OAK RIDGE National Laboratory

A Short Introduction to Kokkos

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ORNL is managed by UT-Battelle LLC
for the US Department of Energy

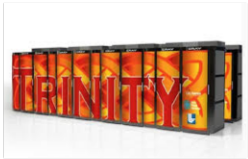
U.S. DEPARTMENT OF ENERGY

A Condensed Short Tutorial

This lecture covers fundamental concepts of Kokkos with Hands-On Exercises as homework.
Slides: https://github.com/kokkos/kokkos-tutorials/Intro-Short/KokkosTutorial_Short.pdf

For the full lectures, with more capabilities covered, and more in-depth explanations visit:
https://github.com/kokkos/kokkos-tutorials/wiki/Kokkos-Lecture-Series

Current Generation: Programming Models OpenMP 3, CUDA and OpenACC depending on machine



LANL/SNL Trinity
Intel Haswell / Intel KNL
OpenMP 3

LLNL SIERRA
IBM Power9 / NVIDIA Volta
CUDA / *OpenMP*[(a)]

ORNL Summit
IBM Power9 / NVIDIA Volta
CUDA / *OpenACC / OpenMP*[(a)]

SNL Astra
ARM CPUs
OpenMP 3

Riken Fugaku
ARM CPUs with SVE
OpenMP 3 / *OpenACC*[(b)]

Upcoming Generation: Programming Models OpenMP 5, CUDA, HIP and DPC++ depending on machine

NERSC Perlmutter
AMD CPU / NVIDIA GPU
CUDA / *OpenMP 5*[(c)]

ORNL Frontier
AMD CPU / AMD GPU
HIP / *OpenMP 5*[(d)]

ANL Aurora
Xeon CPUs / Intel GPUs
DPC++ / *OpenMP 5*[(e)]

LLNL El Capitan
AMD CPU / AMD GPU
HIP / *OpenMP 5*[(d)]

(a) Initially not working. Now more robust for Fortran than C++, but getting better.
(b) Research effort.
(c) OpenMP 5 by NVIDIA.
(d) OpenMP 5 by HPE.
(e) OpenMP 5 by Intel.

Industry Estimate

A full time software engineer writes 10 lines of production code per hour: 20k LOC/year.

- Typical HPC production app: 300k-600k lines
  - Sandia alone maintains a few dozen
- Large Scientific Libraries:
  - E3SM: 1,000k lines
  - Trilinos: 4,000k lines

Conservative estimate: need to rewrite 10% of an app to switch Programming Model

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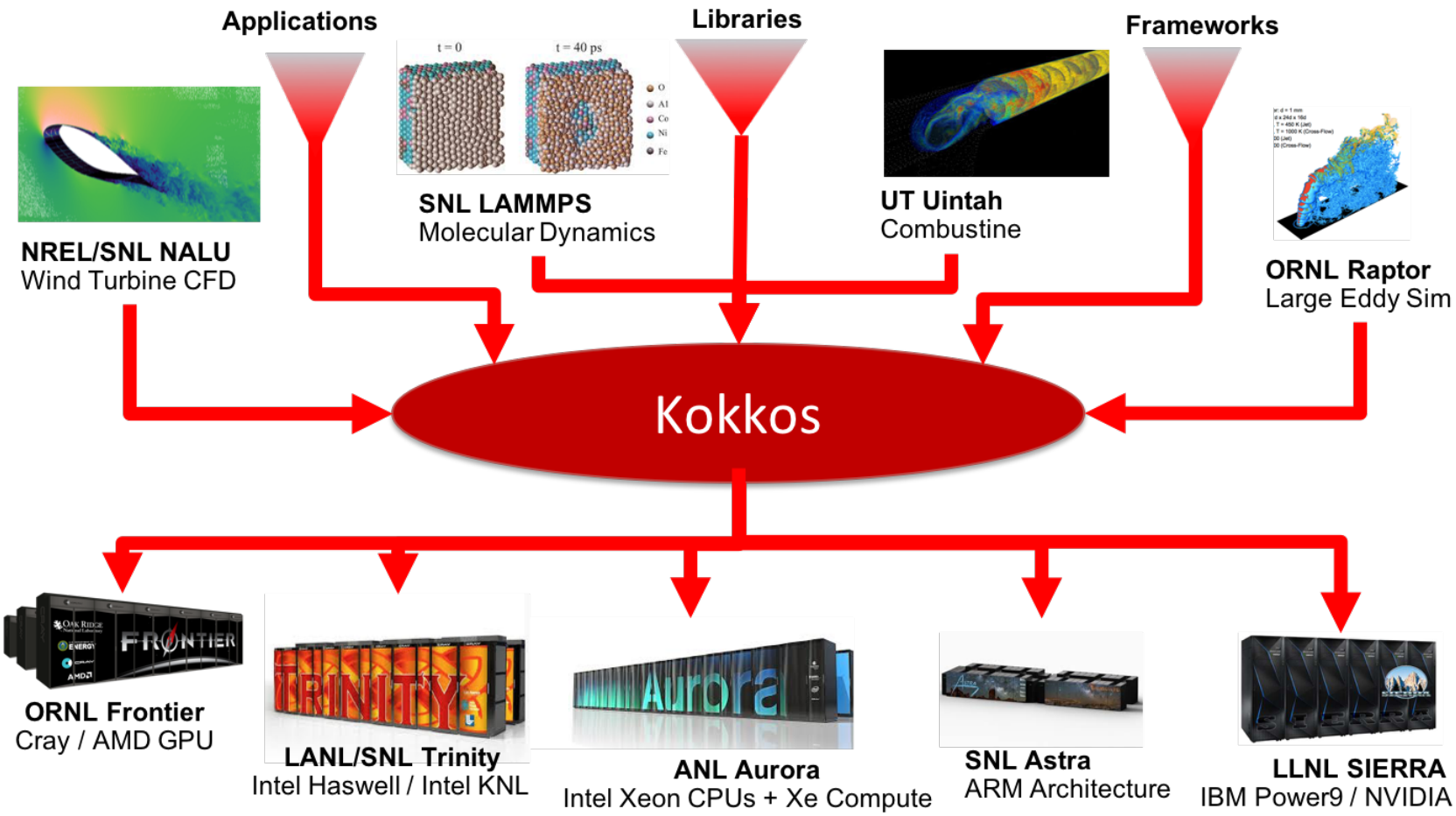
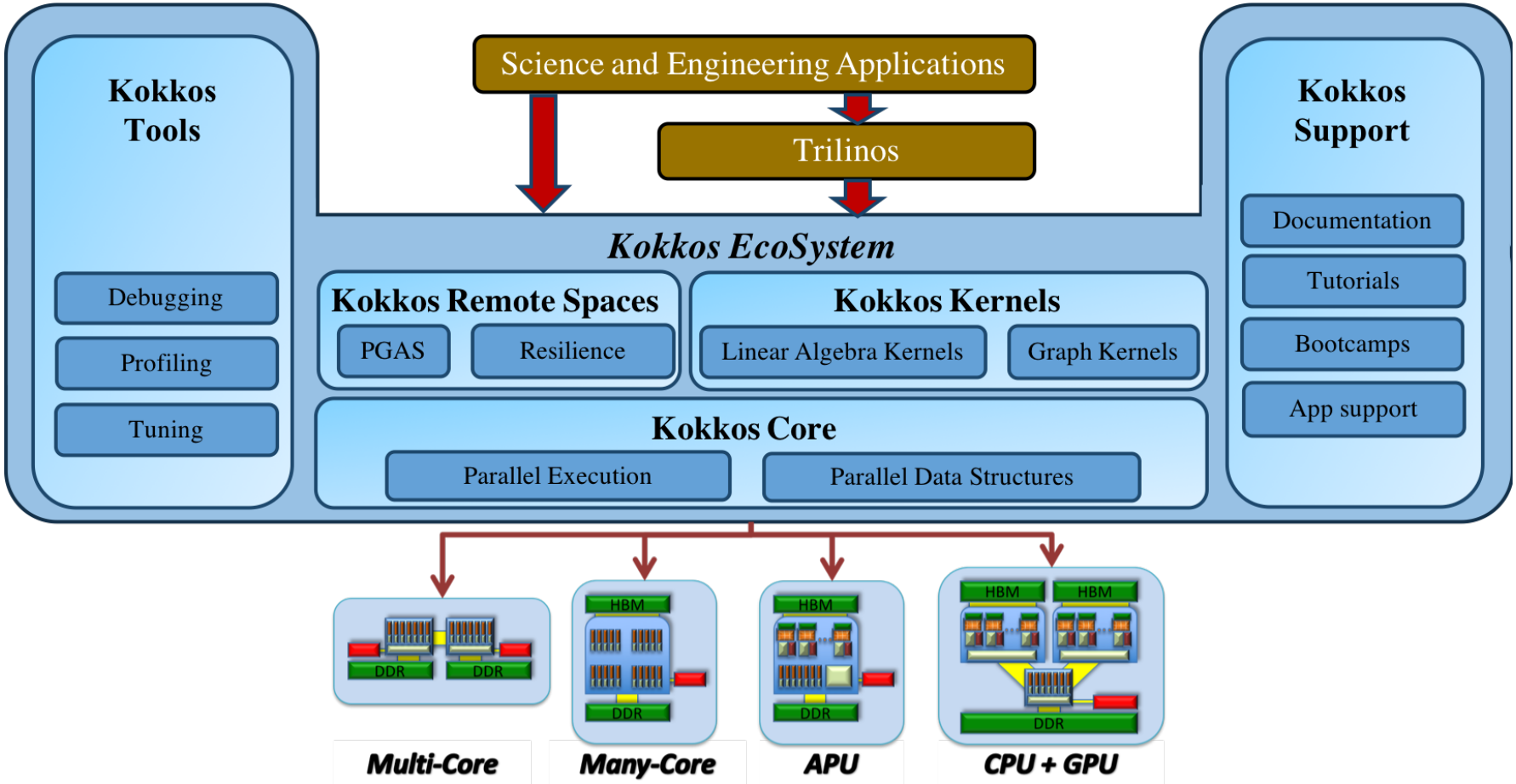
Software Cost Switching Vendors

Just switching Programming Models costs multiple person-years per app!

