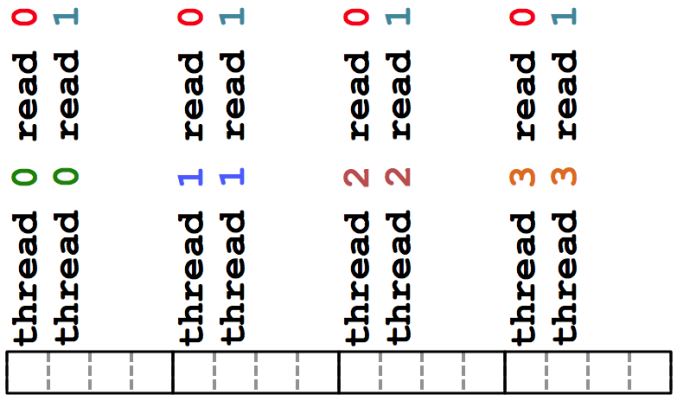
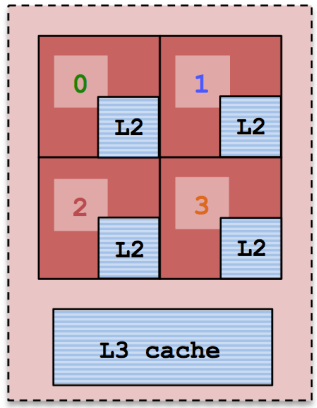
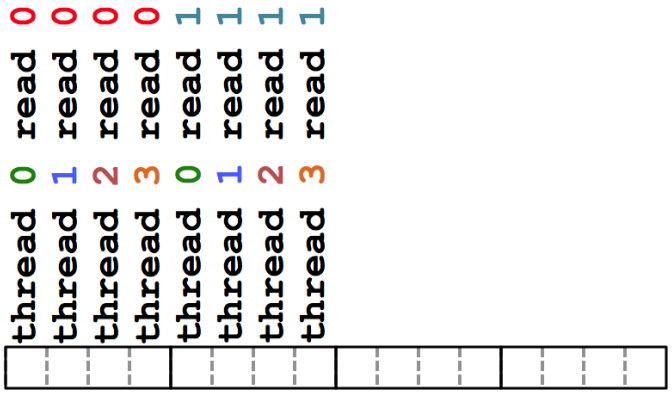
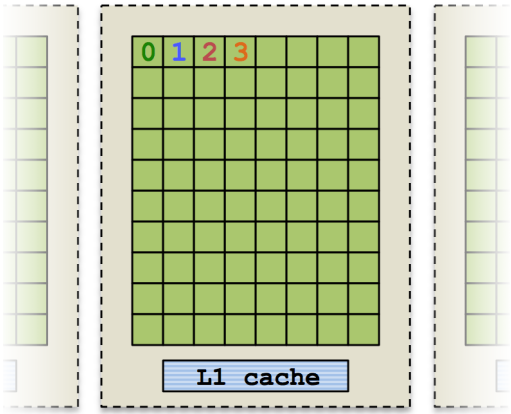




GPUs: many (synchronized) cores with a shared cache:





Important point

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

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

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

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Warning

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

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

Consider the array summation example:

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

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

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

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

Contiguous:	Strided:
`0, 1, 2, ..., N/P`	`0, N/P, 2*N/P, ...`

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Contiguous:	Strided:
`0, 1, 2, ..., N/P`	`0, N/P, 2*N/P, ...`
CPU	**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?

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

Important point

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

Rule of Thumb

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

Example:

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

Important point

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

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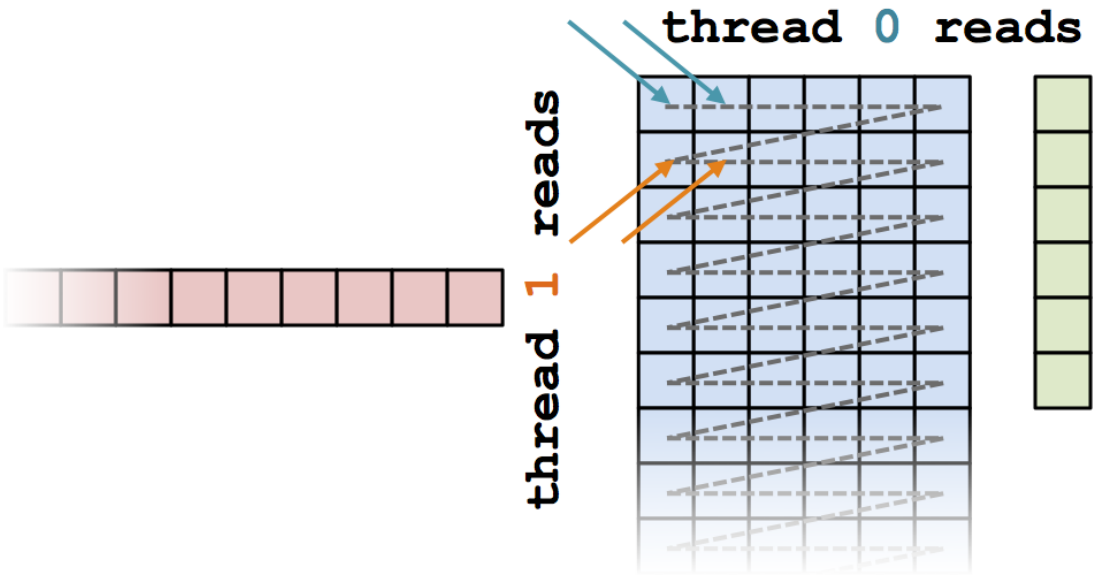
Performant memory access is achieved by Kokkos mapping parallel work indices **and** multidimensional array layout *appropriately for the architecture*.

Analysis: row-major (`LayoutRight`)



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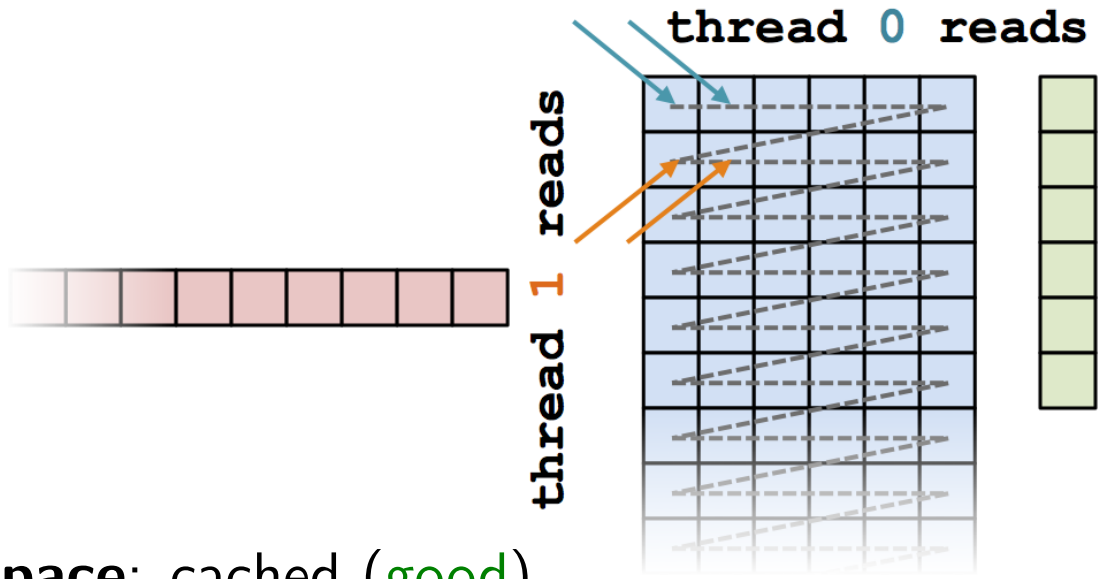
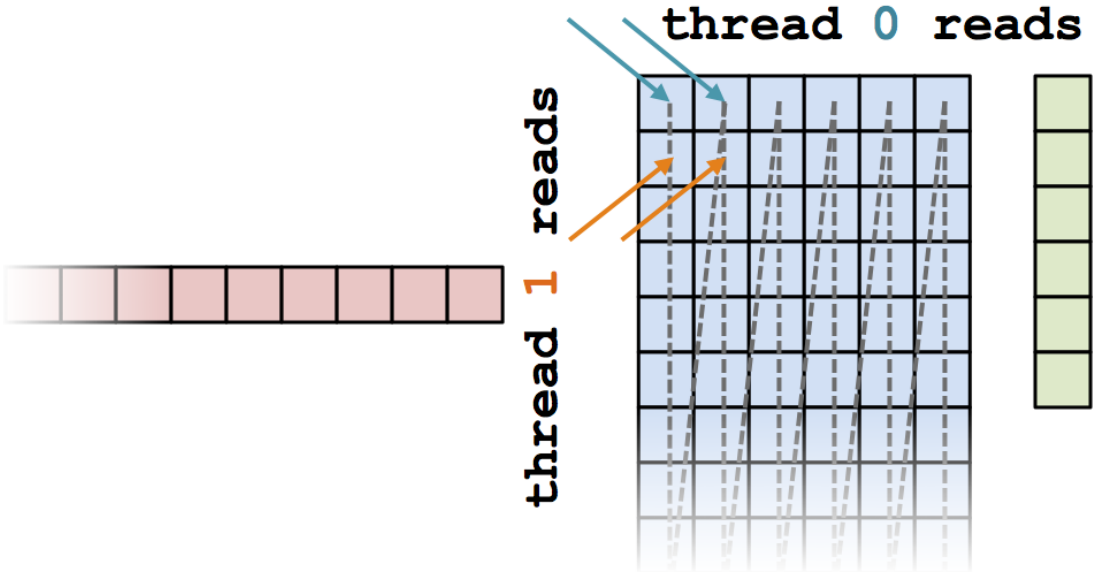


- **HostSpace**: cached (good)
- **CudaSpace**: uncoalesced (bad)

