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/blob/main/Intro-Short/KokkosTutorial_Short.pdf`

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

The Kokkos Lectures

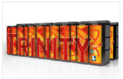
Watch the Kokkos Lectures for all of those and more in-depth explanations or do them on your own.

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

`https://kokkos.link/the-lectures`

The HPC Hardware Landscape

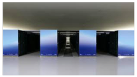
Current Generation: Programming Models OpenMP 3, CUDA and OpenACC depending on machine


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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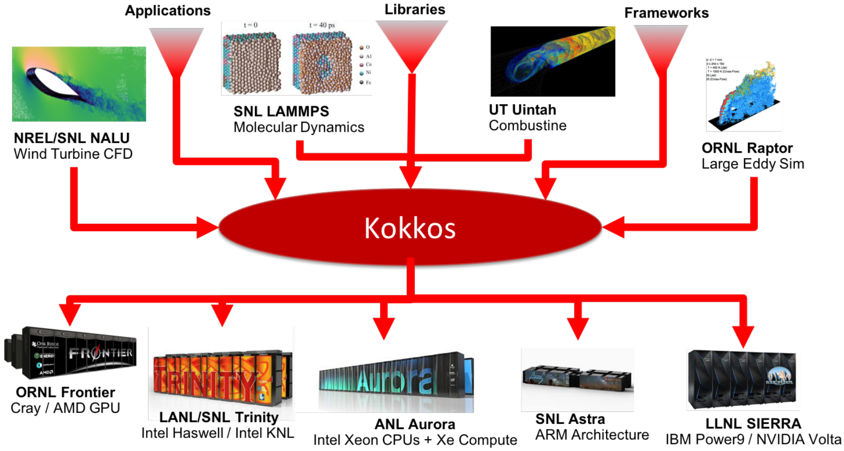
Software Cost Switching Vendors

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

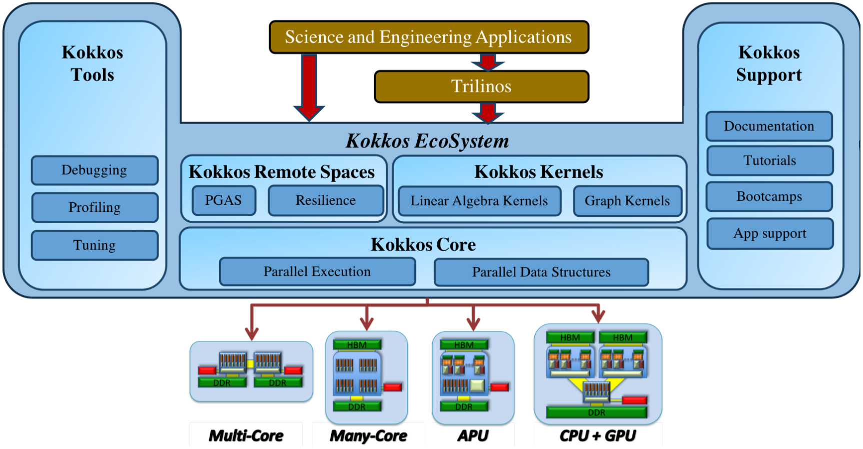
What is Kokkos?

- 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
- 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



