Kokkos Tutorial

H. Carter Edwards [1], Christian R. Trott [1], and Fernanda Foertter [2]

[1]Sandia National Laboratories

[2]Oak Ridge National Laboratory

GPU Tech Conf, May 8-11, 2017

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SAND2017-4683 C

SOFTWARE FOR LAB

Remote Desktop Software:

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

SSH Access Software (optional):

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

CONNECTION INSTRUCTIONS

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

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

Using NVIDIA's NVLABS

- Kokkos pre installed in ${HOME}/kokkos
- Exercises pre installed in ${HOME}/GTC2017

Using your own ${HOME}

- Git
- GCC 4.8.4 (or newer) *OR* Intel 14 (or newer) *OR* Clang 3.5.2 (or newer)
- CUDA nvcc 7.5 (or newer) *AND* NVIDIA compute capability 3.0 (or newer)
- clone github.com/kokkos/kokkos into ${HOME}/kokkos
- clone github.com/kokkos/kokkos-tutorials/GTC2017 into ${HOME}/GTC2017

  makefiles look for ${HOME}/kokkos

Understand Kokkos Programming Model Abstractions

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

Kokkos' basic capabilities covered today:

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

Kokkos' advanced capabilities not covered today:

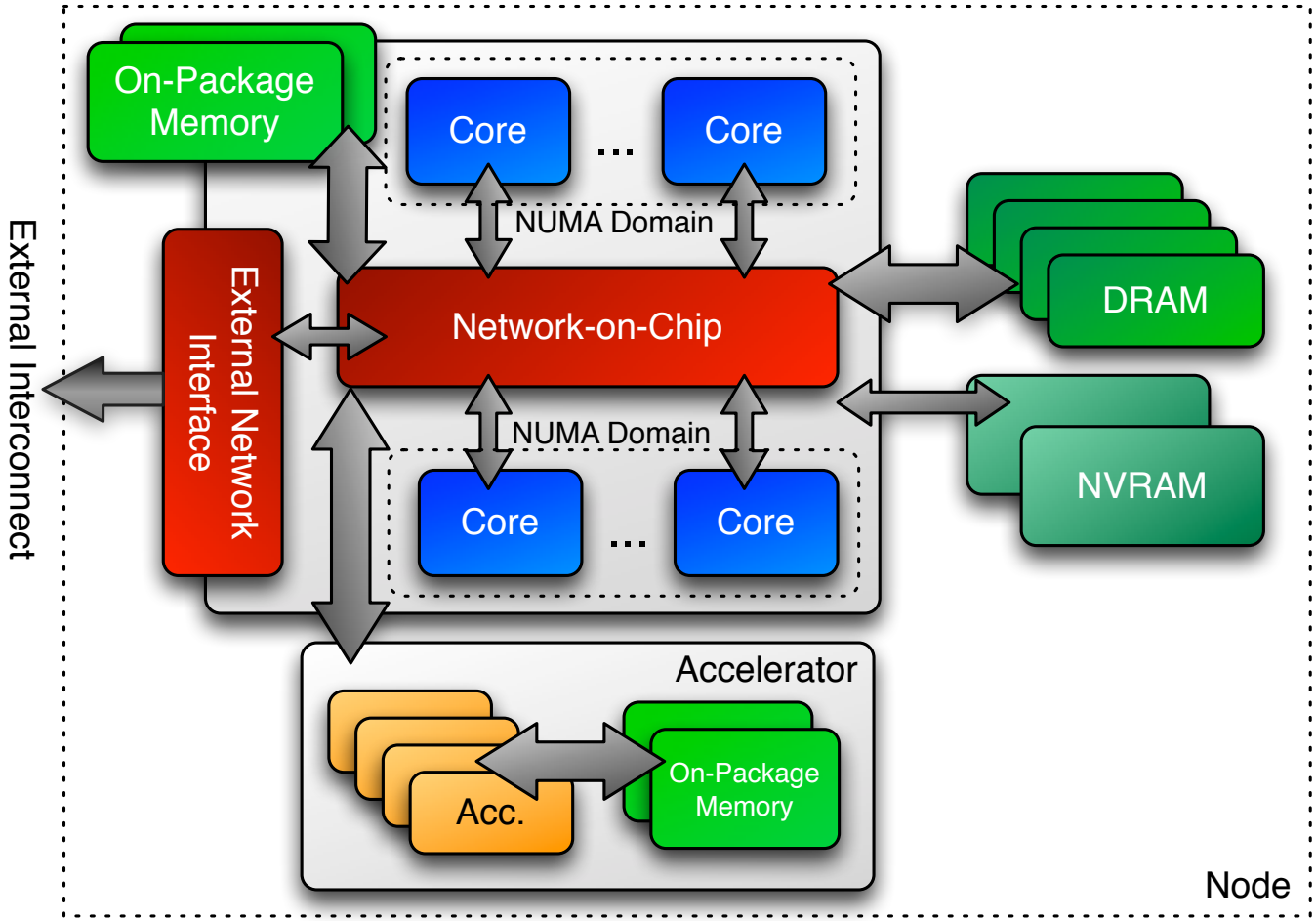
- Thread safety, thread scalability, and atomic operations
- Hierarchical patterns for maximizing parallelism
- Dynamic directed acyclic graph of tasks pattern
- Numerous *pluggin* points for extensibility

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

Target machine:



Important Point

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

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

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

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Goal: write **one implementation** which:

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

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Goal: write **one implementation** which:

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

Kokkos: performance portability across manycore architectures.

Concepts for threaded data parallelism

Learning objectives:

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

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

Pattern 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?

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

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

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

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

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

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

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

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

Option 1: OpenMP 4.0

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

Option 1: OpenMP 4.0

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

Option 2: OpenACC

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

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

But what about performance?

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

But what about performance?

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

Problem: memory access pattern

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

Problem: memory access pattern

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

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    }
  }
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}
```

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

Important Point

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

How does Kokkos address performance portability?

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

- is a C++ **library**, not a new language or language extension.
- supports **clear, concise, thread-scalable** parallel patterns.
- lets you write algorithms once and run on **many architectures**
  e.g. multi-core CPU, NVidia 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

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

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.

Data parallel patterns and work

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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.

Important concept: Work mapping

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

How are computational bodies given to Kokkos?

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

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

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

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

How is work assigned to functor operators?

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

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

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

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

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ParallelFunctor functor;
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and work items are assigned to functors one-by-one:

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

Warning: concurrency and order

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

How is data passed to computational bodies?

```
for (atomIndex = 0; atomIndex < 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?

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

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

How does the body access the data?

Important concept

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

Putting it all together: the complete functor:

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

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

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

Serial

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

Putting it all together: the complete functor:

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struct AtomForceFunctor {
  ForceType _atomForces;
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  void operator()(const size_t atomIndex) const {
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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);
  }
);
```

Functors are tedious $\Rightarrow$ **C++11 Lambdas** are concise

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data already exists
Kokkos::parallel_for(numberOfAtoms,
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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

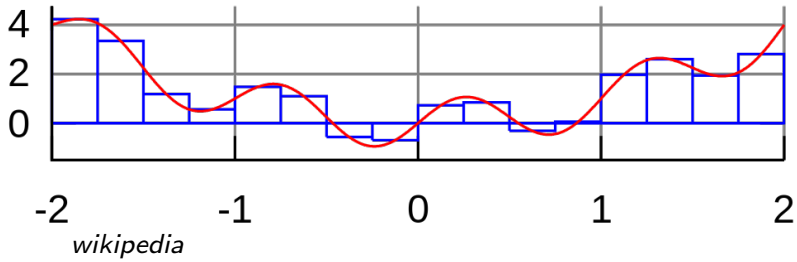
```
parallel_for(N, [=] (const size_t i) {
  /* loop body */
});
```

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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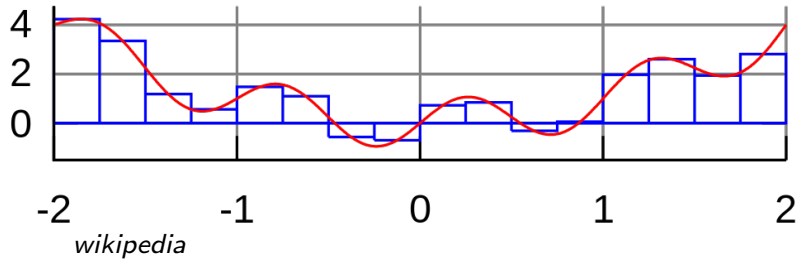


```
double totalIntegral = 0;
for (size_t i = 0; i < numberOfIntervals; ++i) {
  const double x =
    lower + (i/numberOfIntervals) * (upper - lower);
  const double thisIntervalsContribution = function(x);
  totalIntegral += thisIntervalsContribution;
}
totalIntegral *= dx;
```

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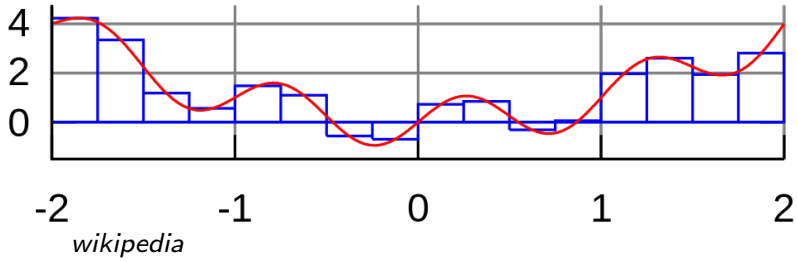


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totalIntegral *= dx;
```

How would we **parallelize** it?

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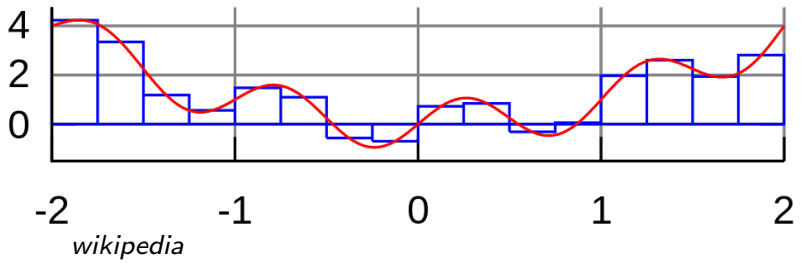

Pattern?

Policy?

Body?

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

How would we **parallelize** it?