- A C++ Programming Model for Performance Portability
  - Implemented as a template library on top CUDA, HIP, OpenMP, ...
  - Aims to be descriptive not prescriptive
  - Aligns with developments in the C++ standard
- Expanding solution for common needs of modern science and engineering codes
  - Math libraries based on Kokkos
  - Tools for debugging, profiling and tuning
  - Utilities for integration with Fortran and Python
- Is is an Open Source project with a growing community
  - Maintained and developed at https://github.com/kokkos
  - Hundreds of users at many large institutions


Applications
Libraries
Frameworks
NREL/SNL NALU
Wind Turbine CFD
t = 0
t = 40 ps
SNL LAMMPS
Molecular Dynamics
UT Uintah
Combustine
ORNL Raptor
Large Eddy Sim
Kokkos
ORNL Frontier
Cray / AMD GPU
LANL/SNL Trinity
Intel Haswell / Intel KNL
ANL Aurora
Intel Xeon CPUs + Xe Compute
SNL Astra
ARM Architecture
LLNL SIERRA
IBM Power9 / NVIDIA Volta

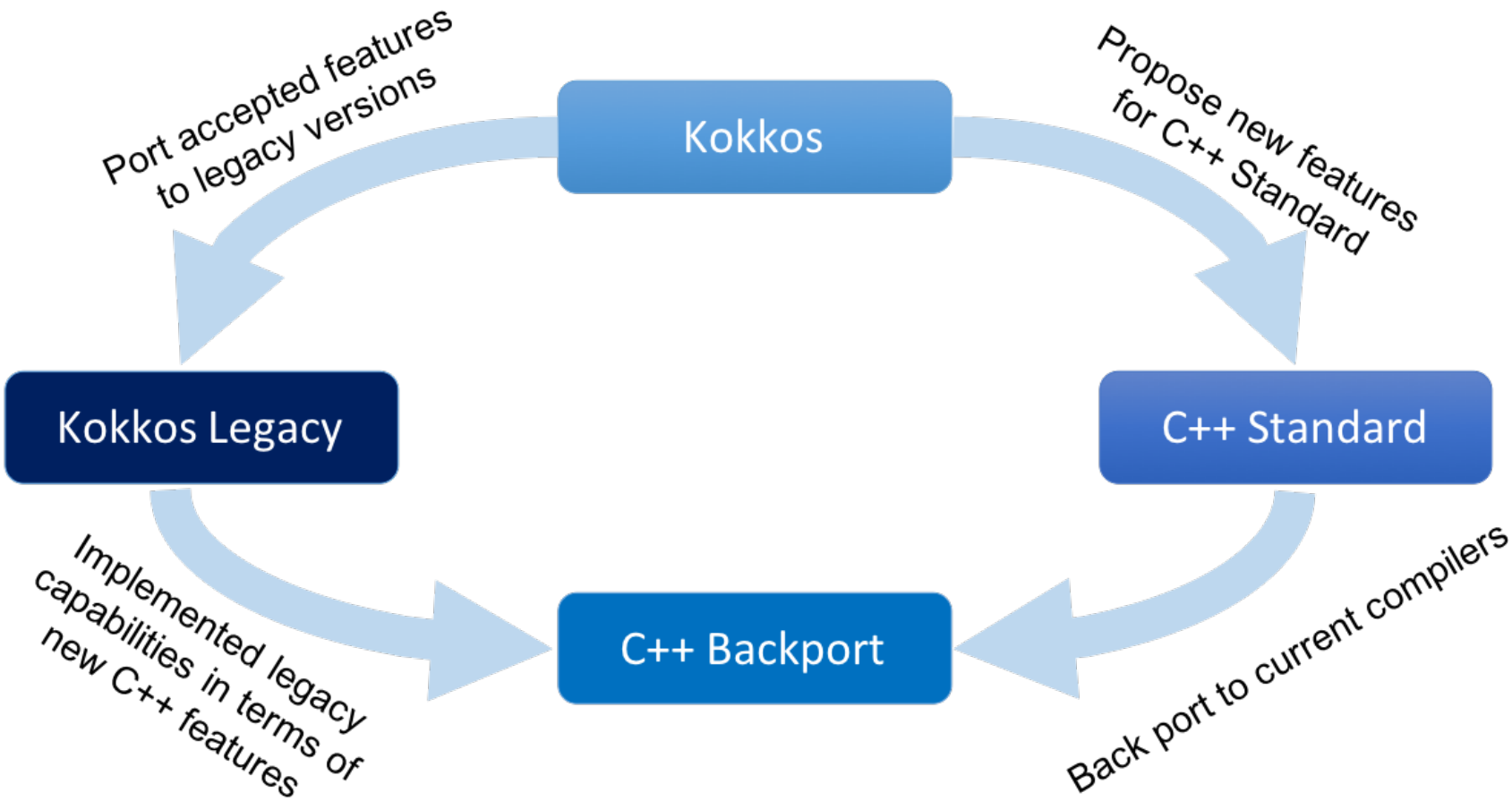
The Kokkos EcoSystem



Kokkos Core: **C. Trott**, **D. Lebrun-Grandié**, D. Arndt, J. Bludau, J. Ciesko, V. Dang, N. Ellingwood, R. Gayatri, D. Ibanez, V. Kale, N. Liber, P. Miller, N. Morales, A. Powell, F. Rizzi, C. Skrzyński, B. Turcksin
`former:` H.C. Edwards, D. Labreche, G. Mackey, S. Bova, D. Sunderland, D.S. Hollman, J. Miles, J. Wilke, J. Madsen, D. Poliakoff, C. Lewis, H. Finkel

Kokkos Kernels: **S. Rajamanickam**, **L. Berger-Vergiat**, V. Dang, N. Ellingwood, J. Foucar, E. Harvey, B. Kelley, K. Kim, J. Loe, C. Pearson
`former:` J. Wilke, S. Acer

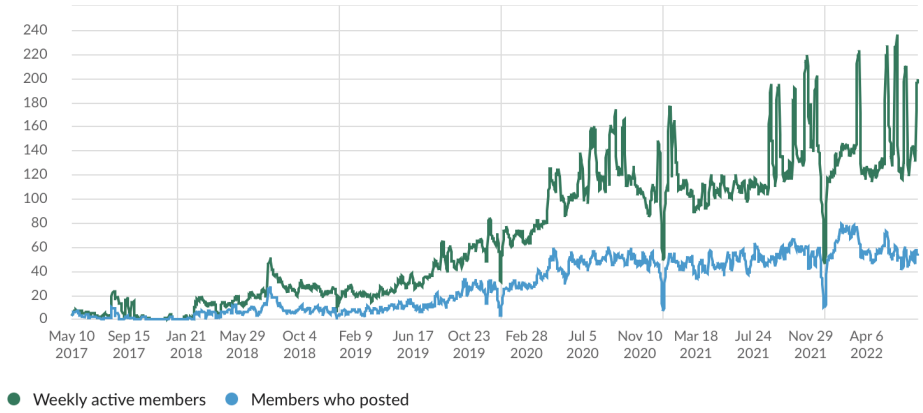
Kokkos helps improve ISO C++



Ten current or former Kokkos team members are members of the ISO C++ standard committee.

Kokkos has a growing OpenSource Community

- 20 ECP projects list Kokkos as Critical Dependency
  - 41 list C++ as critical
  - 25 list Lapack as critical
  - 21 list Fortran as critical
- Slack Channel: 900 members from 90+ institutions
  - 15% Sandia Nat. Lab.
  - 24% other US Labs
  - 22% universities
  - 39% other
- GitHub: 1.1k stars



Online Resources:

- https://github.com/kokkos:
  - Primary Kokkos GitHub Organization
- https://github.com/kokkos/kokkos-tutorials/wiki/Kokkos-Lecture-Series:
  - Slides, recording and Q&A for the Full Lectures
- https://github.com/kokkos/kokkos/wiki:
  - Wiki including API reference
- https://kokkosteam.slack.com:
  - Slack channel for Kokkos.
  - Please join: fastest way to get your questions answered.
  - Can whitelist domains, or invite individual people.