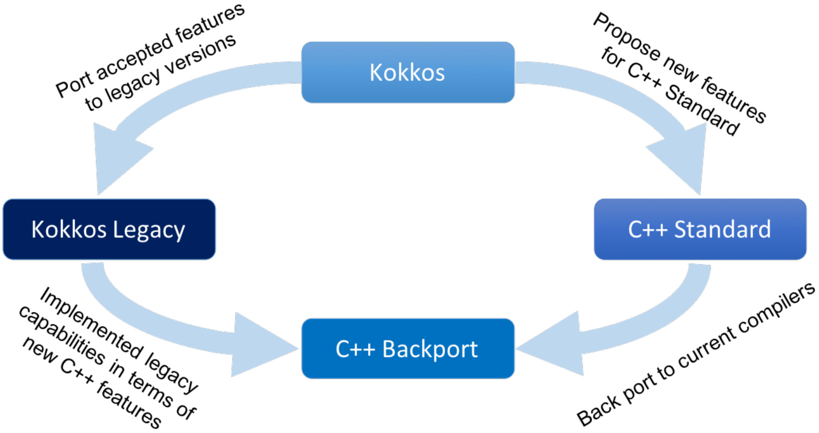
The Kokkos EcoSystem



The Kokkos Team

Kokkos Core:	**C. Trott**, **D. Lebrun-Grandié**, D. Arndt, J. Ciesko, C. Clevenger, N. Ellingwood, R. Gayatri, D. Ibanez, D. Lee, S. Lee, N. Liber, P. Miller, N. Morales, A. Powell, F. Rizzi, M. Simberg, C. Skrzyński, B. Turcksin
Kokkos Kernels:	**S. Rajamanickam**, **L. Berger-Vergiat**, V. Dang, N. Ellingwood, J. Foucar, E. Harvey, B. Kelley, K. Liegeois, C. Pearson, E. Prudencio
Kokkos Support	**C. Trott**, G. Shipmann, G. Womeldorff, and all of the above

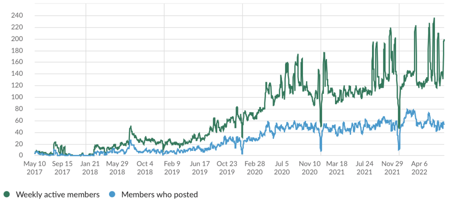
Kokkos helps improve ISO C++


Kokkos
Propose new features for C++ Standard
C++ Standard
Back port to current compilers
C++ Backport
Implemented legacy capabilities in terms of new C++ features
Kokkos Legacy
Port accepted features to legacy versions

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

Kokkos has a growing OpenSource Community

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



Online Resources:

- https://github.com/kokkos:
  - Primary Kokkos GitHub Organization
- https://github.com/kokkos/kokkos-tutorials/wiki/Kokkos-Lecture-Series:
  - Slides, recording and Q&A for the Full Lectures
- https://kokkos.github.io/kokkos-core-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.

Using Kokkos for data parallel patterns (0)

Data parallel patterns and work

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

Kokkos maps **work** to execution resources

Using Kokkos for data parallel patterns (0)

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

Using Kokkos for data parallel patterns (0)

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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.

Using Kokkos for data parallel patterns (2)

How are computational bodies given to Kokkos?

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

Using Kokkos for data parallel patterns (2)

How are computational bodies given to Kokkos?

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

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

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

Using Kokkos for data parallel patterns (3)

How is work assigned to functor operators?

Using Kokkos for data parallel patterns (3)

How is work assigned to functor operators?

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

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

Using Kokkos for data parallel patterns (3)

How is work assigned to functor operators?

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

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

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

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

Warning: concurrency and order

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

Using Kokkos for data parallel patterns (6)

The complete picture (using functors):

1. Defining the functor (operator+data):

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

  AtomForceFunctor(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);
```

Using Kokkos for data parallel patterns (7)

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

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

Using Kokkos for data parallel patterns (7)

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

Using Kokkos for data parallel patterns (7)

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

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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 */
});
```

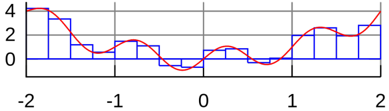
Important concept

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

Scalar integration (0)

Riemann-sum-style numerical integration:

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



Wikipedia

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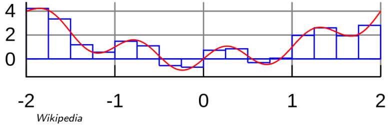

```
double totalIntegral = 0;
for (int64_t i = 0; i < numberOfIntervals; ++i) {
  const double x =
    lower + (i/numberOfIntervals) * (upper - lower);
  const double thisIntervalsContribution = function(x);
  totalIntegral += thisIntervalsContribution;
}
totalIntegral *= dx;
```

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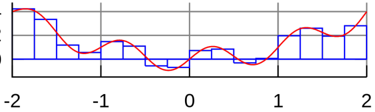

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How do we **parallelize** it? *Correctly?*

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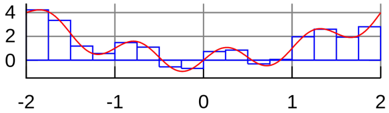

Wikipedia

Pattern?