An (incorrect) attempt:

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

First problem: compiler error; cannot increment `totalIntegral`
(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;
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    *totalIntegralPointer += function(x);},
  );
totalIntegral *= dx;
```

Second problem: race condition

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

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

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Important concept: Reduction

Reductions combine the results contributed by parallel work.

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Reductions combine the results contributed by parallel work.

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

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

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

Important concept: Reduction

Reductions combine the results contributed by parallel work.

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

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

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

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

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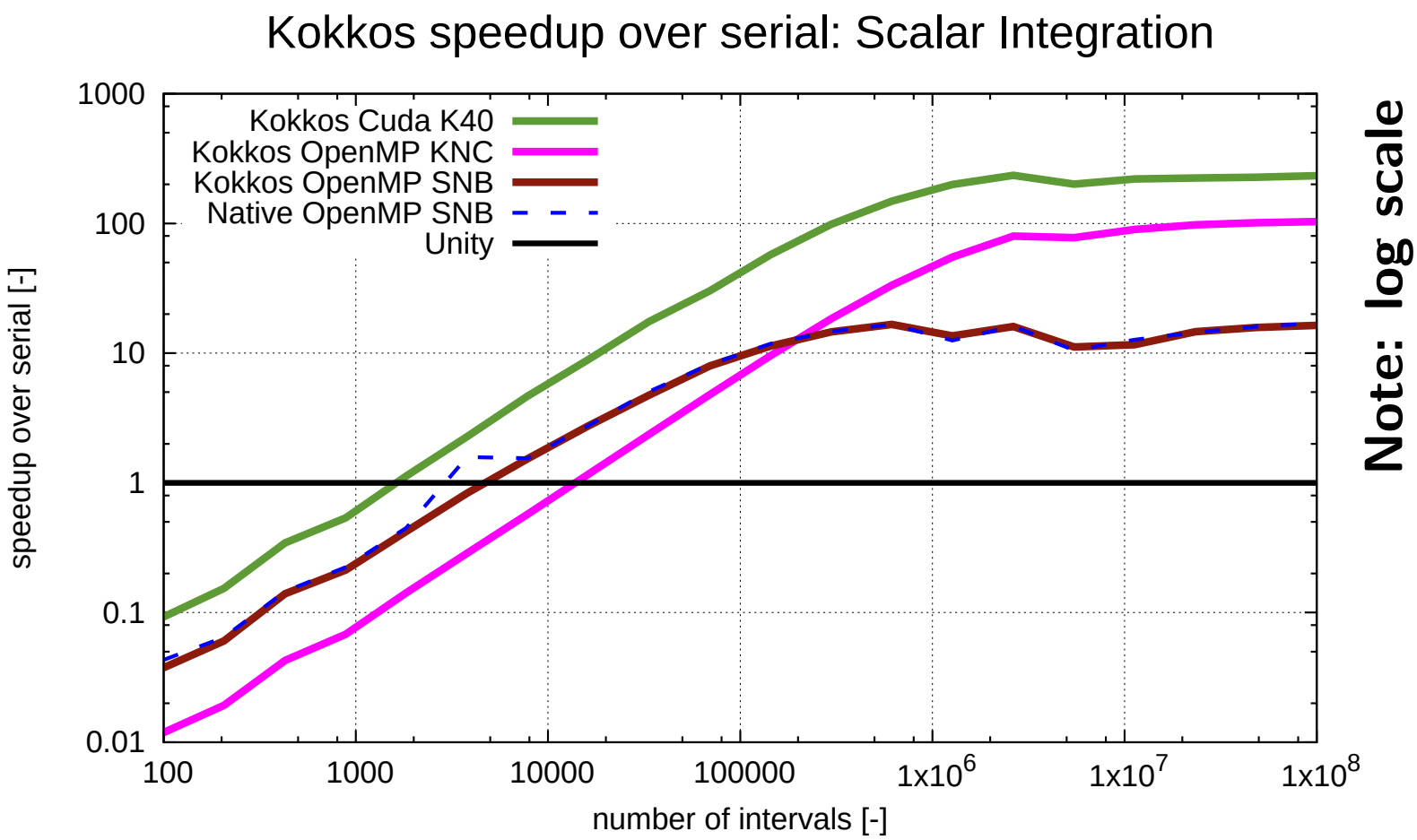
- $\alpha =$ dispatch overhead
- $\beta =$ time for a unit of work
- $N =$ number of units of work
- $P =$ available concurrency

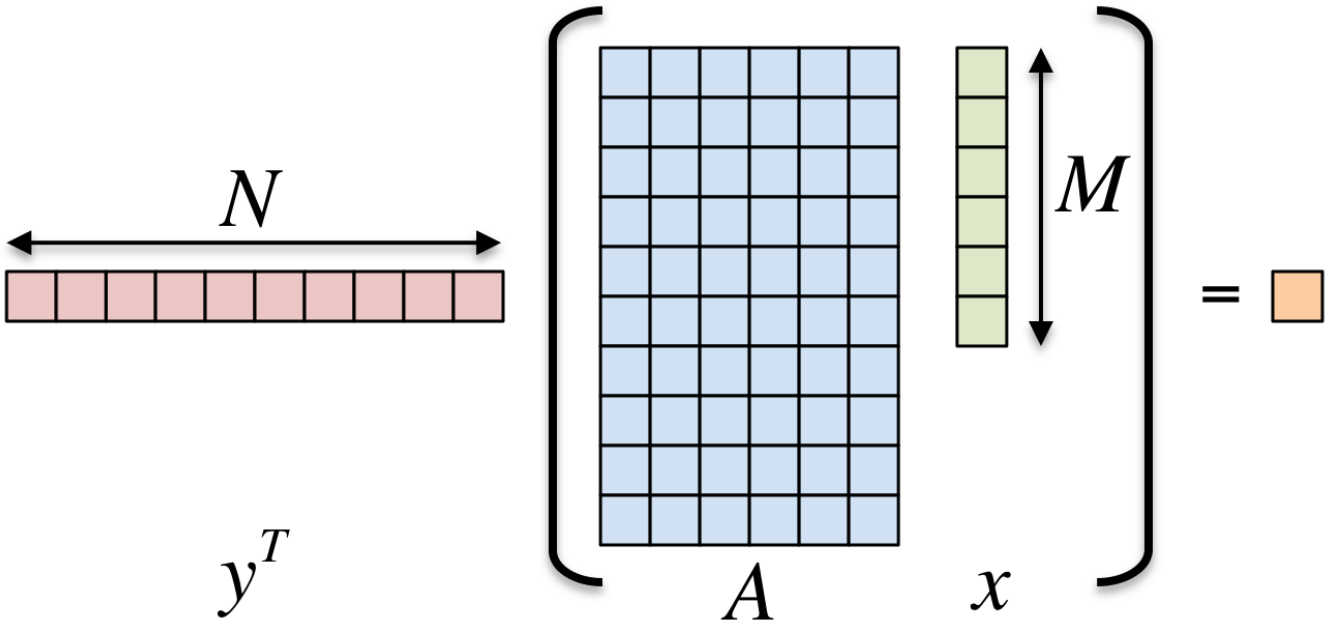
Speedup $= P \div \left(1 + \frac{\alpha * P}{\beta * N}\right)$

- 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

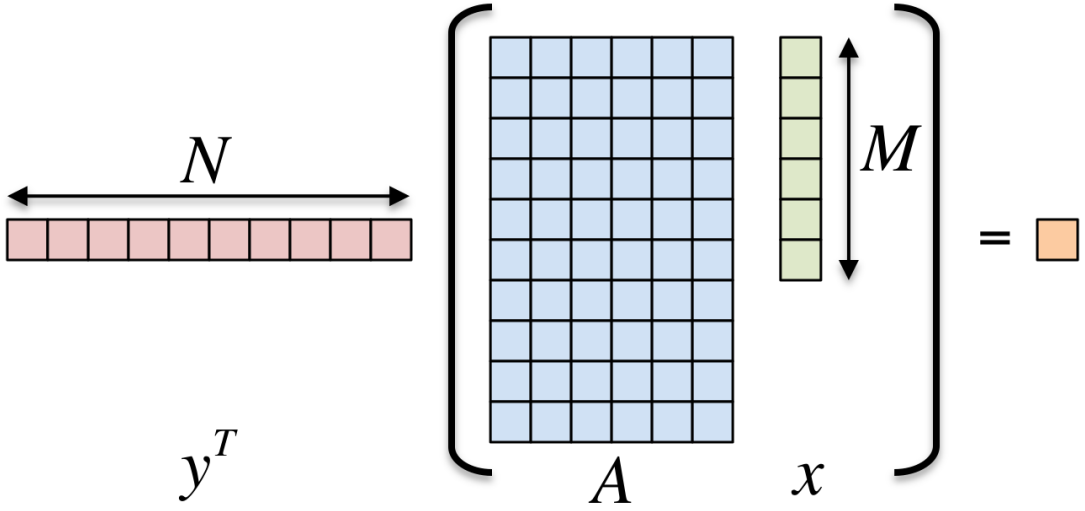
The **first step** in using Kokkos is to include, initialize, and finalize:

```
#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: `~/GTC2017/Exercises/01/`
- Look for comments labeled with "EXERCISE"
- Need to include, initialize, and finalize Kokkos library
- Parallelize loops with `parallel_for` or `parallel_reduce`
- Use lambdas instead of functors for computational bodies.
- For now, this will only use the CPU.

