The Kokkos Lectures

The Fundamentals: A Condensed Short Tutorial

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A Condensed Short Tutorial

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

For the full lectures, with more capabilities covered, and more in-depth explanations visit:
**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 (f)

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(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
Industry Estimate

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Software Cost Switching Vendors

Just switching Programming Models costs multiple person-years per app!
What is Kokkos?

- A C++ Programming Model for Performance Portability
  - Implemented as a template library on top CUDA, HIP, OpenMP, ...
  - Aims to be descriptive not prescriptive
  - Aligns with developments in the C++ standard
- Expanding solution for common needs of modern science and engineering codes
  - Math libraries based on Kokkos
  - Tools for debugging, profiling and tuning
  - Utilities for integration with Fortran and Python
- Is 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

Applications
- NREL/SNL NALU
  Wind Turbine CFD
- SNL LAMMPS
  Molecular Dynamics
- UT Uintah
  Combustine

Frameworks
- ORNL Raptor
  Large Eddy Sim

Kokkos

Hardware
- ORNL Frontier
  Cray / AMD GPU
- LANL/SNL Trinity
  Intel Haswell / Intel KNL
- ANL Aurora
  Intel Xeon CPUs + Xe Compute
- SNL Astra
  ARM Architecture
- LLNL SIERRA
  IBM Power9 / NVIDIA Volta
The Kokkos EcoSystem

Kokkos 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

Science and Engineering Applications

Trilinos

Kokkos Support
- Documentation
- Tutorials
- Bootcamps
- App support

Multi-Core

Many-Core

APU

CPU + GPU
The Kokkos Team


former: J. Wilke, S. Acer


Kokkos Support: C. Trott, G. Shipmann, G. Womeldorff, and all of the above
former: H.C. Edwards, G. Lopez, F. Foertter
Kokkos helps improve ISO C++

Ten current or former Kokkos team members are members of the ISO C++ standard committee.
Kokkos has a growing OpenSource Community

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

Online Resources:

▶ [https://github.com/kokkos/](https://github.com/kokkos/):
  ▶ Primary Kokkos GitHub Organization

▶ [https://github.com/kokkos/kokkos-tutorials/wiki/](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/](https://github.com/kokkos/kokkos/wiki/):
  ▶ Wiki including API reference

▶ [https://kokkosteame.slack.com/](https://kokkosteame.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

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

Kokkos maps **work** to execution resources
Data parallel patterns and work

```
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.
Data parallel patterns and work

```cpp
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.

**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?
How are computational bodies given to Kokkos?

As **functors** or **function objects**, a common pattern in C++. 
How are computational bodies given to Kokkos?

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

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

```cpp
struct ParallelFunctor {
    ...
    void operator() (a work assignment) const {
        /* ... computational body ... */
        ...
    }
};
```
How is work assigned to functor operators?

A total amount of work items is given to a Kokkos pattern, `ParallelFunctor` functor:

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

Warning: concurrency and order

Concurrency and ordering of parallel iterations is not guaranteed by the Kokkos runtime.
How is work assigned to functor operators?

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

```cpp
ParallelFunctor functor;
Kokkos::parallel_for(numberOfIterations, functor);
```
How is work assigned to functor operators?

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

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

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

```cpp
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,

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

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

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

**Warning: concurrency and order**

Concurrency and ordering of parallel iterations is *not* guaranteed by the Kokkos runtime.
The complete picture (using functors):

1. Defining the functor (operator+data):

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

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

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

2. Executing in parallel with Kokkos pattern:
   ```
   AtomForceFunctor functor(atomForces, data);
   Kokkos::parallel_for(numberOfAtoms, functor);
   ```
Functors are tedious ⇒ **C++11 Lambdas** are concise