Policy?

Body?

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

An (incorrect) attempt:

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

First problem: compiler error; cannot increment `totalIntegral` (lambdas capture by value and are treated as const!)

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

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

Second problem: race condition

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

Scalar integration (3)

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

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Important concept: Reduction

Reductions combine the results contributed by parallel work.

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Reductions combine the results contributed by parallel work.

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

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

Scalar integration (3)

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

Important concept: Reduction

Reductions combine the results contributed by parallel work.

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

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

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

Example: Scalar integration

OpenMP

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

Kokkos

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

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

Always name your kernels!

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

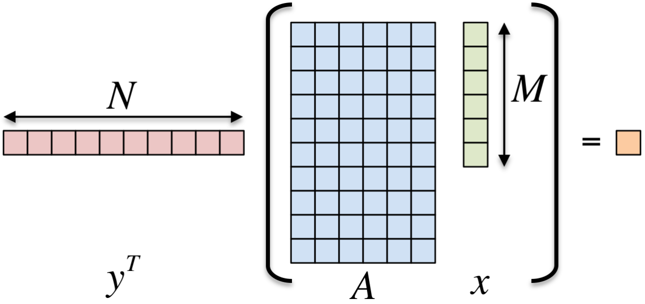
- Non-nested parallel patterns can take an optional string argument.
- The label doesn't need to be unique, but it is helpful.
- Anything convertible to "std::string"
- Used by profiling and debugging tools (see Profiling Tutorial)

Example:

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

Recurring Exercise: Inner Product

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



Details:

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

Using your own ${HOME}

- Git
- GCC 8.2 (or newer) *OR* Intel 19.0.5 (or newer) *OR* Clang 8.0 (or newer)
- CUDA nvcc 11.0 (or newer) *AND* NVIDIA compute capability 6.0 (or newer)
- git clone `https://github.com/kokkos/kokkos`
  into `${HOME}/Kokkos/kokkos`
- git clone `https://github.com/kokkos/kokkos-tutorials`
  into `${HOME}/Kokkos/kokkos-tutorials`

  Slides are in
  `${HOME}/Kokkos/kokkos-tutorials/LectureSeries`

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

  Exercises' makefiles look for `${HOME}/Kokkos/kokkos`

Exercise #1: include, initialize, finalize Kokkos

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

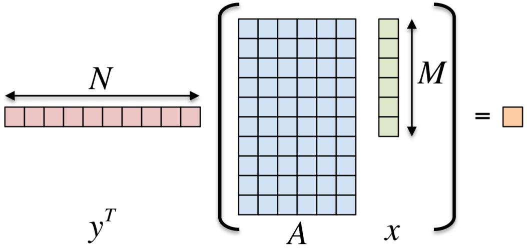
```
#include <Kokkos_Core.hpp>
int main(int argc, char* argv[]) {
  /* ... do any necessary setup (e.g., initialize MPI) ... */
  Kokkos::initialize(argc, argv);
  {
  /* ... do computations ... */
  }
  Kokkos::finalize();
  return 0;
}
```

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

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.

