The Kokkos Lectures

The Compact Course

July 31, 2025

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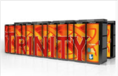
SAND2020-7475 PE

A 1-Day Tutorial

This lecture covers many concepts of Kokkos with Hands-On Exercises as homework.
Slides: https://github.com/kokkos/kokkos-tutorials/Intro-Medium/KokkosTutorial_Medium.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

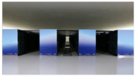


LANL/SNL Trinity
Intel Haswell / Intel KNL
OpenMP 3

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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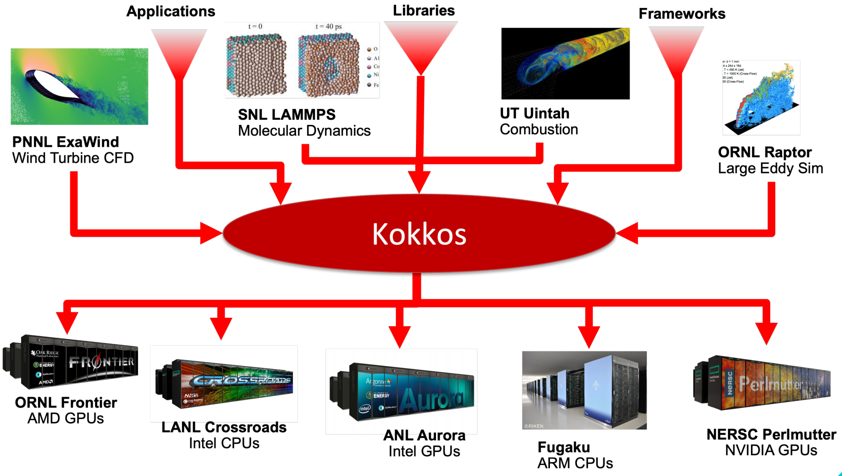
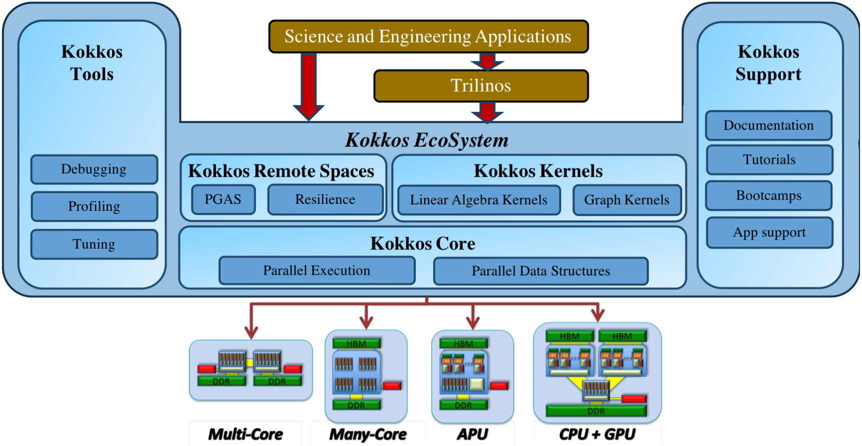
Software Cost Switching Vendors

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
- It is an Open Source project with a growing community
  - Maintained and developed at https://github.com/kokkos
  - Hundreds of users at many large institutions

Kokkos at the Center




Science and Engineering Applications
Trilinos
Kokkos Tools
Debugging
Profiling
Tuning
Kokkos EcoSystem
Kokkos Remote Spaces
PGAS
Resilience
Kokkos Kernels
Linear Algebra Kernels
Graph Kernels
Kokkos Core
Parallel Execution
Parallel Data Structures
Kokkos Support
Documentation
Tutorials
Bootcamps
App support
DDR
HBM
Multi-Core
Many-Core
APU
CPU + GPU

kokkos

Sandia National Laboratories

CSCS

Oak Ridge National Laboratory

Argonne National Laboratory

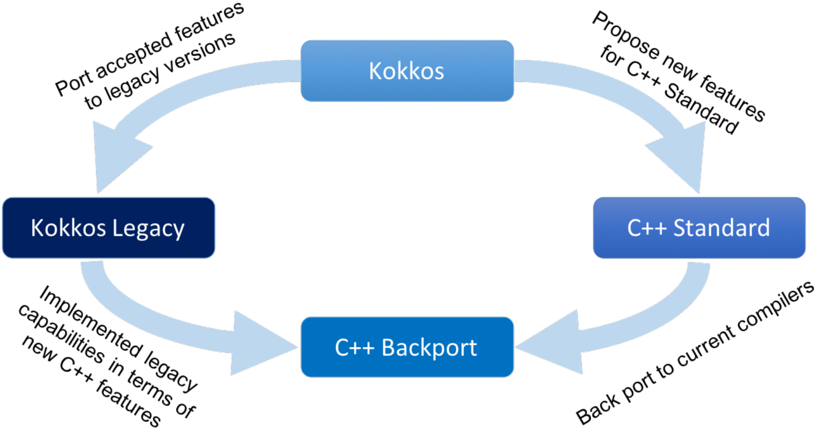
Los Alamos National Laboratory EST. 1943

Berkeley Lab

cea

NGA NexGen Analytics

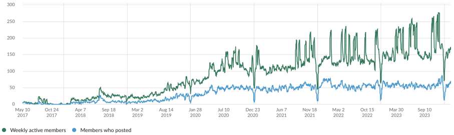
Kokkos helps improve ISO C++



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: 1.7k members from 100+ institutions
  - 15% Sandia Nat. Lab.
  - 24% other US Labs
  - 22% universities
  - 39% other
- GitHub: 1.9k 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) {
  atomForces[atomIndex] = calculateForce(...data...);
}
```

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

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

How is work assigned to functor operators?

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

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

```
struct Functor {
  void operator()(const 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;
  DataType _atomData;

  AtomForceFunctor(ForceType atomForces, DataType 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);
  }
);
```

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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

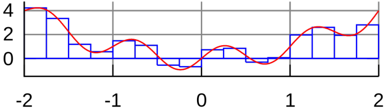
```
parallel_for(N, [=] (const int64_t i) {
  /* loop body */
});
```

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

Riemann-sum-style numerical integration:

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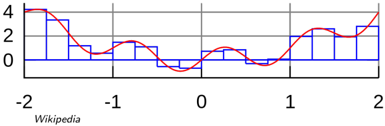


```
double totalIntegral = 0;
for (int64_t i = 0; i < numberOfIntervals; ++i) {
  const double x =
    lower + (i/numberOfIntervals) * (upper - lower);
  const double thisIntervalsContribution = function(x);
  totalIntegral += thisIntervalsContribution;
}
totalIntegral *= dx;
```

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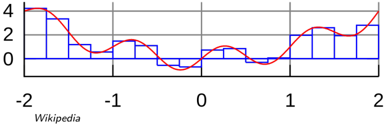


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How do we **parallelize** it? *Correctly?*

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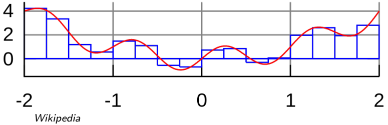

Pattern?

Policy?

Body?

```
double totalIntegral = 0;
for (int64_t i = 0; i < numberOfIntervals; ++i) {
  const double x =
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  const double thisIntervalsContribution = function(x);
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}
totalIntegral *= dx;
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How do we **parallelize** it? *Correctly?*

An (incorrect) attempt:

```
double totalIntegral = 0;
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  [=] (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);
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  );
totalIntegral *= dx;
```

Second problem: race condition

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

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

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Important concept: Reduction

Reductions combine the results contributed by parallel work.

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Reductions combine the results contributed by parallel work.

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

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

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

Important concept: Reduction

Reductions combine the results contributed by parallel work.

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;
#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!

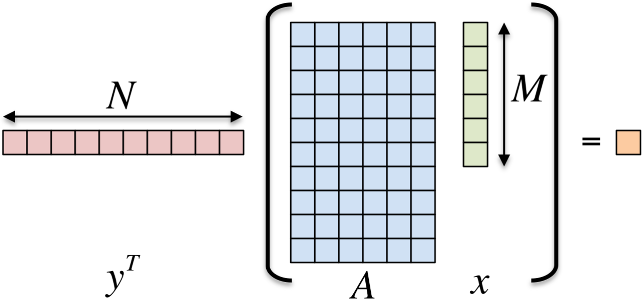
Giving unique names to each kernel is immensely helpful for debugging and profiling. You will regret it if you don't!

- 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

Exercise #1: include, initialize, finalize Kokkos

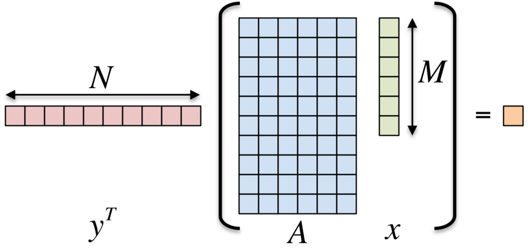
The **first step** in using Kokkos is to include, initialize, and finalize:

```
#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 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

```
cmake -B build_openmp -DKokkos_ENABLE_OPENMP=ON \
    -DCMAKE_BUILD_TYPE=Release
cmake --build build_openmp
```

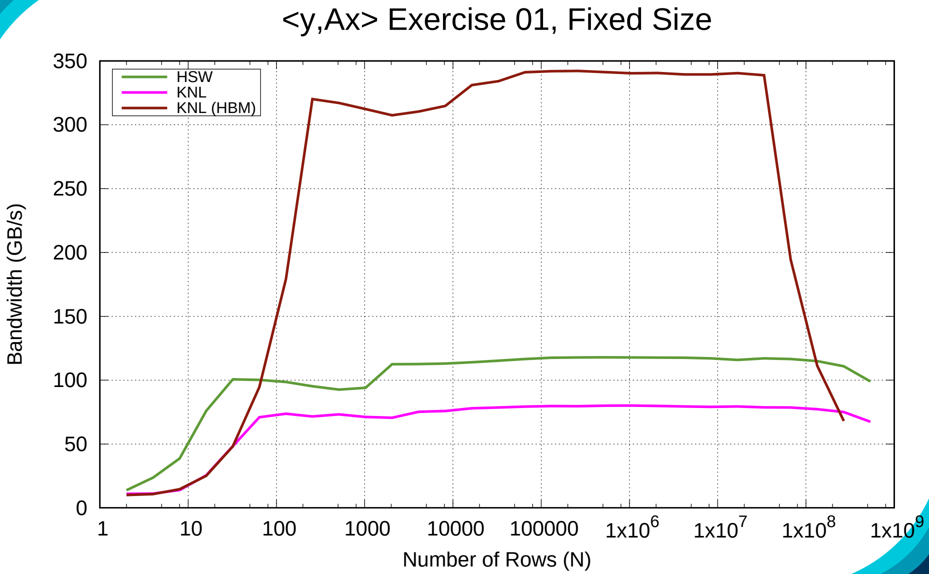
Running on CPU with OpenMP backend

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

Things to try:

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

Exercise #1 results



- **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.

View motivation

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.

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);
  });
```

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    // 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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- 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`

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?