```cpp
atomForces already exists
data already exists
Kokkos::parallel_for(numberOfAtoms,
  [=] (const int64_t atomIndex) {
    atomForces[atomIndex] = calculateForce(data);
  }
);
```
Functors are tedious ⇒ **C++11 Lambdas** are concise

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

A lambda is not *magic*, it is the compiler **auto-generating** a *functor* for you.
Functors are tedious \( \Rightarrow \) **C++11 Lambdas** are concise

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

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

```c
for (int64_t i = 0; i < N; ++i) {
    /* loop body */
}
```

OpenMP

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

Kokkos

```c
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:

\[ y = \int_{\text{lower}}^{\text{upper}} \text{function}(x) \, dx \]
Scalar integration (0)

Riemann-sum-style numerical integration:

\[ y = \int_{\text{lower}}^{\text{upper}} \text{function}(x) \, dx \]

```cpp
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;
```
**Riemann-sum-style numerical integration:**

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

double totalIntegral = 0;
for (int64_t i = 0; i < numberOfIntervals; ++i) {
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How do we **parallelize** it? Correctly?
Riemann-sum-style numerical integration:

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    totalIntegral += thisIntervalsContribution;
}

totalIntegral *= dx;

How do we \textbf{parallelize} it? Correctly?
An (incorrect) attempt:

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

First problem: compiler error; cannot increment totalIntegral
(lambdas capture by value and are treated as const!)
An (incorrect) solution to the (incorrect) attempt:

double totalIntegral = 0;
double * totalIntegralPointer = &totalIntegral;
Kokkos::parallel_for(numberOfIntervals,
    [=] (const int64_t index) {
        const double x =
            lower + (index/numberOfIntervals) * (upper - lower);
        *totalIntegralPointer += function(x);},
    );
totalIntegral *= dx;
An (incorrect) solution to the (incorrect) attempt:

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

Second problem: race condition

<table>
<thead>
<tr>
<th>step</th>
<th>thread 0</th>
<th>thread 1</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>load</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>increment</td>
<td>load</td>
</tr>
<tr>
<td>2</td>
<td>write</td>
<td>increment</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>write</td>
</tr>
</tbody>
</table>
Root problem: we’re using the **wrong pattern**, *for* instead of *reduction*
Root problem: we’re using the **wrong pattern**, for instead of *reduction*

Important concept: Reduction

Reductions combine the results contributed by parallel work.
**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?**

```c
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?**

```c
parallel_reduce(N, functor, 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**?

```c
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**?

```c
double finalReducedValue = 0;
parallel_reduce(N, functor, finalReducedValue);
```
Example: Scalar integration

```c
double totalIntegral = 0;
#pragma omp parallel for reduction(+:totalIntegral)
for (int64_t i = 0; i < numberOfIntervals; ++i) {
    totalIntegral += function(...);
}
```

```cpp
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.
Naming 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:

```cpp
double totalIntegral = 0;
parallel_reduce("Reduction", numberOfIntervals,
    [=] (const int64_t i, double & valueToUpdate) {
        valueToUpdate += function(...);
    },
    totalIntegral);
```
**Exercise:** Inner product $\langle y, A \ast x \rangle$

**Details:**
- $y$ is $N \times 1$, $A$ is $N \times M$, $x$ is $M \times 1$
- We’ll use this exercise throughout the tutorial
The **first step** in using Kokkos is to include, initialize, and finalize:

```cpp
#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:

<table>
<thead>
<tr>
<th>--kokkos-num-threads=INT</th>
<th>total number of threads</th>
</tr>
</thead>
<tbody>
<tr>
<td>KOKKOS_NUM_THREADS</td>
<td></td>
</tr>
<tr>
<td>--kokkos-device-id=INT</td>
<td>device (GPU) ID to use</td>
</tr>
<tr>
<td>KOKKOS_DEVICE_ID</td>
<td></td>
</tr>
</tbody>
</table>
Exercise #1: Inner Product, Flat Parallelism on the CPU

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

**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.
Exercise #1: logistics

Compiling for CPU

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

Running on CPU with OpenMP back-end

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

Things to try:

- Vary problem size with cline arg -S s
- Vary number of rows with cline arg -N n
- Num rows = $2^n$, num cols = $2^m$, total size = $2^s = 2^{n+m}$
Exercise #1 results

<y,Ax> Exercise 01, Fixed Size

Bandwidth (GB/s) vs. Number of Rows (N)

- HSW
- KNL
- KNL (HBM)
Simple usage is similar to OpenMP, advanced features are also straightforward.

Three common data-parallel patterns are parallel_for, parallel_reduce, and parallel_scan.

A parallel computation is characterized by its pattern, policy, and body.

User provides computational bodies as functors or lambdas which handle a single work item.
Views

Learning objectives:
- Motivation behind the View abstraction.
- Key View concepts and template parameters.
- The View life cycle.
Example: running **daxpy on the GPU**:

```c
double * x = new double[N]; // also y
parallel_for("DAXPY", N, [=] (const int64_t i) {
    y[i] = a * x[i] + y[i];
});
```
**Example: running daxpy on the GPU:**

```
double * x = new double[N]; // also y
parallel_for("DAXPY",N, [=] (const int64_t i) {
    y[i] = a * x[i] + y[i];
    
});
```

```
struct Functor {
    double * _x, * _y, a;
    void operator()(const int64_t i) const {
        _y[i] = _a * _x[i] + _y[i];
    }
};
```

**Problem:** x and y reside in CPU memory.
Example: running daxpy on the GPU:

```cpp
double * x = new double[N]; // also y
parallel_for("DAXPY", N, [=] (const int64_t i) {
    y[i] = a * x[i] + y[i];
});
```

```cpp
struct Functor {
    double *_x, *_y, a;
    void operator()(const int64_t i) const {
        _y[i] = _a * _x[i] + _y[i];
    }
};
```

Problem: x and y reside in CPU memory.

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

⇒ 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:

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

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

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```

**Important point**

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

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

---

Example:

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

Note: runtime-sized dimensions must come first.
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**Example:**

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

// Access
```cpp
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`

Example:

```cpp
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?
3.0
**View life cycle:**

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What gets printed? 3.0
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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:**

```cpp
View<double*[5]> a("A", N0);
assert(a.extent(0) == N0);
assert(a.extent(1) == 5);
static_assert(a.static_extent(1) == 5);
assert(a.data() != nullptr);
assert(a.label() == "A");
```
Exercise #2: Inner Product, Flat Parallelism on the CPU, with Views

Location: Exercises/02/Begin/

Assignment: Change data storage from arrays to Views.

Compile and run on CPU, and then on GPU with UVM

make -j KOKKOS_DEVICES=OpenMP  # CPU-only using OpenMP
make -j KOKKOS_DEVICES=Cuda    # GPU - note UVM in Makefile

# Run exercise
./02_Exercise.host -S 26
./02_Exercise.cuda -S 26

# Note the warnings, set appropriate environment variables

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

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

Execution spaces: Serial, Threads, OpenMP, Cuda, HIP, ...
Changing the parallel execution space:

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

Custom

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

Default

```cpp
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.
Changing the parallel execution space:

```cpp
parallel_for("Label",
    RangePolicy< ExecutionSpace >(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

```cpp
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 */
```
Kokkos function and lambda portability annotation macros:

Function annotation with KOKKOS_INLINE_FUNCTION macro

```cpp
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 */
```

Lambda annotation with KOKKOS_LAMBDA macro