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

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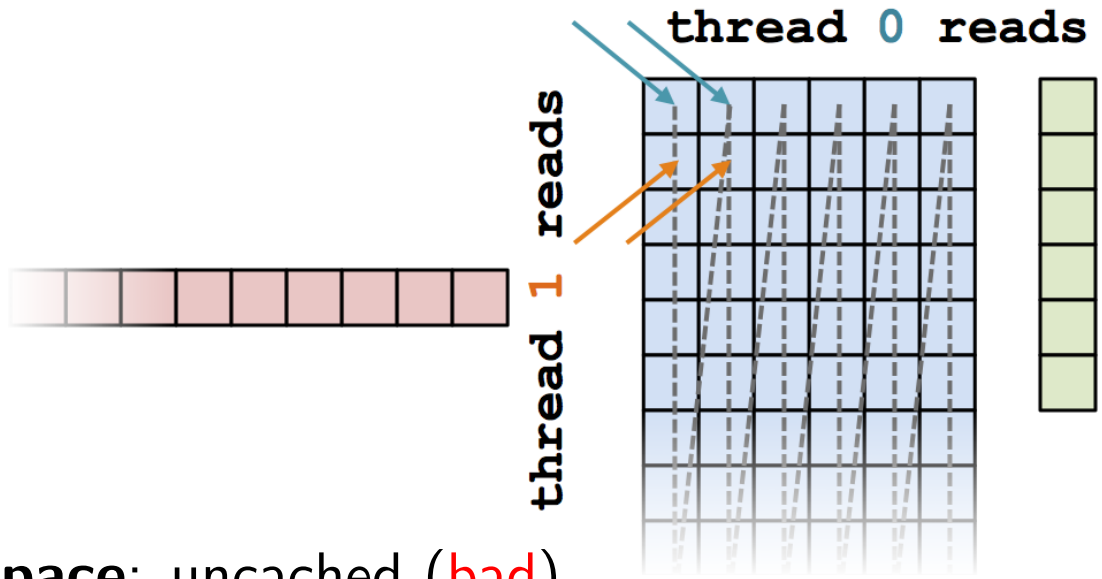
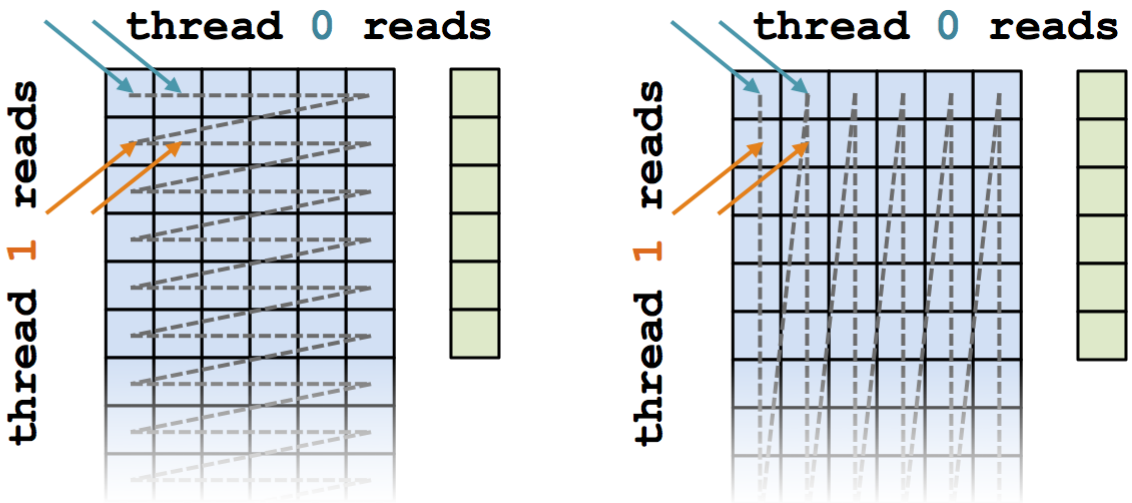
Analysis: column-major (`LayoutLeft`)



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

Analysis: Kokkos architecture-dependent

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



(a) OpenMP (b) Cuda

- **HostSpace**: cached (good)
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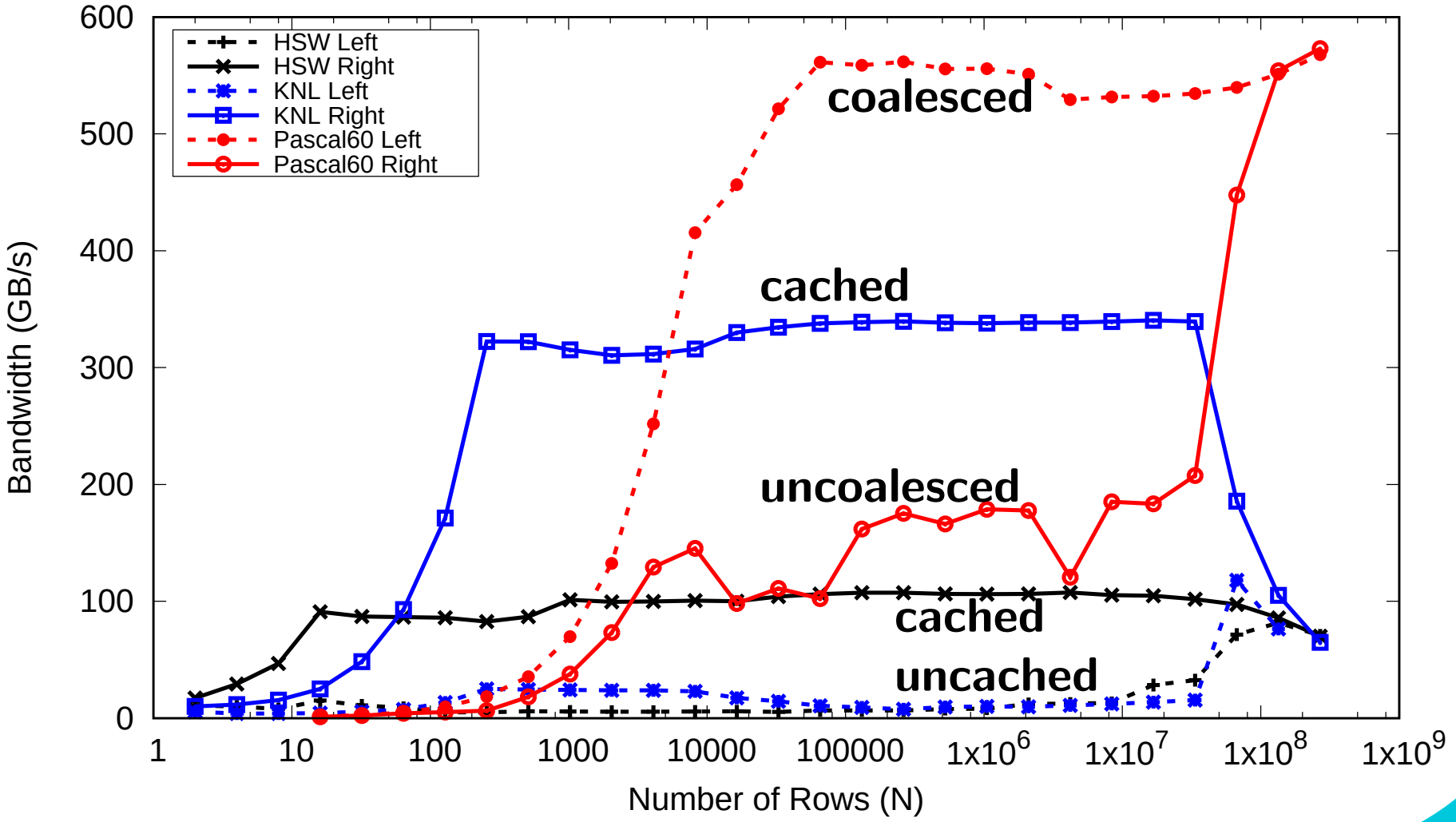
<y|Ax> Exercise 04 (Layout) Fixed Size

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



Memory Access Pattern Summary

- 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.
  $\Rightarrow$ You'll need multiple versions of code or pay the performance penalty.

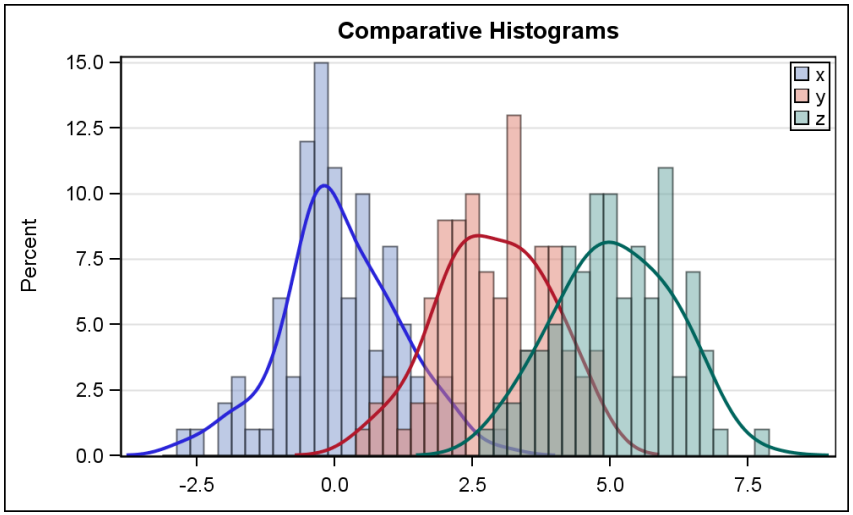
Thread safety and atomic operations

Learning objectives:

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

Histogram kernel:

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



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

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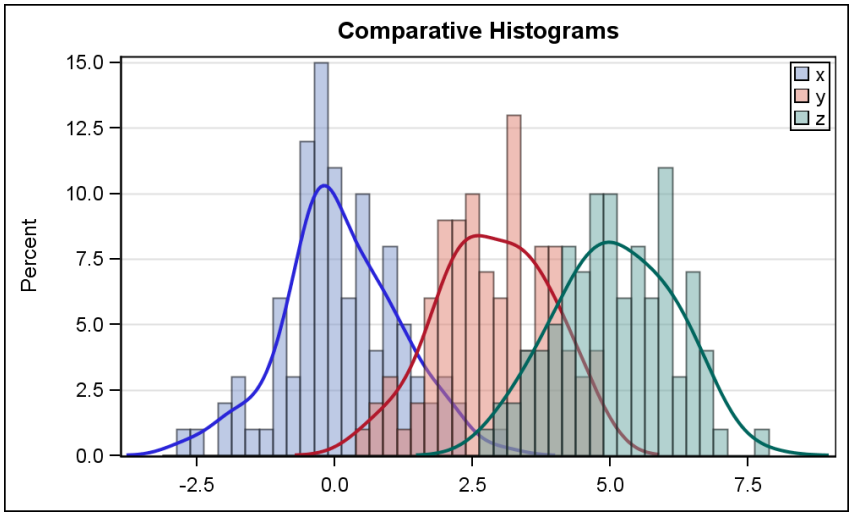
Problem: Multiple threads may try to write to the same location.



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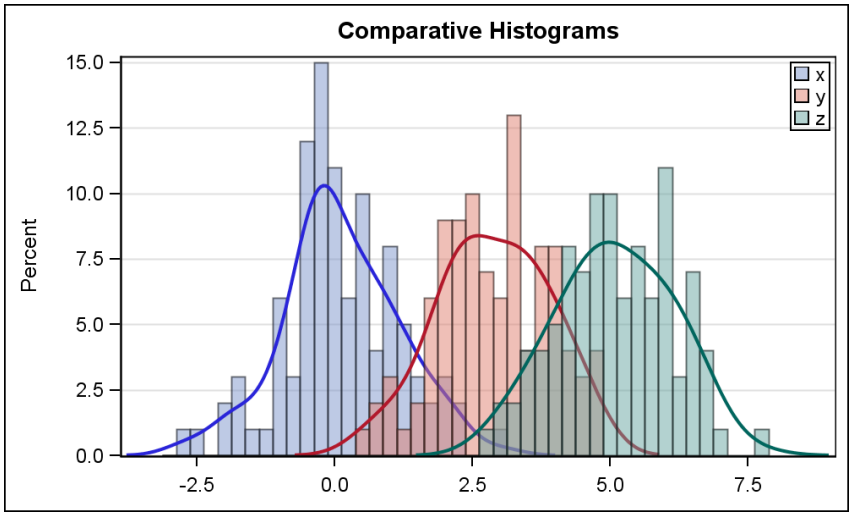
Problem: Multiple threads may try to write to the same location.