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
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Example:

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a = b;
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a(0,2) = 1;
b(0,2) = 2;
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 SharedSpace.

```
# CPU-only using OpenMP
cmake -B build-openmp/  -DKokkos_ENABLE_OPENMP=On \
  -DCMAKE_BUILD_TYPE=Release
cmake --build build_openmp

# GPU build using SYCL
cmake -B build-sycl/ -DKokkos_ENABLE_SYCL=On \
  -DKokkos_ARCH_INTEL_PVC=On \
  -DCMAKE_BUILD_TYPE=Release
cmake --build build_sycl

# Run exercise
./build_openmp/02_Exercise -S 26
./build_sycl/02_Exercise -S 26
```

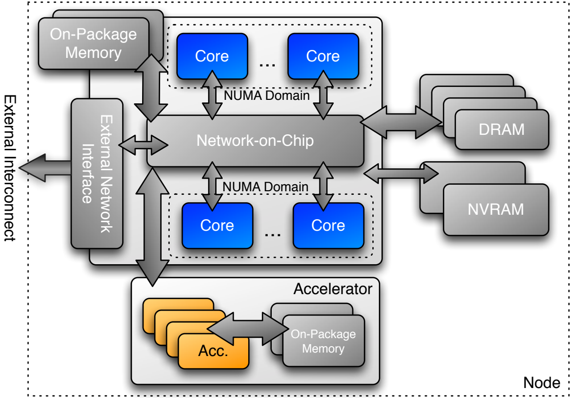
Execution and Memory Spaces

Learning objectives:

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

Execution Space

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



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

Execution spaces (2)

Host

Parallel

```
MPI_Reduce(...);
FILE * file = fopen(...);
runANormalFunction(...data...);
Kokkos::parallel_for("MyKernel", numberOfSomethings,
                     [=] (const int64_t somethingIndex) {
                       const double y = ...;
                       // do something interesting
                     }
                     );
```

Host

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

Parallel

- Where will Host code be run? CPU? GPU?
  ⇒ Always in the **host process**
  also known as **default host execution space**

Host

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MPI_Reduce(...);
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                     [=] (const int64_t somethingIndex) {
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                       // do something interesting
                     }
                     );
```

Parallel

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

  ⇒ Always in the **host process**

  also known as **default host execution space**
- Where will Parallel code be run? CPU? GPU?

  ⇒ The **default execution space**

Host

Parallel

```
MPI_Reduce(...);
FILE * file = fopen(...);
runANormalFunction(...data...);
Kokkos::parallel_for("MyKernel", numberOfSomethings,
                     [=] (const int64_t somethingIndex) {
                       const double y = ...;
                       // do something interesting
                     }
                     );
```

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

Changing the parallel execution space:

Custom

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

Default

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

Changing the parallel execution space:

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Default

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

Requirements for enabling execution spaces:

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

Kokkos function and lambda portability annotation macros:

Function annotation with KOKKOS_INLINE_FUNCTION macro

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

Kokkos function and lambda portability annotation macros:

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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/HIP
```

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/HIP
```

These macros are *already* defined by Kokkos.

Memory space motivating example: summing an array

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

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

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for (int64_t i = 0; i < size; ++i) {
  data(i) = ...read from file...
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Question: Where is the data stored? GPU memory? CPU memory? Both?

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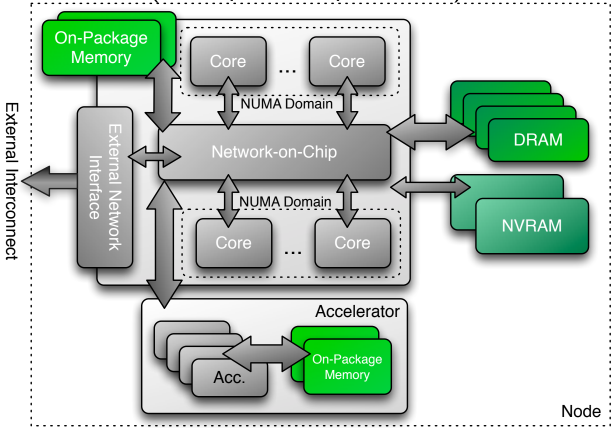

Question: Where is the data stored? GPU memory? CPU memory? Both?

$\Rightarrow$ **Memory Spaces**

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



Important concept: Memory spaces

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

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- Available **memory spaces**:

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

  Portable: `SharedSpace`, `SharedHostPinnedSpace`

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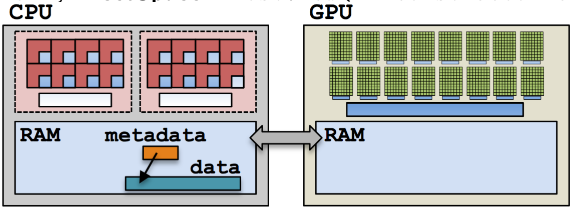
- Each **execution space** has a default memory space, which is used if **Space** provided is actually an execution space
- If no `Space` is provided, the view's data resides in the **default memory space** of the **default execution space**.

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

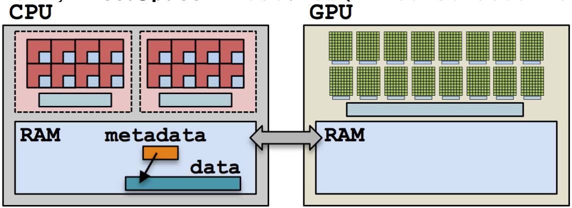
Example: HostSpace

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



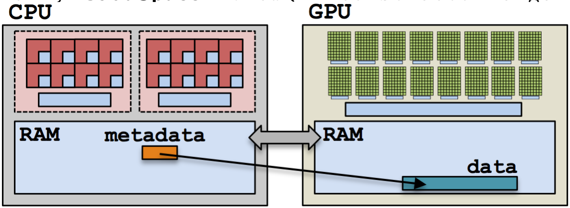
Example: HostSpace

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



Example: CudaSpace

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



Anatomy of a kernel launch:

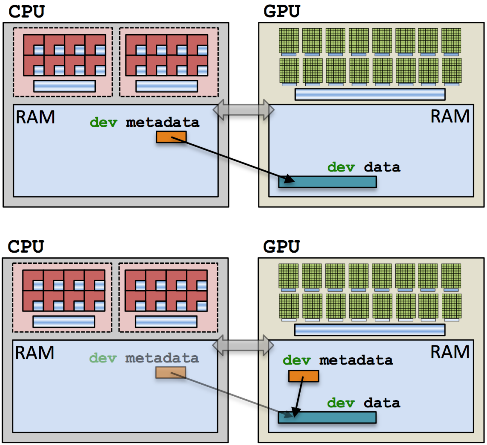
1. User declares views, allocating.
2. User instantiates a functor with views.
3. User launches `parallel_something`:
   - Functor is copied to the device.
   - Kernel is run.
   - Copy of functor on the device is released.

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

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

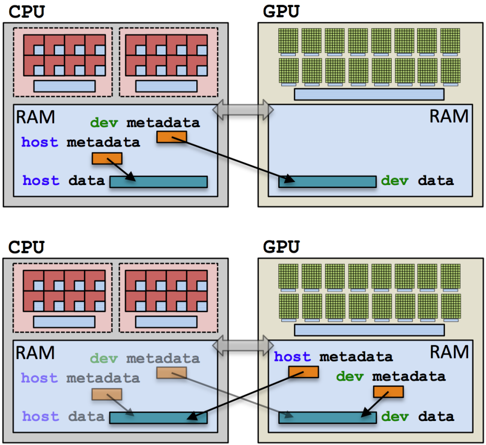
Example: one view

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



Example: two views

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



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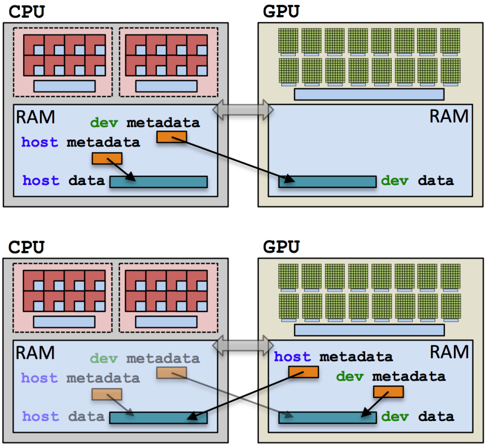
parallel_for("Label",N,
  KL (int i) {
    dev(i)  = ...;
    host(i) = ...;
  });
```



Example (redux): summing an array with the GPU

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

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

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

Example (redux): summing an array with the GPU

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

```
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for (int64_t i = 0; i < size; ++i) {
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}

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

Example (redux): summing an array with the GPU

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

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

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

Example (redux): summing an array with the GPU

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

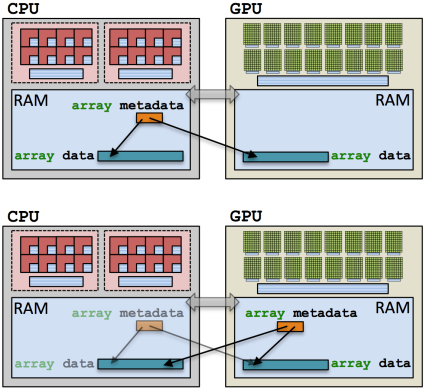
double sum = 0;
Kokkos::parallel_reduce("Label",
  RangePolicy< Cuda>(0, size),
  KOKKOS_LAMBDA (const int64_t index, double & valueToUpdate) {
    valueToUpdate += array(index);                illegal access
  },
  sum);
```

What's the solution?

- SharedSpace
- SharedHostPinnedSpace (skipping)
- Mirroring

SharedSpace

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



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

Important concept: Mirrors

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

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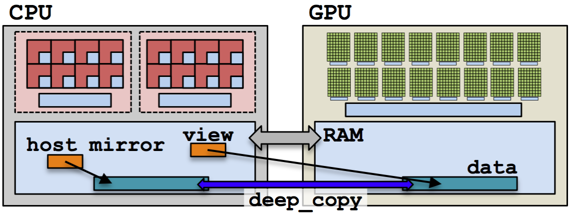
Mirroring schematic

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



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

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

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

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

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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 });
```

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

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

```
Kokkos::View<double*, Space> view("test", 10);
auto 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.
- create_mirror_view_and_copy allocates data if necessary and also **copies** 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

```
# CPU-only using OpenMP
cmake -B build-openmp/  -DKokkos_ENABLE_OPENMP=On \
  -DCMAKE_BUILD_TYPE=Release
cmake --build build_openmp

# GPU build using SYCL
cmake -B build-sycl/ -DKokkos_ENABLE_SYCL=On \
  -DKokkos_ARCH_INTEL_PVC=On \
  -DCMAKE_BUILD_TYPE=Release
cmake --build build_sycl

# Run exercise
./build_openmp/03_Exercise -S 26
./build_sycl/03_Exercise -S 26
```

- 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.

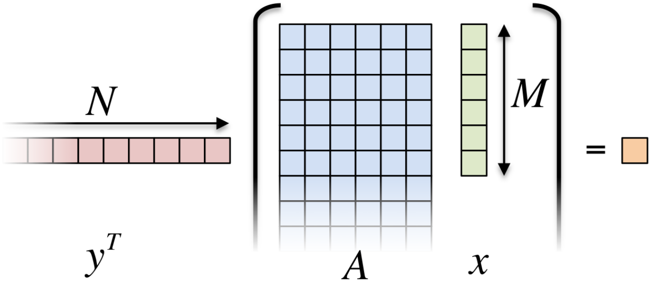
Managing memory access patterns for performance portability

Learning objectives:

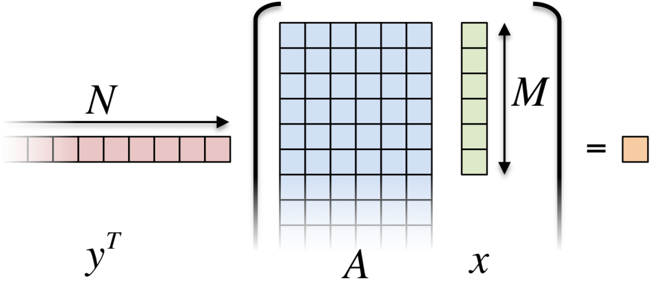
- How the `View`'s `Layout` parameter controls data layout.
- How memory access patterns result from Kokkos mapping parallel work indices **and** layout of multidimensional array data
- Why memory access patterns and layouts have such a performance impact (caching and coalescing).
- See a concrete example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



```
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);
```

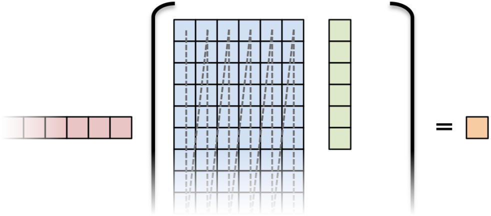


Driving question: How should A be laid out in memory?

Layout is the mapping of multi-index to memory:

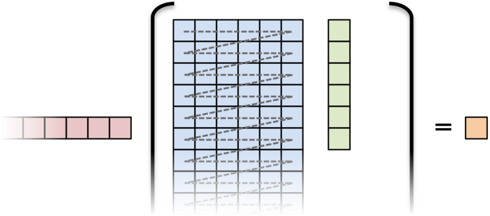
LayoutLeft

in 2D, “column-major”



LayoutRight

in 2D, “row-major”



Important concept: Layout

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

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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: $\approx$ 50 lines
- Advanced layouts: `LayoutStride`, `LayoutTiled`, ...