Compiling for CPU

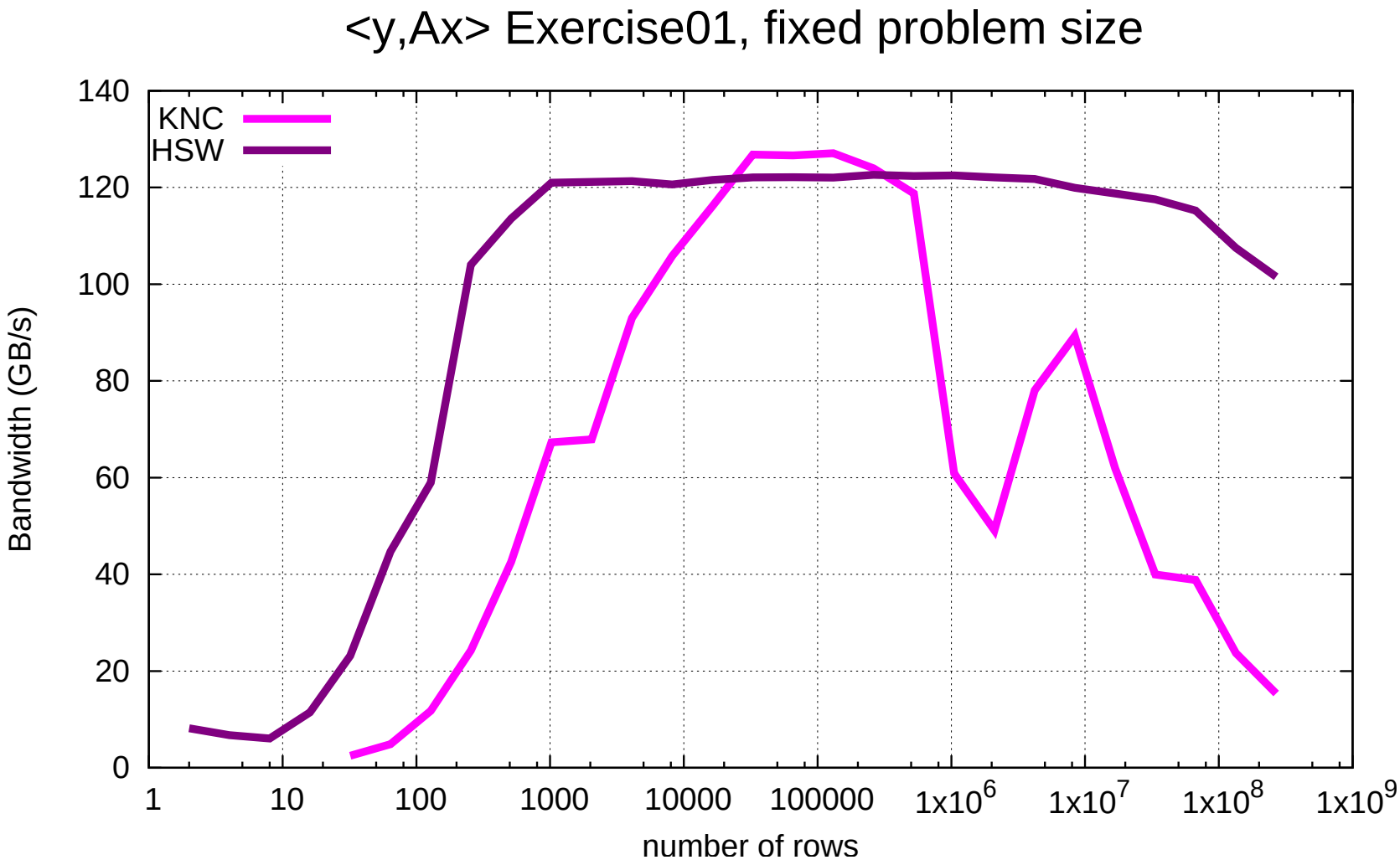
```
cd ~/GTC2017/Exercises/01/Begin
# gcc using OpenMP (default) and Serial back-ends
make -j [KOKKOS_DEVICES=OpenMP,Serial]
```

Running on CPU with OpenMP back-end

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

Things to try:

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


<y,Ax> Exercise01, fixed problem size
KNC
HSW
Bandwidth (GB/s)
0
20
40
60
80
100
120
140
1
10
100
1000
10000
100000
1x10^6
1x10^7
1x10^8
1x10^9
number of rows

Basic capabilities we haven't covered

- 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 {
  double *_x, *_y, a;
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    _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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- Arrays are **rectangular**, not ragged.
- **Sizes of dimensions** set at compile-time or runtime.
  e.g., 2x20, 50x50, etc.

Example:

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

Note: runtime-sized dimensions must come first.

View life cycle:

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

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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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print a(0)
```

What gets printed?

3.0

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

- Location: `~/GTC2017/Exercises/02/`
- Assignment: Change data storage from arrays to Views.
- Compile and run on CPU, and then on GPU with UVM

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

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

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

Execution and Memory Spaces

Learning objectives:

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

Thought experiment: Consider this code:

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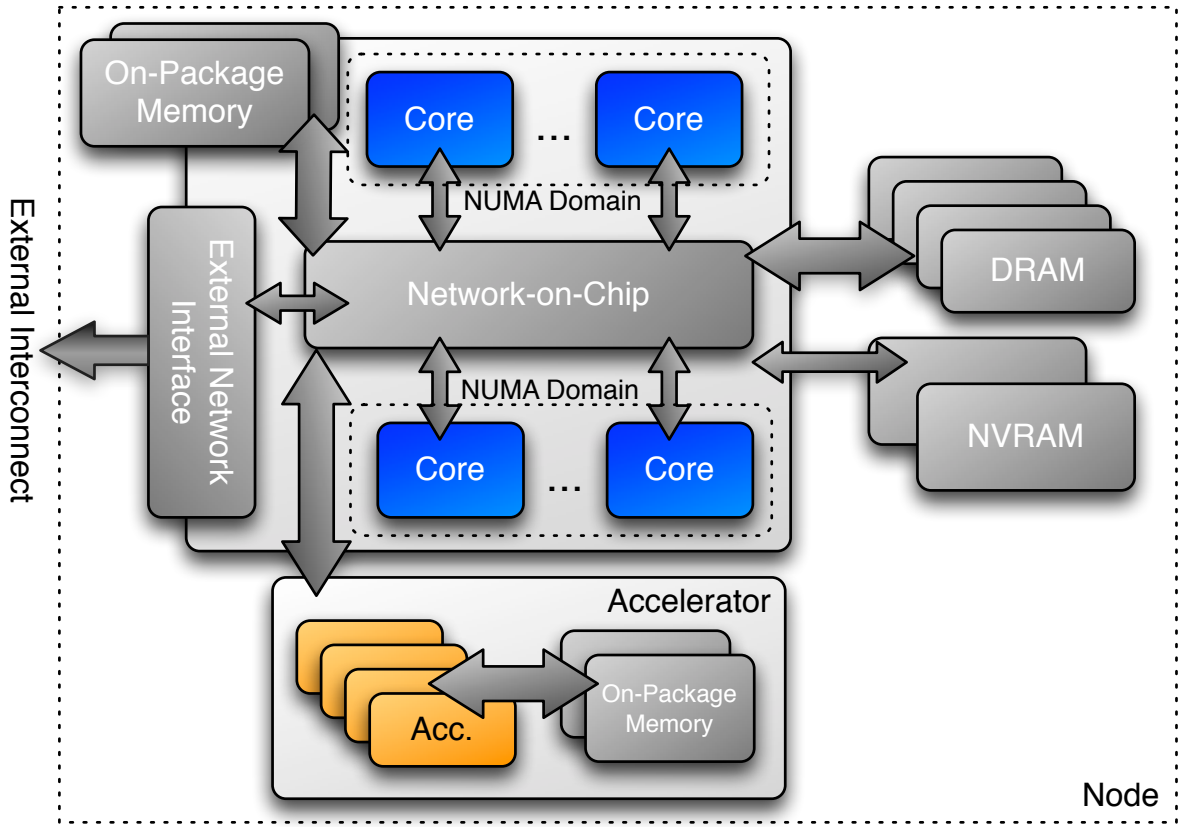
```
section 2
```
Kokkos::parallel_for(numberOfSomethings,
                     [=] (const size_t somethingIndex) {
                       const double y = ...;
                       // do something interesting
                     }
                     );
```

- 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(...);
runANormalFunction(...data...);
```

Parallel

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

- Where will Host code be run? CPU? GPU?
  $\Rightarrow$ Always in the **host process**

Host

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

Parallel

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Kokkos::parallel_for(numberOfSomethings,
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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(...);
FILE * file = fopen(...);
runANormalFunction(...data...);
```
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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**
- 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

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

Requirements for enabling execution spaces:

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

Kokkos function and lambda portability annotation macros:

Function annotation with `KOKKOS_INLINE_FUNCTION` macro

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

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#define KOKKOS_INLINE_FUNCTION inline __device__ __host__ /* #if CPU+Cuda */
```

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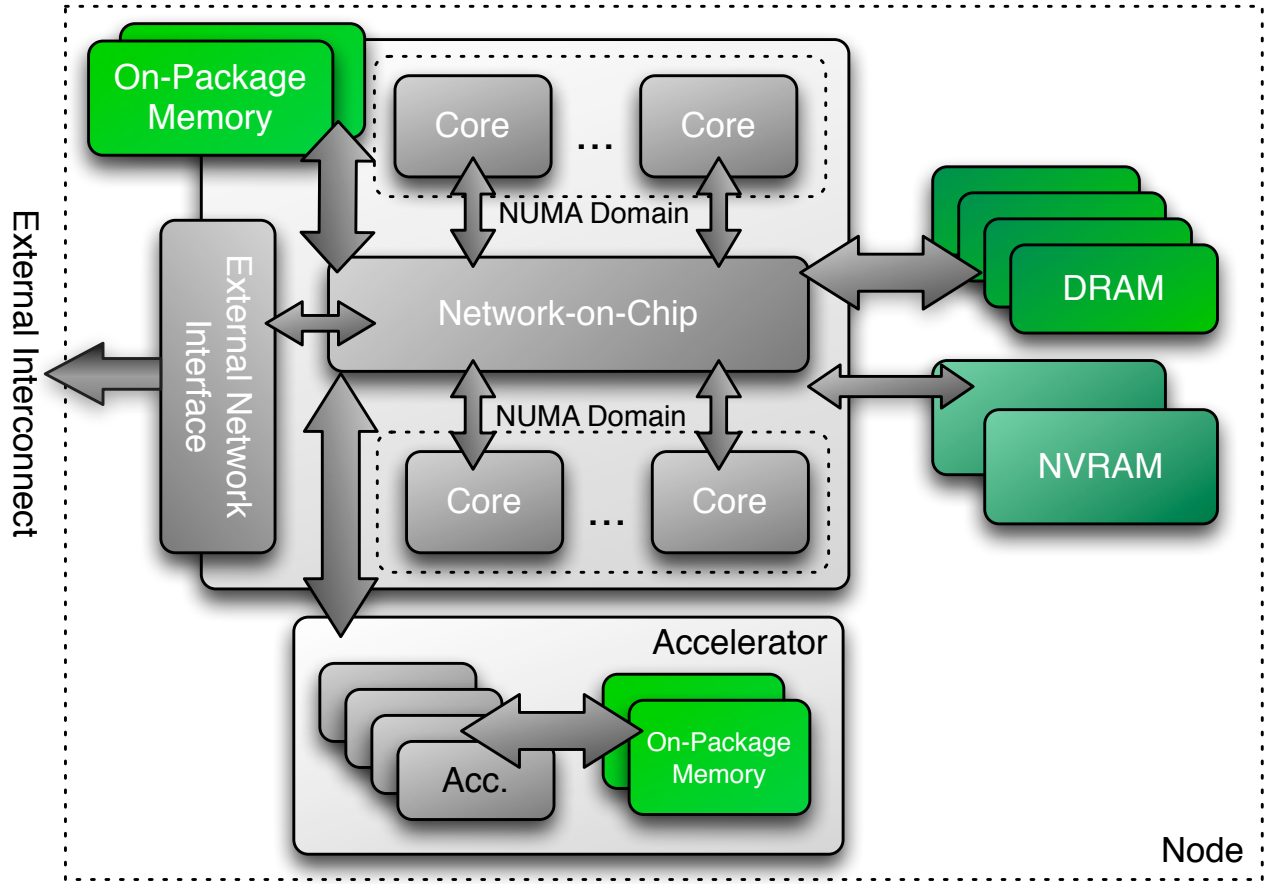
Question: Where is the data stored? GPU memory? CPU memory? Both?

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

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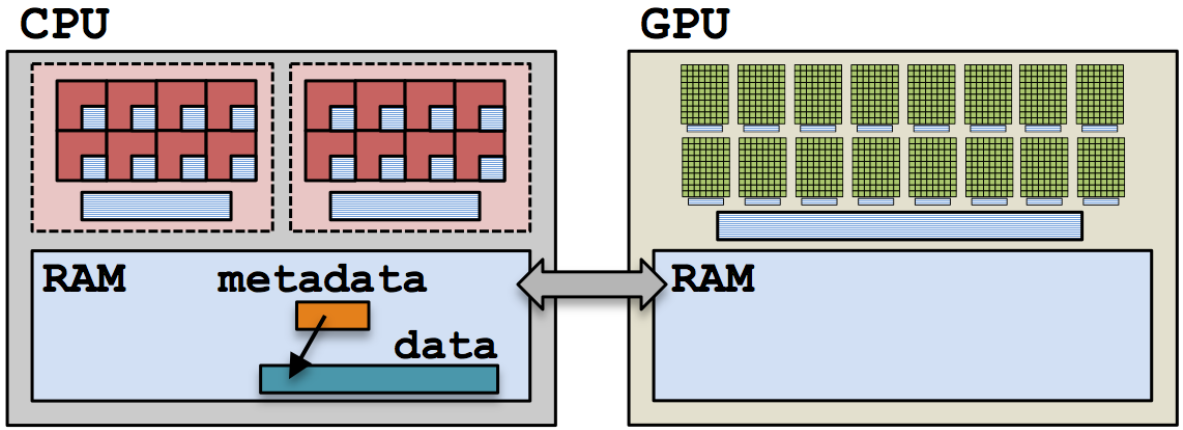
- `View<double***,`*Memory***Space**`> data(...);`
- Available **memory spaces**:

  `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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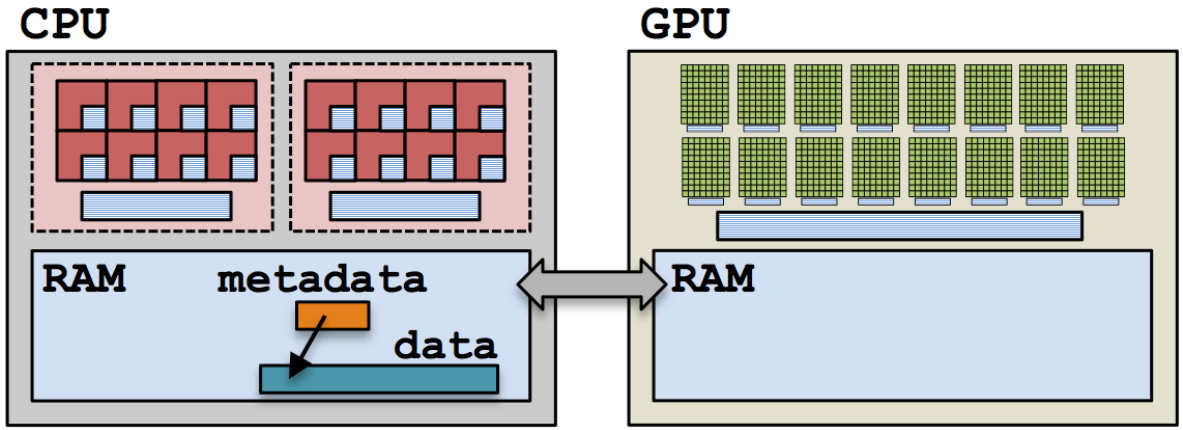
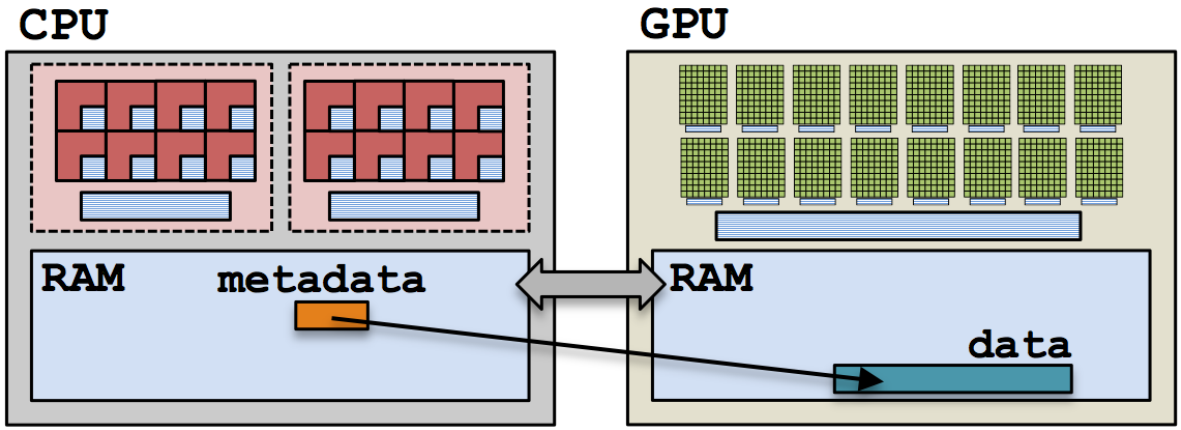


Example: CudaSpace

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



Anatomy of a kernel launch:

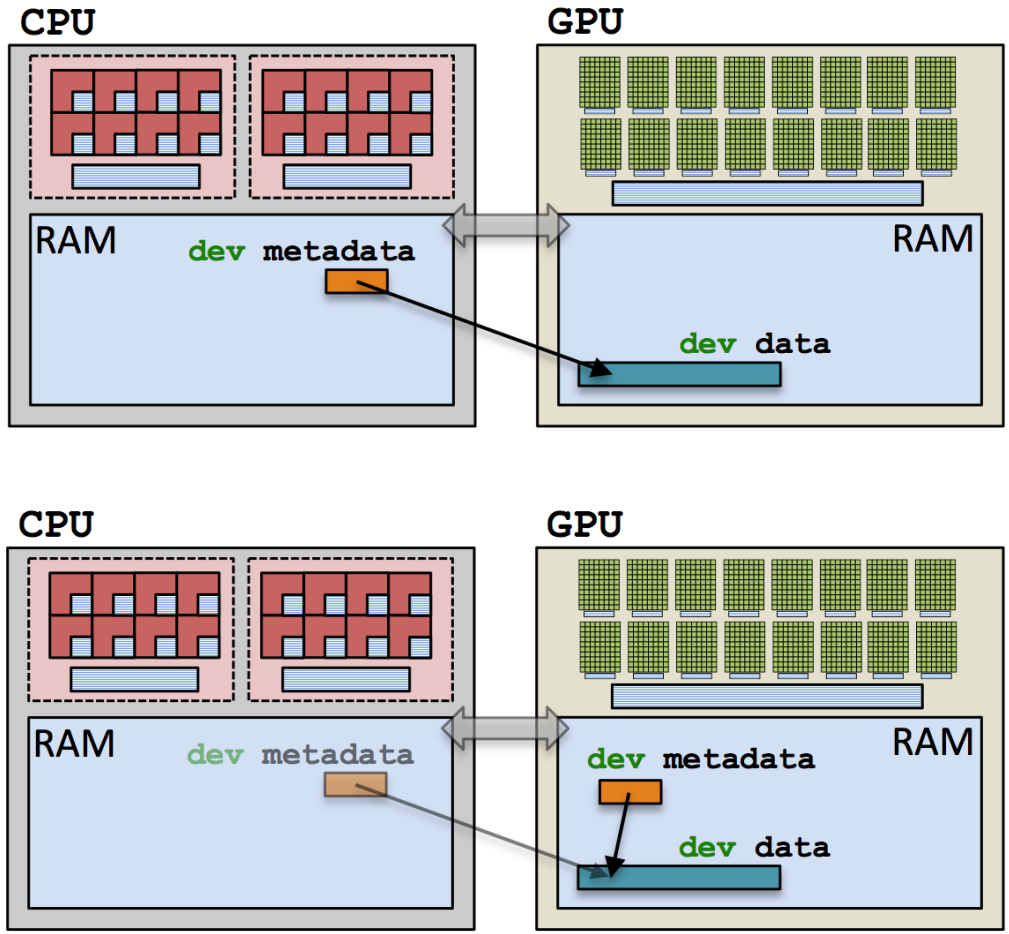
1. User declares views, allocating.
2. User instantiates a functor with views.
3. User launches `parallel_something`:
   - Functor is copied to the device.
   - Kernel is run.
   - Copy of functor on the device is released.

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

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

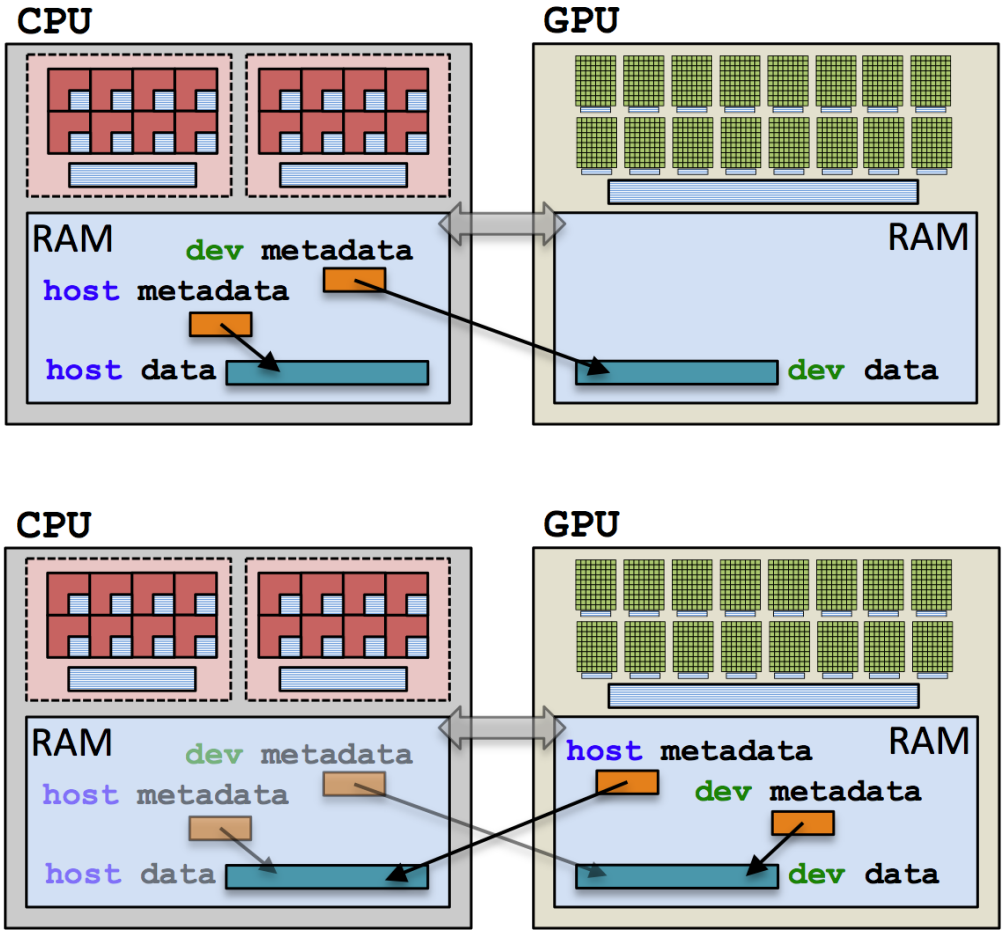
Example: one view