```cpp
Kokkos::parallel_for("Label", numberOfIterations,
    KOKKOS_LAMBDA (const int64_t index) {...});
// Where Kokkos defines:
#define KOKKOS_LAMBDA [=] /* #if CPU-only */
#define KOKKOS_LAMBDA [=] __device__ __host__ /* #if CPU+Cuda */
```
Memory space:
explicitly-manageable memory resource
(i.e., “place to put data”)
Important concept: Memory spaces

Every view stores its data in a memory space set at compile time.
Memory spaces (1)

Important concept: Memory spaces

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

- View<double***, MemorySpace> data(...);

Available memory spaces: HostSpace, CudaSpace, CudaUVMSpace, ...

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);
Important concept: Memory spaces

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

- View<`double***`, `MemorySpace`> data(...);
- Available **memory spaces**:
  - HostSpace, CudaSpace, CudaUVMSpace, ... more
Important concept: Memory spaces

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

- `View<double***, MemorySpace> data(...);`
- Available memory spaces:
  - HostSpace, CudaSpace, CudaUVMSpace, ... more
- Each execution space has a default memory space, which is used if `Space` provided is actually an execution space
Important concept: Memory spaces

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

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

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

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

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

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

Diagram showing memory spaces between CPU and GPU with RAM and metadata.
Example: HostSpace

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

Example: CudaSpace

View<double**, CudaSpace> view(...constructor arguments...);
Example (redux): summing an array with the GPU

(failed) Attempt 1: View lives in CudaSpace

```cpp
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

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

double sum = 0;
Kokkos::parallel_reduce("Label",
    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);
    },
    sum);
Example (redux): summing an array with the GPU

(failed) Attempt 2: View lives in HostSpace

```cpp
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);
```

What's the solution?

- CudaUVMSpace
- CudaHostPinnedSpace (skipping)
- Mirroring

Illegal access
Example (redux): summing an array with the GPU

(failed) Attempt 2: View lives in HostSpace

```cpp
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);
```

What's the solution?

- CudaUVMSpace
- CudaHostPinnedSpace (skipping)
- Mirroring
Important concept: Mirrors

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

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

**Mirroring schematic**

```cpp
using view_type = Kokkos::View<double**, Space>;
view_type view(...);
view_type::HostMirror hostView = Kokkos::create_mirror_view(view);
```
1. **Create** a *view*'s array in some memory space.
   
   ```cpp
   using view_type = Kokkos::View<double*, Space>;
   view_type view(...);
   ```
1. **Create** a `view`'s array in some memory space.
    ```
    using view_type = Kokkos::View<double*, Space>;
    view_type  view(...);
    ```

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

2. **Create** `hostView`, a *mirror* of the `view`'s array residing in the host memory space.
   
   ```cpp
   view_type::HostMirror hostView = Kokkos::create_mirror_view(view);
   ```

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

1. **Create** a `view`'s array in some memory space.
   
   ```cpp
   using view_type = Kokkos::View<double*, Space>;
   view_type view(...);
   ```

2. **Create** `hostView`, a *mirror* of the `view`'s array residing in the host memory space.
   
   ```cpp
   view_type::HostMirror hostView = Kokkos::create_mirror_view(view);
   ```

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

4. **Deep copy** `hostView`'s array to `view`'s array.
   
   ```cpp
   Kokkos::deep_copy(view, hostView);
   ```
Mirroring pattern

1. **Create** a `view`'s array in some memory space.
   
   ```
   using view_type = Kokkos::View<double*, Space>;
   view_type view(...);
   ```

2. **Create** `hostView`, a *mirror* of the `view`'s array residing in the host memory space.
   
   ```
   view_type::HostMirror hostView = 
   Kokkos::create_mirror_view(view);
   ```

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

4. **Deep copy** `hostView`'s array to `view`'s array.
   
   ```
   Kokkos::deep_copy(view, hostView);
   ```

5. **Launch** a kernel processing the `view`'s array.
   
   ```
   Kokkos::parallel_for("Label",
   RangePolicy< Space>(0, size),
   KOKKOS_LAMBDA (...) { use and change view });
   ```
Mirroring pattern

1. **Create** a view’s array in some memory space.
   
   ```cpp
   using view_type = Kokkos::View<double*, Space>;
   view_type view(...);
   ```

2. **Create** hostView, a *mirror* of the view’s array residing in the host memory space.
   