Solution strategies:

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



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Atomics: the portable and thread-scalable solution

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

Atomics: the portable and thread-scalable solution

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

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  });
```

- Atomics are the **only scalable** solution to thread safety.
- Locks 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,
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    valueToUpdate += function(...);
  }, totalIntegral);
```

Experimental setup

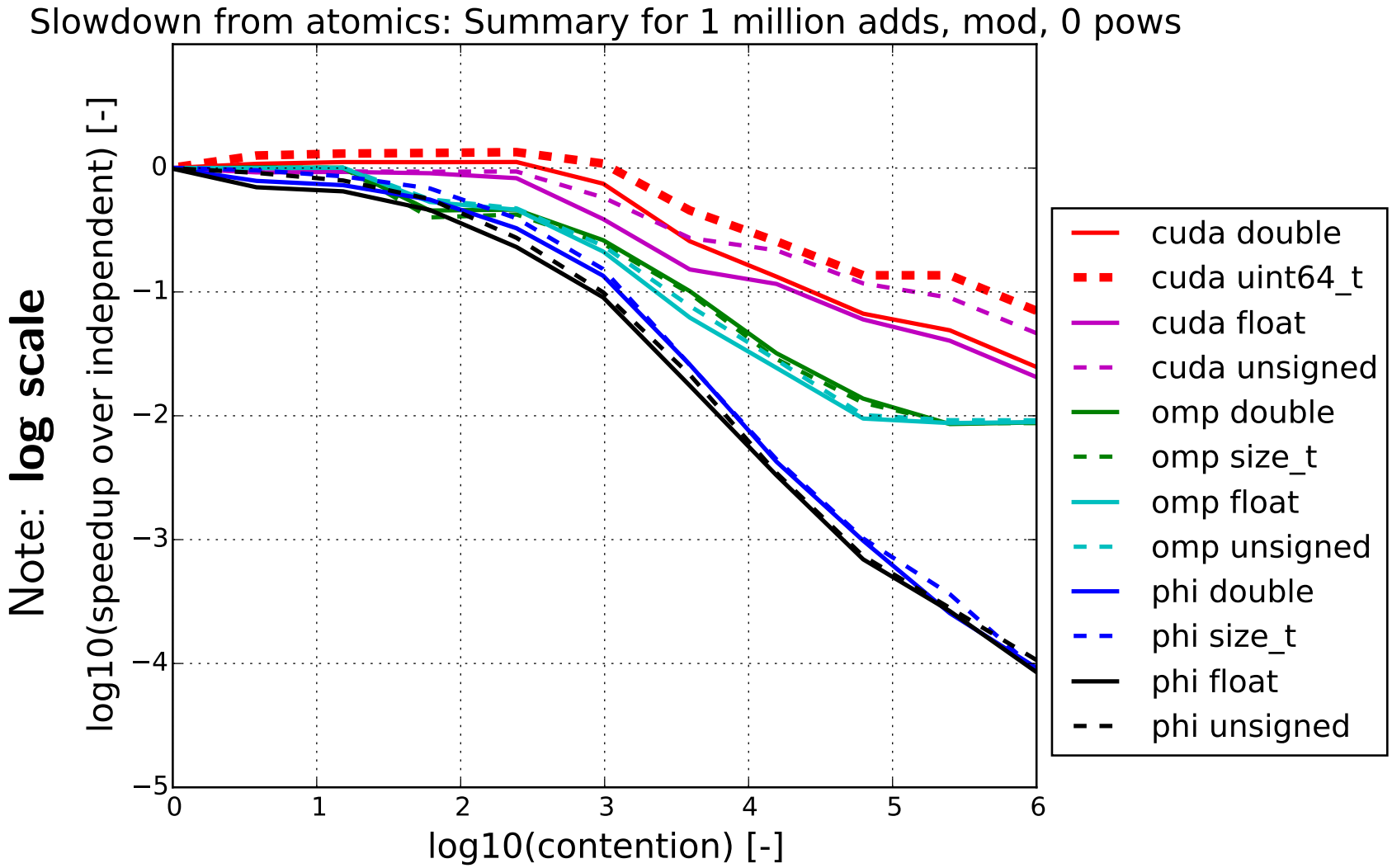
```
operator()(const unsigned int index) const {
  Kokkos::atomic_add(&globalSums[index % atomicStride], 1);
}
```

- This is the most extreme case: all coordination and no work.
- Contention is captured by the `atomicStride`.

  `atomicStride` $\to$ 1 $\Rightarrow$ Scalar integration (bad)

  `atomicStride` $\to$ large $\Rightarrow$ Independent (good)

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



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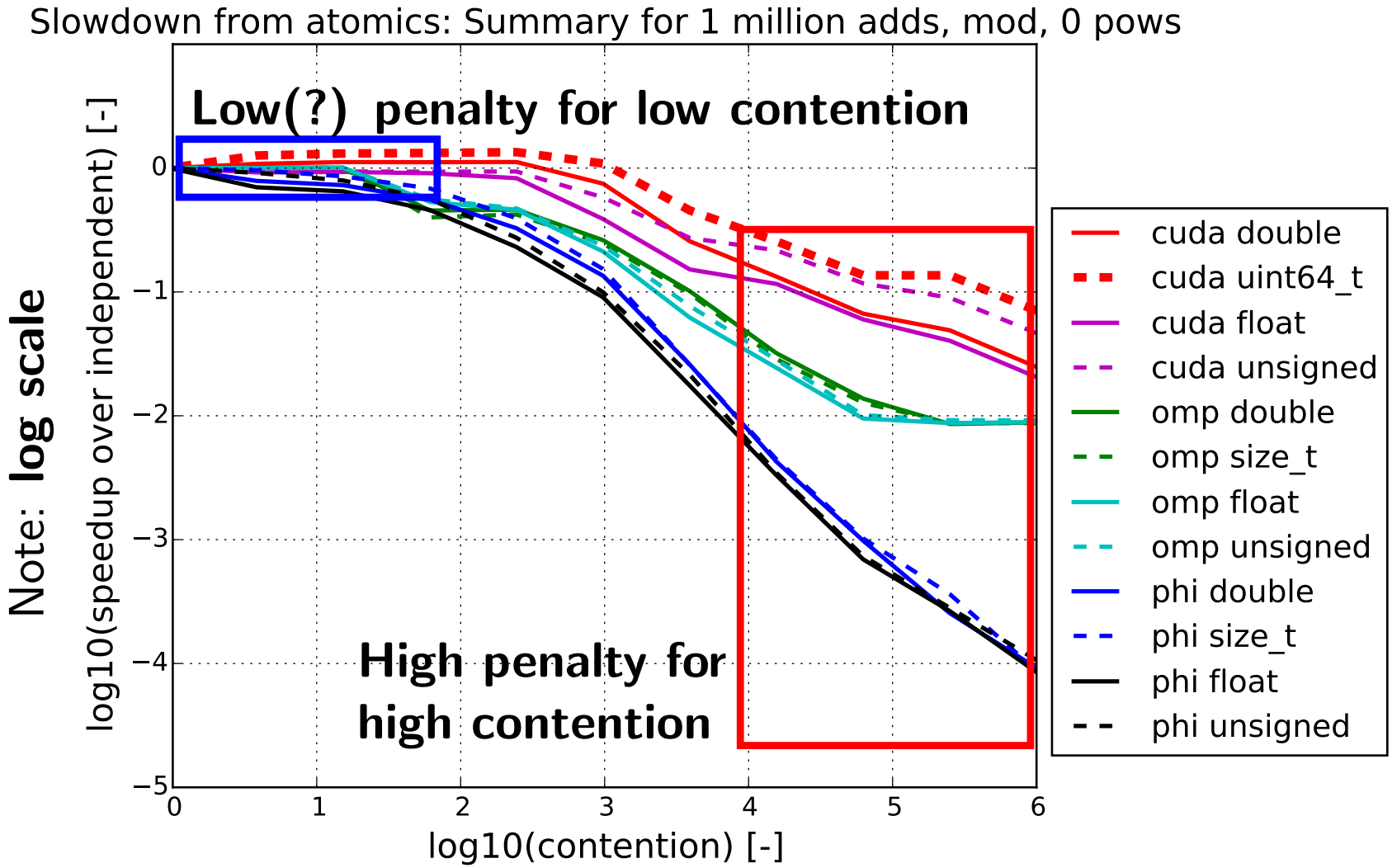
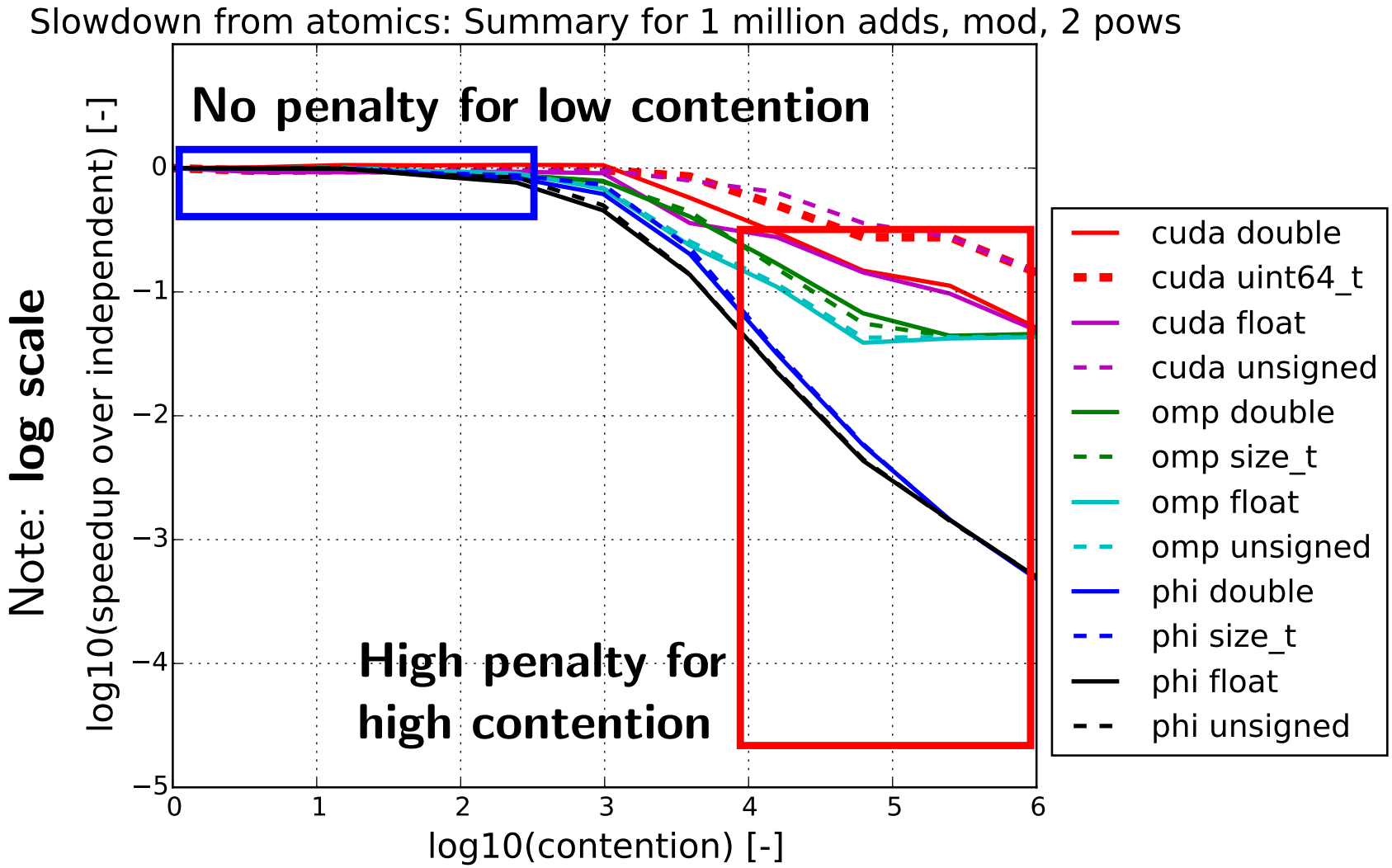
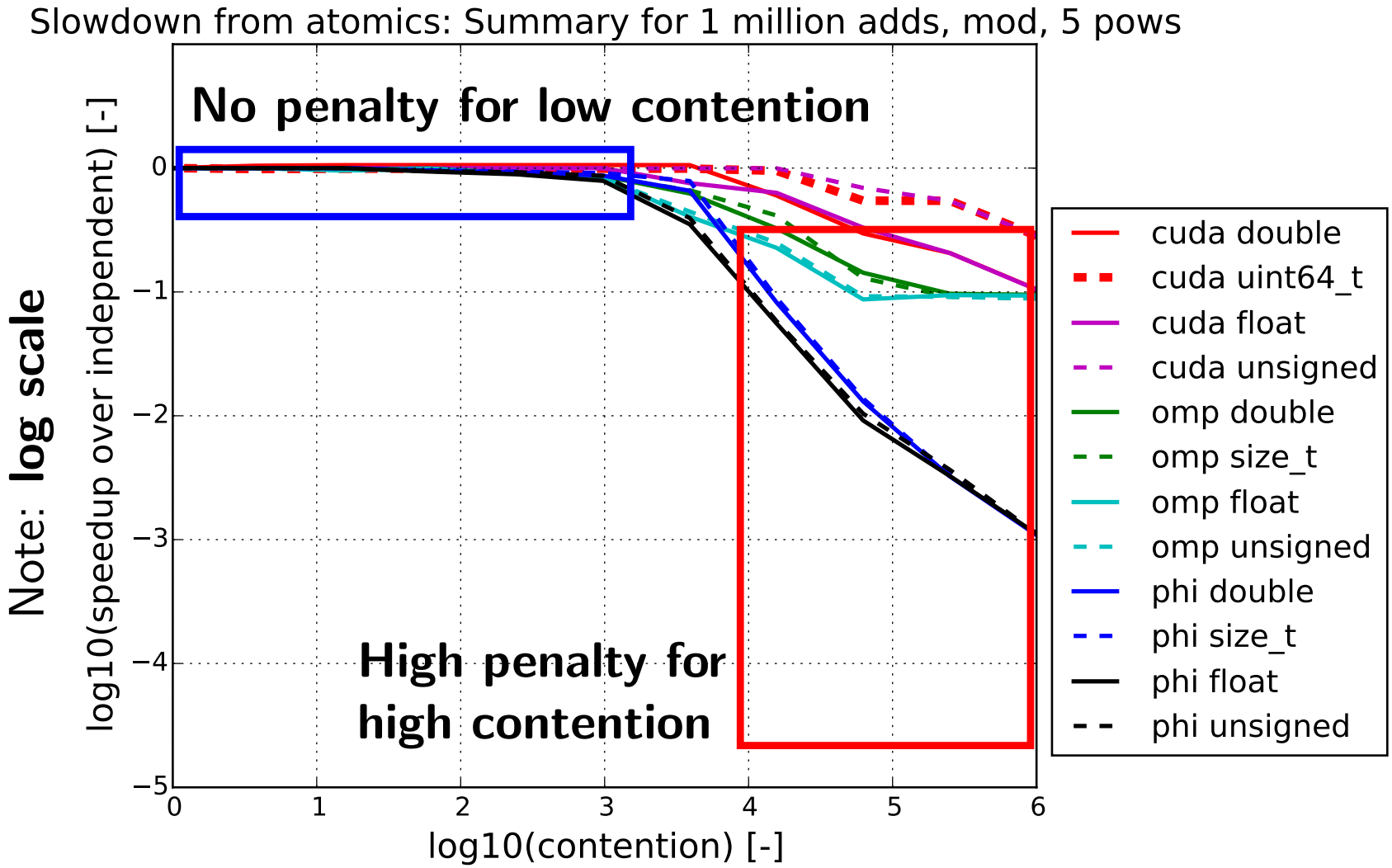