```
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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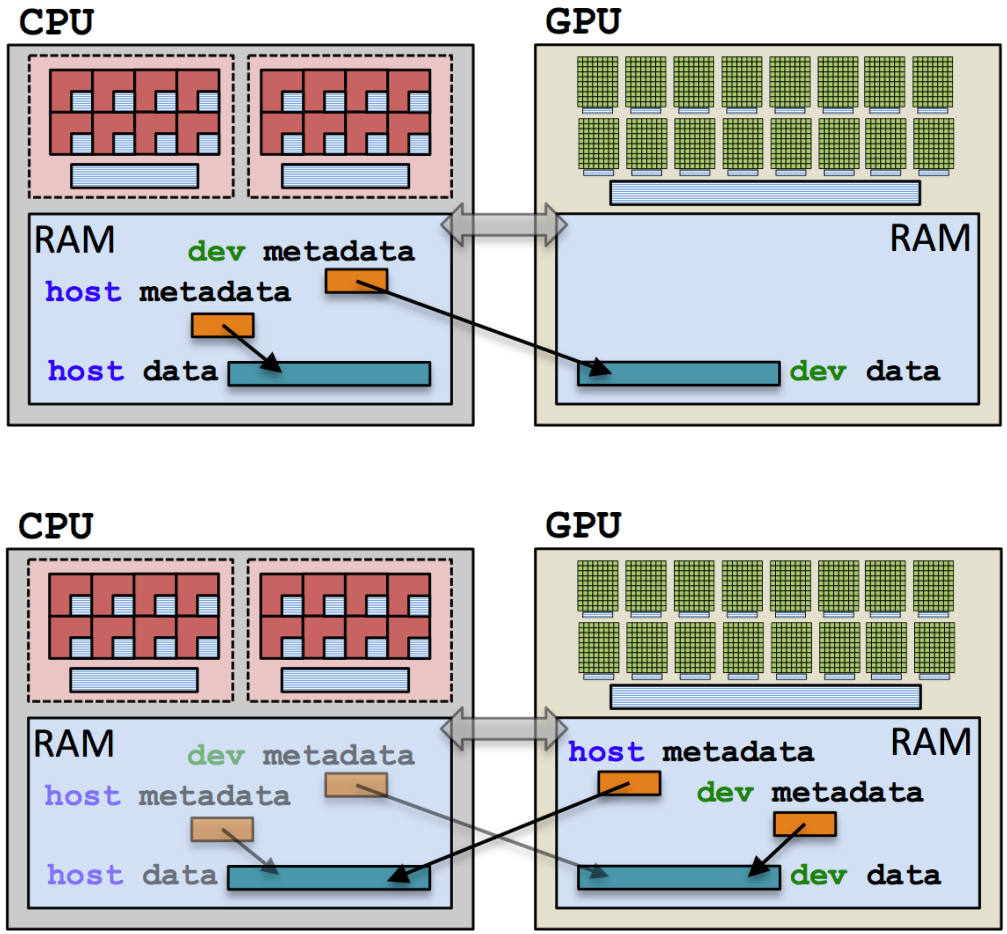
  });
```



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),
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Example (redux): summing an array with the GPU

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}

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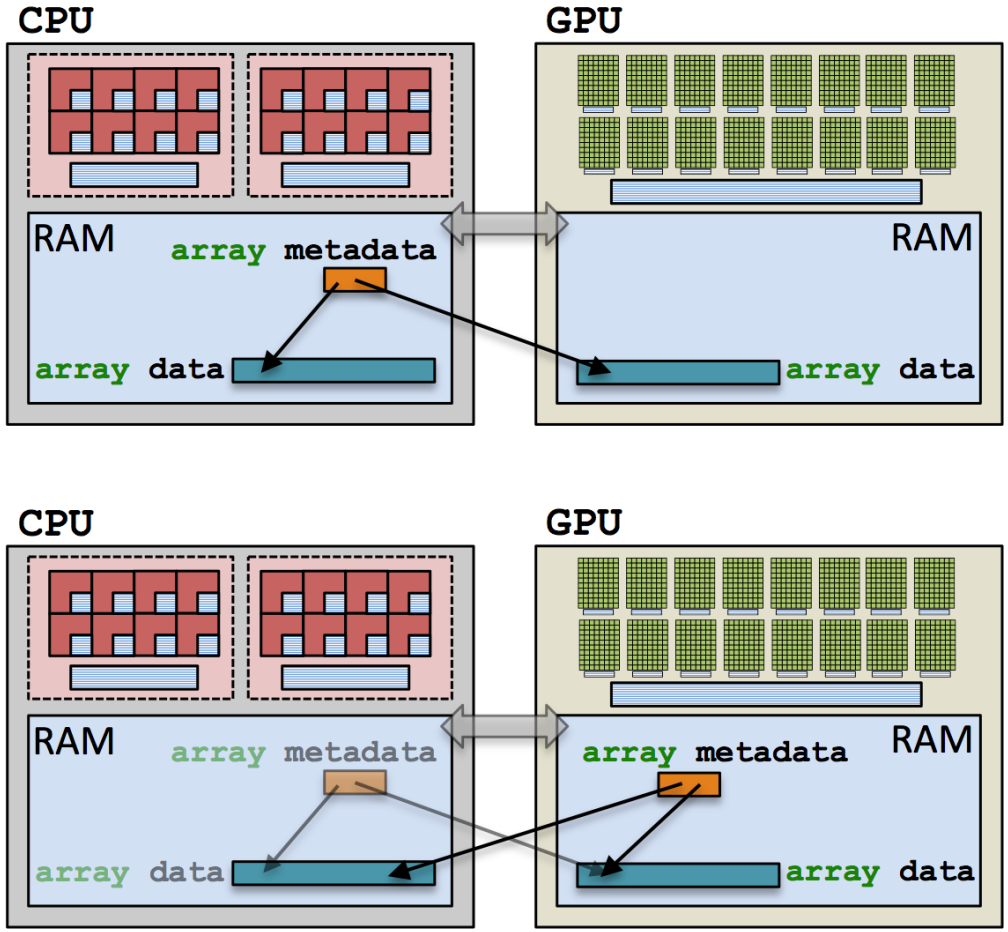
```

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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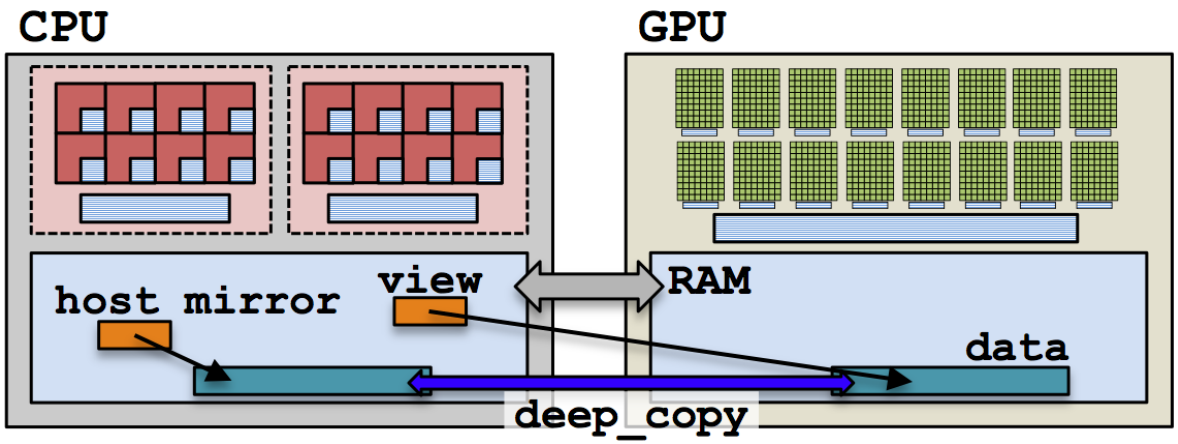
Mirroring schematic

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



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  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: `~/GTC2017/Exercises/03/`
- Add HostMirror Views and deep copy
- Make sure you use the correct view in initialization and Kernel

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

Things to try:

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

View and Spaces Section Summary

- 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.