Exercise #4: Inner Product, Flat Parallelism

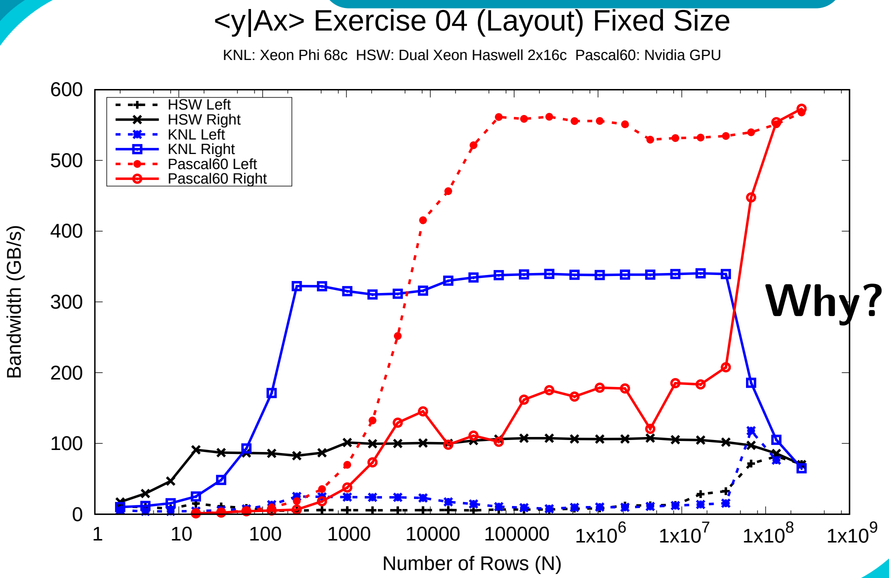
Details:

- 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
- On GPUs, compare using `SharedSpace` vs using the default memory space, i.e, not providing an explicit memory space.
- Check what happens if `MemSpace` and `ExecSpace` do not match.

Exercise #4: Inner Product, Flat Parallelism



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?

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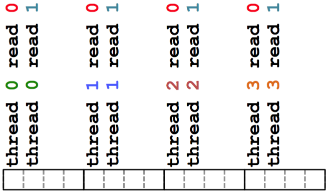
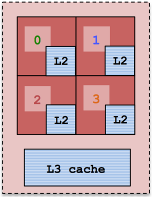
In particular, all threads in a group (*warp* or *wavefront*) must finished their loads before *any* thread can move on.

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

CPUs: few (independent) cores with separate caches:





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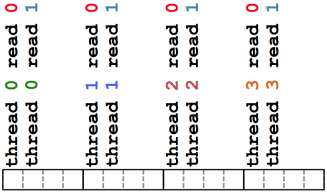
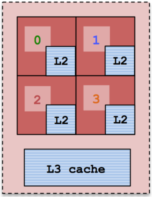
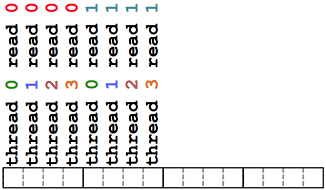
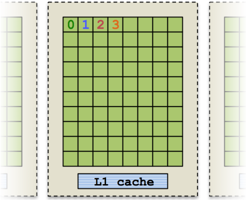




GPUs: many (synchronized) cores with a shared cache:





Important point

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

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

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Warning

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

Consider the array summation example:

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

double sum = 0;
Kokkos::parallel_reduce("Label",
  RangePolicy< Space>(0, size),
  KOKKOS_LAMBDA (const size_t index, double & valueToUpdate) {
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CPU	**GPU**

Why?

Iterating for the execution space:

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

Rule of Thumb

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

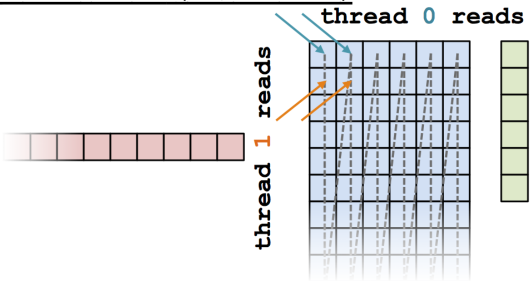
Example:

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

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`)



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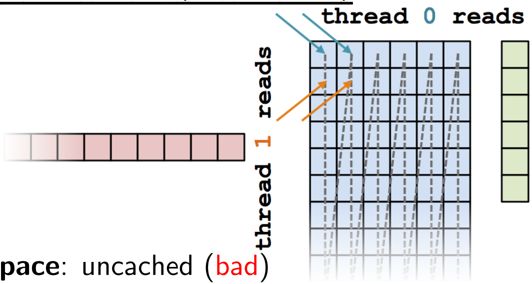
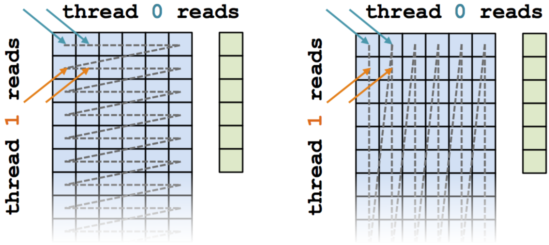


- **HostSpace**: uncached (bad)
- **CudaSpace**: coalesced (good)

Analysis: Kokkos architecture-dependent

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



(a) OpenMP (b) Cuda

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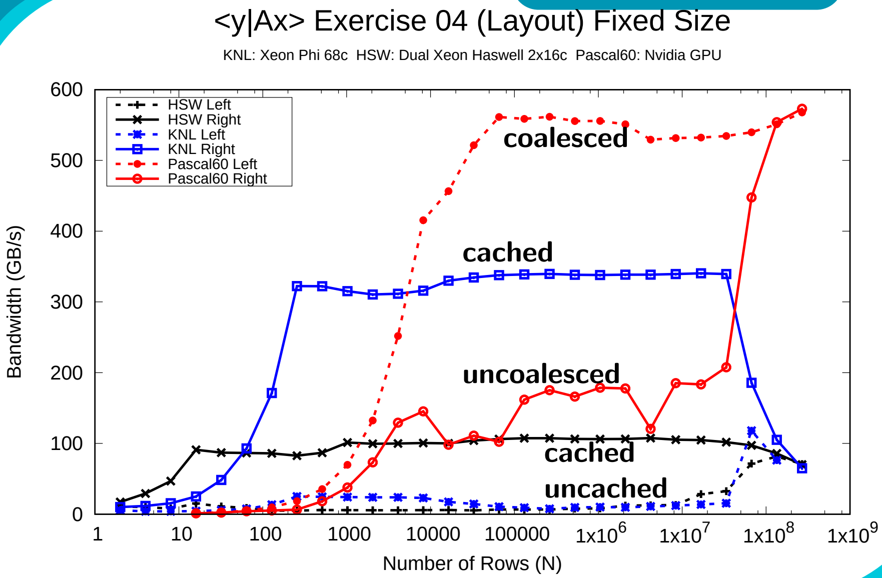
<y|Ax> Exercise 04 (Layout) Fixed Size
KNL: Xeon Phi 68c HSW: Dual Xeon Haswell 2x16c Pascal60: Nvidia GPU
HSW Left
HSW Right
KNL Left
KNL Right
Pascal60 Left
Pascal60 Right
coalesced
cached
uncoalesced
cached
uncached
Bandwidth (GB/s)
Number of Rows (N)
600
500
400
300
200
100
0
1
10
100
1000
10000
100000
1x10^6
1x10^7
1x10^8
1x10^9

- 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.

Advanced Reductions

Learning objectives:

- How to use Reducers to perform different reductions.
- How to do multiple reductions in one kernel.
- Using `Kokkos::View`'s as result for asynchronicity.
- Custom reductions

So far only "sum" reduction. What about other things? Using a Reducer:

```
double max_value = 0;
parallel_reduce("Label", numberOfIntervals,
  KOKKOS_LAMBDA(const int64_t i, double & valueToUpdate) {
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- Some reducers (like `MinLoc`) use special scalar types!
- Custom value types supported via specialization of `reduction_identity`.

Sometimes multiple reductions are needed

- Provide multiple reducers/result arguments
- Functor/Lambda operator takes matching thread-local variables
- Mixing scalar types is fine.

```
float max_value = 0;
double sum = 0;
parallel_reduce("Label", numberOfIntervals,
    KOKKOS_LAMBDA(const int64_t i,float& tl_max,double& tl_sum){
  float a_i = a[i];
  if(a_i > tl_max) tl_max = a_i;
  tl_sum += a_i;
}, Kokkos::Max<float>(max_value),sum);
```

Reducing into a Scalar is blocking!

- Providing a reference to scalar means no lifetime expectation.
  - Call to `parallel_reduce` returns after writing the result.
- `Kokkos::View` can be used as a result, allowing for potentially non-blocking execution.
- Can provide `View` to host memory, or to memory accessible by the `ExecutionSpace` for the reduction.
- Works with Reducers too!

```
View<double,HostSpace> h_sum("sum_h");
View<double,CudaSpace> d_sum("sum_d");
using policy_t = RangePolicy<Cuda>;

parallel_reduce("Label", policy_t(0,N), SomeFunctor,
  h_sum);

parallel_reduce("Label", policy_t(0,N), SomeFunctor,
  Kokkos::Sum<double,CudaSpace>(d_sum));
```

Pseudocode for Kokkos implementation

```
per_thread:
  value& tmp=init(local_tmp);
  for (i in local range)
    functor(i, tmp)
call join for merging values between threads
  in the same thread group
let one (the last) thread group merge all results
  from all thread groups
call final(result) on one thread
```

Three ingredients

- init (optional), default: default constructor
- join (required)
- final (optional), default: no-op

Rules for choosing reduction behavior

1. If a reducer is specified (return type is a functor with `reducer` alias to itself), use that.
2. If functor implements `join`, use functor as reducer.
3. Otherwise, assume `join` behaves like `operator+`.

Note that the functor's `init`, `join`, `final` members must be tagged if the call operator is tagged. The reducers member functions must never be tagged.

```
class Reducer {
  public:
    using reducer     = Reducer;
    using value_type = ... ;
    using result_view_type = Kokkos::View<value_type, ... >;

    KOKKOS_FUNCTION
    void join(value_type& dest, const value_type& src) const;

    //optional
    KOKKOS_INLINE_FUNCTION
    void init(value_type& val) const;

    //optional
    KOKKOS_INLINE_FUNCTION
    void final(value_type& val) const;

    KOKKOS_INLINE_FUNCTION
    value_type& reference() const;

    KOKKOS_INLINE_FUNCTION
    result_view_type view() const;

    KOKKOS_INLINE_FUNCTION
    Reducer(value_type& value_);

    KOKKOS_INLINE_FUNCTION
    Reducer(const result_view_type& value_);
};
```

Subviews: Taking slices of Views

Learning objectives:

- Introduce Kokkos::subview—basic capabilities and syntax
- Suggested usage and practices
- View assignment rules

Sometimes you have to call functions on a subset of data:

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Example: call a frobenius norm on a matrix slice of a rank-3 tensor:

```
double special_norm(View<double***> tensor, int i) {

  auto matrix = ???;
  // Call a function that takes a matrix:
  return some_library::frobenius_norm(matrix);
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```
tensor(i,:,:)
```

Kokkos can do that too!

Subview

`Kokkos::subview` can be used to get a view to a subset of an existing `View`.

Subview description:

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- Can be constructed on host or within a kernel, since no allocation of memory occurs
- Similar capability as provided by Matlab, Fortran, Python, etc., using “colon” notation

Introductory Usage Demo:

Given a `View`:

```
Kokkos::View<double***> v("v", N0, N1, N2);
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slicei0 = v(i0, :, :);
```

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

```
auto sv_i0 =
  Kokkos::subview(v, i0, Kokkos::ALL, Kokkos::ALL);

// Just like in Python, you can do the same thing with
// the equivalent of v(i0, 0:N1, 0:N2)
auto sv_i0_other =
  Kokkos::subview(v, i0, Kokkos::make_pair(0, N1),
                         Kokkos::make_pair(0, N2));
```

Subview can take three types of slice arguments:

- **Index**
  - For every index i the rank of the resulting `View` is decreased by one.
  - Must be between $0 <= i < extent(dim)$
- **Kokkos::pair**
  - References a half-open range of indices.
  - The begin and end must be within the extents of the original view.
- **Kokkos::ALL**
  - References the entire extent in that dimension.
  - Equivalent to providing `make_pair(0,v.extent(dim))`

Usage notes:

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  - The return type of `Kokkos::subview()` is implementation defined for performance reasons
  - You can also use `decltype(subview(/*...*/))` if you really need to spell name of the type somewhere

Usage notes:

- Use `auto` for the type of a subview (unless you can't)
  - The return type of `Kokkos::subview()` is implementation defined for performance reasons
  - You can also use `decltype(subview(/*...*/))` if you really need to spell name of the type somewhere
- Use `Kokkos::pair` for partial ranges if subview created within a kernel

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- Constructing subviews in inner loop code can have performance implications (for now. . .)
  - This will likely be far less of an issue in the future.
  - Prioritize readability and maintainability first, then make changes only if you see a performance impact.

Details:

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

