Kokkos Tutorial

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Location of Materials and Exercises

Tutorial Materials:

- clone github.com/kokkos/kokkos-tutorials into ${HOME}/kokkos-tutorials

  Slides are in ${HOME}/`kokkos-tutorials/Intro-Short`/Slides

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

  Exercises' Makefiles look for ${HOME}/kokkos - suggest clone to ${HOME}
- Advanced Tutorial and Exercises:

  Slides are in ${HOME}/kokkos-tutorials/Intro-Full/Slides

  Additional exercises are in ${HOME}/kokkos-tutorials/Intro-Full/Exercises
- Online Programming Guide, API Reference, Compilation Options - See the Wiki:

  github.com/kokkos/kokkos/wiki

Library Repos and Requirements:

- 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-tools into ${HOME}/kokkos-tools
- clone github.com/kokkos/kokkos-kernels into ${HOME}/kokkos-kernels

What is **Kokkos** and how does it 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**

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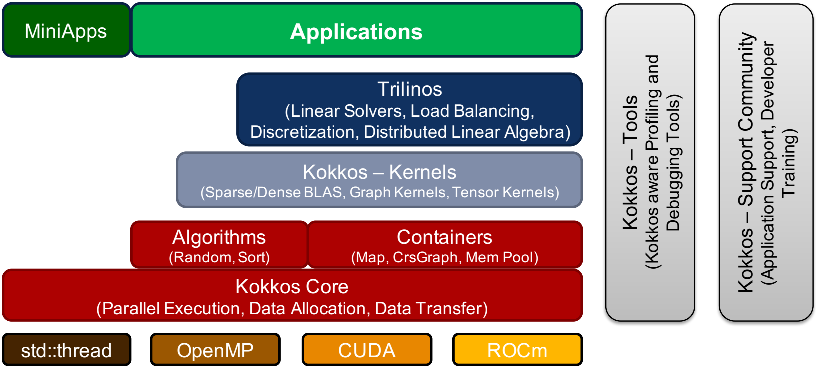
Important Point

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

The Kokkos Ecosystem



MiniApps

Applications

Trilinos
(Linear Solvers, Load Balancing, Discretization, Distributed Linear Algebra)

Kokkos – Kernels
(Sparse/Dense BLAS, Graph Kernels, Tensor Kernels)

Algorithms
(Random, Sort)

Containers
(Map, CrsGraph, Mem Pool)

Kokkos Core
(Parallel Execution, Data Allocation, Data Transfer)

std::thread

OpenMP

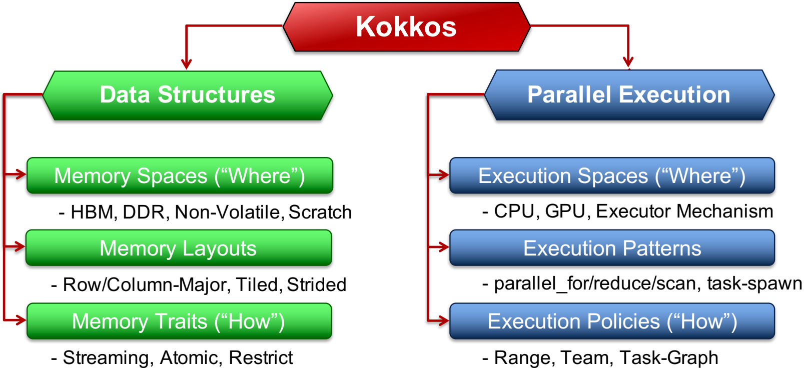
CUDA

ROCm

Kokkos – Tools
(Kokkos aware Profiling and Debugging Tools)

Kokkos – Support Community
(Application Support, Developer Training)

Kokkos Abstractions



Kokkos

Data Structures

Memory Spaces (“Where”)

- HBM, DDR, Non-Volatile, Scratch

Memory Layouts

- Row/Column-Major, Tiled, Strided

Memory Traits (“How”)

- Streaming, Atomic, Restrict

Parallel Execution

Execution Spaces (“Where”)

- CPU, GPU, Executor Mechanism

Execution Patterns

- parallel_for/reduce/scan, task-spawn

Execution Policies (“How”)

- Range, Team, Task-Graph

Concepts: Patterns, Policies, and Bodies

```
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;
}
```

Concepts: Patterns, Policies, and Bodies

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

⇒ The **pattern** and **policy** drive the computational **body**.