Data parallel patterns

Learning objectives:

- How computational bodies are passed to the Kokkos runtime.
- How work is mapped to execution resources.
- 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 execution resources

Data parallel patterns and work

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for (atomIndex = 0; atomIndex < numberOfAtoms; ++atomIndex) {
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Kokkos maps **work** to execution resources

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

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

Important concept: Work mapping

You give an **iteration range** and **computational body** (kernel) to Kokkos, and Kokkos decides how to map that work to execution resources.

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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struct Functor {
  void operator()(const int64_t index) const {...}
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ParallelFunctor functor;
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struct Functor {
  void operator()(const int64_t index) const {...}
}
```

Warning: concurrency and order

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

The complete picture (using functors):

1. Defining the functor (operator+data):

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

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

  void operator()(const int64_t atomIndex) const {
    _atomForces[atomIndex] = calculateForce(_atomData);
  }
}
```

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

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

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

```
atomForces already exists
data already exists
Kokkos::parallel_for(numberOfAtoms,
    [=] (const int64_t atomIndex) {
    atomForces[atomIndex] = calculateForce(data);
  }
);
```

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

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data already exists
Kokkos::parallel_for(numberOfAtoms,
    [=] (const int64_t atomIndex) {
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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 (int64_t i = 0; i < N; ++i) {
  /* loop body */
}
```

OpenMP

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

Kokkos

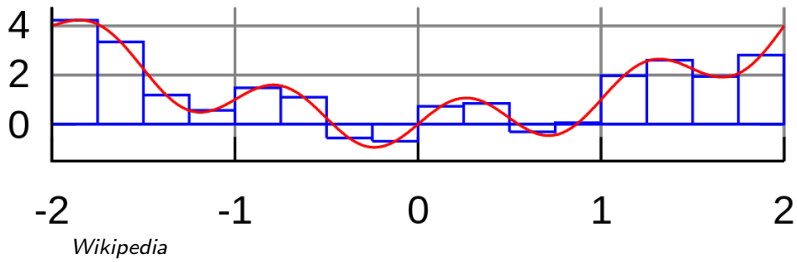
```
parallel_for(N, [=] (const int64_t i) {
  /* loop body */
});
```

Important concept

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

Riemann-sum-style numerical integration:

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



Wikipedia

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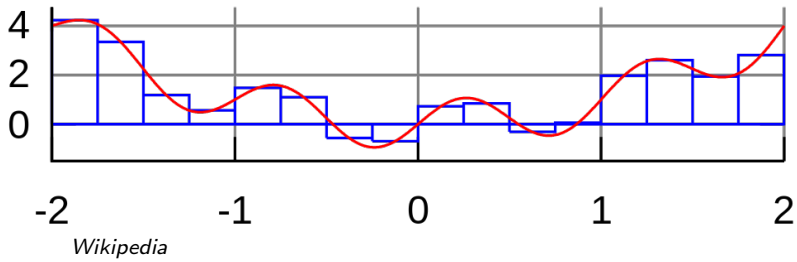

Wikipedia

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

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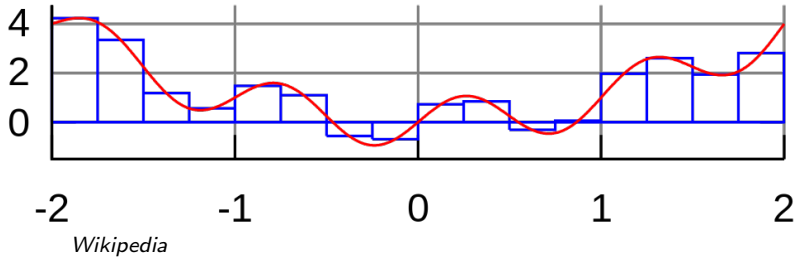


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How do we **parallelize** it? *Correctly?*

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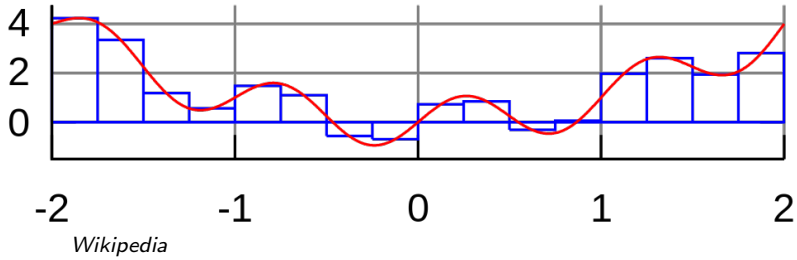

Pattern?

Policy?

Body?

```
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  totalIntegral += thisIntervalsContribution;
}
totalIntegral *= dx;
```

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

An (incorrect) attempt:

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

First problem: compiler error; cannot increment `totalIntegral`
(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 int64_t index) {
    const double x =
      lower + (index/numberOfIntervals) * (upper - lower);
    *totalIntegralPointer += function(x);},
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    const double x =
      lower + (index/numberOfIntervals) * (upper - lower);
    *totalIntegralPointer += function(x);},
  );
totalIntegral *= dx;
```

Second problem: race condition

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

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

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Important concept: Reduction

Reductions combine the results contributed by parallel work.

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Important concept: Reduction

Reductions combine the results contributed by parallel work.

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

```
double finalReducedValue = 0;
#pragma omp parallel for reduction(+:finalReducedValue)
for (int64_t i = 0; i < N; ++i) {
  finalReducedValue += ...
}
```

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

Important concept: Reduction

Reductions combine the results contributed by parallel work.

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

```
double finalReducedValue = 0;
#pragma omp parallel for reduction(+:finalReducedValue)
for (int64_t i = 0; i < N; ++i) {
  finalReducedValue += ...
}
```

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 (int64_t i = 0; i < numberOfIntervals; ++i) {
  totalIntegral += function(...);
}
```

Kokkos

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

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

Always name your kernels!

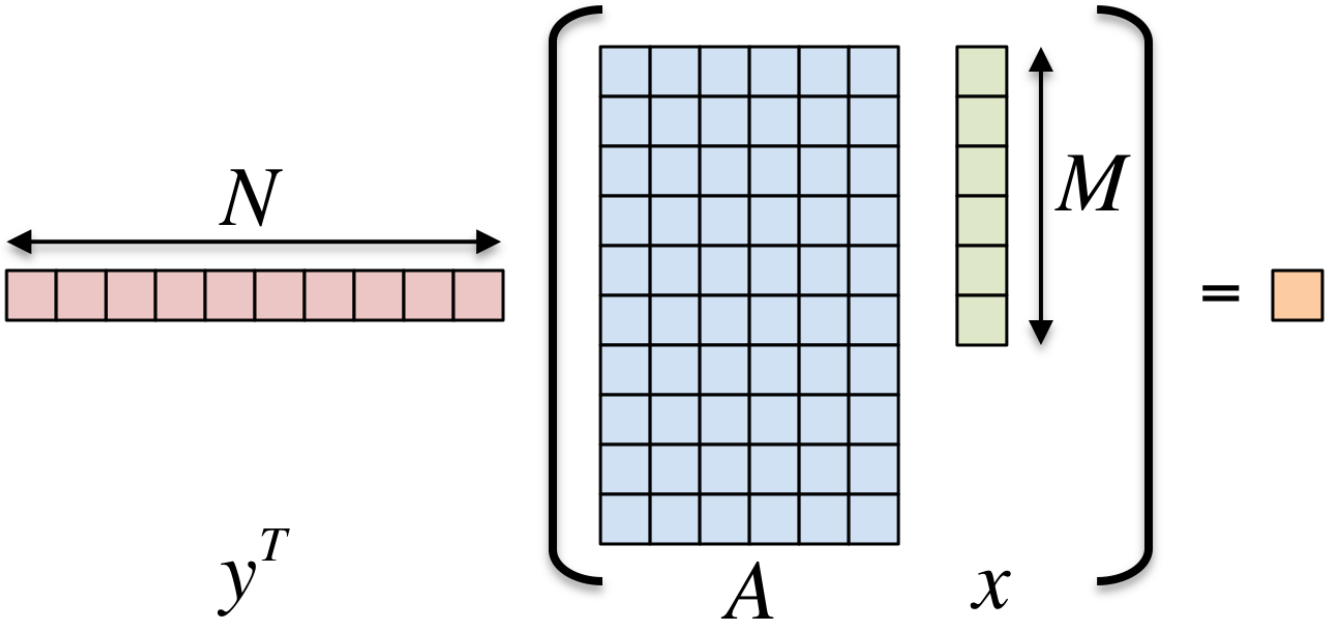
Giving unique names to each kernel is immensely helpful for debugging and profiling. You will regret it if you don't!

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

Example:

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

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



Details:

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

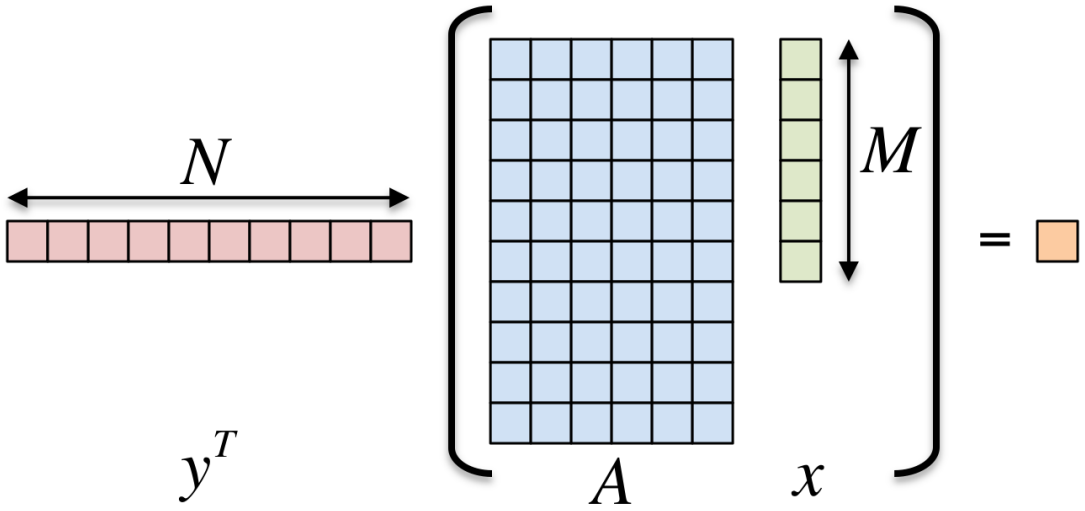
The **first step** in using Kokkos is to include, initialize, and finalize:

```
#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 or environment variables:

`--kokkos-num-threads=INT` or `KOKKOS_NUM_THREADS`	total number of threads
`--kokkos-device-id=INT` or `KOKKOS_DEVICE_ID`	device (GPU) ID to use

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



Details:

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

Compiling for CPU

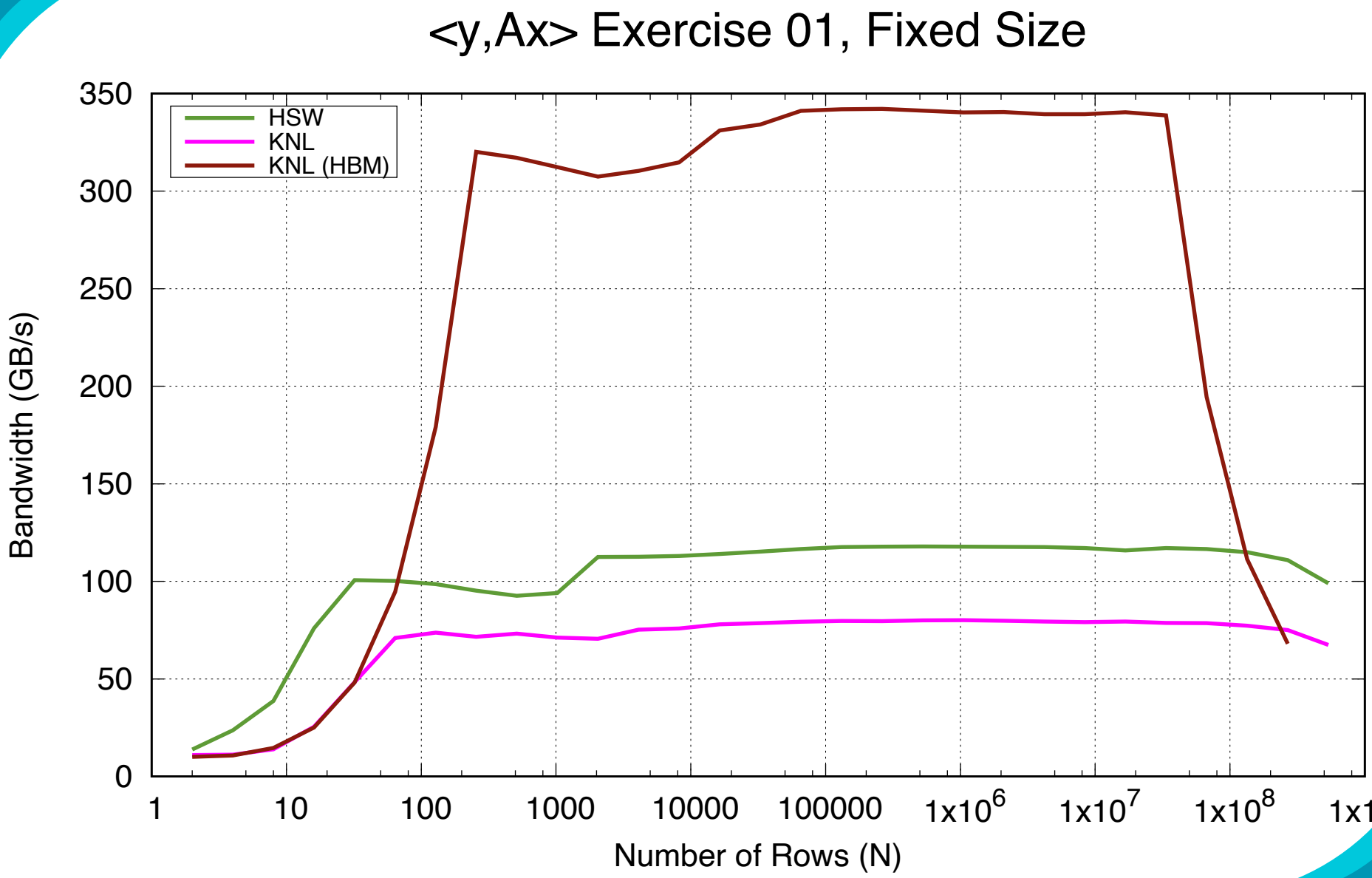
```
# gcc using OpenMP (default) and Serial back-ends,
# (optional) change non-default arch with KOKKOS_ARCH
  make -j KOKKOS_DEVICES=OpenMP,Serial KOKKOS_ARCH=...
```

Running on CPU with OpenMP back-end

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

Things to try:

- Vary problem size with cline arg -S s
- Vary number of rows with cline arg -N n
- Num rows $= 2^n$, num cols $= 2^m$, total size $= 2^s == 2^{n+m}$


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

- **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("DAXPY",N, [=] (const int64_t i) {
    y[i] = a * x[i] + y[i];
  });
```

Functor

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

View abstraction

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

High-level example of Views for daxpy using lambda:

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

parallel_for("DAXPY",N, [=] (const int64_t i) {
    // Views x and y are captured by value (shallow copy)
    y(i) = a * x(i) + y(i);
  });
```

Important point

Views are **like pointers**, so copy them in your functors.

View overview:

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

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  e.g., 2x20, 50x50, etc.
- Access elements via "(...)" operator.

Example:

```
View<double***> data("label", N0, N1, N2); //3 run, 0 compile
View<double**[N2]> data("label", N0, N1);  //2 run, 1 compile
View<double*[N1][N2]> data("label", N0);   //1 run, 2 compile
View<double[N0][N1][N2]> data("label");    //0 run, 3 compile
//Access
data(i,j,k) = 5.3;
```

Note: runtime-sized dimensions must come first.

View life cycle:

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

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Example:

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

What gets printed?

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c(0,2) = 3;
print_value( a(0,2) );
```

What gets printed?

3.0

View Properties:

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

Example:

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

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

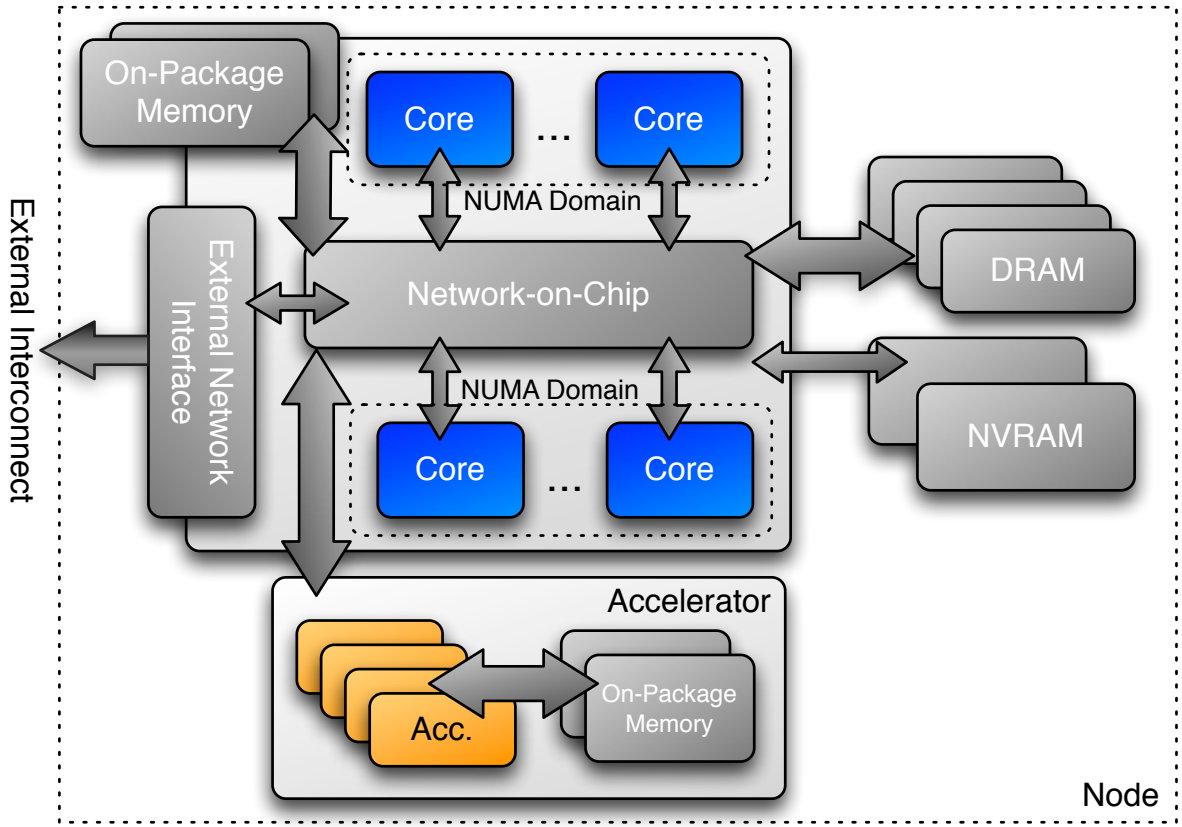
- Location: `Exercises/02/Begin/`
- Assignment: Change data storage from arrays to Views.
- Compile and run on CPU, and then on GPU with UVM