```
# Compile for CPU
cmake -B build_openmp -DKokkos_ENABLE_OPENMP=ON
cmake --build build_openmp
# Run on CPU
./build_openmp/subview_exercise -S 26
# Note the warnings, set appropriate environment variables
# Compile for GPU
cmake -B build_cuda -DKokkos_ENABLE_CUDA=ON
cmake --build build_cuda
# Run on GPU
./build_cuda/subview_exercise -S 26
```

`View::operator=()` **just does the "Right Thing"™**

- `View<int**> a; a = View<int*[5]>("b", 4)`

`View::operator=()` just does the "Right Thing"™

- `View<int**> a; a = View<int*[5]>("b", 4)` => Okay

`View::operator=()` **just does the "Right Thing"™**

- `View<int**> a; a = View<int*[5]>("b", 4)` => Okay
- `View<int*[5]> a; a = View<int**>("b", 4, 5)`

`View::operator=()` **just does the "Right Thing"™**

- `View<int**> a; a = View<int*[5]>("b", 4)` => Okay
- `View<int*[5]> a; a = View<int**>("b", 4, 5)` => Okay, checked at runtime

`View::operator=()` just does the "Right Thing"™

- `View<int**> a; a = View<int*[5]>("b", 4)` => Okay
- `View<int*[5]> a; a = View<int**>("b", 4, 5)`
  => Okay, checked at runtime
- `View<int*[5]> a; a = View<int*[3]>("b", 4)`

`View::operator=()` **just does the "Right Thing"™**

- `View<int**> a; a = View<int*[5]>("b", 4)` => Okay
- `View<int*[5]> a; a = View<int**>("b", 4, 5)`
  => Okay, checked at runtime
- `View<int*[5]> a; a = View<int*[3]>("b", 4)`
  => Compilation error

`View::operator=()` **just does the "Right Thing"™**

- `View<int**> a; a = View<int*[5]>("b", 4)` => Okay
- `View<int*[5]> a; a = View<int**>("b", 4, 5)`
  => Okay, checked at runtime
- `View<int*[5]> a; a = View<int*[3]>("b", 4)`
  => Compilation error
- `View<int*[5]> a; a = View<int**>("b", 4, 3)`

`View::operator=()` **just does the "Right Thing"™**

- `View<int**> a; a = View<int*[5]>("b", 4)` => Okay
- `View<int*[5]> a; a = View<int**>("b", 4, 5)`
  => Okay, checked at runtime
- `View<int*[5]> a; a = View<int*[3]>("b", 4)`
  => Compilation error
- `View<int*[5]> a; a = View<int**>("b", 4, 3)`
  => Runtime error

Aside: View Assignment (1)

`View::operator=()` **just does the “Right Thing”™**

- `View<int**> a; a = View<int*[5]>("b", 4)` => Okay
- `View<int*[5]> a; a = View<int**>("b", 4, 5)` => Okay, checked at runtime
- `View<int*[5]> a; a = View<int*[3]>("b", 4)` => Compilation error
- `View<int*[5]> a; a = View<int**>("b", 4, 3)` => Runtime error
- `View<int*, CudaSpace> a;`
  `a = View<int*, HostSpace>("b", 4)`

`View::operator=()` **just does the "Right Thing"™**

- `View<int**> a; a = View<int*[5]>("b", 4)` => Okay
- `View<int*[5]> a; a = View<int**>("b", 4, 5)`
  => Okay, checked at runtime
- `View<int*[5]> a; a = View<int*[3]>("b", 4)`
  => Compilation error
- `View<int*[5]> a; a = View<int**>("b", 4, 3)`
  => Runtime error
- `View<int*, CudaSpace> a;`
  `a = View<int*, HostSpace>("b", 4)`
  => Compilation error
- `View<int**, LayoutLeft> a;`
  `a = View<int**, LayoutRight>("b", 4, 5)`

`View::operator=()` **just does the "Right Thing"™**

- `View<int**> a; a = View<int*[5]>("b", 4)` => Okay
- `View<int*[5]> a; a = View<int**>("b", 4, 5)`
  => Okay, checked at runtime
- `View<int*[5]> a; a = View<int*[3]>("b", 4)`
  => Compilation error
- `View<int*[5]> a; a = View<int**>("b", 4, 3)`
  => Runtime error
- `View<int*, CudaSpace> a;`
  `a = View<int*, HostSpace>("b", 4)`
  => Compilation error
- `View<int**, LayoutLeft> a;`
  `a = View<int**, LayoutRight>("b", 4, 5)`
  => Compilation error

Aside: View Assignment (2)

`View::operator=()` **just does the "Right Thing"™**

- `View<const int*> a; a = View<int*>("b", 4)`

`View::operator=()` **just does the "Right Thing"™**

- `View<const int*> a; a = View<int*>("b", 4)`
  => Okay

`View::operator=()` **just does the "Right Thing"™**

- `View<const int*> a; a = View<int*>("b", 4)`
  => Okay
- `View<int*> a; a = View<const int*>("b", 4)`

`View::operator=()` **just does the "Right Thing"™**

- `View<const int*> a; a = View<int*>("b", 4)`
  => Okay
- `View<int*> a; a = View<const int*>("b", 4)`
  => Compilation error

`View::operator=()` **just does the "Right Thing"™**

- `View<const int*> a; a = View<int*>("b", 4)`
  => Okay
- `View<int*> a; a = View<const int*>("b", 4)`
  => Compilation error
- `View<int*[5], LayoutStride> a;`
  `a = View<int*[5], LayoutLeft>("b", 4)`

`View::operator=()` **just does the "Right Thing"™**

- `View<const int*> a; a = View<int*>("b", 4)` => Okay
- `View<int*> a; a = View<const int*>("b", 4)` => Compilation error
- `View<int*[5], LayoutStride> a;`
  `a = View<int*[5], LayoutLeft>("b", 4)` => Okay, converting compile-time strides into runtime strides

`View::operator=()` **just does the "Right Thing"™**

- `View<const int*> a; a = View<int*>("b", 4)`
  => Okay
- `View<int*> a; a = View<const int*>("b", 4)`
  => Compilation error
- `View<int*[5], LayoutStride> a;`
  `a = View<int*[5], LayoutLeft>("b", 4)` => Okay, converting compile-time strides into runtime strides
- `View<int*[5], LayoutLeft> a;`
  `a = View<int*[5], LayoutStride>("b", 4)`

`View::operator=()` just does the "Right Thing"™

- `View<const int*> a; a = View<int*>("b", 4)`
  => Okay
- `View<int*> a; a = View<const int*>("b", 4)`
  => Compilation error
- `View<int*[5], LayoutStride> a;`
  `a = View<int*[5], LayoutLeft>("b", 4)` => Okay,
  converting compile-time strides into runtime strides
- `View<int*[5], LayoutLeft> a;`
  `a = View<int*[5], LayoutStride>("b", 4)` => Okay,
  but only if strides match layout left (checked at runtime)

Given a `View`:

```
Kokkos::View<int***> v("v", n0, n1, n2);
```

- ```
  View<int***> a;
  a = Kokkos::subview(v, ALL, 42, ALL);
  ```
  ```

Given a `View`:

```
Kokkos::View<int***> v("v", n0, n1, n2);
```

- `View<int***> a;`
  `a = Kokkos::subview(v, ALL, 42, ALL);`
  => Compilation error

Given a View:

```
Kokkos::View<int***> v("v", n0, n1, n2);
```

- `View<int***> a;`
  `a = Kokkos::subview(v, ALL, 42, ALL);`
  => Compilation error
- `View<int*> a;`
  `a = Kokkos::subview(v, ALL, 5, 42);`

Given a `View`:

```
Kokkos::View<int***> v("v", n0, n1, n2);
```

- `View<int***> a;`
  `a = Kokkos::subview(v, ALL, 42, ALL);`
  => Compilation error
- `View<int*> a;`
  `a = Kokkos::subview(v, ALL, 5, 42);`
  => Okay for LayoutLeft but => Compilation error for LayoutRight

Given a `View`:

```
Kokkos::View<int***> v("v", n0, n1, n2);
```

- `View<int***> a;`
  `a = Kokkos::subview(v, ALL, 42, ALL);`
  => Compilation error
- `View<int*> a;`
  `a = Kokkos::subview(v, ALL, 5, 42);`
  => Okay for LayoutLeft but => Compilation error for LayoutRight
- `View<int**> a;`
  `a = Kokkos::subview(v, ALL, 15, ALL);`

Given a View:

```
Kokkos::View<int***> v("v", n0, n1, n2);
```

- `View<int***> a;`
  `a = Kokkos::subview(v, ALL, 42, ALL);`
  => Compilation error
- `View<int*> a;`
  `a = Kokkos::subview(v, ALL, 5, 42);`
  => Okay for LayoutLeft but => Compilation error for LayoutRight
- `View<int**> a;`
  `a = Kokkos::subview(v, ALL, 15, ALL);`
  => Runtime error (!)

Given a View:

```
Kokkos::View<int***> v("v", n0, n1, n2);
```

- `View<int***> a;`
  `a = Kokkos::subview(v, ALL, 42, ALL);`
  => Compilation error
- `View<int*> a;`
  `a = Kokkos::subview(v, ALL, 5, 42);`
  => Okay for LayoutLeft but => Compilation error for LayoutRight
- `View<int**> a;`
  `a = Kokkos::subview(v, ALL, 15, ALL);`
  => Runtime error (!)
- `View<int**, LayoutStride> a;`
  `a = Kokkos::subview(v, ALL, 15, ALL);`

Given a View:

```
Kokkos::View<int***> v("v", n0, n1, n2);
```

- `View<int***> a;`
  `a = Kokkos::subview(v, ALL, 42, ALL);`
  => Compilation error
- `View<int*> a;`
  `a = Kokkos::subview(v, ALL, 5, 42);`
  => Okay for LayoutLeft but => Compilation error for LayoutRight
- `View<int**> a;`
  `a = Kokkos::subview(v, ALL, 15, ALL);`
  => Runtime error (!)
- `View<int**, LayoutStride> a;`
  `a = Kokkos::subview(v, ALL, 15, ALL);`
  => Okay

- Use subviews to get a portion of a `View`. Helps with:
  - code reuse
  - code readability
  - library function compatibility

- Use subviews to get a portion of a `View`. Helps with:
  - code reuse
  - code readability
  - library function compatibility
- Kokkos supports slicing Views similar to Python/Matlab/Fortran slicing syntax

```
auto sv = Kokkos::subview(v, 42, ALL, std::make_pair(3, 17));
```

Subview Summary

- Use subviews to get a portion of a `View`. Helps with:
  - code reuse
  - code readability
  - library function compatibility
- Kokkos supports slicing Views similar to Python/Matlab/Fortran slicing syntax

```
auto sv = Kokkos::subview(v, 42, ALL, std::make_pair(3, 17));
```

- The return type of `subview` is complicated. Use **auto**!!
- `View::operator=()` just does the “Right Thing”™
  - So generally don’t worry about it at first! This is advanced stuff, and more for future reference.

Tightly Nested Loops with MDRangePolicy

Learning objectives:

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

Motivating example: Consider the nested for loops:

```
for ( int i = 0; i < N0; ++i )
for ( int j = 0; j < N1; ++j )
for ( int k = 0; k < N2; ++k )
  some_init_fcn(i, j, k);
```

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

```
Kokkos::parallel_for("Label", N0,
                     KOKKOS_LAMBDA (const i) {
                       for ( int j = 0; j < N1; ++j )
                       for ( int k = 0; k < N2; ++k )
                        some_init_fcn(i, j, k);
                     }
                     );
```

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

OpenMP has a solution: the collapse clause

```
#pragma omp parallel for collapse(3)
for (int64_t i = 0; i < N0; ++i) {
  for (int64_t j = 0; j < N1; ++j) {
    for (int64_t k = 0; k < N2; ++k) {
      /* loop body */
    }
  }
}
```

OpenMP has a solution: the collapse clause

```
#pragma omp parallel for collapse(3)
for (int64_t i = 0; i < N0; ++i) {
  for (int64_t j = 0; j < N1; ++j) {
    for (int64_t k = 0; k < N2; ++k) {
      /* loop body */
    }
  }
}
```

Note this changed the policy by adding a ‘collapse‘ clause.