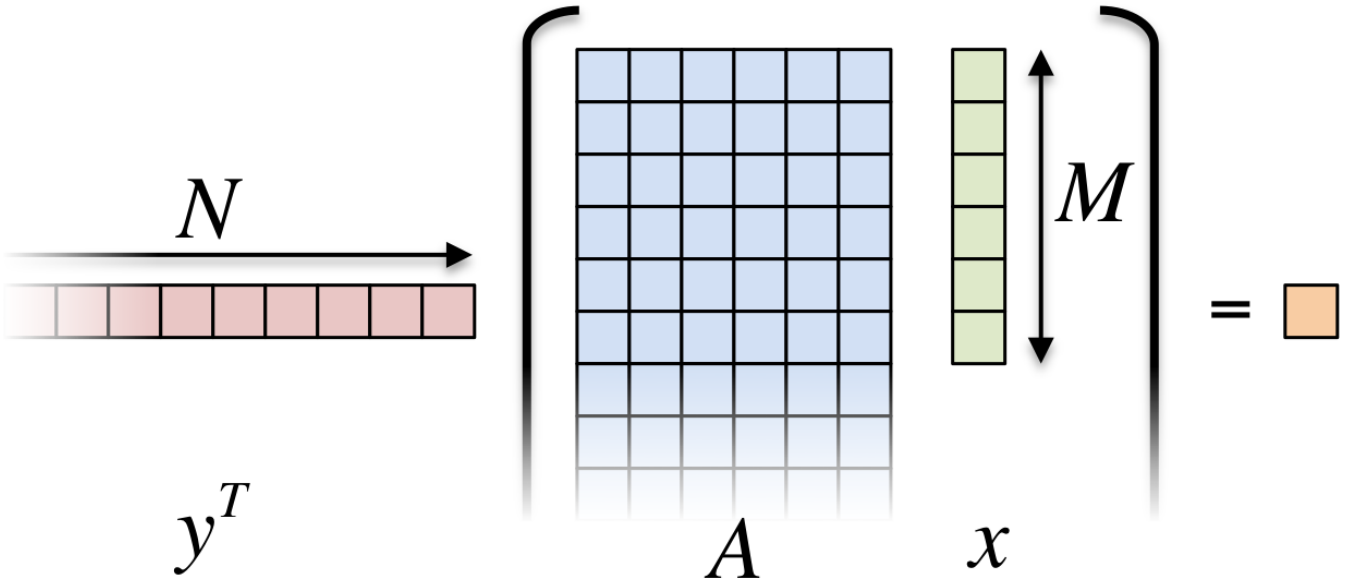
Managing memory access patterns for performance portability

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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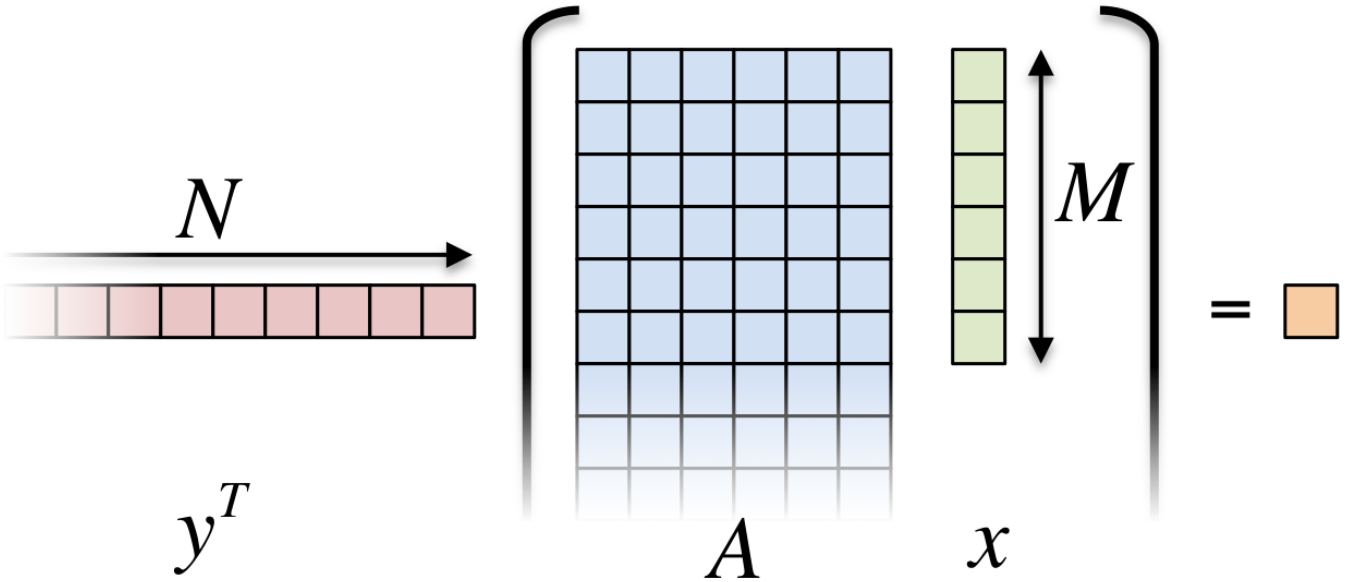
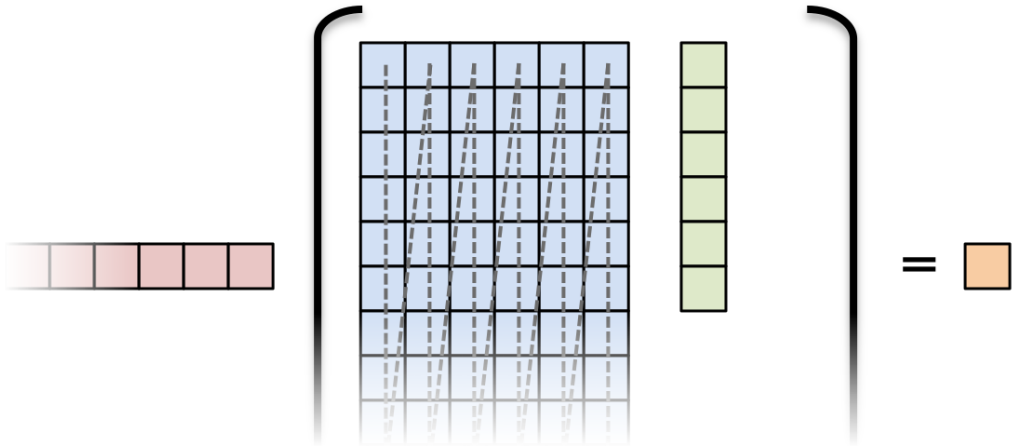


Driving question: How should A be laid out in memory?

Layout is the mapping of multi-index to memory:

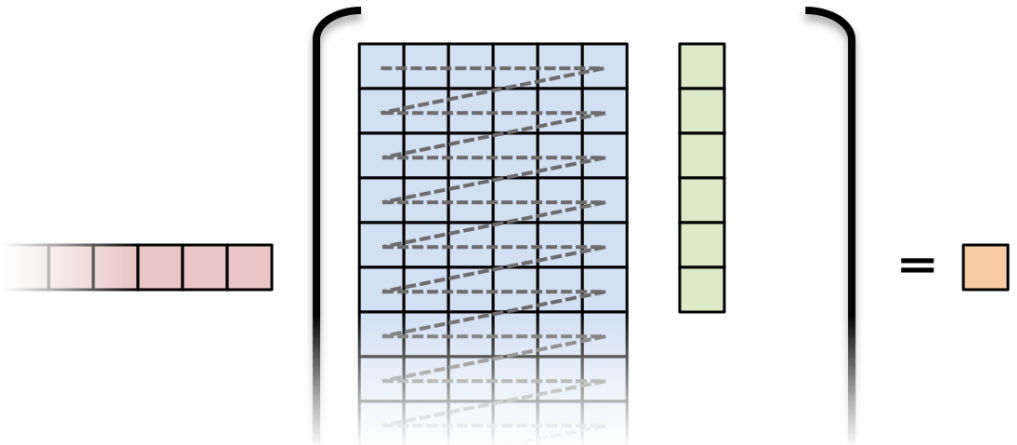
LayoutLeft

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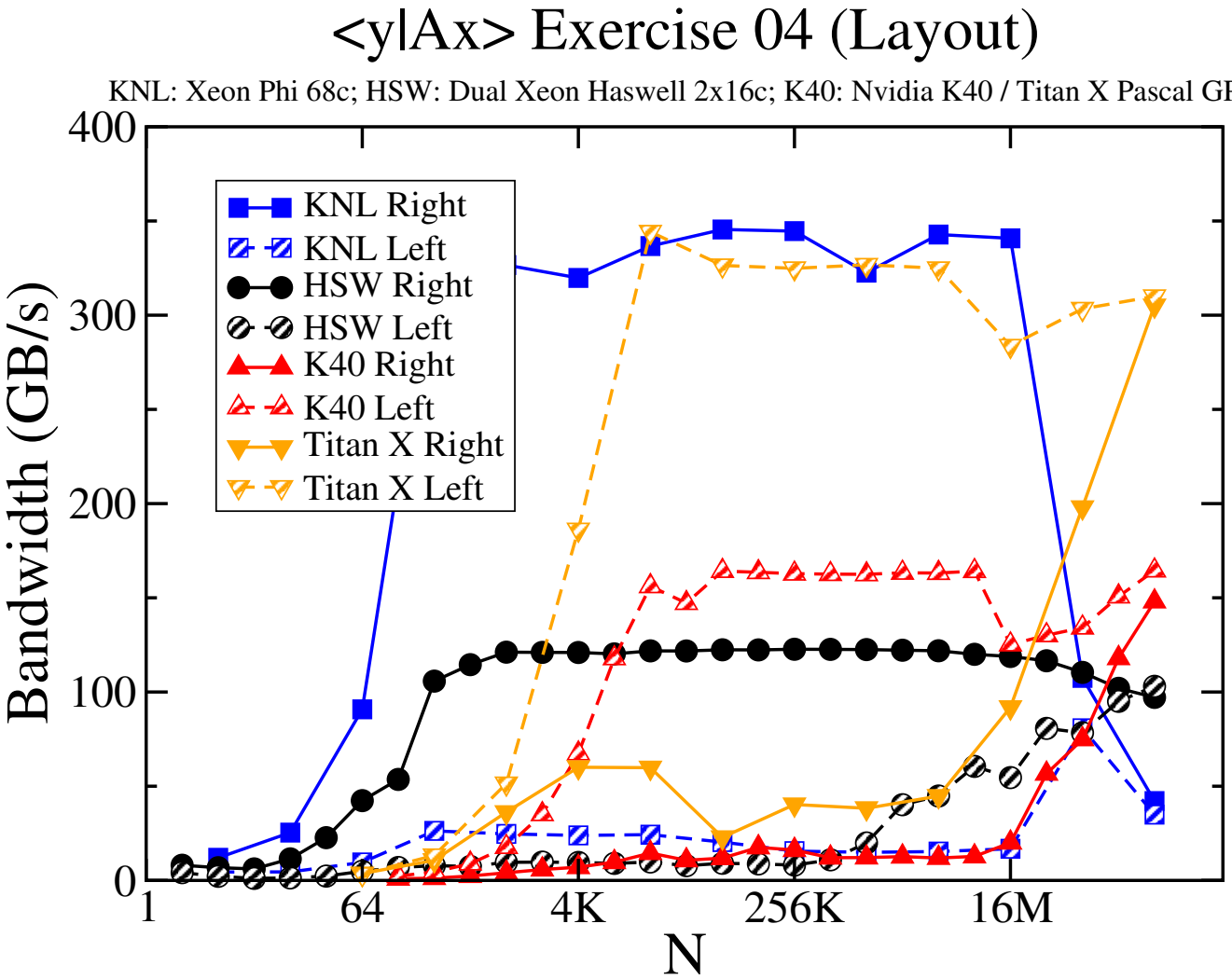
- Most-common layouts are `LayoutLeft` and `LayoutRight`.
  `LayoutLeft`: left-most index is stride 1.
  `LayoutRight`: right-most index is stride 1.
- If no layout specified, default for that memory space is used.
  `LayoutLeft` for `CudaSpace`, `LayoutRight` for `HostSpace`.
- Layouts are extensible: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

Details:

- Location: `~/GTC2017/Exercises/04/`
- Replace ‘‘`N`’’ in parallel dispatch with `RangePolicy<ExecSpace>`
- Add `MemSpace` to all `Views` and `Layout` to `A`
- Experiment with the combinations of `ExecSpace`, `Layout` to view performance

Things to try:

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


<y|Ax> Exercise 04 (Layout)
KNL: Xeon Phi 68c; HSW: Dual Xeon Haswell 2x16c; K40: Nvidia K40 / Titan X Pascal GPU
Bandwidth (GB/s)
400
300
200
100
0
1
64
4K
256K
16M
N
KNL Right
KNL Left
HSW Right
HSW Left
K40 Right
K40 Left
Titan X Right
Titan X Left

Why?