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=...
```

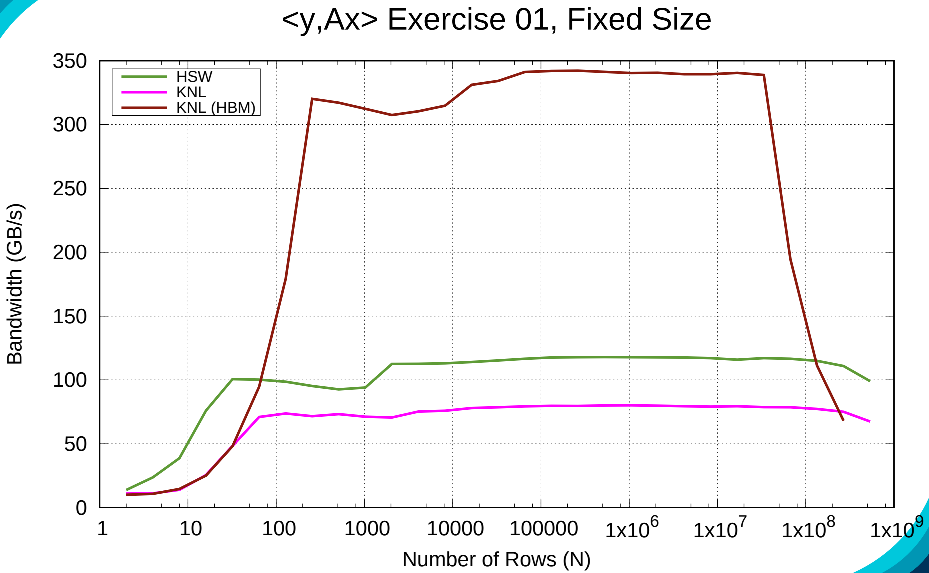
Running on CPU with OpenMP back-end

```
# 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



Section Summary

- **Simple** usage is similar to OpenMP, advanced features are also straightforward
- Three common **data-parallel patterns** are `parallel_for`, `parallel_reduce`, and `parallel_scan`.
- A parallel computation is characterized by its **pattern**, **policy**, and **body**.
- User provides **computational bodies** as functors or lambdas which handle a single work item.

Views

Learning objectives:

- Motivation behind the `View` abstraction.
- Key `View` concepts and template parameters.
- The `View` life cycle.

Example: running daxpy on the GPU:

Lambda

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

Functor

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

View motivation

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struct Functor {
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    _y[i] = _a * _x[i] + _y[i];
  }
};
```

Problem: x and y reside in CPU memory.

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

$\Rightarrow$ **Views**

View abstraction

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

High-level example of Views for daxpy using lambda:

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

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

Views (0)

View abstraction

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

High-level example of Views for daxpy using lambda:

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

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

Important point

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

Views (1)

View overview:

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

Views (1)

View overview:

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- Arrays are **rectangular**, not ragged.
- **Sizes of dimensions** set at compile-time or runtime.
  e.g., 2x20, 50x50, etc.
- 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.

Views (2)

View life cycle:

- Allocations only happen when *explicitly* specified.

  i.e., there are **no hidden allocations**.
- Copy construction and assignment are **shallow** (like pointers).

  so, you pass `Views` by value, *not* by reference
- Reference counting is used for **automatic deallocation.**
- They behave like `std::shared_ptr`

Views (2)

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  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:

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  i.e., there are **no hidden allocations**.
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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

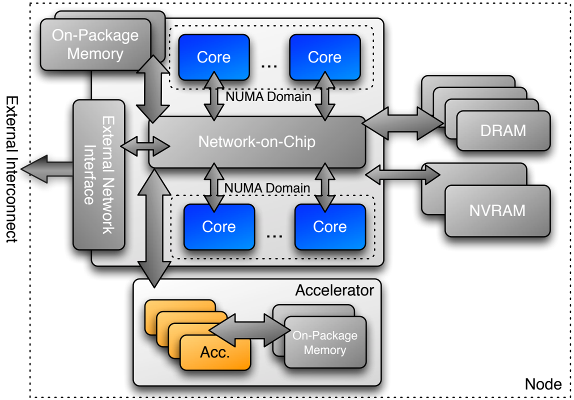
- Location: `Exercises/02/Begin/`
- Assignment: Change data storage from arrays to Views.
- Compile and run on CPU, and then on GPU with UVM

```
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`, `OpenMP`, `Cuda`, `HIP`, `SYCL`, ...