Kokkos Core Capabilities

Concept	Example
Parallel Loops	parallel_for(N, KOKKOS_LAMBDA (int i) { ...BODY… });

Parallel Reduction	parallel_reduce(RangePolicy<ExecSpace>(0,N), KOKKOS_LAMBDA (int i, double& upd) {
	…BODY...
	upd += ...
	}, result);

Tightly Nested Loops	parallel_for(MDRangePolicy<Rank<3> > ({0,0,0},{N1,N2,N3},{T1,T2,T3}, KOKKOS_LAMBDA (int i, int j, int k) {…BODY...});

Non-Tightly Nested Loops	parallel_for(TeamPolicy<Schedule<Dynamic>>(N, TS), KOKKOS_LAMBDA (Team team) {
	… COMMON CODE 1 ...
	parallel_for(TeamThreadRange(team, M(N)), [&] (int j) { ... INNER BODY... });
	… COMMON CODE 2 ...
	});

Task Dag	task_spawn(TaskTeam(scheduler , priority), KOKKOS_LAMBDA (Team team) { … BODY });
Data Allocation	View<double**, Layout, MemSpace> a(“A”,N,M);
Data Transfer	deep_copy(a,b);
Exec Spaces	Serial, Threads, OpenMP, Cuda, ROCm *(experimental)*

Tutorial Prerequisites and Objectives:

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

Kokkos' basic capabilities - today's objectives:

- 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 not covered today:

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

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.

Using Kokkos for data parallel patterns (0)

Data parallel patterns and work

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

Kokkos maps **work** to cores

Using Kokkos for data parallel patterns (0)

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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.

Using Kokkos for data parallel patterns (0)

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    for (atomIndex = 0; atomIndex < numberOfAtoms; ++atomIndex) {
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- each iteration of a computational body is a **unit of work**.
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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.

Using Kokkos for data parallel patterns (0)

Data parallel patterns and work

```
    for (atomIndex = 0; atomIndex < numberOfAtoms; ++atomIndex) {
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Preview of `Kokkos::parallel_for` API:

```
    parallel_for (numberOfAtoms, ... );
```

Using Kokkos for data parallel patterns (2)

How are computational bodies given to Kokkos?

Using Kokkos for data parallel patterns (2)

How are computational bodies given to Kokkos?

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

Using Kokkos for data parallel patterns (2)

How are computational bodies given to Kokkos?

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 ... */
  ...
};
```

Using Kokkos for data parallel patterns (3)

How is work assigned to functor operators?

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

```
ParallelFunctor functor;
Kokkos::parallel_for(numberOfIterations, functor);
```

Using Kokkos for data parallel patterns (3)

How is work assigned to functor operators?

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

```
ParallelFunctor functor;
Kokkos::parallel_for(numberOfIterations, functor);
```

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

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

Using Kokkos for data parallel patterns (3)

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

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```

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

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

Warning: concurrency and order

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

Using Kokkos for data parallel patterns (4)

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...);
  }
  ...
}
```

Using Kokkos for data parallel patterns (4)

How is data passed to computational bodies?

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

Using Kokkos for data parallel patterns (5)

Putting it all together: the complete functor:

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

Using Kokkos for data parallel patterns (5)

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

Serial

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

Functor

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

Using Kokkos for data parallel patterns (6)

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);
```

Using Kokkos for data parallel patterns (7)

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);
  }
);
```

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

Using Kokkos for data parallel patterns (7)

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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

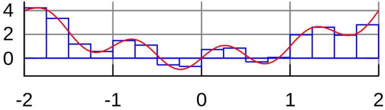
```
parallel_for(N, [=] (const size_t i) {
  /* loop body */
});
```

Important concept

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

Riemann-sum-style numerical integration:

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



wikipedia

Scalar integration (0)

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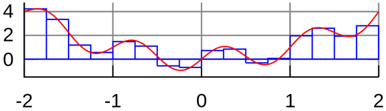

wikipedia

```
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;
```

Riemann-sum-style numerical integration:

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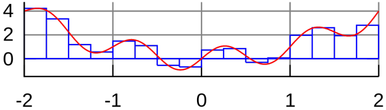

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How do we **parallelize** it? *Correctly?*

Scalar integration (0)

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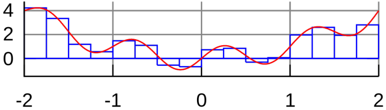

wikipedia

Pattern?

Policy?

Body?

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

Scalar integration (1)

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!)

Scalar integration (2)

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

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

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    *totalIntegralPointer += function(x);},
  );
totalIntegral *= dx;
```

Second problem: race condition

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

Scalar integration (3)

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 += ...
}
```

Scalar integration (3)

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Important concept: Reduction

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}
```

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

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

Scalar integration (4)

Comparison using lambda

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.

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

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];
  }
};
```

View motivation

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Problem: x and y reside in CPU memory.

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  }
};
```

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**

Views (0)

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.

Views (1)

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.

Views (1)

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  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.

Views (2)

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`

Views (2)

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`

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?

Views (2)

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.**
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a(0) = 1;
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c(0) = 3;
print a(0)
```

What gets printed?

`3.0`

Execution and Memory Spaces

Learning objectives:

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

Execution spaces (0)

Thought experiment: Consider this code:

section 1

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

```
Kokkos::parallel_for(numberOfSomethings,
                     [=] (const size_t somethingIndex) {
```

section 2

```
                       const double y = ...;
                       // do something interesting
```

```
                     }
                     );
```

Execution spaces (0)

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
                     }
                     );
```

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

Execution spaces (0)