Thread independence:

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

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

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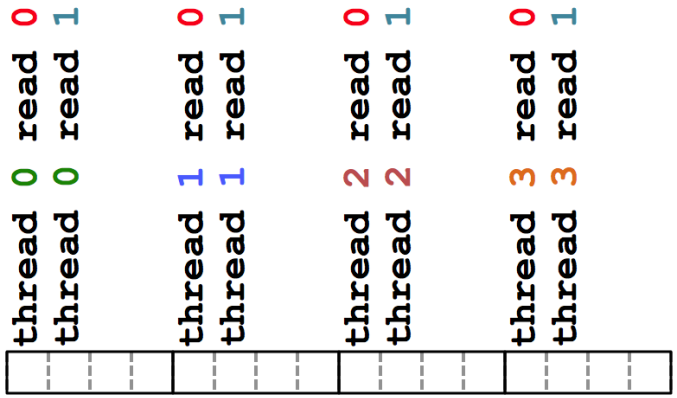
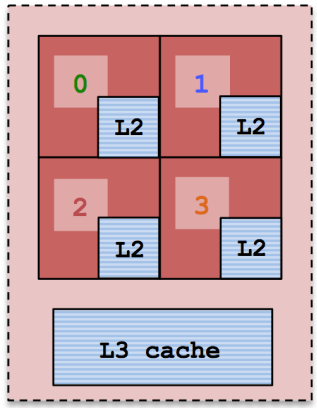
In particular, all threads in a group (*warp*) must finished their loads before *any* thread can move on.

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

CPUs: few (independent) cores with separate caches:





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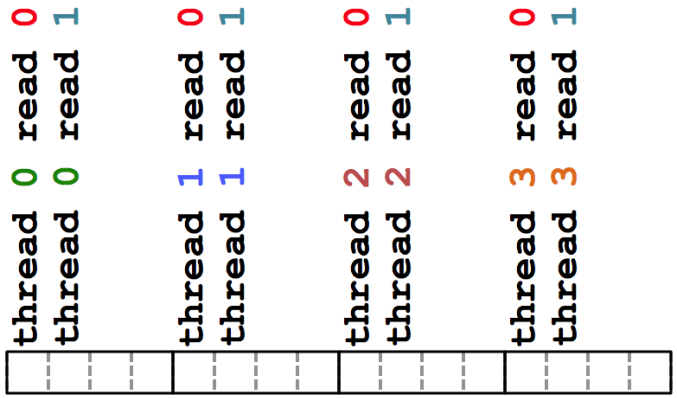
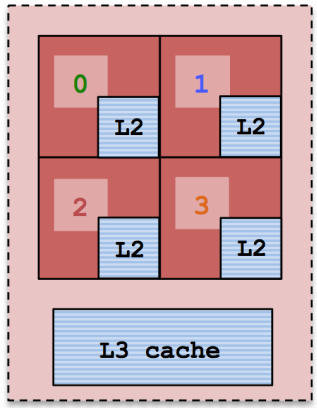
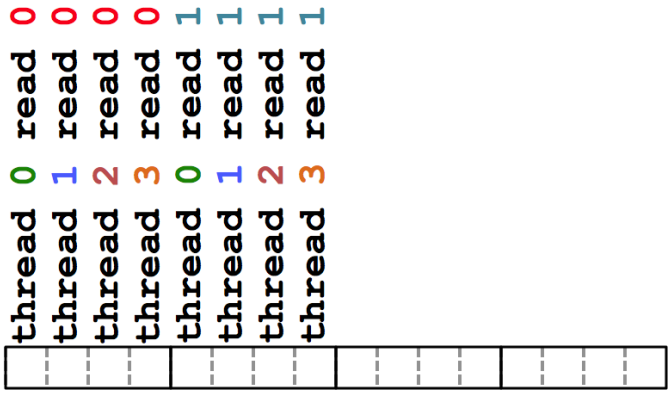
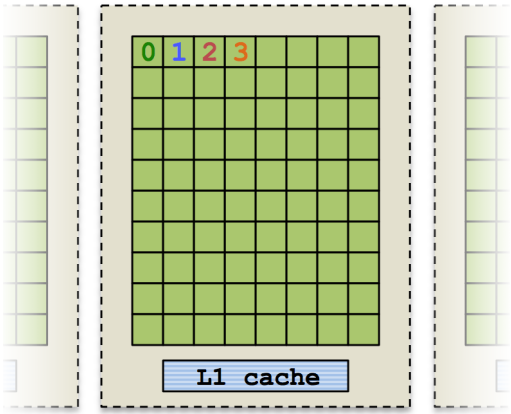




GPUs: many (synchronized) cores with a shared cache:





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

Consider the array summation example:

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

double sum = 0;
Kokkos::parallel_reduce(
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Question: is this cached (for `OpenMP`) and coalesced (for `Cuda`)?

Mapping indices to cores (0)

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

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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`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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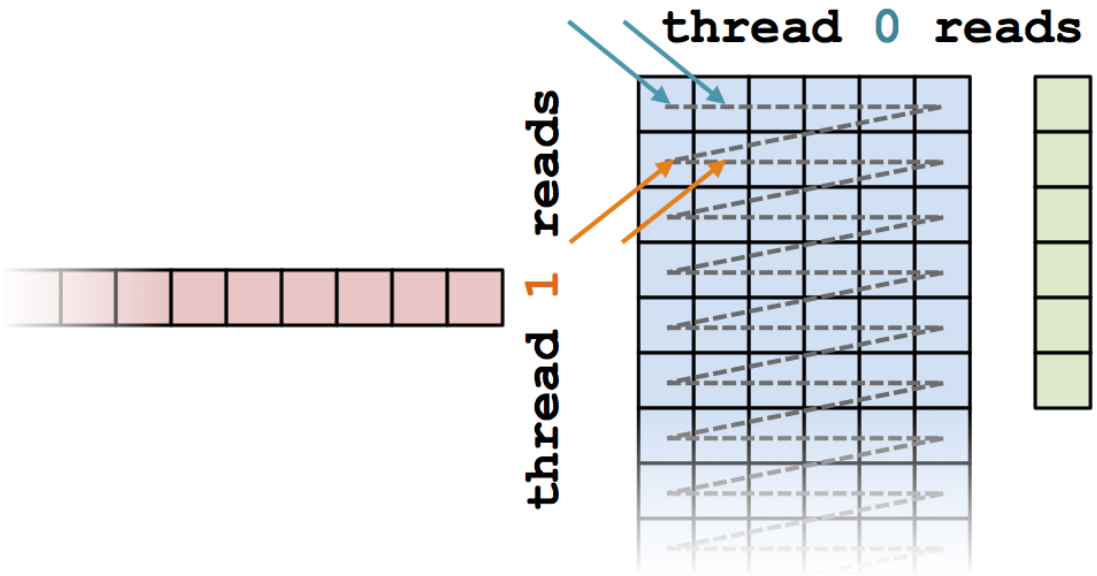
Analysis: row-major (`LayoutRight`)



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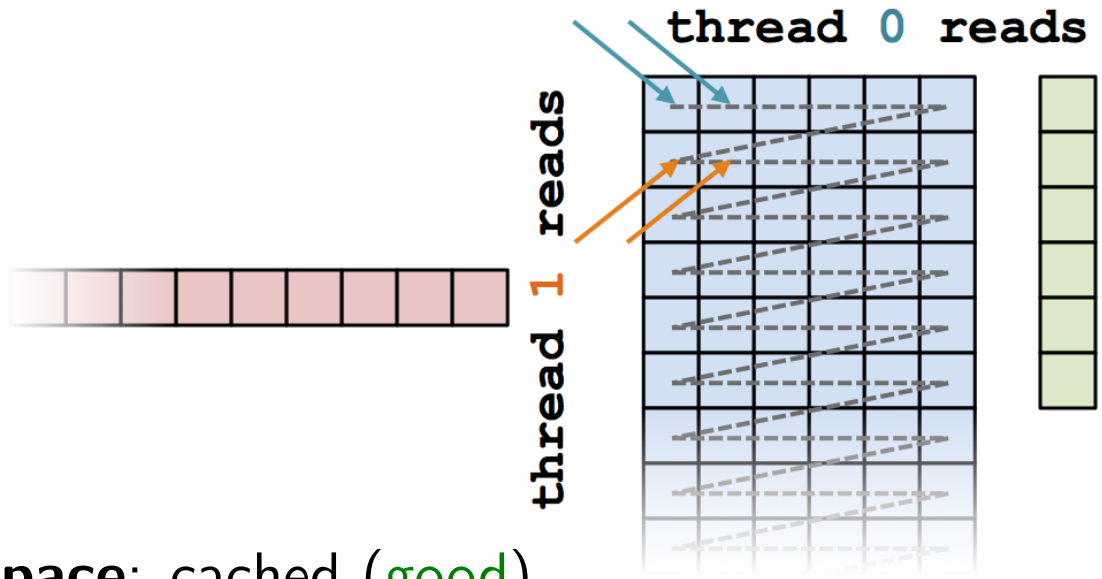
Performant memory access is achieved by Kokkos mapping parallel work indices **and** multidimensional array layout *appropriately for the architecture*.