   ```cpp
   view_type::HostMirror hostView =
   Kokkos::create_mirror_view(view);
   ```

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

4. **Deep copy** hostView’s array to view’s array.
   
   ```cpp
   Kokkos::deep_copy(view, hostView);
   ```

5. **Launch** a kernel processing the view’s array.
   
   ```cpp
   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.
   
   ```cpp
   Kokkos::deep_copy(hostView, view);
   ```
What if the View is in HostSpace too? Does it make a copy?

typedef Kokkos::View<double*, Space> ViewType;
ViewType view("test", 10);
ViewType::HostMirror hostView =
   Kokkos::create_mirror_view(view);

- create_mirror_view allocates data only if the host process cannot access view’s data, otherwise hostView references the same data.
- create_mirror always allocates data.
- Reminder: Kokkos never performs a hidden deep copy.
Exercise #3: Flat Parallelism on the GPU, Views and Host Mirrors

**Details:**

- **Location:** Exercises/03/Begin/
- **Add HostMirror Views and deep copy**
- **Make sure you use the correct view in initialization and Kernel**

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

**Things to try:**

- Vary problem size and number of rows (-S ...; -N ...)
- Change number of repeats (-nrepeat ...)
- Compare behavior of CPU vs GPU
Data is stored in Views that are “pointers” to multi-dimensional arrays residing in memory spaces.

Views abstract away platform-dependent allocation, (automatic) deallocation, and access.

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.
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.

```c
View<double***, Layout, Space> name(...);
```
Important concept: Layout

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

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

- Most-common layouts are LayoutLeft and LayoutRight.
  - LayoutLeft: left-most index is stride 1.
  - LayoutRight: right-most index is stride 1.
- If no layout specified, default for that memory space is used.
  - LayoutLeft for CudaSpace, LayoutRight for HostSpace.
- Layouts are extensible: ≈ 50 lines
- Advanced layouts: LayoutStride, LayoutTiled, ...
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
- Compare using UVM vs not using UVM on GPUs
- Check what happens if MemSpace and ExecSpace do not match.
Exercise #4: Inner Product, Flat Parallelism

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

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

Bandwidth (GB/s)

Number of Rows (N)

Why?
**Thread independence:**

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

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

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

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

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

CPU threads are independent. i.e., threads may execute at any rate.
### 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?

- **CPU** threads are independent.
  - i.e., threads may execute at any rate.
- **GPU** threads execute synchronized.
  - i.e., threads in groups can/must execute instructions together.
Thread independence:

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

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

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

▶ **GPU** threads execute synchronized.
  ▶ i.e., threads in groups can/must execute instructions together.

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

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

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

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

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

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?
**Important point**

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

**Caching**: if thread $t$’s current access is at position $i$, thread $t$’s next access should be at position $i+1$.

**Coalescing**: if thread $t$’s current access is at position $i$, thread $t+1$’s current access should be at position $i+1$. 
Important point

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

**Caching**: if thread $t$’s current access is at position $i$, thread $t$’s next access should be at position $i+1$.

**Coalescing**: if thread $t$’s current access is at position $i$, thread $t+1$’s current access should be at position $i+1$.

**Warning**

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

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

Example:

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

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

(a) OpenMP
- HostSpace: cached (good)
- CudaSpace: coalesced (good)

(b) Cuda
Example: inner product (5)

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

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

Bandwidth (GB/s) vs. Number of Rows (N)

- Coalesced
- Cached
- Uncached

Graph showing bandwidth performance for different architectures and layouts with coalesced, cached, and uncached data access patterns.
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.

⇒ You’ll need multiple versions of code or pay the performance penalty.
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);

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

Solutions:
▶ Atomics
▶ Thread teams
Example: inner product (0)

(Flat parallel) Kernel:

```cpp
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);
```

Problem: What if we don’t have enough rows to saturate the GPU?
(Flat parallel) Kernel:

```cpp
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);
```

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

Solutions?
Example: inner product (0)

(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);

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.