OpenMP has a solution: the collapse clause

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for (int64_t i = 0; i < N0; ++i) {
  for (int64_t j = 0; j < N1; ++j) {
    for (int64_t k = 0; k < N2; ++k) {
      /* loop body */
    }
  }
}
```

Note this changed the policy by adding a ‘collapse‘ clause.

With Kokkos you also change the policy:

```
parallel_for("L", MDRangePolicy<Rank<3>>({0,0,0},{N0,N1,N2}),
   KOKKOS_LAMBDA(int64_t i, int64_t j, int64_t k) {
      /* loop body */
});
```

MDRangePolicy

MDRangePolicy can parallelize tightly nested loops of 2 to 6 dimensions.

```
parallel_for("L", MDRangePolicy<Rank<3>>({0,0,0},{N0,N1,N2}),
   KOKKOS_LAMBDA(int64_t i, int64_t j, int64_t k) {
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- Specify the dimensionality of the loop with $Rank < DIM >$.

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- Specify the dimensionality of the loop with $Rank < DIM >$.
- As with Kokkos Views: only rectangular iteration spaces.

MDRangePolicy

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   KOKKOS_LAMBDA(int64_t i, int64_t j, int64_t k) {
      /* loop body */
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```

- Specify the dimensionality of the loop with $Rank < DIM >$.
- As with Kokkos Views: only rectangular iteration spaces.
- Provide initializer lists for begin and end values.

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parallel_for("L", MDRangePolicy<Rank<3>>({0,0,0},{N0,N1,N2}),
   KOKKOS_LAMBDA(int64_t i, int64_t j, int64_t k) {
      /* loop body */
});
```

- Specify the dimensionality of the loop with $Rank < DIM >$.
- As with Kokkos Views: only rectangular iteration spaces.
- Provide initializer lists for begin and end values.
- The functor/lambda takes matching number of indicies.

You can also do Reductions:

```
double result;
parallel_reduce("Label",
  MDRangePolicy<Rank<3>>({0,0,0},{N0,N1,N2}),
  KOKKOS_LAMBDA(int i, int j, int k, double& lsum) {
     /* loop body */
  lsum += something;
}, result);
```

You can also do Reductions:

```
double result;
parallel_reduce("Label",
  MDRangePolicy<Rank<3>>({0,0,0},{N0,N1,N2}),
  KOKKOS_LAMBDA(int i, int j, int k, double& lsum) {
      /* loop body */
  lsum += something;
}, result);
```

- The Policy doesn't change the rules for ‘parallel_reduce‘.

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  lsum += something;
}, result);
```

- The Policy doesn't change the rules for ‘parallel_reduce‘.
- Additional Thread Local Argument.

You can also do Reductions:

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double result;
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```

- The Policy doesn't change the rules for ‘parallel_reduce‘.
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- Can do other reductions with reducers.

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- The Policy doesn't change the rules for ‘parallel_reduce‘.
- Additional Thread Local Argument.
- Can do other reductions with reducers.
- Can use ‘View‘s as reduction argument.

You can also do Reductions:

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double result;
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     /* loop body */
  lsum += something;
}, result);
```

- The Policy doesn't change the rules for 'parallel_reduce'.
- Additional Thread Local Argument.
- Can do other reductions with reducers.
- Can use 'View's as reduction argument.
- Multiple reducers not yet implemented though.

In structured grid applications a **tiling** strategy is often used to help with caching.

Tiling

MDRangePolicy uses a tiling strategy for the iteration space.

- Specified as a third initializer list.
- For GPUs a tile is handled by a single thread block.
  - If you provide too large a tile size this will fail!
- In Kokkos 3.3 we will add auto tuning for tile sizes.

```
double result;
parallel_reduce("Label",
  MDRangePolicy<Rank<3>>({0,0,0},{N0,N1,N2},{T0,T1,T2}),
  KOKKOS_LAMBDA(int i, int j, int k, double& lsum) {
     /* loop body */
  lsum += something;
}, result);
```

Initializing a Matrix:

```
View<double**,LayoutLeft> A("A",N0,N1);
parallel_for("Label",
  MDRangePolicy<Rank<2>>({0,0},{N0,N1}),
  KOKKOS_LAMBDA(int i, int j) {
    A(i,j) = 1000.0 * i + 1.0*j;
});

View<double**,LayoutRight> B("B",N0,N1);
parallel_for("Label",
  MDRangePolicy<Rank<2>>({0,0},{N0,N1}),
  KOKKOS_LAMBDA(int i, int j) {
    B(i,j) = 1000.0 * i + 1.0*j;
});
```

Initializing a Matrix:

```
View<double**,LayoutLeft> A("A",N0,N1);
parallel_for("Label",
  MDRangePolicy<Rank<2>>({0,0},{N0,N1}),
  KOKKOS_LAMBDA(int i, int j) {
    A(i,j) = 1000.0 * i + 1.0*j;
});

View<double**,LayoutRight> B("B",N0,N1);
parallel_for("Label",
  MDRangePolicy<Rank<2>>({0,0},{N0,N1}),
  KOKKOS_LAMBDA(int i, int j) {
    B(i,j) = 1000.0 * i + 1.0*j;
});
```

How do I make sure that I get the right access pattern?

Iteration Pattern

MDRangePolicy provides compile time control over iteration patterns.

```
Kokkos::Rank< N, IterateOuter, IterateInner >
```

- **N: (Required)** the rank of the index space (limited from 2 to 6)
- **IterateOuter (Optional)** iteration pattern between tiles
  - **Options:** Iterate::Left, Iterate::Right, Iterate::Default
- **IterateInner (Optional)** iteration pattern within tiles
  - **Options:** Iterate::Left, Iterate::Right, Iterate::Default

Initializing a Matrix fast:

```
View<double**,LayoutLeft> A("A",N0,N1);
parallel_for("Label",
  MDRangePolicy<Rank<2,Iterate::Left,Iterate::Left>>(
        {0,0},{N0,N1}),
  KOKKOS_LAMBDA(int i, int j) {
    A(i,j) = 1000.0 * i + 1.0*j;
});

View<double**,LayoutRight> B("B",N0,N1);
parallel_for("Label",
  MDRangePolicy<Rank<2,Iterate::Right,Iterate::Right>>(
        {0,0},{N0,N1}),
  KOKKOS_LAMBDA(int i, int j) {
    B(i,j) = 1000.0 * i + 1.0*j;
});
```

Initializing a Matrix fast:

```
View<double**,LayoutLeft> A("A",N0,N1);
parallel_for("Label",
  MDRangePolicy<Rank<2,Iterate::Left,Iterate::Left>>(
        {0,0},{N0,N1}),
  KOKKOS_LAMBDA(int i, int j) {
    A(i,j) = 1000.0 * i + 1.0*j;
});

View<double**,LayoutRight> B("B",N0,N1);
parallel_for("Label",
  MDRangePolicy<Rank<2,Iterate::Right,Iterate::Right>>(
        {0,0},{N0,N1}),
  KOKKOS_LAMBDA(int i, int j) {
    B(i,j) = 1000.0 * i + 1.0*j;
});
```

Default Patterns Match

Default iteration patterns match the default memory layouts!

Exercise - mdrange: Initialize multi-dim views with MDRangePolicy

Details:

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

```
# Compile for CPU
cmake -B build_openmp -DKokkos_ENABLE_OPENMP=ON
cmake --build build_openmp
# Run on CPU
./build_openmp/mdrange_exercise -S 26
# Note the warnings, set appropriate environment variables
# Compile for GPU
cmake -B build_cuda -DKokkos_ENABLE_CUDA=ON
cmake --build build_cuda
# Run on GPU
./build_cuda/mdrange_exercise -S 26
```

Template Parameters common to ALL policies.

- `ExecutionSpace`: control where code executes
  - **Options:** Serial, OpenMP, Threads, Cuda, HIP, ...
- `Schedule<Options>`: set scheduling policy.
  - **Options:** Static, Dynamic
- `IndexType<Options>`: control internal indexing type
  - **Options:** int, long, etc
- `WorkTag`: enables multiple operators in one functor

```
struct Foo {
  struct Tag1{}; struct Tag2{};
  KOKKOS_FUNCTION void operator(Tag1, int i) const {...}
  KOKKOS_FUNCTION void operator(Tag2, int i) const {...}
  void run_both(int N) {
    parallel_for(RangePolicy<Tag1>(0,N),*this);
    parallel_for(RangePolicy<Tag2>(0,N),*this);
  }
});
```

MDRangePolicy

- allows for tightly nested loops similar to OpenMP's collapse clause.
- requires functors/lambdas with as many parameters as its rank is.
- works with `parallel_for` and `parallel_reduce`.
- uses a tiling strategy for the iteration space.
- provides compile time control over iteration patterns.

Hierarchical parallelism

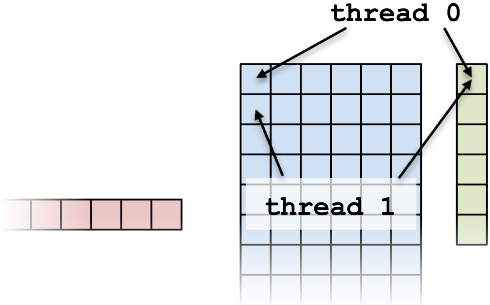
Finding and exploiting more parallelism in your computations.

Learning objectives:

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

(Flat parallel) Kernel:

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



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      thisRowsSum += A(row,col) * x(col);
    }
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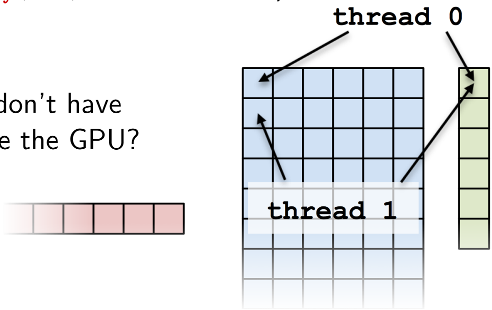
  }, result);
```

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



(Flat parallel) Kernel:

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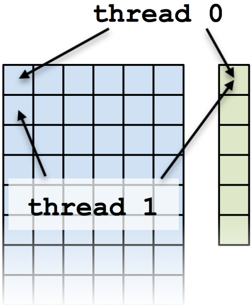
  }, result);
```



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

Solutions?

(Flat parallel) Kernel:

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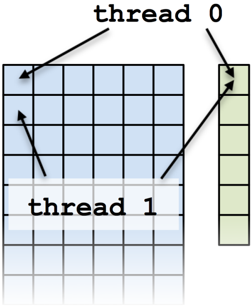
    double thisRowsSum = 0;
    for (int col = 0; col < M; ++col) {
      thisRowsSum += A(row,col) * x(col);
    }
    valueToUpdate += y(row) * thisRowsSum;
  }, result);
```



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

Solutions?

- Atomics
- Thread teams

Using an atomic with every element is doing scalar integration with atomics. (See module 3)

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

```
for each row
  Functor functor(row, ...);
  parallel_reduce(M, functor);
}
```

Using an atomic with every element is doing scalar integration with atomics. (See module 3)

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

```
for each row
  Functor functor(row, ...);
  parallel_reduce(M, functor);
}
```

This is an example of *hierarchical work*.

Important concept: Hierarchical parallelism

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

Important concept: Thread team

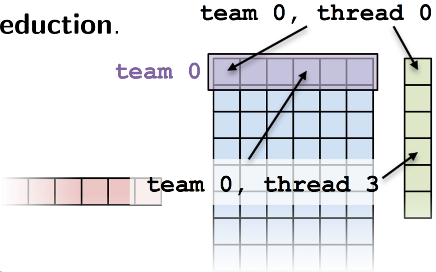
A collection of threads which are guaranteed to be executing **concurrently** and **can synchronize**.

Important concept: Thread team

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

High-level **strategy**:

1. Do **one parallel launch** of `N` teams.
2. Each team handles a row.
3. The threads within **teams perform a reduction**.
4. The thread teams **perform a reduction**.



The final hierarchical parallel kernel:

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

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

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

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

Important point

Using teams is changing the execution *policy*.

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

We specify a *total amount of work*.

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

Important point

Using teams is changing the execution *policy*.

“**Flat** parallelism” uses `RangePolicy`:

We specify a *total amount of work*.