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
                     }
                     );
```

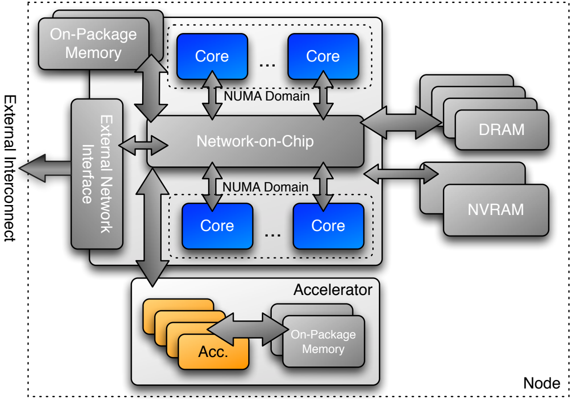
- Where will section 1 be run? CPU? GPU?
- Where will section 2 be run? CPU? GPU?
- How do I **control** where code is executed?

⇒ **Execution spaces**

Execution Space

a homogeneous set of cores and an execution mechanism

(i.e., “place to run code”)



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

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
                     }
                     );
```

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
                     }
                     );
```

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

  ⇒ Always in the **host process**

Execution spaces (2)

Host

Parallel

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

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

  ⇒ Always in the **host process**

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

  ⇒ The **default execution space**

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
                     }
                     );
```

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

Execution spaces (3)

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 ... */
  });
```

Execution spaces (3)

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 ... */
  });
```

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.

Execution spaces (5)

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 */
```

Execution spaces (5)

Kokkos function and lambda portability annotation macros:

Function annotation with `KOKKOS_INLINE_FUNCTION` macro

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

Memory space motivating example: summing an array

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View<double*> data("data", size);
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  sum);
```

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

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...
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Kokkos::parallel_reduce(
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    valueToUpdate += data(index);
  },
  sum);
```

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

Memory Space Motivation

Memory space motivating example: summing an array

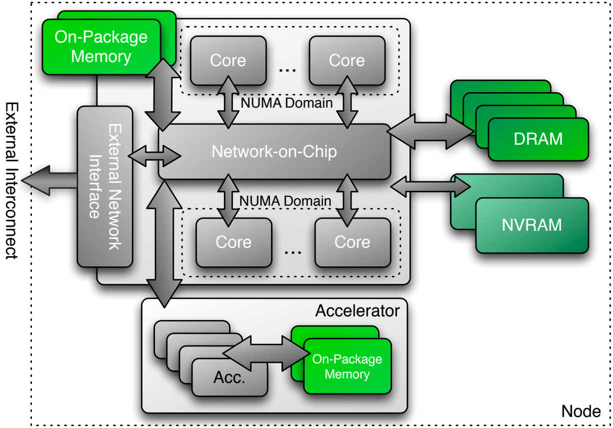
```
View<double*> data("data", size);
for (size_t i = 0; i < size; ++i) {
  data(i) = ...read from file...
}

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

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

⇒ **Memory Spaces**

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



Memory spaces (1)

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(...);`

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

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

Memory spaces (1)

Important concept: Memory spaces

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

- `View<double***,`*Memory***Space**`> data(...);`
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  `HostSpace, CudaSpace, CudaUVMSpace, ...` more
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Every view stores its data in a **memory space** set at compile time.

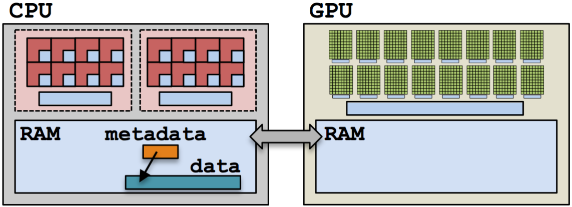
- `View<double***,`*Memory***Space**`> data(...);`
- Available **memory spaces**:

  `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**.

Memory spaces (2)

Example: HostSpace

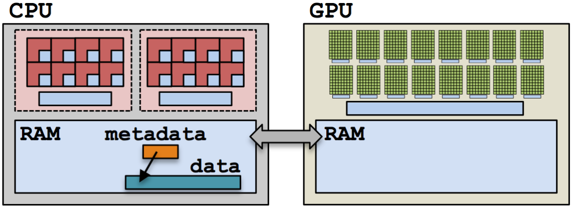
```
View<double**, HostSpace> hostView(...constructor arguments...);
```



Memory spaces (2)

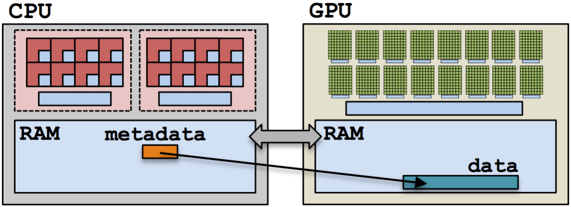
Example: HostSpace

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



Example: CudaSpace

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



Anatomy of a kernel launch:

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

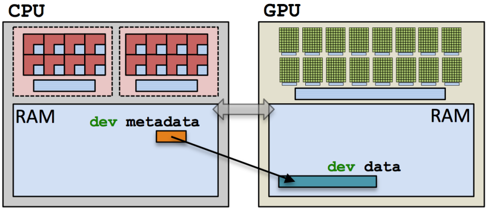
```
View<int*, Cuda> v("v",N);
parallel_for(N,
  KOKKOS_LAMBDA (int i) {
    v(i) = ...;
  });
```

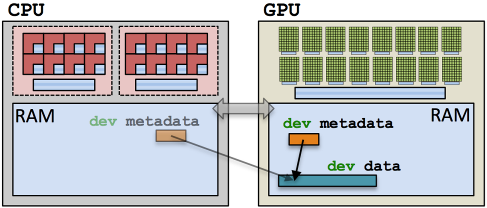
Note: **no deep copies** of array data are performed;
views are like pointers.