Analysis: row-major (`LayoutRight`)

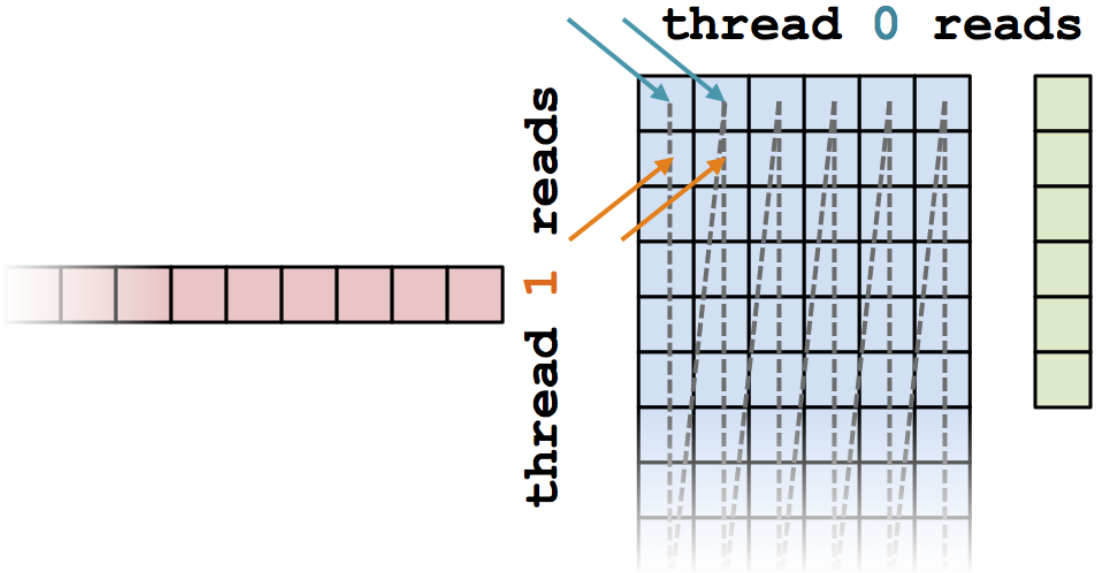


- **HostSpace**: cached (good)
- **CudaSpace**: uncoalesced (bad)

Important point

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

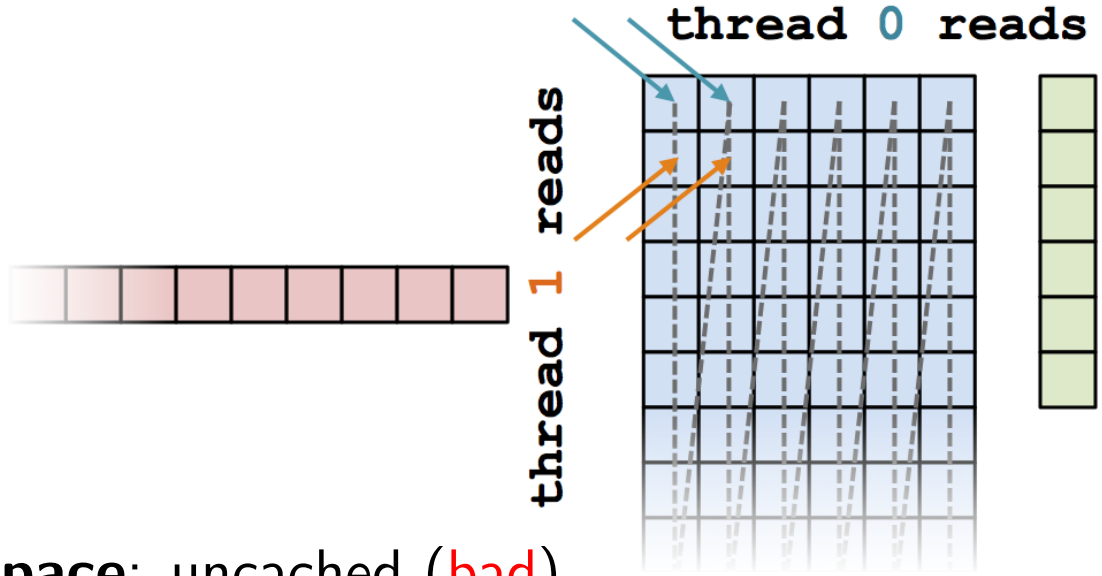
Analysis: column-major (`LayoutLeft`)



Important point

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

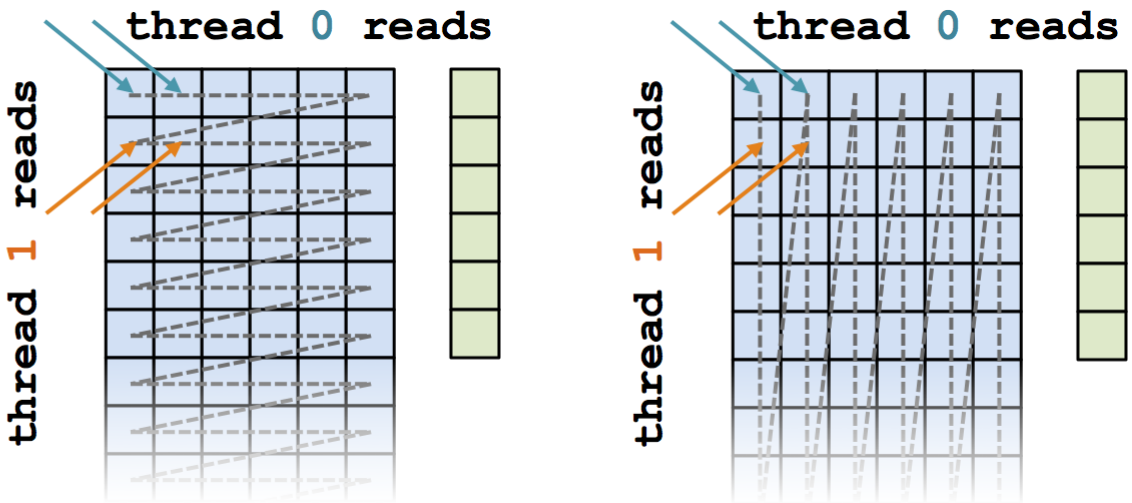
Analysis: column-major (`LayoutLeft`)



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

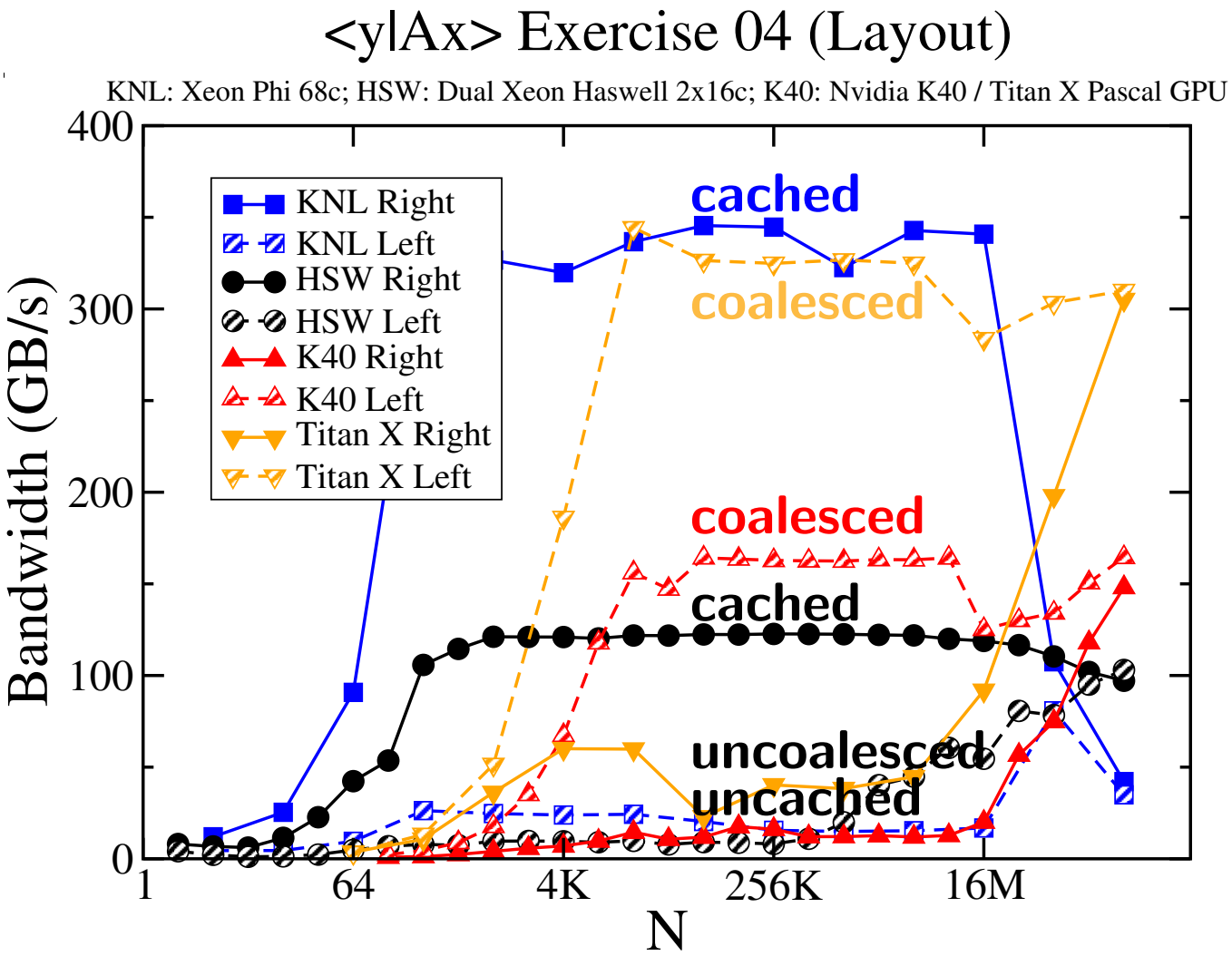
Analysis: Kokkos architecture-dependent

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



(a) OpenMP (b) Cuda

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


<y|Ax> Exercise 04 (Layout)
KNL: Xeon Phi 68c; HSW: Dual Xeon Haswell 2x16c; K40: Nvidia K40 / Titan X Pascal GPU
Bandwidth (GB/s)
N
400
300
200
100
0
1
64
4K
256K
16M
KNL Right
KNL Left
HSW Right
HSW Left
K40 Right
K40 Left
Titan X Right
Titan X Left
cached
coalesced
coalesced
cached
uncoalesced
uncached

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.

Kokkos capabilities NOT covered today, only 2 hours

- Atomic operations and their scalability
- Multidimensional range policy (heirarchical pattern)
- Thread-team policy (hierarchical pattern) with intra-team shared memory
  CUDA grid-block parallelism, but easier and portable
- Dynamic directed acyclic graph (DAG) of tasks pattern
- 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.