```
make -j KOKKOS_DEVICES=OpenMP  # CPU-only using OpenMP
make -j KOKKOS_DEVICES=Cuda    # GPU - note UVM in Makefile
# Run exercise
./02_Exercise.host -S 26
./02_Exercise.cuda -S 26
# Note the warnings, set appropriate environment variables
```

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

Execution Space

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



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

Changing the parallel execution space:

Custom

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

Default

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

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  [=] (const int64_t i) {
    /* ... body ... */
  });
```

Requirements for enabling execution spaces:

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

Kokkos function and lambda portability annotation macros:

Function annotation with `KOKKOS_INLINE_FUNCTION` macro

```
struct ParallelFunctor {
  KOKKOS_INLINE_FUNCTION
  double helperFunction(const int64_t s) const {...}
  KOKKOS_INLINE_FUNCTION
  void operator()(const int64_t index) const {
    helperFunction(index);
  }
}
// Where kokkos defines:
#define KOKKOS_INLINE_FUNCTION inline                              /* #if CPU-only */
#define KOKKOS_INLINE_FUNCTION inline __device__ __host__ /* #if CPU+Cuda */
```

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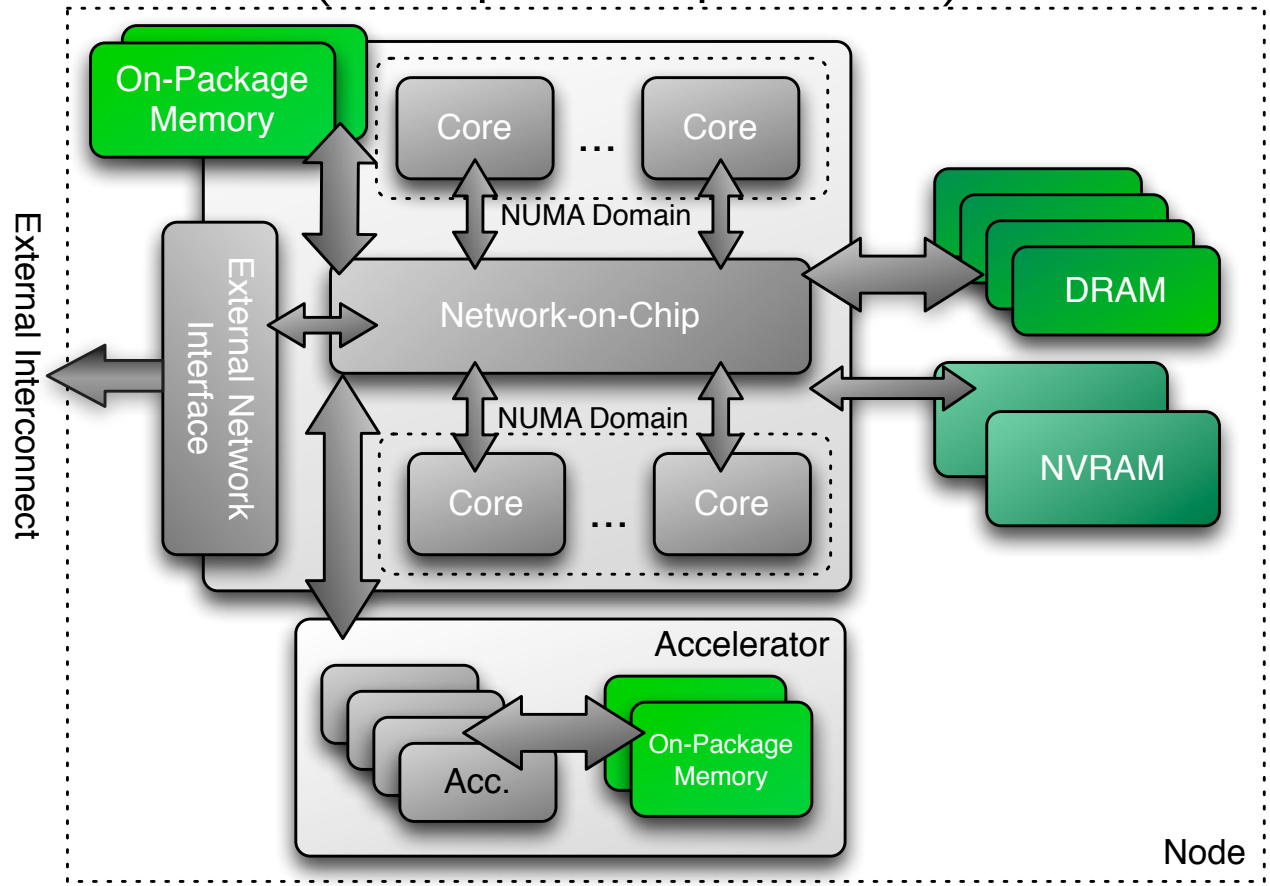
}
// Where kokkos defines:
#define KOKKOS_INLINE_FUNCTION inline                          /* #if CPU-only */
#define KOKKOS_INLINE_FUNCTION inline __device__ __host__ /* #if CPU+Cuda */
```

Lambda annotation with KOKKOS_LAMBDA macro

```
Kokkos::parallel_for("Label",numberOfIterations,
  KOKKOS_LAMBDA (const int64_t index) {...});

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

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



Important concept: Memory spaces

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

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- Available **memory spaces**:

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

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

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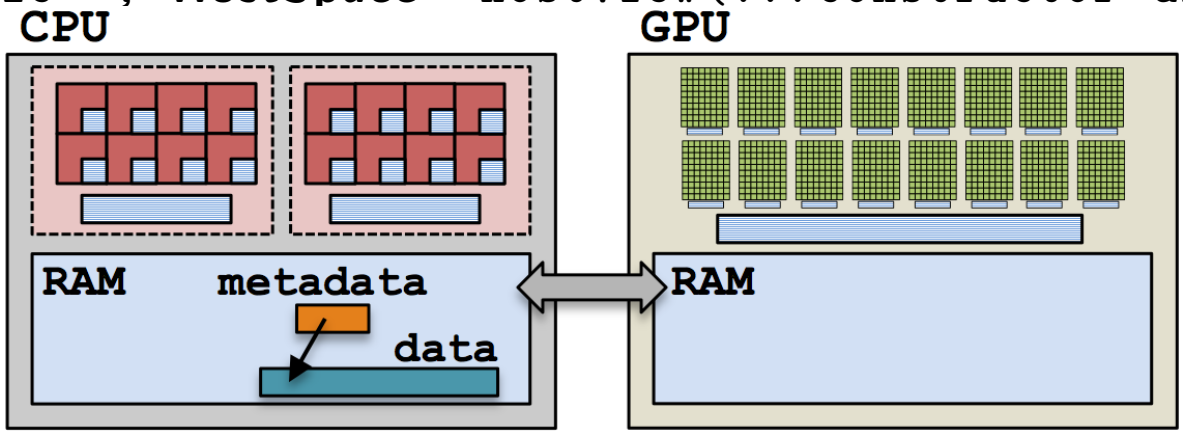
  `HostSpace, CudaSpace, CudaUVMSpace, ...` more
- Each **execution space** has a default memory space, which is used if **Space** provided is actually an execution space
- If no `Space` is provided, the view's data resides in the **default memory space** of the **default execution space**.

```
// Equivalent:
View<double*> a("A",N);
View<double*,DefaultExecutionSpace::memory_space> b("B",N);
```