Atomics performance: 1 million adds, **some** work per kernel



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



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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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.

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

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texDesc.readMode = cudaReadModeElementType;

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

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

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

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

Hierarchical parallelism

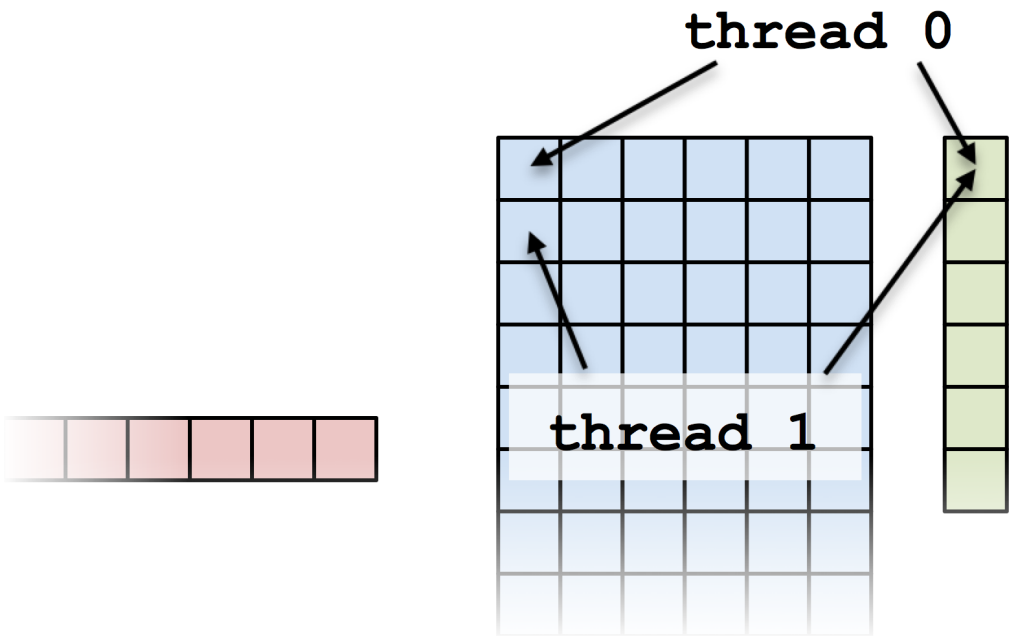
Finding and exploiting more parallelism in your computations.

Learning objectives:

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

(Flat parallel) Kernel:

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



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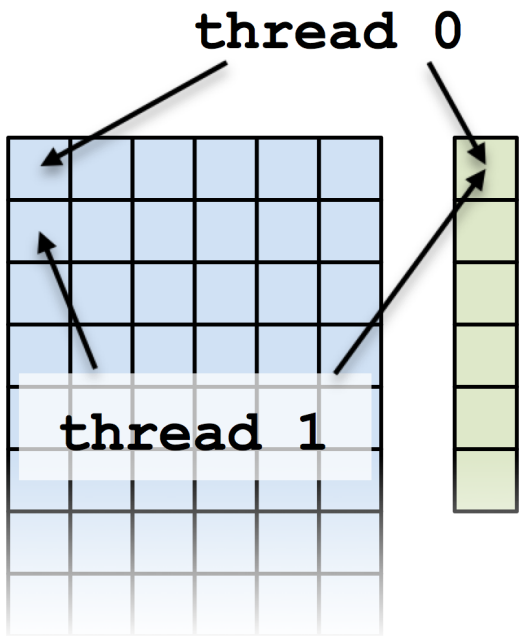
Problem: What if we don't have enough rows to saturate the GPU?



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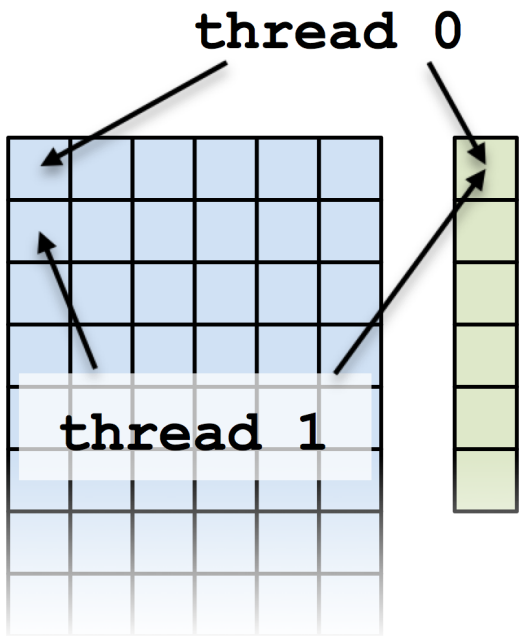
Solutions?



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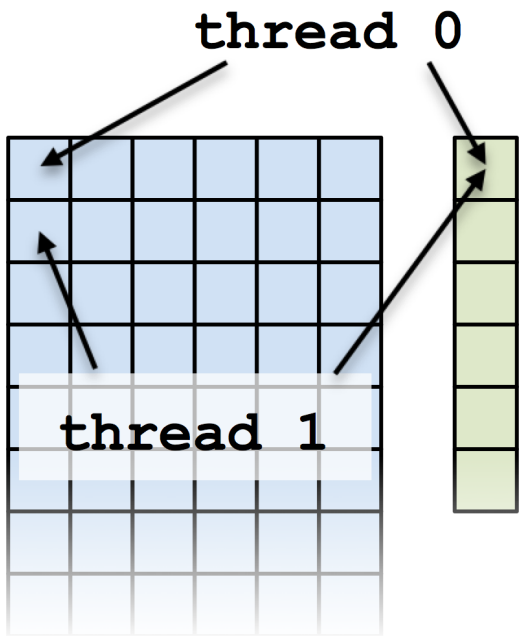


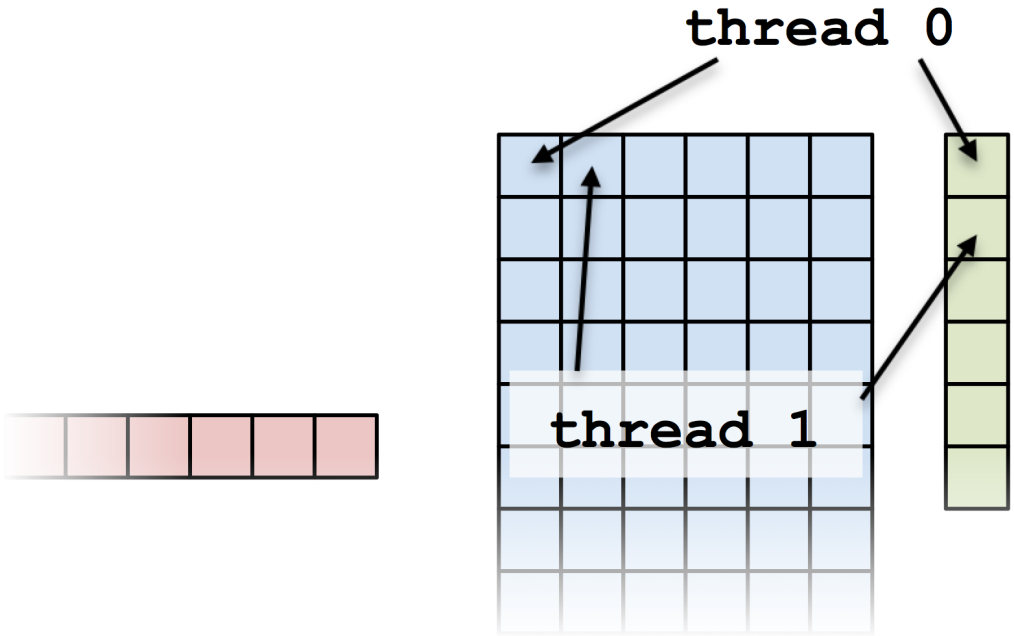
Problem: What if we don't have enough rows to saturate the GPU?