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

“**Hierarchical** parallelism” uses `TeamPolicy`:

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

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

Important point

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

```
using member_type = typename TeamPolicy<ExecSpace>::member_type;

void operator()(const member_type & teamMember) {
  // How many teams are there?
  const unsigned int league_size = teamMember.league_size();

  // Which team am I on?
  const unsigned int league_rank = teamMember.league_rank();

  // How many threads are in the team?
  const unsigned int team_size = teamMember.team_size();

  // Which thread am I on this team?
  const unsigned int team_rank = teamMember.team_rank();

  // Make threads in a team wait on each other:
  teamMember.team_barrier();
}
```

We shouldn't be hard-coding the work mapping...

```
operator() (member_type & teamMember, double & update) {
  const int row = teamMember.league_rank();
  double thisRowsSum;
  ''do a reduction''(''over M columns'',
    [=] (const int col) {
      thisRowsSum += A(row,col) * x(col);
    });
  if (teamMember.team_rank() == 0) {
    update += (row) * thisRowsSum;
  }
}
```

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If this were a parallel execution,

we'd use `Kokkos::parallel_reduce`.

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Key idea: this *is* a parallel execution.

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}
```

If this were a parallel execution,

we'd use `Kokkos::parallel_reduce`.

Key idea: this *is* a parallel execution.

$\Rightarrow$ **Nested parallel patterns**

TeamThreadRange:

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

TeamThreadRange:

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

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

Anatomy of nested parallelism:

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

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

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

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

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```
parallel_something(
  TeamPolicy<ExecutionSpace>(numberOfTeams, Kokkos::AUTO),
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```

GPUs

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

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```

GPUs

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

Intel Xeon Phi:

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

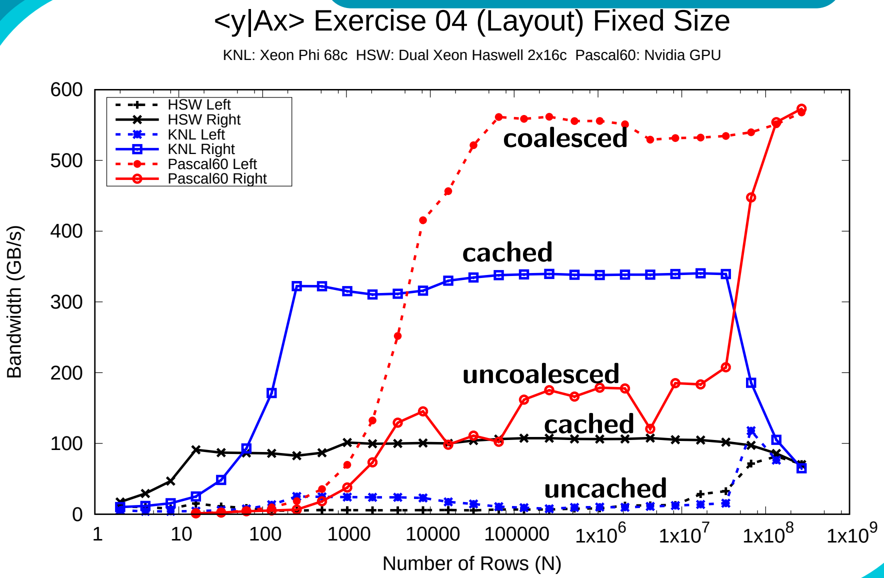
Details:

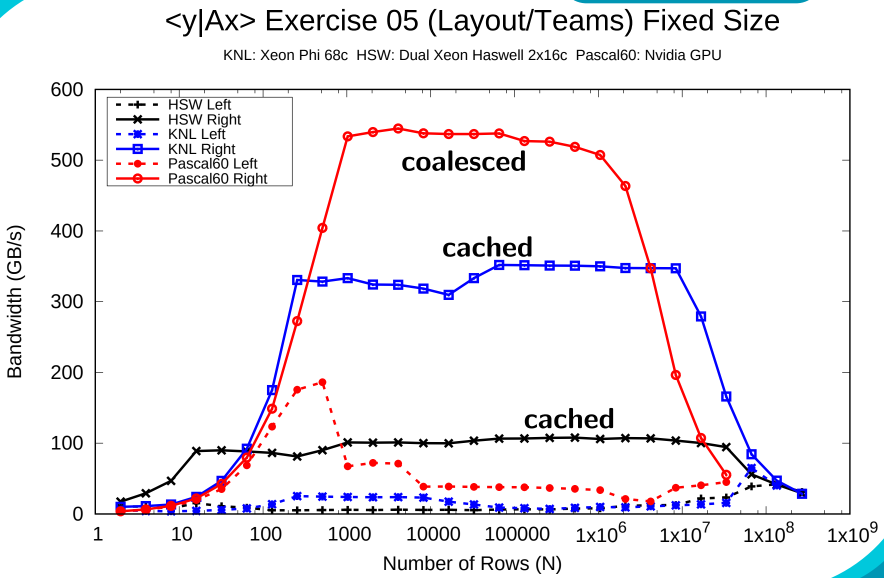
- Location: `Exercises/team_policy/`
- Replace `RangePolicy<Space>` with `TeamPolicy<Space>`
- Use `AUTO` for `team_size`
- Make the inner loop a `parallel_reduce` with `TeamThreadRange` policy
- Experiment with the combinations of `Layout`, `Space`, `N` to view performance
- Hint: what should the layout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

Things to try:

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

Reminder, Exercise #4 with Flat Parallelism




<y|Ax> Exercise 05 (Layout/Teams) Fixed Size
KNL: Xeon Phi 68c HSW: Dual Xeon Haswell 2x16c Pascal60: Nvidia GPU
Bandwidth (GB/s)
Number of Rows (N)
HSW Left
HSW Right
KNL Left
KNL Right
Pascal60 Left
Pascal60 Right
coalesced
cached
cached
0
100
200
300
400
500
600
1
10
100
1000
10000
100000
1x10^6
1x10^7
1x10^8
1x10^9

Exposing Vector Level Parallelism

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

Anatomy of nested parallelism:

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

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

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

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

`totalSum = numberOfThreads * 10`

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

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

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    int thisThreadsSum = 0;
    for (int i = 0; i < 10; ++i) {
      ++thisThreadsSum;
    }
    partialSum += thisThreadsSum;
}, totalSum);
```

`totalSum = numberOfTeams * team_size * 10`

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

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

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

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

`totalSum = numberOfTeams * team_size * team_size * 10`

The `single` pattern can be used to restrict execution

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

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

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

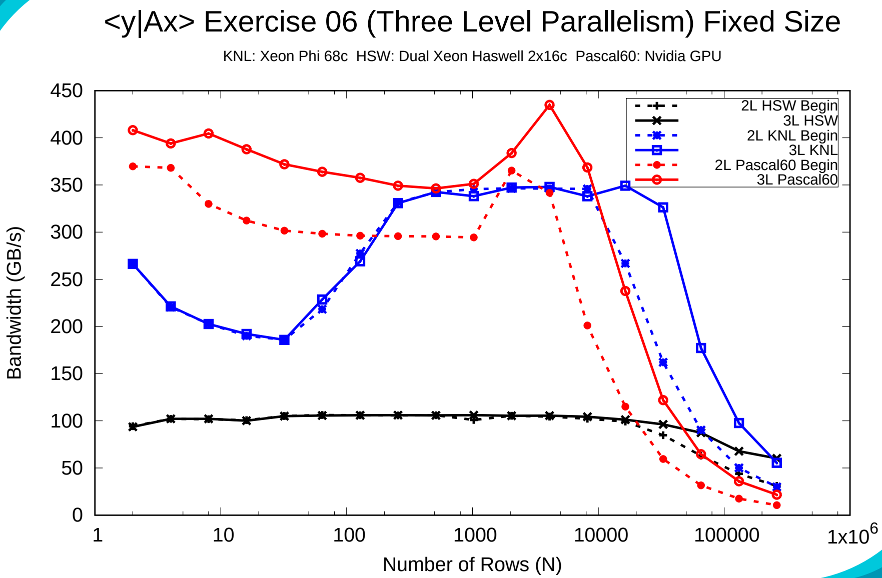
The previous example was extended with an outer loop over "Elements" to expose a third natural layer of parallelism.

Details:

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

Things to try:

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


<y|Ax> Exercise 06 (Three Level Parallelism) Fixed Size
KNL: Xeon Phi 68c HSW: Dual Xeon Haswell 2x16c Pascal60: Nvidia GPU
Bandwidth (GB/s)
Number of Rows (N)
450
400
350
300
250
200
150
100
50
0
1
10
100
1000
10000
100000
1x10^6
2L HSW Begin
3L HSW
2L KNL Begin
3L KNL
2L Pascal60 Begin
3L Pascal60

- **Hierarchical work** can be parallelized via hierarchical parallelism.
- Hierarchical parallelism is leveraged using **thread teams** launched with a `TeamPolicy`.
- Team "worksets" are processed by a team in nested `parallel_for` (or `reduce` or `scan`) calls with a `TeamThreadRange`, `ThreadVectorRange`, and `TeamVectorRange` policy.
- Execution can be restricted to a subset of the team with the `single` pattern using either a `PerTeam` or `PerThread` policy.

Kokkos Tools

Leveraging Kokkos' built-in instrumentation.

Learning objectives:

- The need for Kokkos-aware tools.
- How instrumentation helps.
- Simple profiling tools.
- Simple debugging tools.

Output from NVIDIA NVProf for Trilinos Tpetra

```
==278743== Profiling application: ./TpetraCore_Performance-CGSolve.exe --size=200
==278743== Profiling result:
            Type  Time(%)      Time     Calls       Avg       Min       Max  Name
 GPU activities:   26.09%  380.32ms         1  380.32ms  380.32ms  380.32ms  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::ParallelFor<Tpetra::CrsMatrix<double, int, __int64, Kokkos::Compat::KokkosDeviceWrapperNode<Kokkos::Cuda, Kokkos::CudaUVMSpace>>::pack_functor<Kokkos::View<double*>, Kokkos::View<unsigned long const *>>, Kokkos::RangePolicy<>, Kokkos::Cuda>>(double)
                   22.28%  324.77ms         1  324.77ms  324.77ms  324.77ms  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::ParallelReduce<Kokkos::Impl::CudaFunctorAdapter<Tpetra::Details::Impl::ConvertColumnIndicesFromGlobalToLocal<int, __int64, Kokkos::Device<Kokkos::Cuda, Kokkos::CudaUVMSpace>, unsigned long, unsigned long>, Kokkos::RangePolicy<>, unsigned long, void>, Kokkos::RangePolicy<>, Kokkos::InvalidType, Kokkos::Cuda>>(int)
                   21.83%  318.26ms        77  4.1332ms  3.8786ms  22.643ms  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::ParallelFor<KokkosSparse::Impl::SPMV_Functor<KokkosSparse::CrsMatrix<double const , int const , Kokkos::Device<Kokkos::Cuda, Kokkos::CudaUVMSpace>, Kokkos::MemoryTraits<unsigned int=1>, unsigned long const >, Kokkos::View<double const *>, Kokkos::View<double*>, int=0, bool=0>, Kokkos::TeamPolicy<>, Kokkos::Cuda>>(double const )
                   15.51%  226.15ms         1  226.15ms  226.15ms  226.15ms  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::ParallelFor<Tpetra::CrsMatrix<double, int, __int64, Kokkos::Compat::KokkosDeviceWrapperNode<Kokkos::Cuda, Kokkos::CudaUVMSpace>>::pack_functor<Kokkos::View<int*>, Kokkos::View<unsigned long const *>>, Kokkos::RangePolicy<>, Kokkos::Cuda>>(double)
                    3.60%  52.486ms       227  231.22us  230.17us  232.93us  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::ParallelFor<KokkosBlas::Impl::Axpby_Functor<double, Kokkos::View<double const *>, double, Kokkos::View<double*>, int=2, int=2, int>, Kokkos::RangePolicy<>, Kokkos::Cuda>>(double)
                    1.86%  27.174ms        13  2.0903ms  1.0560us  27.157ms  [CUDA memcpy HtoD]
                    1.81%  26.350ms       153  172.22us  138.27us  206.08us  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::ParallelReduce<KokkosBlas::Impl::DotFunctor<Kokkos::View<double>, Kokkos::View<double const *>, Kokkos::View<double const *>, int>, Kokkos::RangePolicy<>, Kokkos::InvalidType, Kokkos::Cuda>>(double)
                    1.61%  23.431ms         1  23.431ms  23.431ms  23.431ms  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::ParallelFor<KokkosBlas::Impl::V_Update_Functor<Kokkos::View<double const *>, Kokkos::View<double const *>, Kokkos::View<double*>, int=2, int=0, int=0, int>, Kokkos::RangePolicy<>, Kokkos::Cuda>>(double const *)
                    1.39%  20.299ms         1  20.299ms  20.299ms  20.299ms  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::ParallelFor<KokkosBlas::Impl::V_Update_Functor<Kokkos::View<double const *>, Kokkos::View<double const *>, Kokkos::View<double*>, int=2, int=2, int=0, int>, Kokkos::RangePolicy<>, Kokkos::Cuda>>(double const *)
```