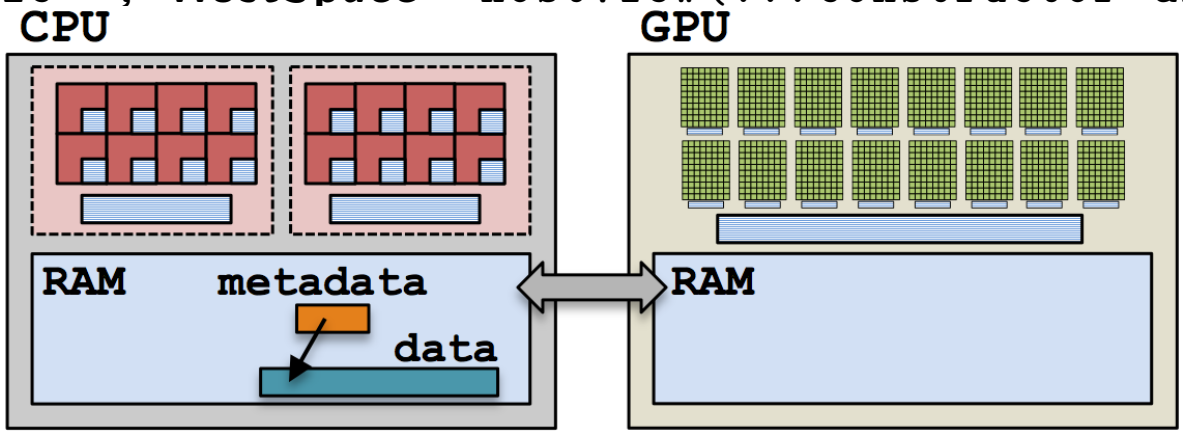
Example: HostSpace

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



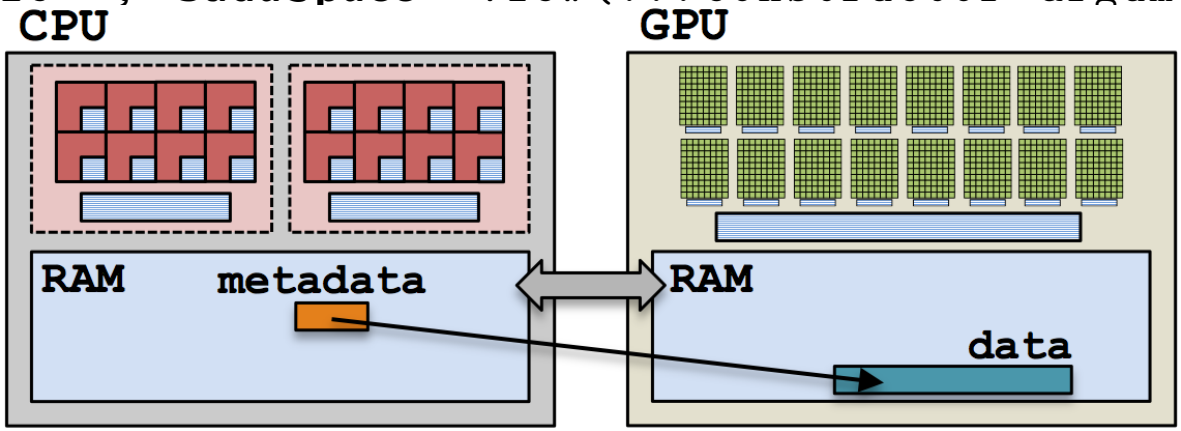
Example: HostSpace

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



Example: CudaSpace

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



Example (redux): summing an array with the GPU

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

```
View<double*, CudaSpace> array("array", size);
for (int64_t i = 0; i < size; ++i) {
  array(i) = ...read from file...
}

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

Example (redux): summing an array with the GPU

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

```
View<double*, CudaSpace> array("array", size);
for (int64_t i = 0; i < size; ++i) {
  array(i) = ...read from file...                    fault
}

double sum = 0;
Kokkos::parallel_reduce("Label",
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    valueToUpdate += array(index);
  },
  sum);
```

Example (redux): summing an array with the GPU

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

```
View<double*, HostSpace> array("array", size);
for (int64_t i = 0; i < size; ++i) {
  array(i) = ...read from file...
}

double sum = 0;
Kokkos::parallel_reduce("Label",
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  },
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```

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

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

What's the solution?

- `CudaUVMSpace`
- `CudaHostPinnedSpace` (skipping)
- Mirroring

Important concept: Mirrors

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

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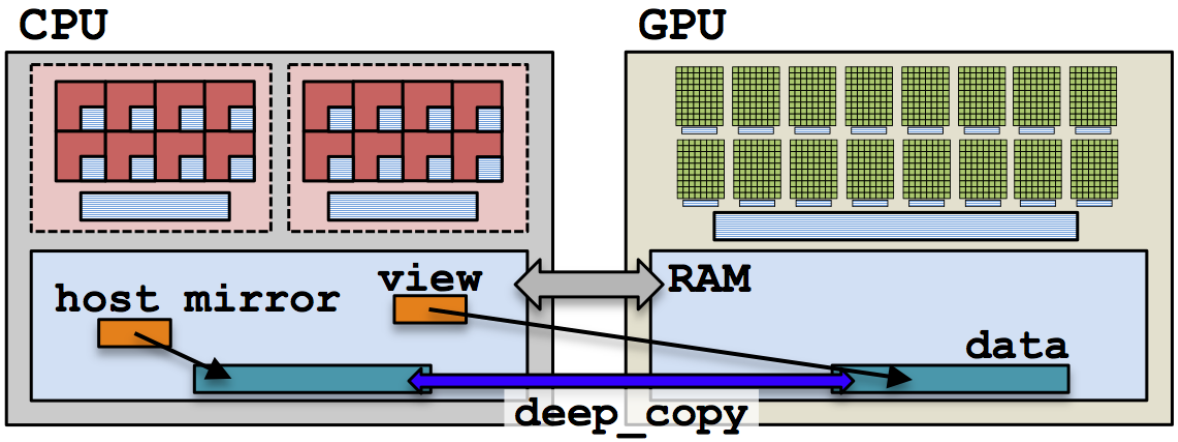
Mirroring schematic

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



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

```
using view_type = Kokkos::View<double*, Space>;
view_type view(...);
```

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```
using view_type = Kokkos::View<double*, Space>;
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2. **Create** `hostView`, a *mirror* of the `view`'s array residing in the host memory space.

```
view_type::HostMirror hostView =
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```

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

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

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

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```
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```
Kokkos::parallel_for("Label",
  RangePolicy< Space>(0, size),
  KOKKOS_LAMBDA (...) { use and change view });
```
6. If needed, **deep copy** the `view`'s updated array back to the `hostView`'s array to write file, etc.
```
Kokkos::deep_copy(hostView, view);
```