Solutions?

- Atomics
- Thread teams

Atomics kernel:

```
Kokkos::parallel_for(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));
  });
```



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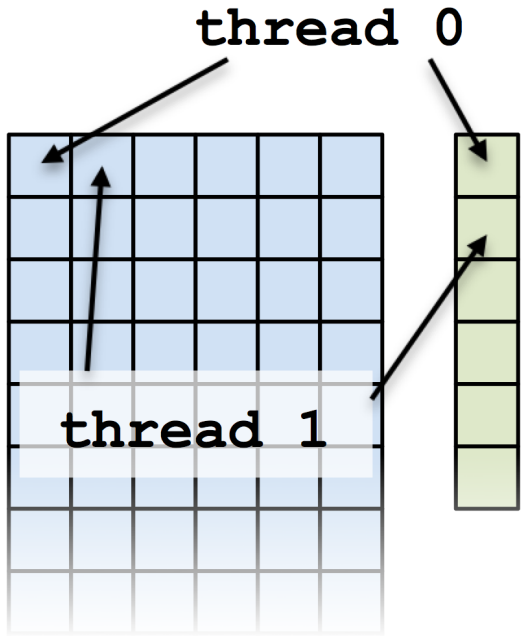
Problem: Poor performance



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

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```

This is an example of *hierarchical work*.

Important concept: Hierarchical parallelism

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

Important concept: Thread team

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

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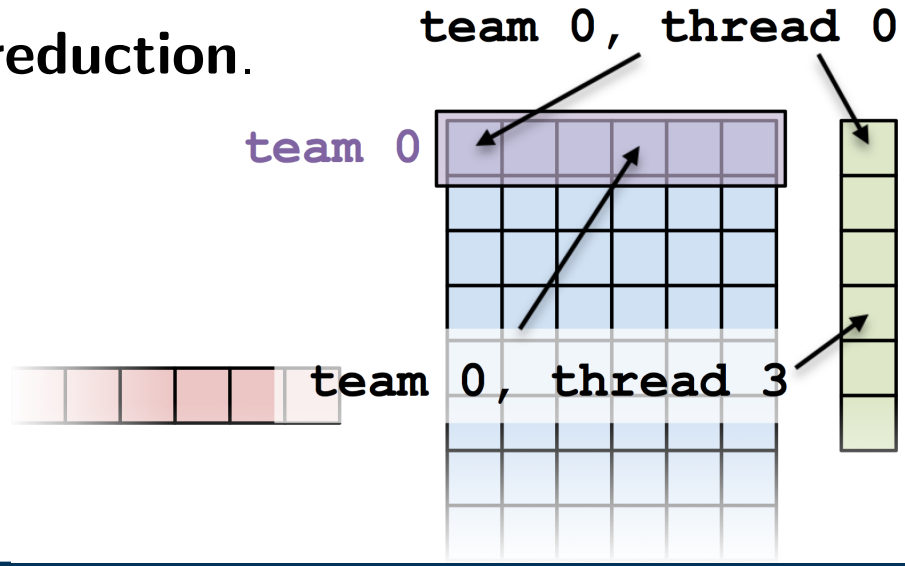
A collection of threads which are guaranteed to be executing **concurrently** and **can synchronize**.

High-level **strategy**:

1. Do **one parallel launch** of `N` teams of `M` threads.
2. Each thread performs **one** entry in the row.
3. The threads within **teams perform a reduction**.
4. The thread teams **perform a reduction**.



The final hierarchical parallel kernel:

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

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

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

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

Important point

Using teams is changing the execution *policy*.

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

We specify a *total amount of work*.

```
// total work = N
parallel_for(
  RangePolicy<ExecutionSpace>(0,N), functor);
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We specify a *total amount of work*.

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

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

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

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

Important point

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

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

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

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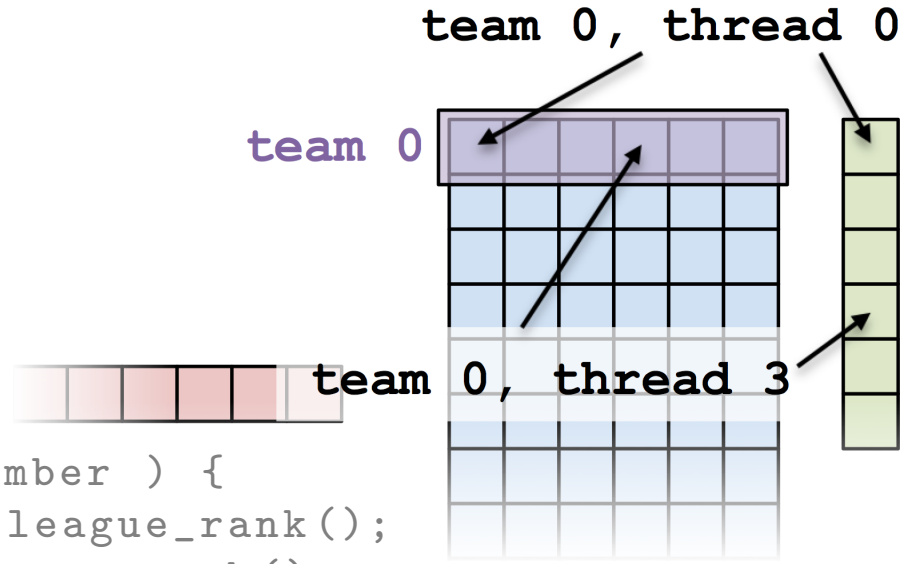
Warning

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

TeamThreadRange (0)



First attempt at exercise:

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

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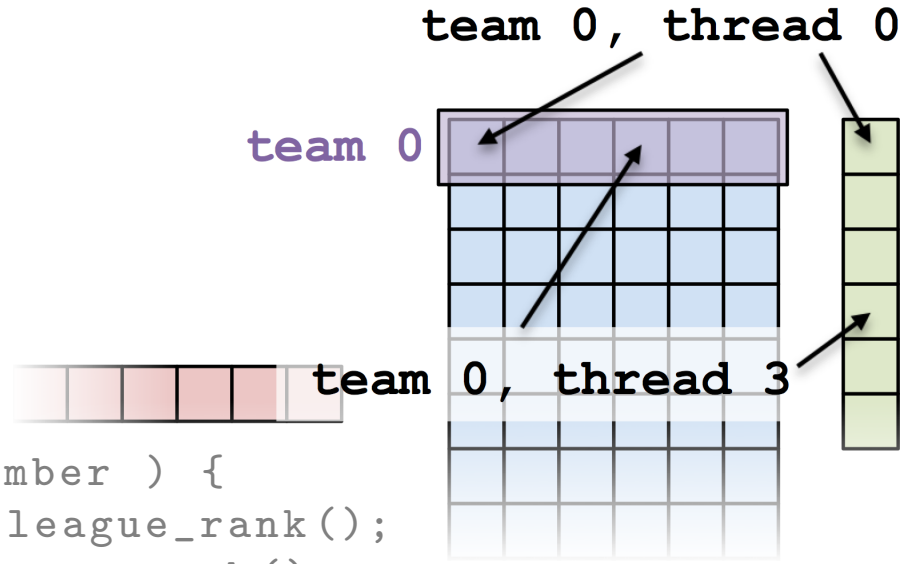

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```

- When team size $\neq$ number of columns, how are units of work mapped to team's member threads? Is the mapping architecture-dependent?
- `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 thisRowsSum;
  ``do a reduction''(``over M columns'',
    [=] (const int col) {
      thisRowsSum += A(row,col) * x(col);
    });
  if (teamMember.team_rank() == 0) {
    update += (row) * thisRowsSum;
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}
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If this were a parallel execution,

we'd use `Kokkos::parallel_reduce`.

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Key idea: this *is* a parallel execution.

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$\Rightarrow$ **Nested parallel patterns**

TeamThreadRange:

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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;
  }
}
```

TeamThreadRange:

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

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

Anatomy of nested parallelism:

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

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

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

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

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parallel_something(
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NVIDIA GPU:

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

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- Within a team 32 threads (*warp*) execute "lock step."
- Maximum team size: **1024**; Recommended team size: **256**

Intel Xeon Phi:

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

Details:

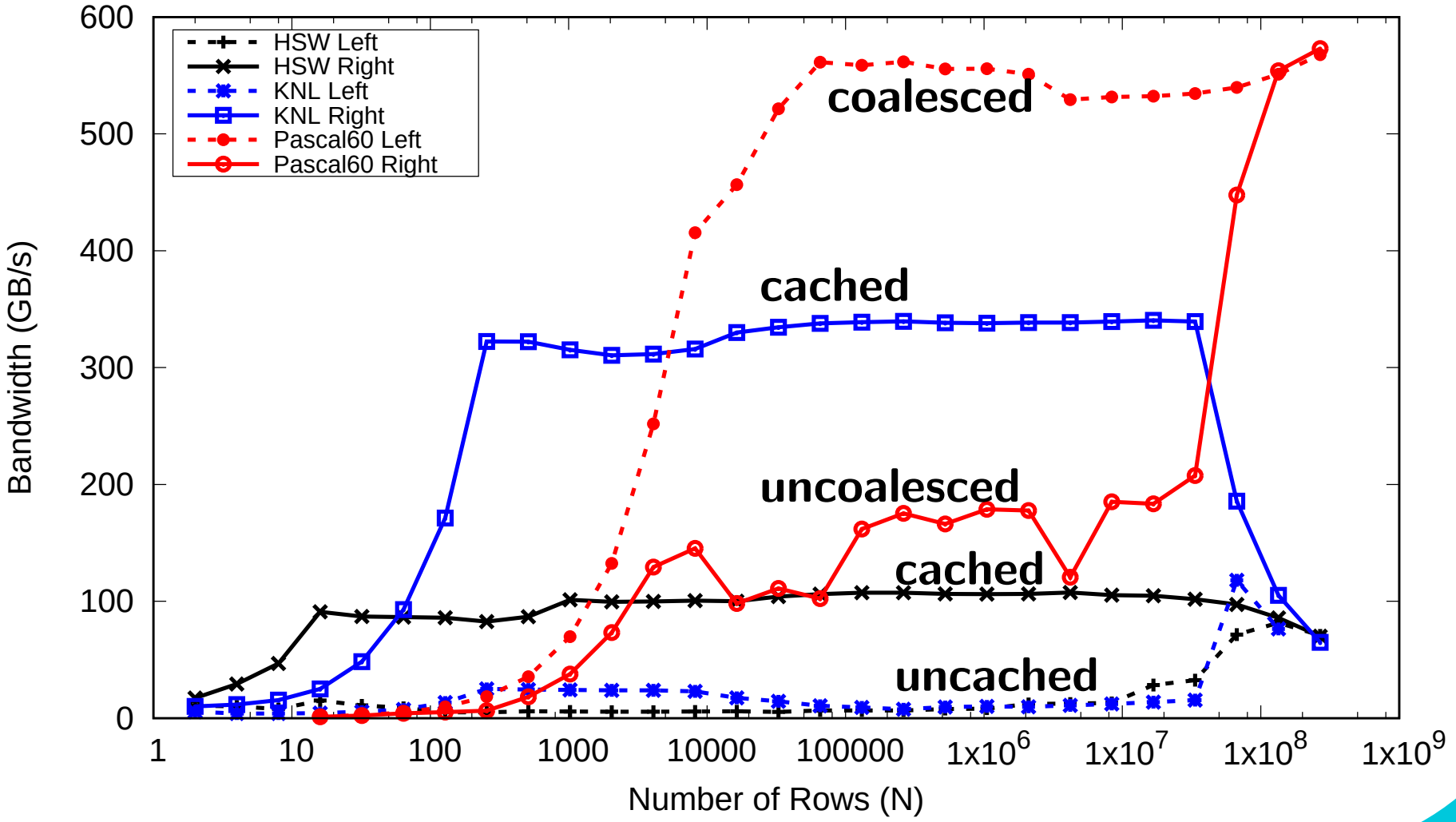
- Location: `SNL2017/Exercises/05/`
- Replace `RangePolicy<Space>` with `TeamPolicy<Space>`
- Use `AUTO` for `team_size`
- Make the inner loop a `parallel_reduce` with `TeamThreadRange` policy
- Experiment with the combinations of `Layout`, `Space`, `N` to view performance
- Hint: what should the layout of `A` be?