Execution and Memory spaces (1)

Example: one view

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

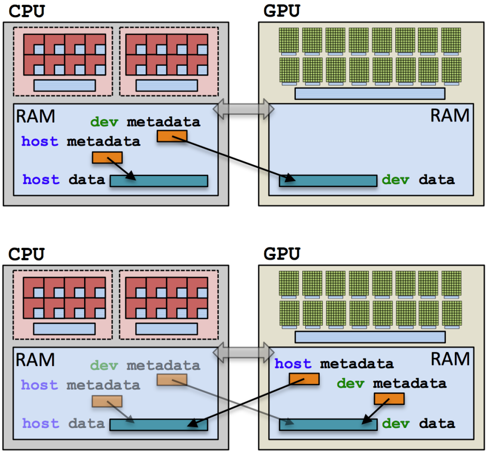




Execution and Memory spaces (2)

Example: two views

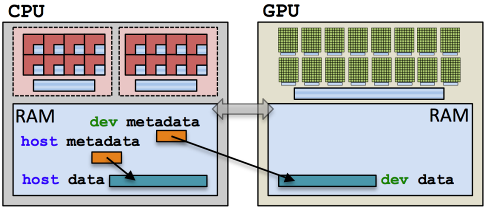
```
View<int*, Cuda> dev;
View<int*, Host> host;
parallel_for(N,
  KOKKOS_LAMBDA (int i)
    dev(i)  = ...;
    host(i) = ...;
  });
```

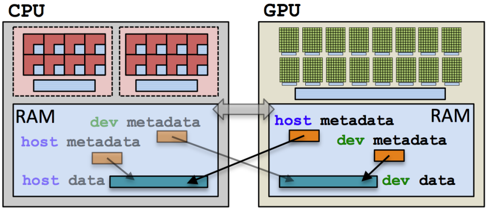


Execution and Memory spaces (2)

Example: two views

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





Execution and Memory spaces (3)

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);
```

Execution and Memory spaces (3)

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...                   fault
}

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

Execution and Memory spaces (4)

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);
```

Execution and Memory spaces (4)

Example (redux): summing an array with the GPU

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

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

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

Execution and Memory spaces (4)

Example (redux): summing an array with the GPU

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

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

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

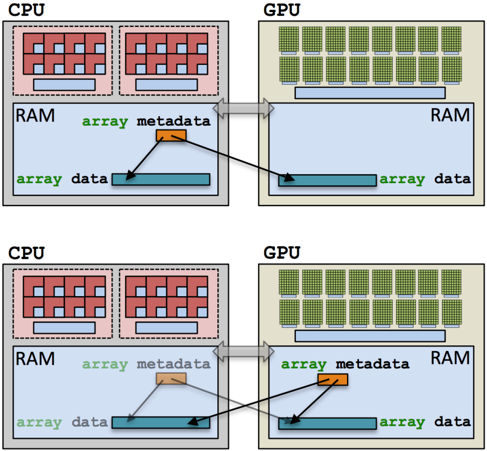
What's the solution?

- CudaUVMSpace
- CudaHostPinnedSpace (skipping)
- Mirroring

Execution and Memory spaces (5)

CudaUVMSpace

```
View<double*,
     CudaUVMSpace> array
array = ...from file...
double sum = 0;
parallel_reduce(N,
  KOKKOS_LAMBDA (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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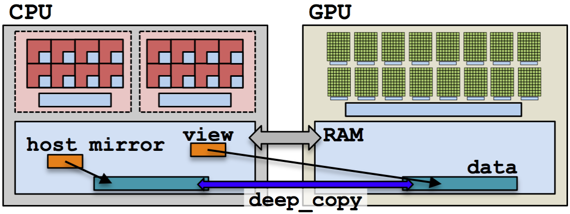
Mirrors are views of equivalent arrays residing in possibly different memory spaces.

Mirroring schematic

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



Mirroring pattern

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

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

Mirroring pattern

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

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

2. **Create** hostView, a *mirror* of the view's array residing in the host memory space.

   ```
   ViewType::HostMirror hostView =
     Kokkos::create_mirror_view(view);
   ```

Mirroring pattern

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

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

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ViewType::HostMirror hostView =
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```

3. **Populate** hostView on the host (from file, etc.).

Mirroring pattern

1. **Create** a view's array in some memory space.
   ```
   typedef Kokkos::View<double*, Space> ViewType;
   ViewType view(...);
   ```
2. **Create** hostView, a *mirror* of the view's array residing in the host memory space.
   ```
   ViewType::HostMirror hostView =
     Kokkos::create_mirror_view(view);
   ```
3. **Populate** hostView on the host (from file, etc.).
4. **Deep copy** hostView's array to view's array.
   ```
   Kokkos::deep_copy(view, hostView);
   ```

Mirroring pattern

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

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   ```
   ViewType::HostMirror hostView =
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3. **Populate** hostView on the host (from file, etc.).

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

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

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

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

Mirroring pattern

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

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

2. **Create** `hostView`, a *mirror* of the `view`'s array residing in the host memory space.