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

```
using ViewType = Kokkos::View<double*, Space>;
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: `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

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

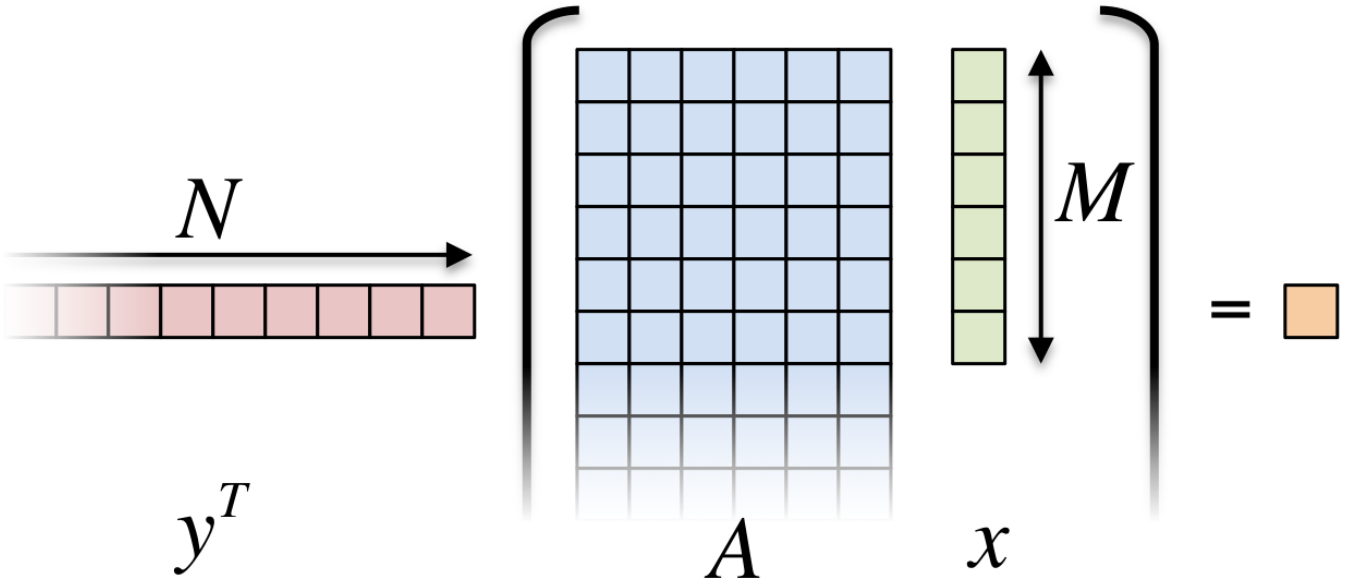
Managing memory access patterns for performance portability

Learning objectives:

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

Example: inner product (0)

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



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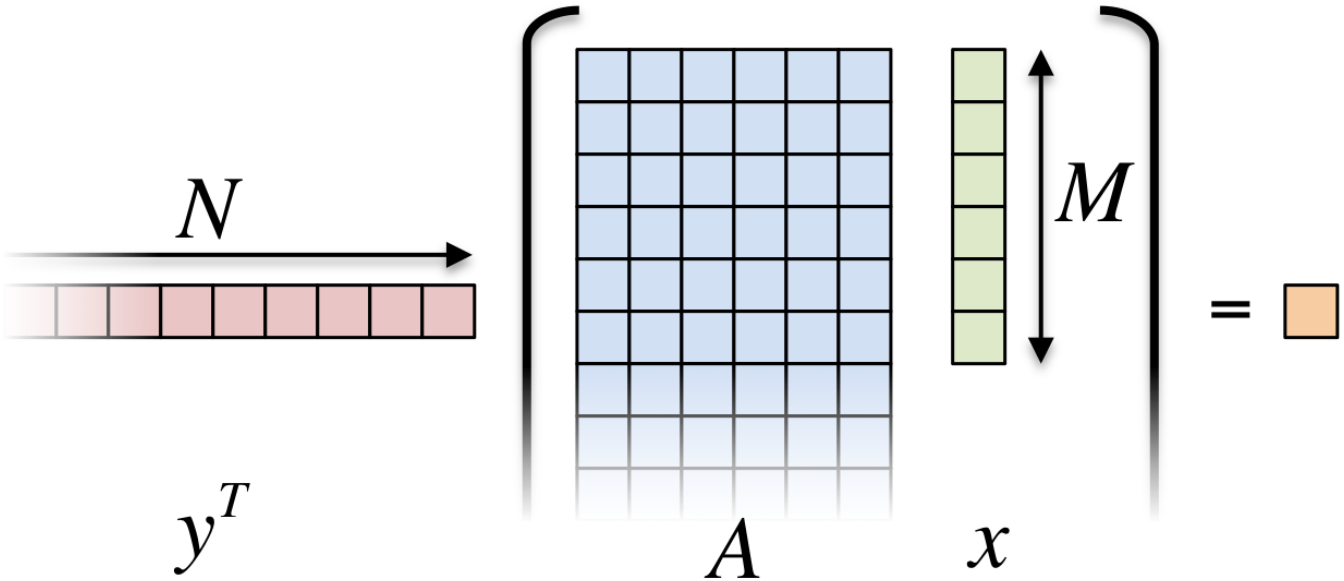
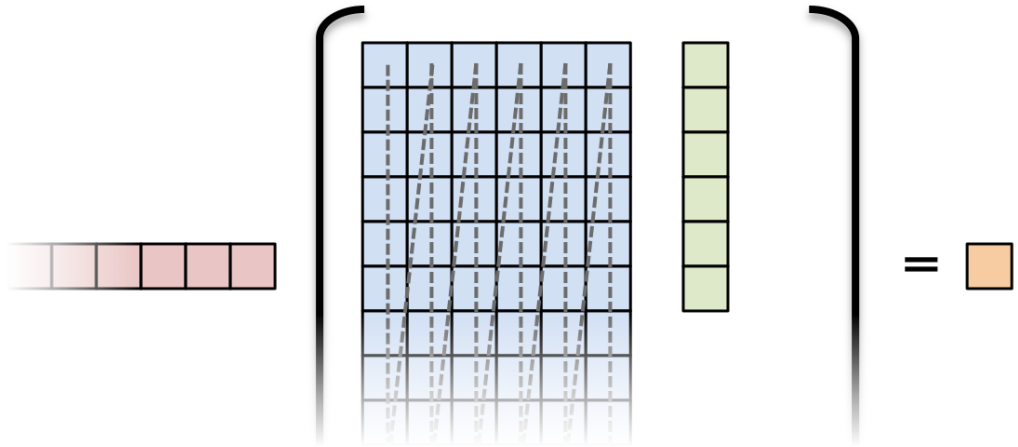


Driving question: How should A be laid out in memory?

Layout is the mapping of multi-index to memory:

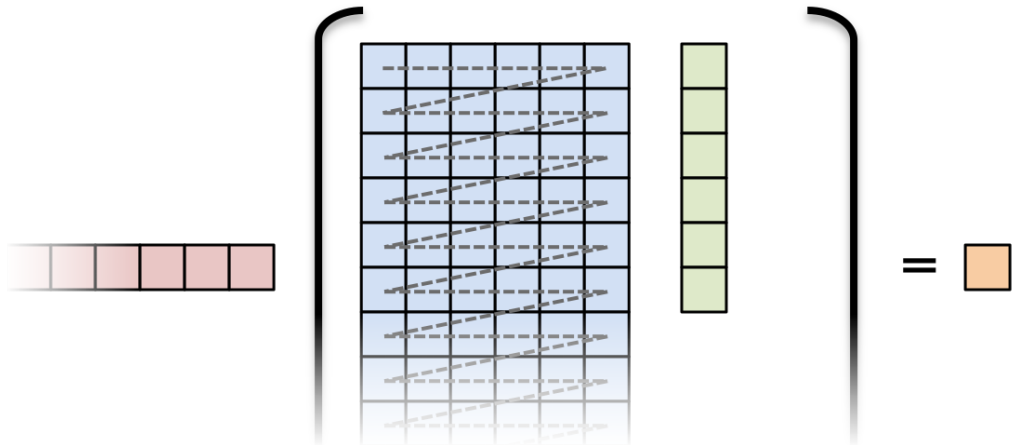
LayoutLeft

in 2D, "column-major"



LayoutRight

in 2D, "row-major"



Important concept: Layout

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

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

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

```
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```

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

Details:

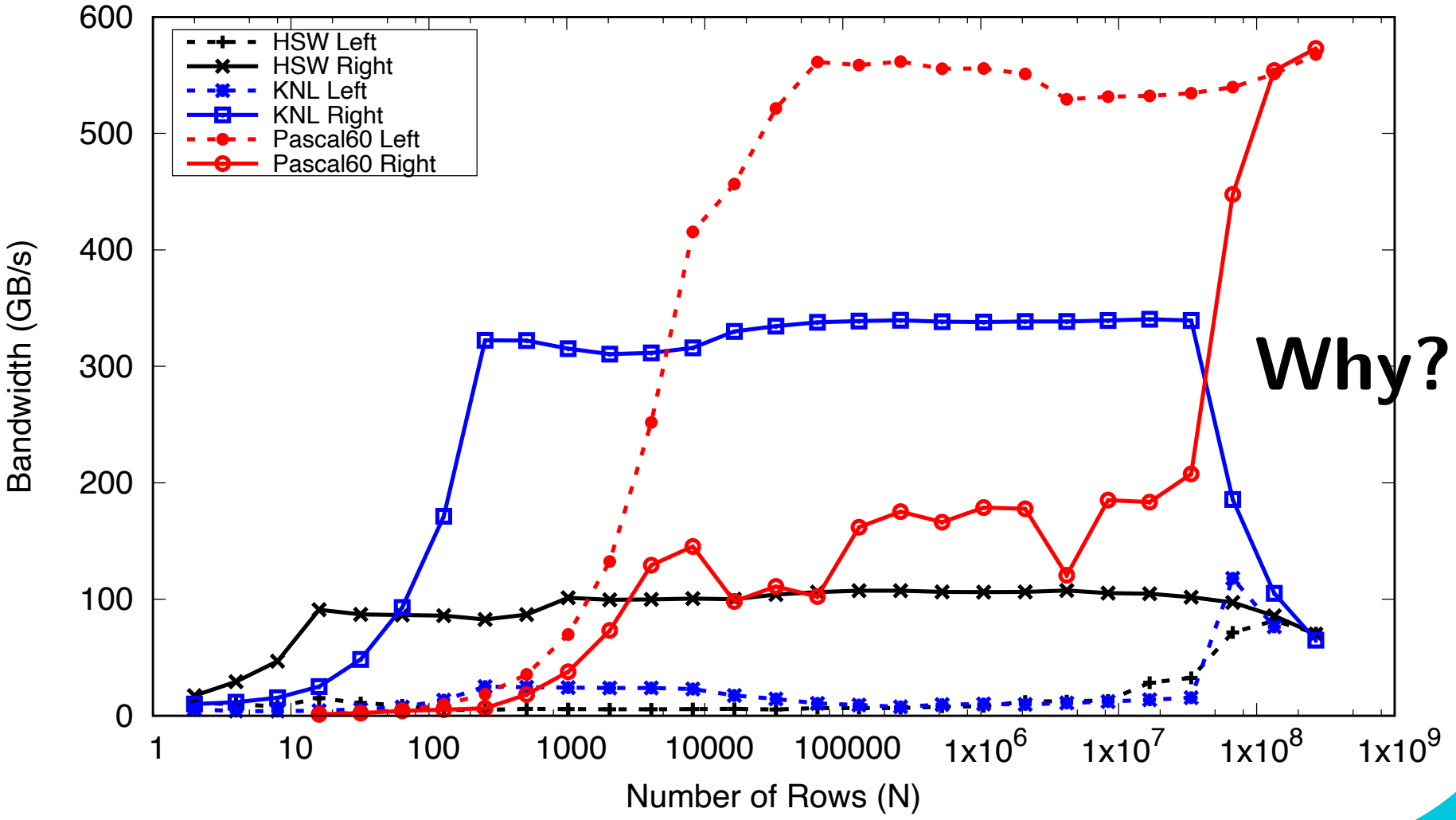
- Location: `Exercises/04/Begin/`
- Replace ‘‘`N`’’ in parallel dispatch with `RangePolicy<ExecSpace>`
- Add `MemSpace` to all `Views` and `Layout` to `A`
- Experiment with the combinations of `ExecSpace`, `Layout` to view performance

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.