Things to try:

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

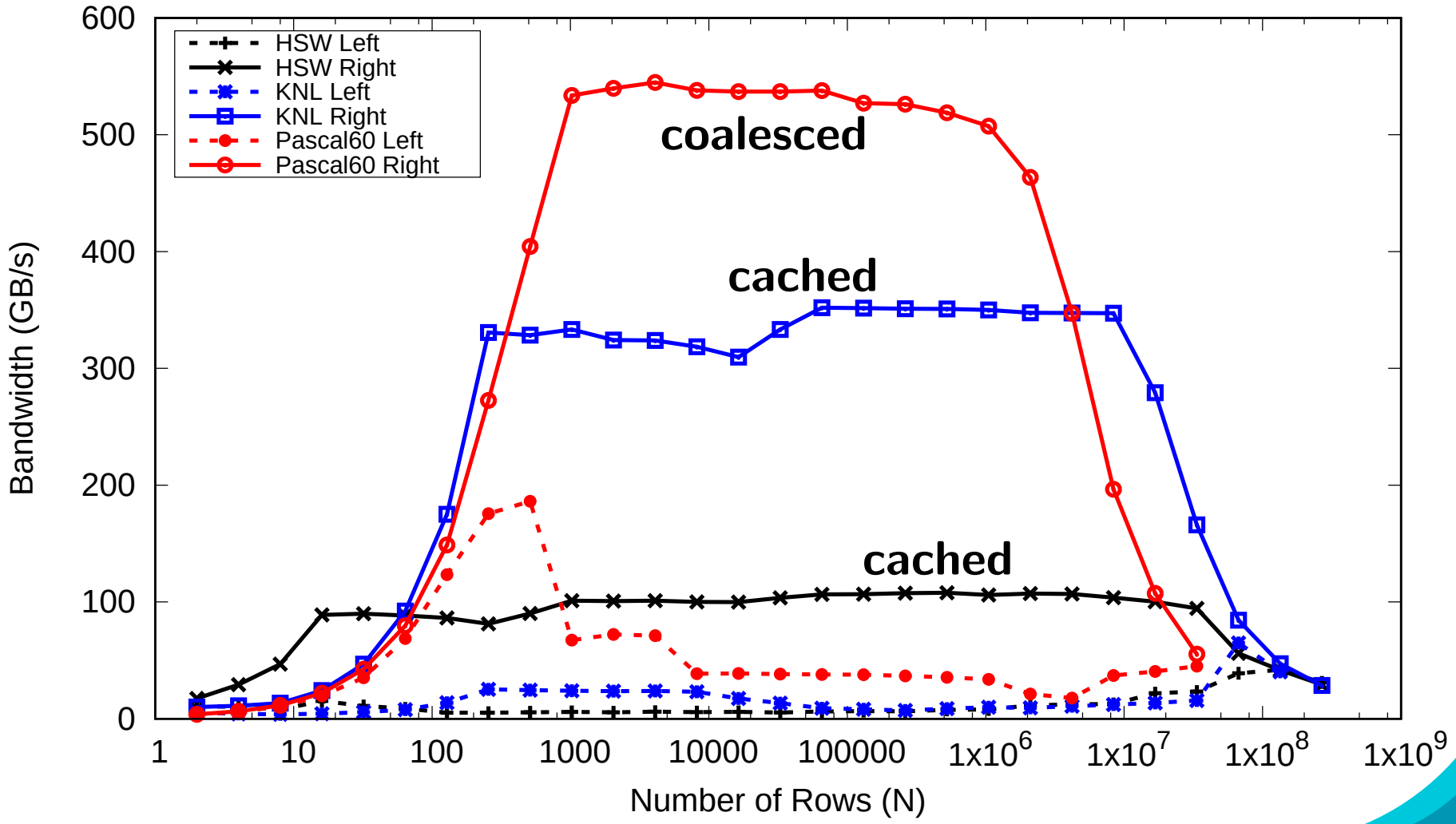
<y|Ax> Exercise 04 (Layout) Fixed Size

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



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

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.

Anatomy of nested parallelism:

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

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

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

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

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

`totalSum = numberOfThreads * 10`

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

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

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

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

`totalSum = numberOfTeams * team_size * 10`

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

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

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

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

`totalSum = numberOfTeams * team_size * team_size * 10`

The `single` pattern can be used to restrict execution

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

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

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

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

Details:

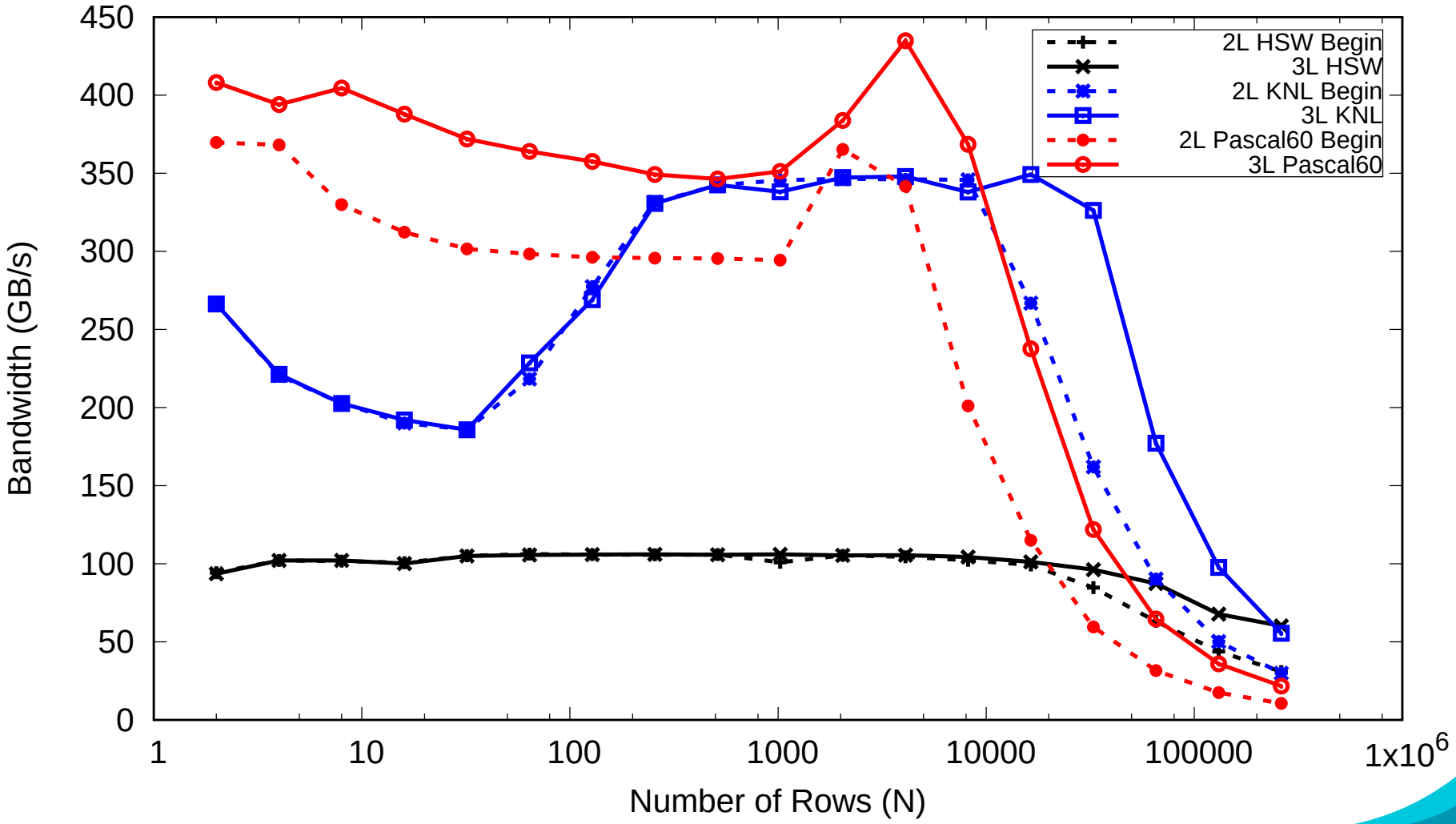
- Location: `SNL2017/Exercises/06/`
- Use the `single` policy instead of checking team rank
- Parallelize all three loop levels.

Things to try:

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

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

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



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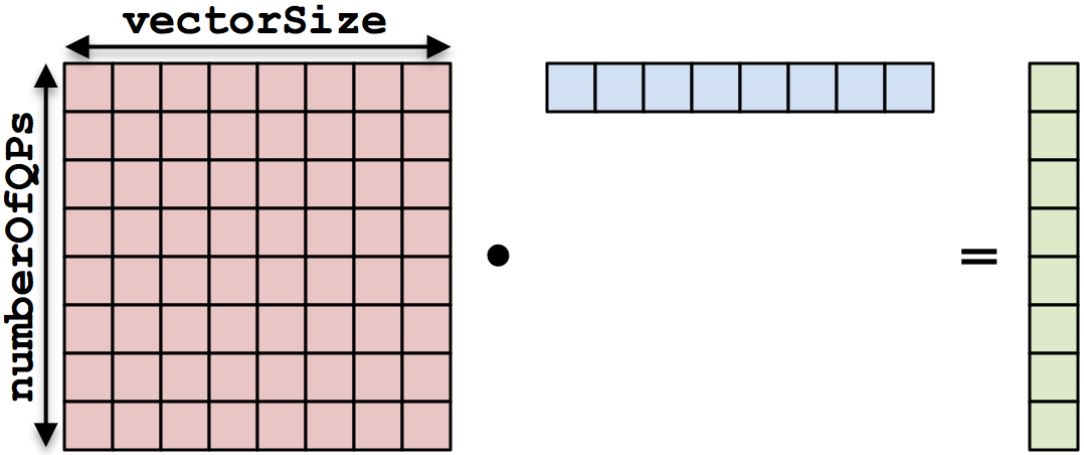
Manually Managed Cache