```
ViewType::HostMirror hostView =
  Kokkos::create_mirror_view(view);
```

3. **Populate** `hostView` on the host (from file, etc.).
4. **Deep copy** `hostView`'s array to `view`'s array.

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

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

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

Mirrors of Views in HostSpace

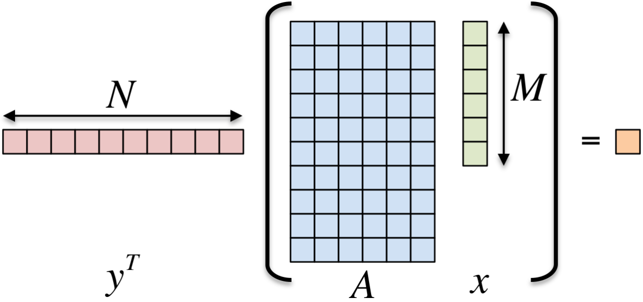
What if the View is in HostSpace too? Does it make a copy?

```
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**.

Recurring Exercise: Inner Product

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



Details:

- y is $Nx1$, A is NxM, x is $Mx1$
- We'll use this exercise throughout the tutorial
- Optional: Try Exercises 1-4 during break or evening hands-on session

Exercise #1: include, initialize, finalize Kokkos

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

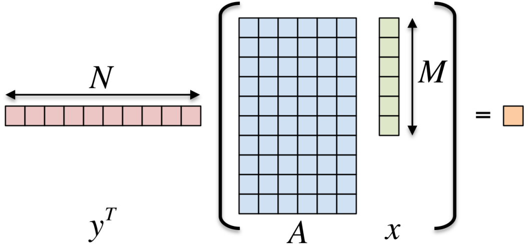
```
#include <Kokkos_Core.hpp>
int main(int argc, char** argv) {
  /* ... do any necessary setup (e.g., initialize MPI) ... */
  Kokkos::initialize(argc, argv);
  {
  /* ... do computations ... */
  }
  Kokkos::finalize();
  return 0;
}
```

(Optional) Command-line arguments:

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

Exercise #1: Inner Product, Flat Parallelism on the CPU

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



Details:

- Location: `Intro-Short/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.

Exercise #1: logistics

Compiling for CPU

```
# gcc using OpenMP (default) and Serial back-ends,
# (optional) non-default arch set with KOKKOS_ARCH
  make -j KOKKOS_DEVICES=OpenMP,Serial KOKKOS_ARCH=SNB
# KOKKOS_ARCH Options: See the wiki at
# https://github.com/kokkos/kokkos/wiki/Compiling
```

Running on CPU with OpenMP back-end

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

Things to try:

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

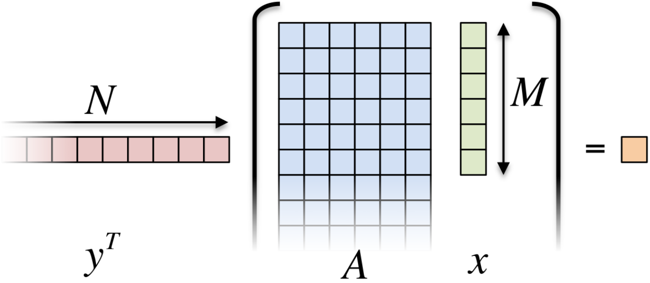
Managing memory access patterns for performance portability

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)

```
double result = 0.0;
for ( size_t row = 0; row < N; ++row ) {
  double thisRowsSum = 0;
  for (size_t entry = 0; entry < M; ++entry) {
    thisRowsSum += A(row, entry) * x(entry);
  }
  result += y(row) * thisRowsSum;
}
```



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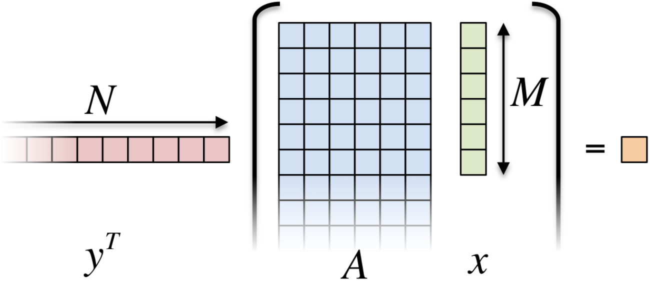