Output from NVIDIA NVProf for Trilinos Tpetra

```
==278743== Profiling application: ./TpetraCore_Performance-CGSolve.exe --size=200
==278743== Profiling result:
            Type  Time(%)      Time     Calls       Avg       Min       Max  Name
 GPU activities:   26.09%  380.32ms         1  380.32ms  380.32ms  380.32ms  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::
ParallelFor<Tpetra::CrsMatrix<double, int, __int64, Kokkos::Compat::KokkosDeviceWrapperNode<Kokkos::Cuda, Kokkos::CudaUVMSpace>>::pack_functor<K
okkos::View<double*>, Kokkos::View<unsigned long const *>>, Kokkos::RangePolicy<>, Kokkos::Cuda>>(double)
                   22.28%  324.77ms         1  324.77ms  324.77ms  324.77ms  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::
ParallelReduce<Kokkos::Impl::CudaFunctorAdapter<Tpetra::Details::Impl::ConvertColumnIndicesFromGlobalToLocal<int, __int64, Kokkos::Device<Kokkos
::Cuda, Kokkos::CudaUVMSpace>, unsigned long, unsigned long>, Kokkos::RangePolicy<>, unsigned long, void>, Kokkos::RangePolicy<>, Kokkos::Invali
dType, Kokkos::Cuda>>(int)
                   21.83%  318.26ms        77  4.1332ms  3.8786ms  22.643ms  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::
ParallelFor<KokkosSparse::Impl::SPMV_Functor<KokkosSparse::CrsMatrix<double const , int const , Kokkos::Device<Kokkos::Cuda, Kokkos::CudaUVMSpac
e>, Kokkos::MemoryTraits<unsigned int=1>, unsigned long const >, Kokkos::View<double const *>, Kokkos::View<double*>, int=0, bool=0>, Kokkos::Te
amPolicy<>, Kokkos::Cuda>>(double const )
                   15.51%  226.15ms         1  226.15ms  226.15ms  226.15ms  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::
ParallelFor<Tpetra::CrsMatrix<double, int, __int64, Kokkos::Compat::KokkosDeviceWrapperNode<Kokkos::Cuda, Kokkos::CudaUVMSpace>>::pack_functor<K
okkos::View<int*>, Kokkos::View<unsigned long const *>>, Kokkos::RangePolicy<>, Kokkos::Cuda>>(double)
                    3.60%  52.486ms       227  231.22us  230.17us  232.93us  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::
ParallelFor<KokkosBlas::Impl::Axpby_Functor<double, Kokkos::View<double const *>, double, Kokkos::View<double*>, int=2, int=2, int>, Kokkos::Ran
gePolicy<>, Kokkos::Cuda>>(double)
                    1.86%  27.174ms        13  2.0903ms  1.0560us  27.157ms  [CUDA memcpy HtoD]
                    1.81%  26.350ms       153  172.22us  138.27us  206.08us  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::
ParallelReduce<KokkosBlas::Impl::DotFunctor<Kokkos::View<double>, Kokkos::View<double const *>, Kokkos::View<double const *>, int>, Kokkos::Rang
ePolicy<>, Kokkos::InvalidType, Kokkos::Cuda>>(double)
                    1.61%  23.431ms         1  23.431ms  23.431ms  23.431ms  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::
ParallelFor<KokkosBlas::Impl::V_Update_Functor<Kokkos::View<double const *>, Kokkos::View<double const *>, Kokkos::View<double*>, int=2, int=0,
int=0, int>, Kokkos::RangePolicy<>, Kokkos::Cuda>>(double const *)
                    1.39%  20.299ms         1  20.299ms  20.299ms  20.299ms  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos::Impl::
ParallelFor<KokkosBlas::Impl::V_Update_Functor<Kokkos::View<double const *>, Kokkos::View<double const *>, Kokkos::View<double*>, int=2, int=2,
int=0, int>, Kokkos::RangePolicy<>, Kokkos::Cuda>>(double const *)
```

What are those Kernels doing?

Generic code obscures what is happening from the tools

Historically a lot of profiling tools are coming from a Fortran and C world:

- Focused on functions and variables
- C++ has a lot of other concepts:
  - Classes with member functions
  - Inheritance
  - Template Metaprogramming
- Abstraction Models (Generic Programming) obscure things
  - From a profiler perspective interesting stuff happens in the abstraction layer (e.g. `#pragma omp parallel`)
  - Symbol names get really complex due to deep template layers

Instrumentation enables context information to reach tools.

Most profiling tools have an instrumentation interface

- E.g. nvtx for NVIDIA, ITT for Intel.
- Allows to name regions
- Sometimes can mark up memory operations.

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- Allows to name regions
- Sometimes can mark up memory operations.

KokkosP

Kokkos has its own instrumentation interface KokkosP, which can be used to write tools.

- Knows about parallel dispatch
- Knows about allocations, deallocations and deep_copy
- Provides region markers
- Leverages naming information (kernels, Views)

There are two components to Kokkos Tools: the KokkosP instrumentation interface and the actual Tools.

KokkosP Interface

- The internal instrumentation layer of Kokkos.
- Always available even in release builds.
- Zero overhead if no tool is loaded.

Kokkos Tools

- Tools leveraging the KokkosP instrumentation layer.
- Are loaded at runtime by Kokkos.
  - Set `KOKKOS_TOOLS_LIBS` environment variable to load a shared library.
  - Compile tools into the executable and use the API callback setting mechanism.

Download tools from
https://github.com/kokkos/kokkos-tools

- Tools are largely independent of the Kokkos configuration
  - May need to use the same C++ standard library.
  - Use the same tool for CUDA and OpenMP code for example.
- We recommend you build the tools with CMake

```
cd kokkos-tools && cmake -B build
cmake --build build --parallel 4
cmake --install build --prefix /where/to/install/the/tools
```

Loading Tools:

- Set `KOKKOS_TOOLS_LIBS` environment variable to the full path to the shared library of the tool.
- Kokkos dynamically loads symbols from the library during `initialize` and fills function pointers.
- If no tool is loaded the overhead is a function pointer comparison to `nullptr`.

```
View<double*> a("A",N);
View<double*, HostSpace> h_a = create_mirror_view(a);

Profiling::pushRegion("Setup");
parallel_for("Init_A",RangePolicy<h_exec_t>(0,N),
  KOKKOS_LAMBDA(int i) { h_a(i) = i; });
deep_copy(a,h_a);
Profiling::popRegion();

Profiling::pushRegion("Iterate");
for(int r=0; r<10; r++) {
  View<double*> tmp("Tmp",N);
  parallel_scan("K_1",RangePolicy<exec_t>(0,N),
    KOKKOS_LAMBDA(int i, double& lsum, bool f) {
      if(f) tmp(i) = lsum;
      lsum += a(i);
  });
  double sum;
  parallel_reduce("K_2",N, KOKKOS_LAMBDA(int i, double& lsum) {
    lsum += tmp(i);
  },sum);
}
Profiling::popRegion();
```

Output of: `nvprof ./test.cuda`

```
==141309== Profiling application: ./test.cuda
==141309== Profiling result:
            Type  Time(%)      Time     Calls       Avg       Min       Max  Name
 GPU activities:   40.95%  1.4516ms        20  72.580us  65.215us  81.663us  _ZN6Kokkos4Impl33cuda_parallel_launch_local_memoryINS0_12Pa
rallelScanIZ4mainEUliRdbE_NS_11RangePolicyIJNS_4CudaEEEES6_EEEEvT_
                   40.75%  1.4444ms        18  80.246us  1.1520us  1.4186ms  [CUDA memcpy HtoD]
                    8.84%  313.34us        11  28.485us  28.415us  28.703us  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos
::Impl::ParallelFor<Kokkos::Impl::ViewValueFunctor<Kokkos::Cuda, double, bool=1>, Kokkos::RangePolicy<>, Kokkos::Cuda>>(Kokkos::Cuda)
                    7.91%  280.25us        10  28.025us  27.423us  29.024us  _ZN6Kokkos4Impl33cuda_parallel_launch_local_memoryINS0_14Pa
rallelReduceINS0_18CudaFunctorAdapterIZ4mainEUliRdE_NS_11RangePolicyIJNS_4CudaEEEEdvEES8_NS_11InvalidTypeES7_EEEEvT_
                    1.20%  42.592us        28  1.5210us  1.3440us  2.1760us  [CUDA memcpy DtoH]
                    0.13%  4.5760us         1  4.5760us  4.5760us  4.5760us  Kokkos::_GLOBAL__N__52_tmpxft_0001ee3d_00000000_6_Kokkos_Cu
da_Locks_cpp1_ii_915ea793::init_lock_array_kernel_atomic(void)
                    0.08%  2.8480us         1  2.8480us  2.8480us  2.8480us  Kokkos::Impl::_GLOBAL__N__55_tmpxft_0001ee3b_00000000_6_Kok
kos_Cuda_Instance_cpp1_ii_a8bc5097::query_cuda_kernel_arch(int*)
                    0.08%  2.6880us         1  2.6880us  2.6880us  2.6880us  Kokkos::_GLOBAL__N__52_tmpxft_0001ee3d_00000000_6_Kokkos_Cu
da_Locks_cpp1_ii_915ea793::init_lock_array_kernel_threadid(int)
                    0.06%  2.1440us         2  1.0720us  1.0560us  1.0880us  [CUDA memset]
```

Output of: `nvprof ./test.cuda`

```
==141309== Profiling application: ./test.cuda
==141309== Profiling result:
            Type  Time(%)      Time     Calls       Avg       Min       Max  Name
 GPU activities:   40.95%  1.4516ms        20  72.580us  65.215us  81.663us  _ZN6Kokkos4Impl33cuda_parallel_launch_local_memoryINS0_12Pa
rallelScanIZ4mainEUliRdbE_NS_11RangePolicyIJNS_4CudaEEEES6_EEEvT_
                   40.75%  1.4444ms        18  80.246us  1.1520us  1.4186ms  [CUDA memcpy HtoD]
                    8.84%  313.34us        11  28.485us  28.415us  28.703us  void Kokkos::Impl::cuda_parallel_launch_local_memory<Kokkos
::Impl::ParallelFor<Kokkos::Impl::ViewValueFunctor<Kokkos::Cuda, double, bool=1>, Kokkos::RangePolicy<>, Kokkos::Cuda>>(Kokkos::Cuda)
                    7.91%  280.25us        10  28.025us  27.423us  29.024us  _ZN6Kokkos4Impl33cuda_parallel_launch_local_memoryINS0_14Pa
rallelReduceINS0_18CudaFunctorAdapterIZ4mainEUliRdE_NS_11RangePolicyIJNS_4CudaEEEEdvEES8_NS_11InvalidTypeES7_EEEEvT_
                    1.20%  42.592us        28  1.5210us  1.3440us  2.1760us  [CUDA memcpy DtoH]
                    0.13%  4.5760us         1  4.5760us  4.5760us  4.5760us  Kokkos::_GLOBAL__N__52_tmpxft_0001ee3d_00000000_6_Kokkos_Cu
da_Locks_cpp1_ii_915ea793::init_lock_array_kernel_atomic(void)
                    0.08%  2.8480us         1  2.8480us  2.8480us  2.8480us  Kokkos::Impl::_GLOBAL__N__55_tmpxft_0001ee3b_00000000_6_Kok
kos_Cuda_Instance_cpp1_ii_a8bc5097::query_cuda_kernel_arch(int*)
                    0.08%  2.6880us         1  2.6880us  2.6880us  2.6880us  Kokkos::_GLOBAL__N__52_tmpxft_0001ee3d_00000000_6_Kokkos_Cu
da_Locks_cpp1_ii_915ea793::init_lock_array_kernel_threadid(int)
                    0.06%  2.1440us         2  1.0720us  1.0560us  1.0880us  [CUDA memset]
```

Let us make one larger:

```
_ZN6Kokkos4Impl33cuda_parallel_launch_local_memoryINS0
_14ParallelReduceINS0_18CudaFunctorAdapterIZ4mainEUliRdE
_NS_11RangePolicyIJNS_4CudaEEEEdvEES8_NS_11InvalidTypeES7_EEEEvT_
```

And demangled:

```
void Kokkos::Impl::cuda_parallel_launch_local_memory
<Kokkos::Impl::ParallelReduce<Kokkos::Impl::CudaFunctorAdapter
<main::{lambda(int, double&)#1}, Kokkos::RangePolicy<Kokkos::Cuda>
double, void>, Kokkos::Cuda, Kokkos::InvalidType, Kokkos::RangePol
(Kokkos::Impl::ParallelReduce<Kokkos::Impl::CudaFunctorAdapter<
main::{lambda(int, double&)#1}, Kokkos::RangePolicy<Kokkos::Cuda>,
double, void>, Kokkos::Cuda, Kokkos::InvalidType, Kokkos::RangePol
```

Aaa this is horrifying can't we do better??