```c
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 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.

```cpp
// 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.

```cpp
// total work = numberOfTeams * teamSize
parallel_for("Label",
    TeamPolicy<ExecutionSpace>(numberOfTeams, teamSize), functor);
```
typedef typename TeamPolicy<ExecSpace>::member_type 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;
    }
}
We shouldn’t be hard-coding the work mapping...

```cpp
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;
    }
}
```

If this were a parallel execution,
we'd use Kokkos::parallel_reduce.
We shouldn’t be hard-coding the work mapping...

```cpp
operator() (member_type & teamMember, double & update) {
    const int row = teamMember.league_rank();
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}
```

If this were a parallel execution, we’d use Kokkos::parallel_reduce.

**Key idea:** this is a parallel execution.
We shouldn’t be hard-coding the work mapping...

```cpp
operator () (member_type & teamMember, double & update) {
    const int row = teamMember.league_rank();
    double thisRowsSum;
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        [=] (const int col) {
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    }
}
```

If this were a parallel execution,
we’d use Kokkos::parallel_reduce.

**Key idea**: this is a parallel execution.

⇒ **Nested parallel patterns**
TeamThreadRange:

```cpp
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.
TeamThreadRange:

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

- The **mapping** of work indices to threads is architecture-dependent.
- The **amount of work** given to the TeamThreadRange **need not be a multiple** of the team size.
- Intrateam **reduction handled** by Kokkos.
**Anatomy** of nested parallelism:

```cpp
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:

```cpp
class TeamPolicy<ExecutionSpace>
```
In practice, you can let Kokkos decide:

\[
\text{parallel\_something}(\\ 
\quad \text{TeamPolicy<ExecutionSpace>}(\text{numberOfTeams}, \text{Kokkos::AUTO}),\\ 
\quad /* \text{functor} */);\\
\]

**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**
What should the team size be?

In practice, you can let Kokkos decide:

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

**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
Exercise: TeamPolicy

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

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

Bandwidth (GB/s) vs. Number of Rows (N)

- Coalesced
- Cached
- Uncoalesced
- Uncached
Exercise: TeamPolicy

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

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

Bandwidth (GB/s) vs Number of Rows (N)

- HSW Left
- HSW Right
- KNL Left
- KNL Right
- Pascal60 Left
- Pascal60 Right

Bandwidth patterns:
- coalesced
- cached
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.
Three-level parallelism (1)

**Anatomy** of nested parallelism:

```cpp
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 */
      }[, ...]);
    /* end middle body */
    parallel_middle(
      TeamVectorRange(teamMember, someSize),
      [=] (const int indexTeamVector[, ...]) {
        /* nested body */
        }[, ...]);
    /* end of outer body */
  }[, ...]);
```
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`

```c
// 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
Exercise: TeamVectorLoop

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

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

Bandwidth (GB/s) vs. Number of Rows (N)
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.
**Exercise:** Find $x$ in $b = A \times x$

Getting set up in your home directory:

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

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

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

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

Things to try:
- Compare with previous exercise on GPU with low iteration count.
- Compare performance for small problems.
- Compare performance dependent on Layout of col_idx and values.
This was a short introduction
Didn’t cover many things:

▶ Full BuildSystem integration.
▶ Non-Sum reductions / multiple reductions.
▶ Multidimensional loops.
▶ Advanced data structures.
▶ Subviews.
▶ Atomic operations and Scatter Contribute patterns.
▶ Team Scratch memory (GPU shared memory).
▶ SIMD vectorization.
▶ MPI and PGAS integration.
▶ Tools for Profiling, Debugging and Tuning.
▶ Math Kernels.
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Watch the Kokkos Lectures for all of those and more in-depth explanations or do them on your own.

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

https://kokkos.link/the-lectures
Online Resources:

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