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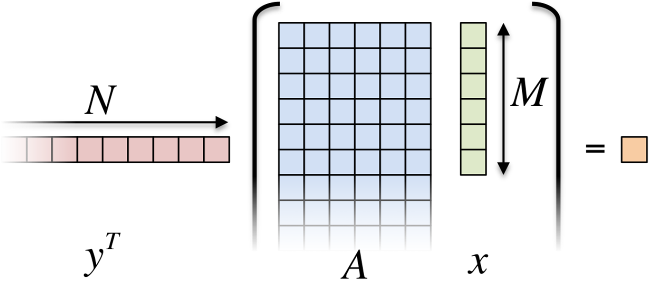


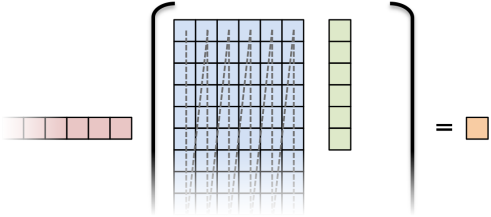
Driving question: How should `A` be laid out in memory?

Example: inner product (1)

Layout is the mapping of multi-index to memory:

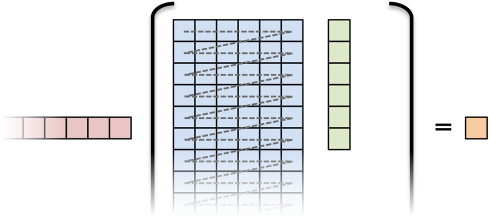
LayoutLeft

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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View<double***, Layout, Space> name(...);
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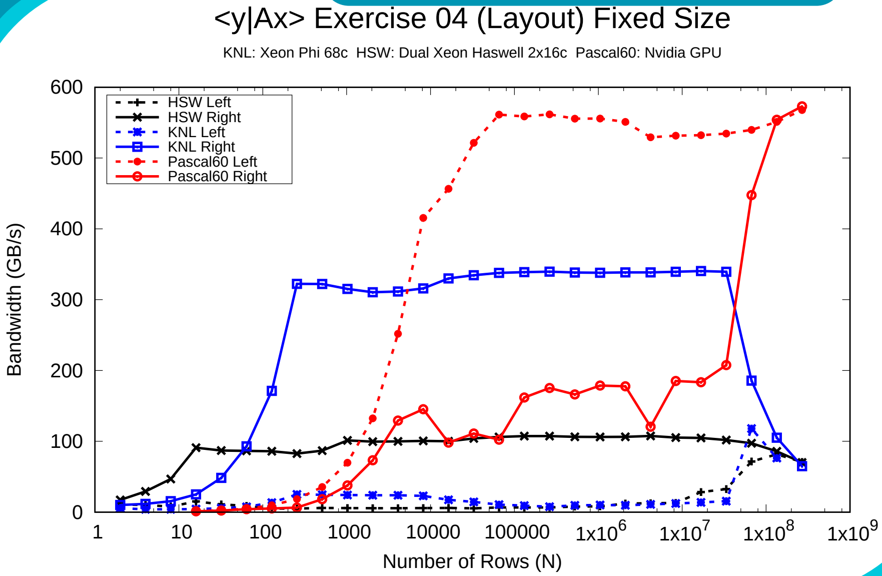
- Most-common layouts are LayoutLeft and LayoutRight.
  LayoutLeft: left-most index is stride 1.
  LayoutRight: right-most index is stride 1.
- If no layout specified, default for that memory space is used.
  LayoutLeft for CudaSpace, LayoutRight for HostSpace.
- Layouts are extensible: ˜50 lines
- Advanced layouts: LayoutStride, LayoutTiled, ...

Memory Layout Affect on Performance

Exercise 4 Summary:

- Added `parallel_reduce` and replaced `‘‘N’’` in parallel dispatch with `RangePolicy<ExecSpace>`
- Replaced raw pointer allocations with Kokkos::View’s for x, y, and A
- Added HostMirror Views and deep copy
- Added `MemSpace` to all `Views` and `Layout` to `A`

Exercise #4: Inner Product, Flat Parallelism



Caching and coalescing (0)

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?

- **CPU** threads are independent.

  i.e., threads may execute at any rate.
- **GPU** threads are synchronized in groups (of 32).

  i.e., threads in groups must execute instructions together.

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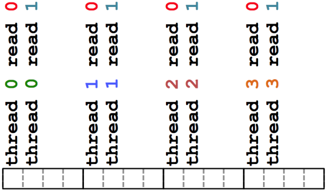
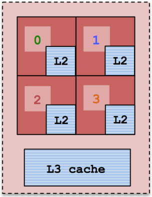
In particular, all threads in a group (*warp*) must finished their loads before *any* thread can move on.

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

CPUs: few (independent) cores with separate caches:





Caching and coalescing (1)

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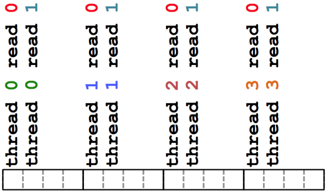
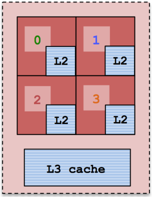
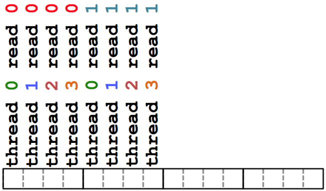
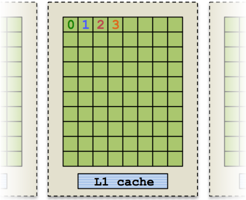




GPUs: many (synchronized) cores with a shared cache:





Caching and coalescing (2)

Important point

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

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

Coalescing: if thread `t'`s current access is at position `i`,
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Note: uncoalesced *read-only, random* access in `CudaSpace` is okay through Kokkos `const RandomAccess` views (*advanced tutorial*).