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

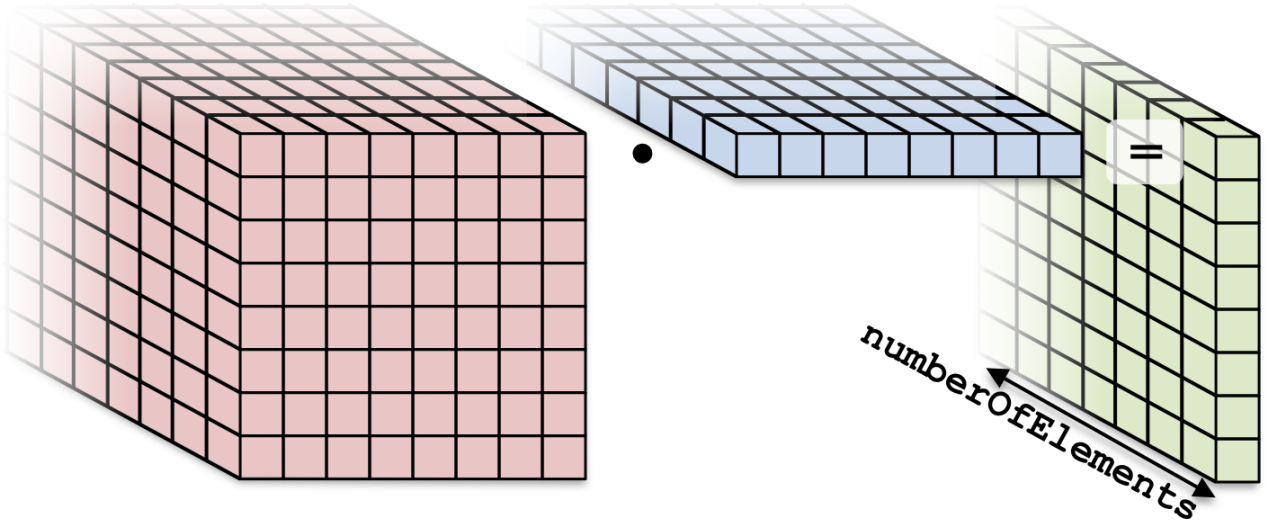
Now: Discuss Manually Managed Cache Usecase.

One slice of contractDataFieldScalar:




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

contractDataFieldScalar:




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

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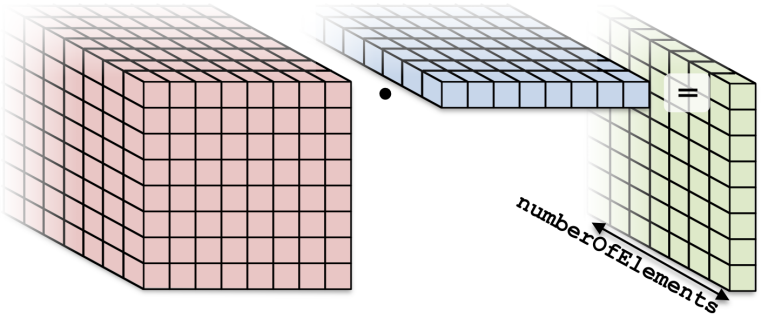
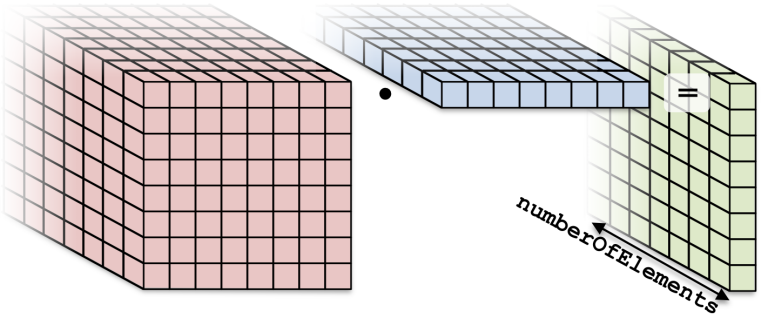



Parallelization approaches:

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

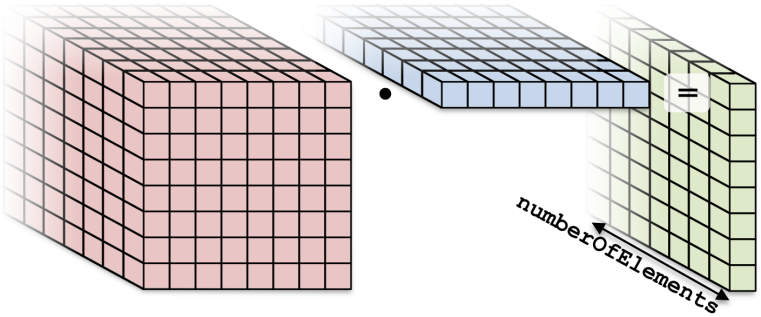
```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```



Parallelization approaches:

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

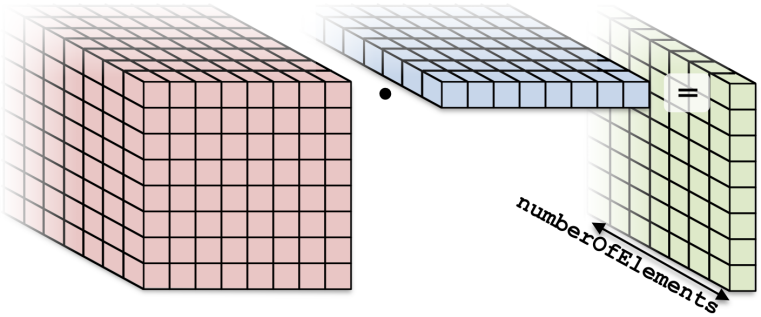
```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```



Parallelization approaches:

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

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



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

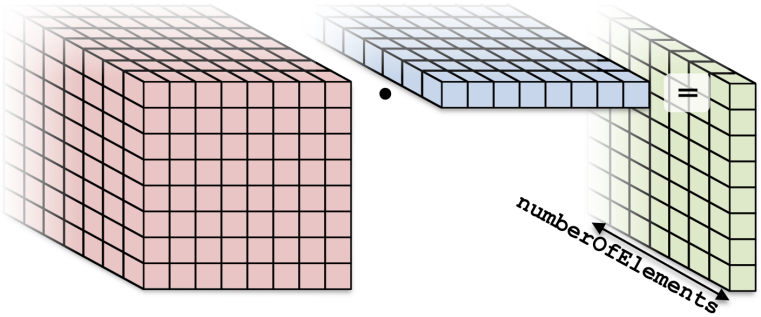

Flat kernel: Each thread handles a quadrature point

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

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

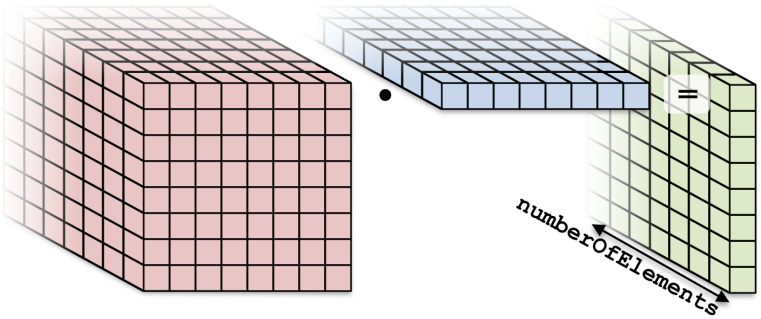

Teams kernel: Each team handles an element

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

Example: contractDataFieldScalar (6)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
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    }
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  }
}
```

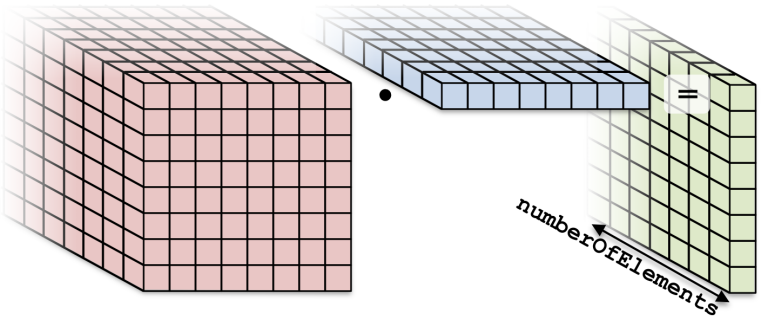

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  parallel_for(
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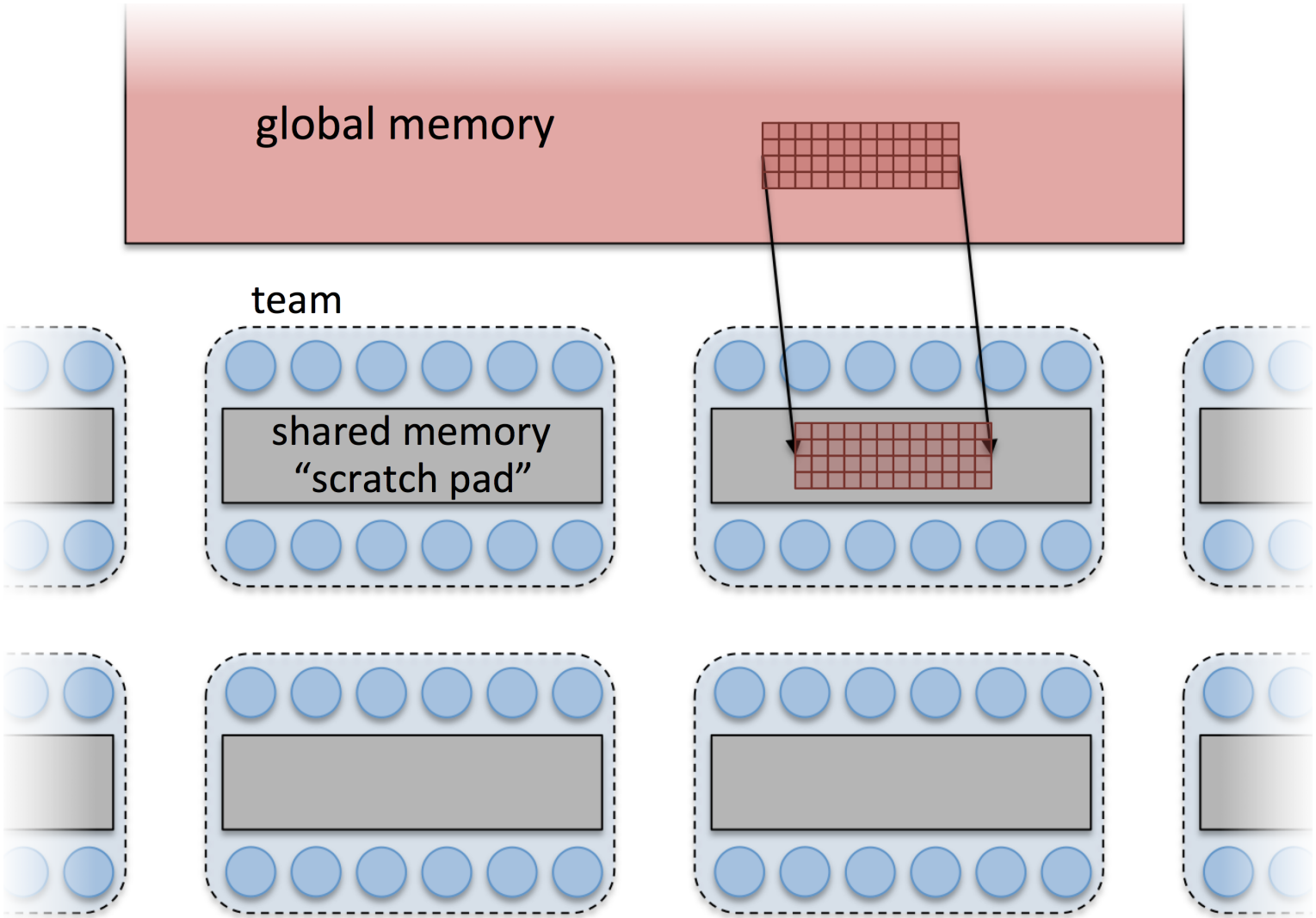
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * B(element, i);
      }
      result(element, qp) = total;
    });
}
```

No real advantage (yet)

Each team has access to a "scratch pad".