Aaa this is horrifying can't we do better??

Lets use SimpleKernelTimer from Kokkos Tools:

- Simple tool producing a summary similar to nvprof
- Good way to get a rough overview of whats going on
- Writes a file `HOSTNAME-PROCESSID.dat` per process
- Use the reader accompanying the tool to read the data

Usage:

```
git clone git@github.com:kokkos/kokkos-tools
cd kokkos-tools/profiling/simple_kernel_timer
make
export KOKKOS_TOOLS_LIBS=${PWD}/kp_kernel_timer.so
export PATH=${PATH}:${PWD}
cd ${WORKDIR}
./text.cuda
kp_reader *.dat
```

Output from SimpleKernelTimer:

```
Regions:

-                                                                        Iterate
 (Region)          0.02977          4         0.00744 147.131  60.772
-                                                                          Setup
 (Region)          0.00769          4         0.00192  38.010  15.700

-------------------------------------------------------------------------
Kernels:

-                                          Kokkos::View::initialization [A_mirror]
 (ParFor)          0.00878          4         0.00220  43.402  17.927
-                                                                            K_1
 (ParScan)         0.00651         40         0.00016  32.178  13.291
-                                               Kokkos::View::initialization [Tmp]
 (ParFor)          0.00191         40         0.00005   9.454   3.905
-                                                                            K_2
 (ParRed)          0.00169         40         0.00004   8.372   3.458
-                                                                         Init_A
 (ParFor)          0.00100          4         0.00025   4.965   2.051
-                                                 Kokkos::View::initialization [A]
 (ParFor)          0.00033          4         0.00008   1.629   0.673

-------------------------------------------------------------------------
Summary:

Total Execution Time (incl. Kokkos + non-Kokkos):                  0.04899 seconds
Total Time in Kokkos kernels:                                      0.02024 seconds
   -> Time outside Kokkos kernels:                                 0.02876 seconds
   -> Percentage in Kokkos kernels:                                  41.31 %
Total Calls to Kokkos Kernels:                                         132
```

Output from SimpleKernelTimer:

```
Regions:

-                                                                       Iterate
 (Region)          0.02977           4         0.00744 147.131  60.772
-                                                                         Setup
 (Region)          0.00769           4         0.00192  38.010  15.700

-------------------------------------------------------------------------
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-                                               Kokkos::View::initialization [A_mirror]
 (ParFor)          0.00878           4         0.00220  43.402  17.927
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-                                                    Kokkos::View::initialization [Tmp]
 (ParFor)          0.00191          40         0.00005   9.454   3.905
-                                                                           K_2
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-                                                                        Init_A
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Total Calls to Kokkos Kernels:                                         132
```

Will introduce *Regions* later.

Kernel Naming

Naming Kernels avoid seeing confusing Profiler output!

Lets look at Tpetra again with the Simple Kernel Timer Loaded:

At the top we get Region output:

```
Regions:

- CG: global
 (REGION)   0.547101 1 0.547101 26.922698 5.470153
- CG: spmv
 (REGION)   0.323189 77 0.004197 15.904024 3.231379
- CG: axpby
 (REGION)   0.091971 154 0.000597 4.525865 0.919565
- KokkosBlas::axpby[ETI]
 (REGION)   0.055017 228 0.000241 2.707360 0.550081
- KokkosBlas::update[ETI]
 (REGION)   0.030842 2 0.015421 1.517718 0.308370
- CG: dot
 (REGION)   0.028661 153 0.000187 1.410413 0.286568
- KokkosBlas::dot[ETI]
 (REGION)   0.028120 153 0.000184 1.383756 0.281152
```

Then we get kernel output:

```
Kernels:

- Tpetra::CrsMatrix::sortAndMergeIndicesAndValues
 (ParRed)   0.708770 1 0.708770 34.878388 7.086590
- KokkosSparse::spmv<NoTranspose,Dynamic>
 (ParFor)   0.319268 77 0.004146 15.711118 3.192184
- Tpetra::Details::Impl::ConvertColumnIndicesFromGlobalToLocal
 (ParRed)   0.292309 1 0.292309 14.384452 2.922633
- Tpetra::CrsMatrix pack values
 (ParFor)   0.267800 1 0.267800 13.178373 2.677581
- Tpetra::CrsMatrix pack column indices
 (ParFor)   0.157867 1 0.157867 7.768592 1.578422
- KokkosBlas::Axpby::S15
 (ParFor)   0.054251 227 0.000239 2.669699 0.542429
- Kokkos::View::initialization [Tpetra::CrsMatrix::val]
 (ParFor)   0.033584 2 0.016792 1.652666 0.335789
- Kokkos::View::initialization [lgMap]
 (ParFor)   0.033417 2 0.016708 1.644441 0.334118
- KokkosBlas::dot<1D>
 (ParRed)   0.027782 153 0.000182 1.367155 0.277778
```

Understanding MemorySpace Utilization is critical

Three simple tools for understanding memory utilization:

- MemoryHighWaterMark: just the maximum utilization for each memory space.
- MemoryUsage: Timeline of memory usage.
- MemoryEvents: allocation, deallocation and deep_copy.
  - Name, Memory Space, Pointer, Size

```
# Memory Events
# Time      Ptr                   Size        MemSpace       Op         Name
0.000776   0x7f095f600000         8000000              Cuda Allocate   A
0.000910        0x1cb4680         8000000              Host Allocate   A_mirror
0.001571 PushRegion Setup {
0.003754 } PopRegion
0.003756 PushRegion Iterate {
0.004100   0x7f0960000000         8000000              Cuda Allocate   Tmp
0.004451   0x7f0960000000        -8000000              Cuda DeAllocate Tmp
...
0.010350   0x7f0960000000         8000000              Cuda Allocate   Tmp
0.010605   0x7f0960000000        -8000000              Cuda DeAllocate Tmp
0.010753 } PopRegion
0.010753        0x1cb4680        -8000000              Host DeAllocate A_mirror
0.010766   0x7f095f600000        -8000000              Cuda DeAllocate A
```

Adding region markers to capture more code structure

Region Markers are helpful to:

- Find where time is spent outside of kernels.
- Group Kernels which belong together.
- Structure code profiles.
  - For example bracket *setup* or *solve* phase.

Adding region markers to capture more code structure

Region Markers are helpful to:

- Find where time is spent outside of kernels.
- Group Kernels which belong together.
- Structure code profiles.
  - For example bracket *setup* or *solve* phase.

Simple Push/Pop interface:

```
Kokkos::Profiling::pushRegion("Label");
...
Kokkos::Profiling::popRegion();
```

The simplest tool to leverage regions is the **Space Time Stack**:

- **Bottom Up** and **Top Down** data representation
- Can do MPI aggregation if compiled with MPI support
- Also aggregates memory utilization info.

```
BEGIN KOKKOS PROFILING REPORT:
TOTAL TIME: 0.0100131 seconds
TOP-DOWN TIME TREE:
<average time> <percent of total time> <percent time in Kokkos> <percent MPI imbalance> <remainder> <kernels per second> <number of calls> <name> [type]

===================
|-> 6.90e-03 sec 68.9% 33.9% 0.0% 66.1% 4.35e+03 1 Iterate [region]
|   |-> 1.55e-03 sec 15.5% 100.0% 0.0% ------ 10 K_1 [scan]
|   |-> 4.04e-04 sec 4.0% 100.0% 0.0% ------ 10 Kokkos::View::initialization [Tmp] [for]
|   |-> 3.80e-04 sec 3.8% 100.0% 0.0% ------ 10 K_2 [reduce]
|-> 1.84e-03 sec 18.4% 98.6% 0.0% 1.4% 1.09e+03 1 Setup [region]
|   |-> 1.59e-03 sec 15.9% 100.0% 0.0% ------ 1 "A"="A_mirror" [copy]
|   |-> 2.21e-04 sec 2.2% 100.0% 0.0% ------ 1 Init_A [for]
|-> 6.64e-04 sec 6.6% 100.0% 0.0% ------ 1 Kokkos::View::initialization [A_mirror] [for]
|-> 6.68e-05 sec 0.7% 100.0% 0.0% ------ 1 Kokkos::View::initialization [A] [for]

BOTTOM-UP TIME TREE:
...

KOKKOS HOST SPACE:
===================
MAX MEMORY ALLOCATED: 7812.5 kB
ALLOCATIONS AT TIME OF HIGH WATER MARK:
  100.0% A_mirror

KOKKOS CUDA SPACE:
===================
MAX MEMORY ALLOCATED: 15625.0 kB
ALLOCATIONS AT TIME OF HIGH WATER MARK:
  50.0% A
  50.0% Iterate/Tmp

Host process high water mark memory consumption: 161668 kB

END KOKKOS PROFILING REPORT.
```

Non-Blocking Dispatch implies asynchronous error reporting!

```
Profiling::pushRegion("Iterate");
for(int r=0; r<10; r++) {
  parallel_for("K_1",2*N, KOKKOS_LAMBDA(int i) {a(i) = i;});
  printf("Passed␣point␣A\n");
  double sum;
  parallel_reduce("K_2",N, KOKKOS_LAMBDA(int i, double& lsum) {
    lsum += a(i); },sum);
}
Profiling::popRegion();
```

Output of the run:

```
./test.cuda
Passed point A
terminate called after throwing an instance of 'std::runtime_error
  what():  cudaStreamSynchronize(m_stream) error( cudaErrorIllegal
  an illegal memory access was encountered
    Kokkos/kokkos/core/src/Cuda/Kokkos_Cuda_Instance.cpp:312
Traceback functionality not available
Aborted (core dumped)
```

Debugging with Tools

Kokkos Tools can be used to implement Debugging functionality.

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Kokkos Tools can be used to implement Debugging functionality.

The KernelLogger is a tool to localize errors and check the actual runtime flow of a code.

- As other tools it inserts fences - which check for errors.
- Prints out Kokkos operations as they happen.

Debugging with Tools

Kokkos Tools can be used to implement Debugging functionality.

The KernelLogger is a tool to localize errors and check the actual runtime flow of a code.

- As other tools it inserts fences - which check for errors.
- Prints out Kokkos operations as they happen.

Output from the above test case with KernelLogger:

```
KokkosP: Allocate<Cuda> name: A pointer: 0x7f598b800000 size: 8000
KokkosP: Executing parallel-for kernel on device 0 with unique exe
KokkosP: Kokkos::View::initialization [A]
KokkosP: Execution of kernel 0 is completed.
KokkosP: Entering profiling region: Iterate
KokkosP: Executing parallel-for kernel on device 0 with unique exe
KokkosP: Iterate
KokkosP:   K_1
terminate called after throwing an instance of 'std::runtime_error
  what():  cudaDeviceSynchronize() error( cudaErrorIllegalAddress)
Traceback functionality not available
```

The standard Kokkos profiling approach

Understand Kokkos Utilization (SimpleKernelTimer)

- Check how much time in kernels
- Identify HotSpot Kernels

Run Memory Analysis (MemoryEvents)

- Are there many allocations/deallocations - 5000/s is OK.
- Identify temporary allocations which could be hoisted

Identify Serial Code Regions (SpaceTimeStack)

- Add Profiling Regions
- Find Regions with low fraction of time spend in Kernels

Dive into individual Kernels

- Use connector tools (next subsection) to analyze kernels.
- E.g. use roof line analysis to find underperforming code.

Analyse a MiniMD variant with a serious performance issue.

Details:

- Location: `Exercises/tools_minimd/`
- Use standard Profiling Approach.
- Find the code location which causes the performance issue.
- Run with `miniMD.exe -s 20`

What should happen:

- Performance should be
- About 50% of time in a Force compute kernel
- About 25% in neighbor list creation

- Kokkos Tools provide an instrumentation interface **KokkosP** and **Tools** to leverage it.
- The interface is **always available** - even in release builds.
- Zero overhead if no tool is loaded during the run.
- Dynamically load a tool via setting `KOKKOS_TOOLS_LIBS` environment variable.
- Set callbacks directly in code for tools compiled into the executable.

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- Full BuildSystem integration.
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- Team Scratch memory (GPU shared memory).
- SIMD vectorization.
- MPI and PGAS integration.
- All Tools for Profiling, Debugging and Tuning.

The Kokkos Lectures

Join 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

Find More

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.