Mapping indices to cores (0)

Consider the array summation example:

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

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

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

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

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

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

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

Why?

Mapping indices to cores (1)

Iterating for the execution space:

```
operator()(const size_t index, double & valueToUpdate) {
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As users we don't control how indices are mapped to threads, so how do we achieve good memory access?

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

Important point

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

Mapping indices to cores (2)

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, ... , ... ) = ...;
  });
...
```

Example: inner product (2)

Important point

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

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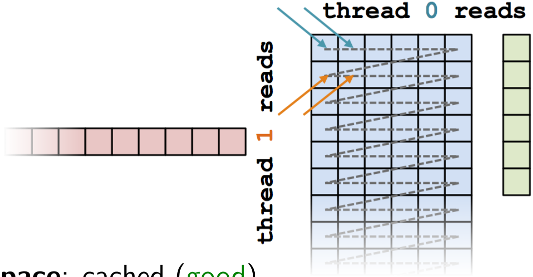
Analysis: row-major (`LayoutRight`)

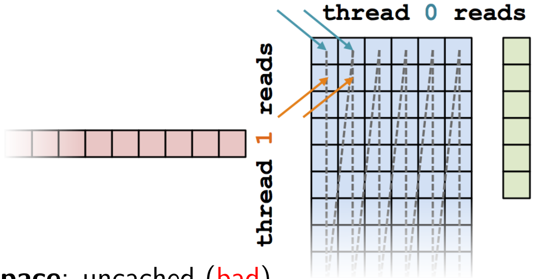


- **HostSpace**: cached (good)
- **CudaSpace**: uncoalesced (bad)

Important point

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

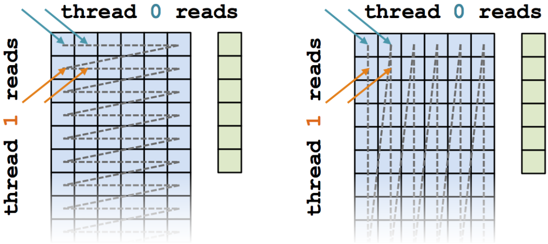
Analysis: column-major (`LayoutLeft`)



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

Analysis: Kokkos architecture-dependent

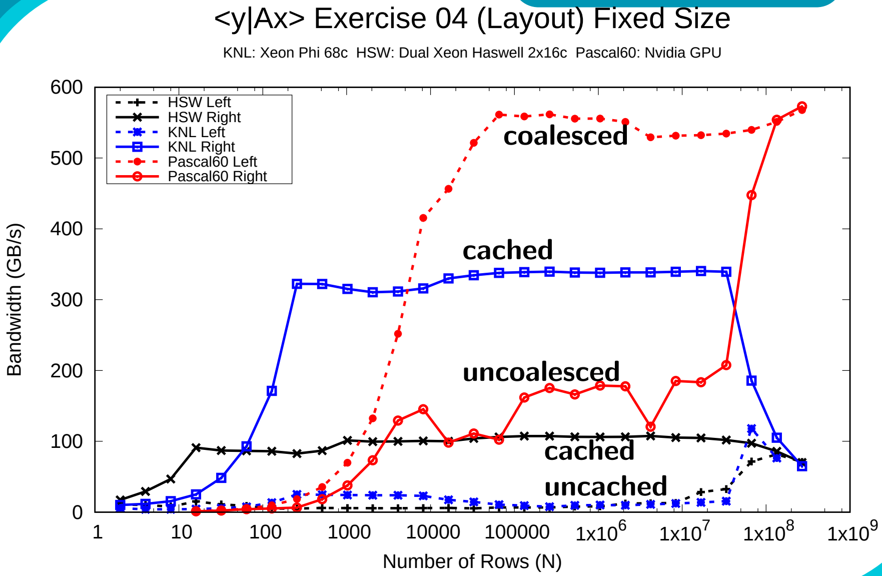
```
View<double**, ExecutionSpace> A(N, M);
parallel_reduce(RangePolicy< ExecutionSpace>(0, N),
  ... thisRowsSum += A(j, i) * x(i);
```



(a) OpenMP (b) Cuda

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

Example: inner product (5)