Scratch memory (scratch pad) as manual cache:

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

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Important concept

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

Scratch memory for temporary per work-item storage:

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

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- Scenario: Algorithm requires temporary workspace of size W.
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- `PerThread` and `PerTeam` scratch can be used concurrently.
- Level 0 and Level 1 scratch memory can be used concurrently.

Important concept

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

To use scratch memory, you need to:

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

To use scratch memory, you need to:

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

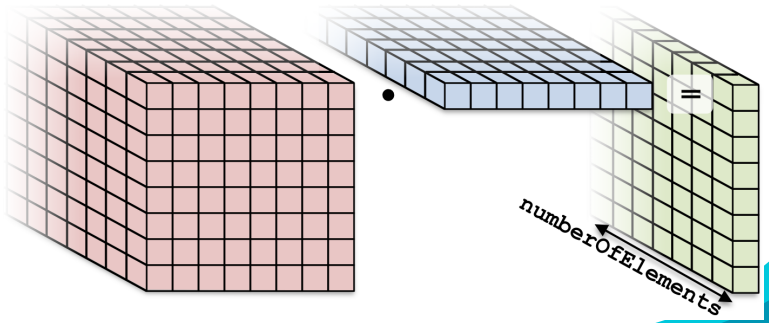
    // Create a view from the pre-existing scratch memory
    ScratchPadView scratch(teamMember.team_scratch(0),
                           vectorSize);
});
```

Kernel outline for teams with scratch memory:

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

  // TODO: load slice of B into scratch

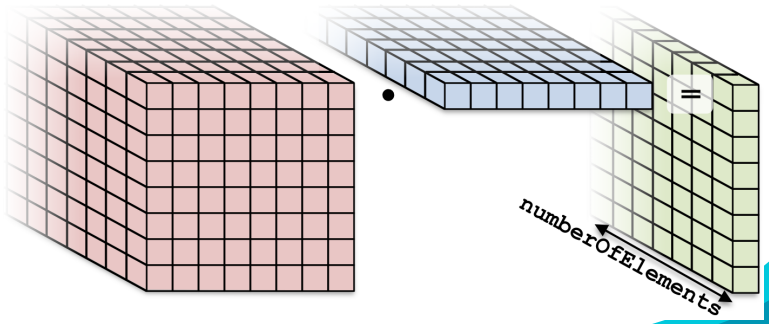
  parallel_for(
    TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * scratch(i);
      }
      result(element, qp) = total;
    });
}
```



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);
  }
}
```



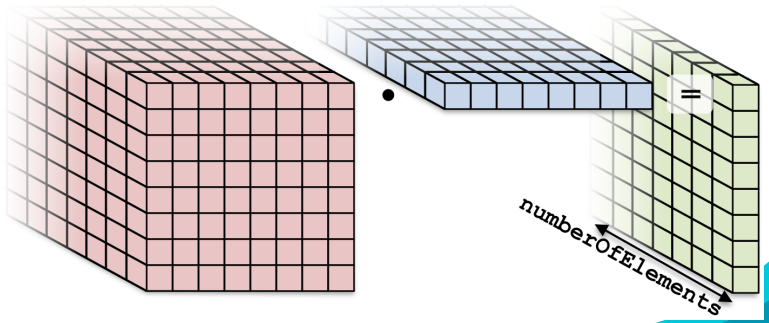
How to populate the scratch memory?

- ~~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);
```



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  }
}
```
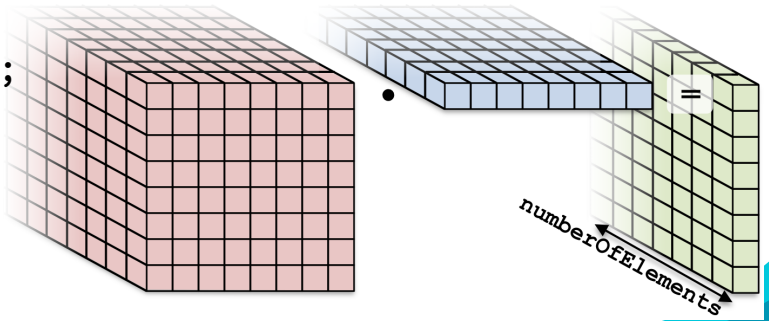

- ~~Each thread loads one entry?~~ teamSize $\neq$ vectorSize

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

- TeamThreadRange

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



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- TeamThreadRange

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  });
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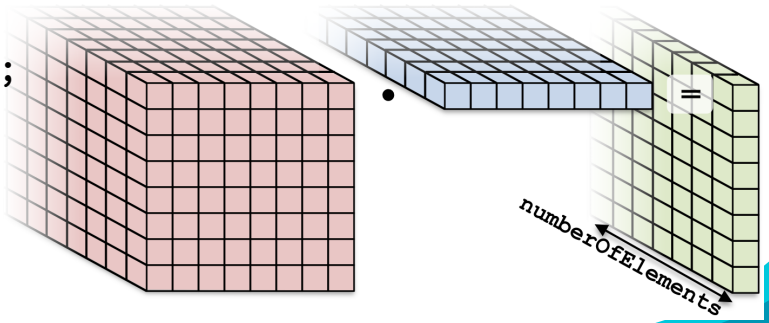

(incomplete) Kernel for teams with scratch memory:

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

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

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

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

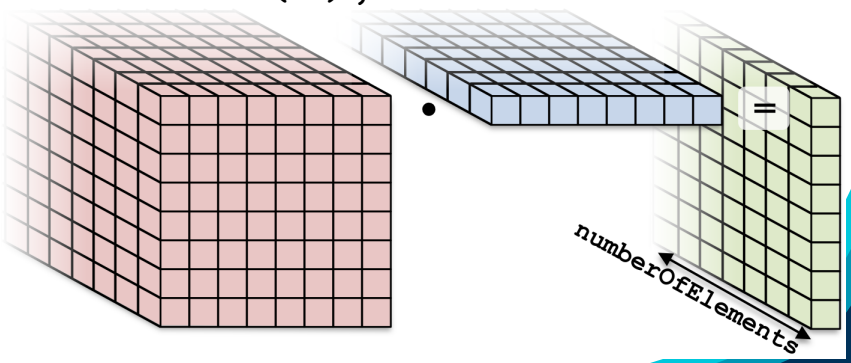
Problem: threads may start to use `scratch` before all threads are done loading.

Kernel for teams with scratch memory:

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

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

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



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

Details:

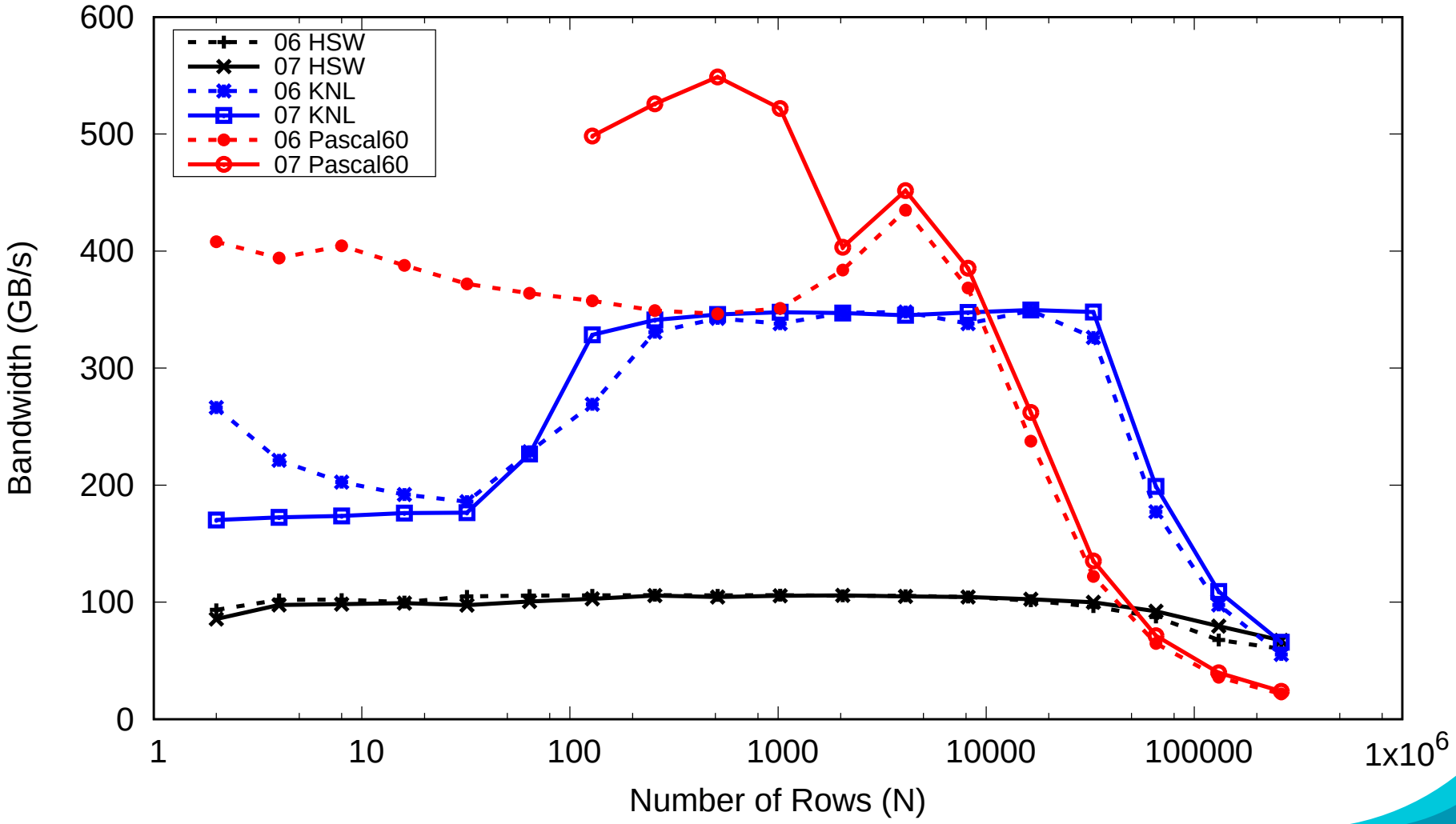
- Location: `SNL2017/Exercises/07/`
- Use the `single` policy instead of checking team rank
- Parallelize all three loop levels.

Things to try:

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

Exercise 07 (Scratch Memory) 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));
```

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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:

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policy.set_scratch_size(level,PerTeam(bytes));
```

Using PerThread, PerTeam or both:

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

Using both levels of scratch:

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

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

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

Kokkos advanced capabilities NOT covered today

- Multidimensional range policy for tightly nested loops
  similar to OpenMP loop collapse
- 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 multdimensional array data layout
  e.g., arbitrarily strided, heirarchical 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*