<ylAx> Exercise 04 (Layout) Fixed Size

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



Thread independence:

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

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

Thread independence:

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

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

- **CPU** threads are independent.
  - i.e., threads may execute at any rate.

Thread independence:

```
operator()(int index, double & valueToUpdate) const {
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}
```

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 execute synchronized.
  - i.e., threads in groups can/must execute instructions together.

Thread independence:

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

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

Important point

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

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

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

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Warning

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

Rule of Thumb

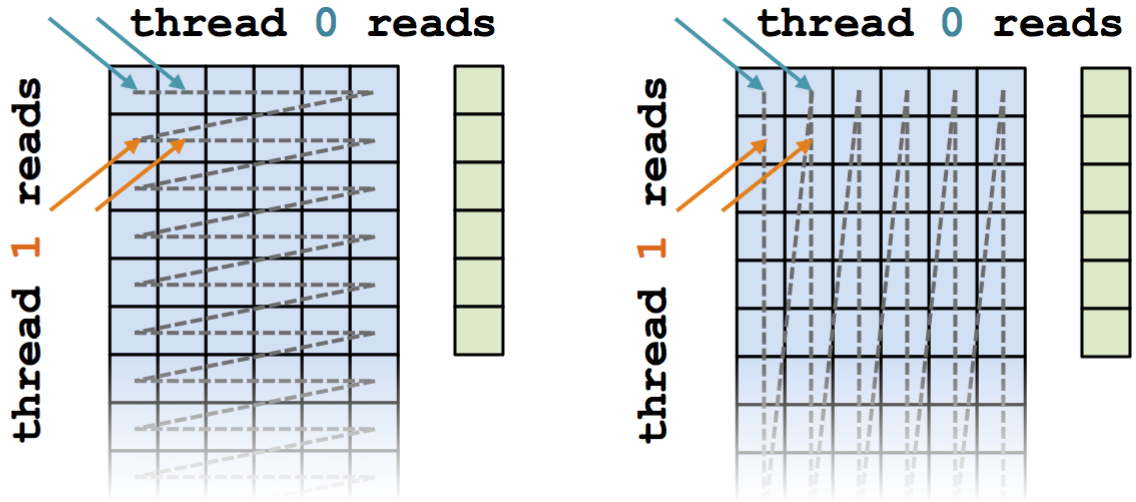
Kokkos index mapping and default layouts provide efficient access if **iteration indices** correspond to the **first index** of array.

Example:

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

Analysis: Kokkos architecture-dependent

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

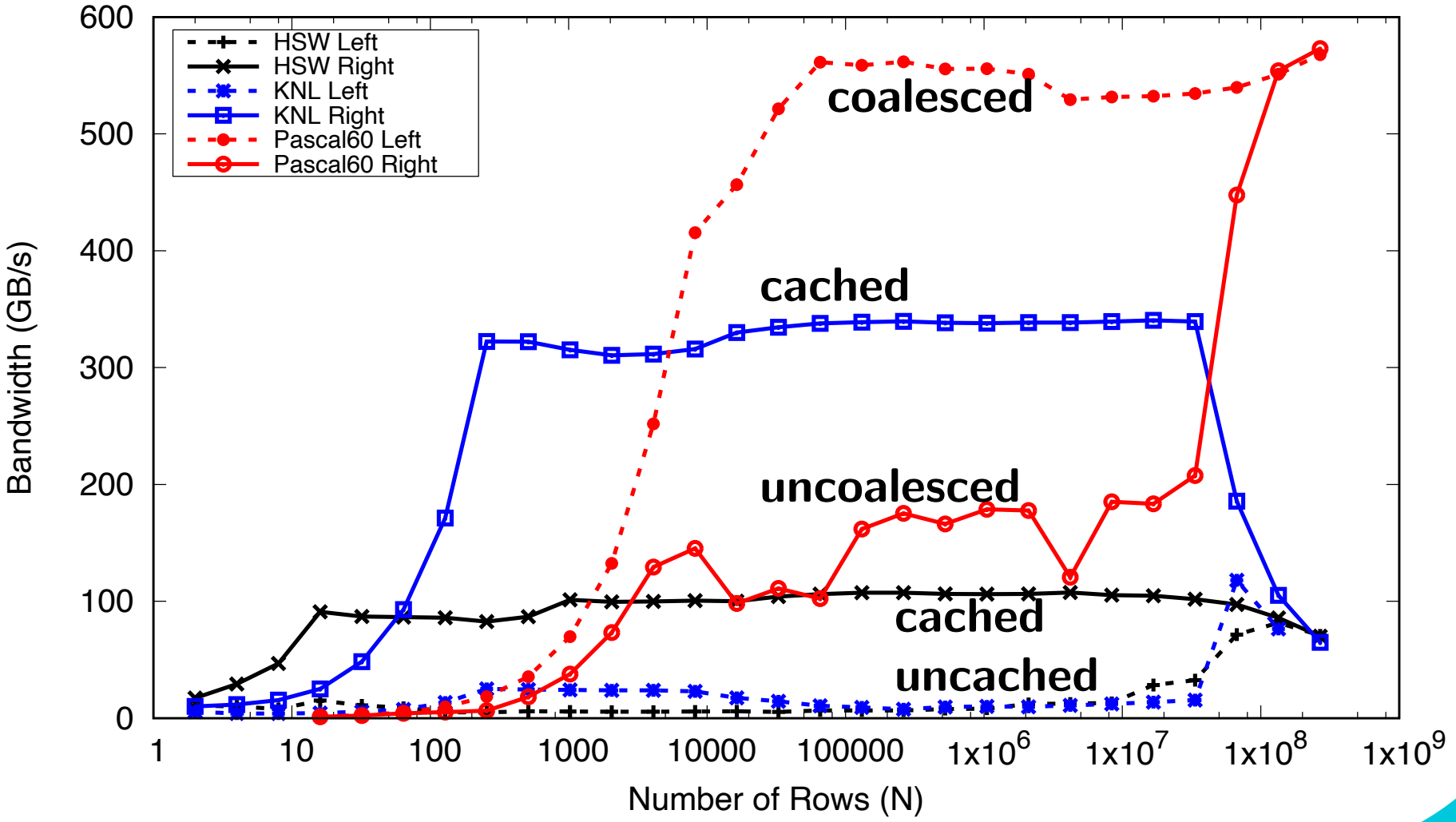


(a) OpenMP (b) Cuda

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

<ylAx> Exercise 04 (Layout) Fixed Size

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



Memory Access Pattern Summary

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

Exercise: Find x in $b = A * x$
Getting set up in your home directory:

```
mkdir Kokkos
cd Kokkos
git clone https://github.com/kokkos/kokkos
git clone https://github.com/kokkos/kokkos-tutorials
```

Find the exercise in the kokkos-tutorials/Exercises/cg-solve-hp folder.

The Begin subdirectory contains the code. Only cg_solve.cpp needs modifications.

Look for EXERCISE comments to find places to modify. Note: this contains the same Exercise components as the first cg-solve. So you can just start with the solution of that and add the new things! To make it clearer they are marked as EXERCISE-HP.

Tasks:

- Use HostMirrors instead of Unified Memory for GPUs.
- Use a hierarchical parallelism SPMV.

Things to try:

- Compare with previous exercise on GPU with low iteration count.
- Compare performance for small problems.
- Compare performance dependent on Layout of col_idx and values.

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- Tools for Profiling, Debugging and Tuning.
- Math Kernels.

The Kokkos Lectures

Watch the Kokkos Lectures for all of those and more in-depth explanations or do them on your own.

- Module 1: Introduction, Building and Parallel Dispatch
- Module 2: Views and Spaces
- Module 3: Data Structures + MultiDimensional Loops
- Module 4: Hierarchical Parallelism
- Module 5: Tasking, Streams and SIMD
- Module 6: Internode: MPI and PGAS
- Module 7: Tools: Profiling, Tuning and Debugging
- Module 8: Kernels: Sparse and Dense Linear Algebra

https://kokkos.link/the-lectures

Online Resources:

- https://github.com/kokkos:
  - Primary Kokkos GitHub Organization
- https://kokkos.link/the-lectures:
  - Slides, recording and Q&A for the Full Lectures
- https://github.com/kokkos/kokkos/wiki:
  - Wiki including API reference
- https://kokkosteam.slack.com:
  - Slack channel for Kokkos.
  - Please join: fastest way to get your questions answered.
  - Can whitelist domains, or invite individual people.