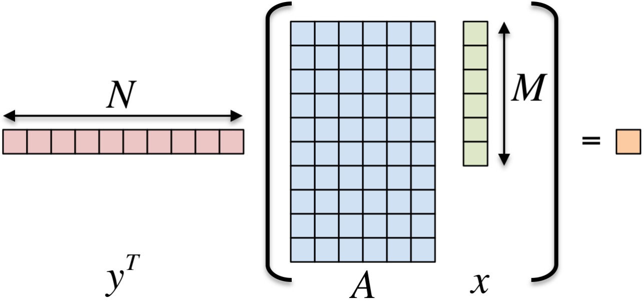
End Short Intro

Kokkos advanced capabilities NOT covered today

- Thread safety, thread scalability, and atomic operations
- Hierarchical parallelism via team policies for thread teams
- 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

Recurring Exercise: Inner Product

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



Details:

- y is Nx1, A is NxM, x is Mx1
- We'll use this exercise throughout the tutorial
- Optional: Try Exercises 1-4 during break or evening hands-on session

Exercise #1: include, initialize, finalize Kokkos

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

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

(Optional) Command-line arguments:

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

Exercise #1: Inner Product, Flat Parallelism on the CPU

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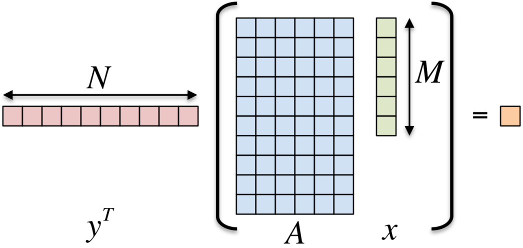

Details:

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Running on CPU with OpenMP back-end

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# Run larger problem
./01_Exercise.host -S 26
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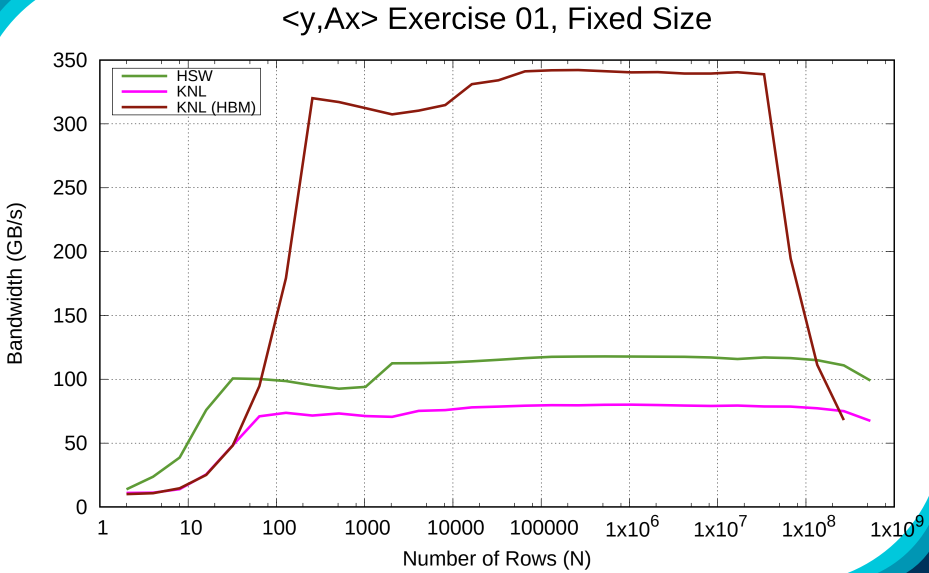
Things to try:

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

Exercise #1 results



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

- Location: `Intro-Short/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

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

Details:

- Location: `Intro-Short/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

Exercise #4: Inner Product, Flat Parallelism

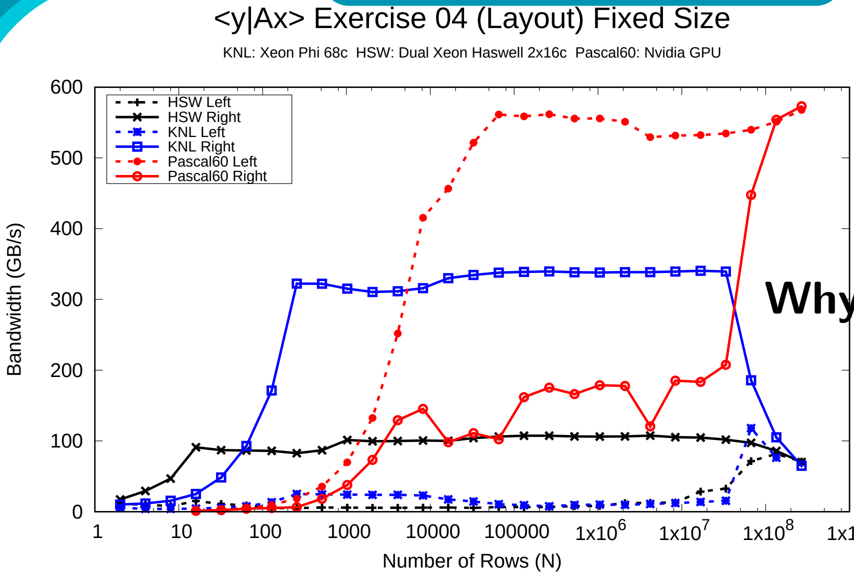
Details:

- Location: `Intro-Short/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.

Exercise #4: Inner Product, Flat Parallelism



Why?