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
                     }
                     );
```

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
                     }
                     );
```

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

  $\Rightarrow$ Always in the **host process**

Execution spaces (2)

Host

Parallel

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Kokkos::parallel_for("MyKernel", numberOfSomethings,
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                     );
```

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

Execution spaces (2)

Host

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

Changing the parallel execution space:

Custom

```
parallel_for("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:

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 ... */
  });
```

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 */
```

Kokkos function and lambda portability annotation macros:

Function annotation with `KOKKOS_INLINE_FUNCTION` macro

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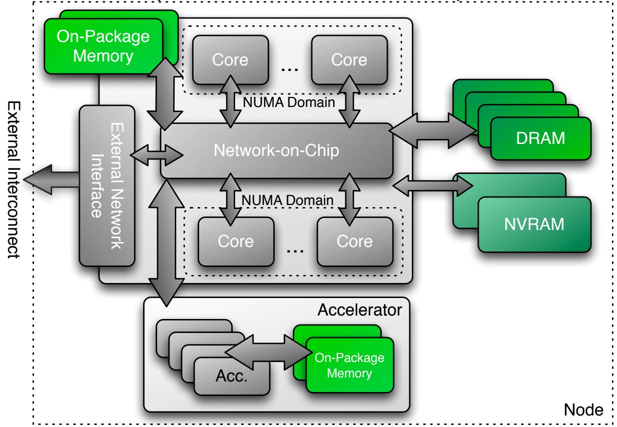
  void operator()(const int64_t index) const {
    helperFunction(index);
  }
}
// Where kokkos defines:
#define KOKKOS_INLINE_FUNCTION inline                     /* #if CPU-only */
#define KOKKOS_INLINE_FUNCTION inline __device__ __host__ /* #if CPU+Cuda */
```

Lambda annotation with `KOKKOS_LAMBDA` macro

```
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”)



Memory spaces (1)

Important concept: Memory spaces

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

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

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

Memory spaces (1)

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

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

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- Each **execution space** has a default memory space, which is used if **Space** provided is actually an execution space

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- `View<double***,`*Memory***Space**`> data(...);`
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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**.

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

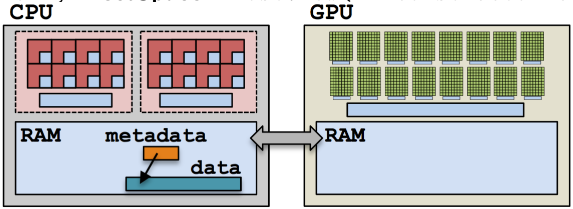
- `View<double***,`*Memory***Space**`> data(...);`
- Available **memory spaces**:

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

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

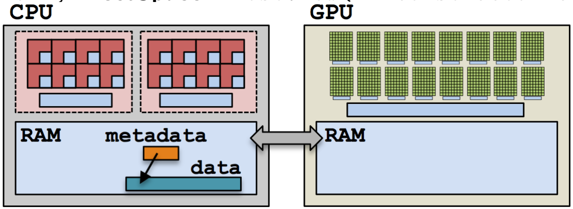
Example: HostSpace

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



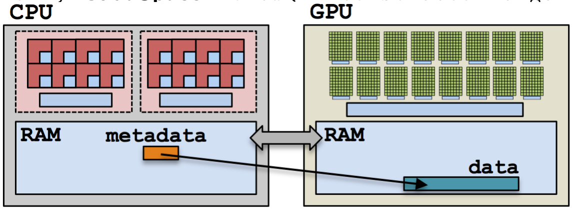
Example: HostSpace

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



Example: CudaSpace

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



Example (redux): summing an array with the GPU

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

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

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

Example (redux): summing an array with the GPU

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

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

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

```
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

(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);
```

What's the solution?

- CudaUVMSpace
- CudaHostPinnedSpace (skipping)
- Mirroring

Important concept: Mirrors

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

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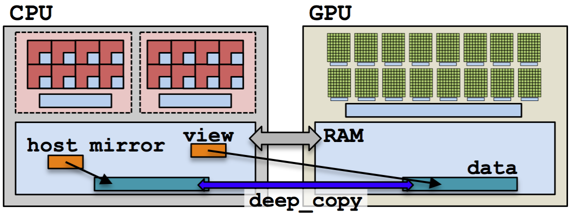
Mirroring schematic

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



Mirroring pattern

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

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

Mirroring pattern

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   ```
   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);
   ```

Mirroring pattern

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

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   view_type::HostMirror hostView =
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   ```
3. **Populate** `hostView` on the host (from file, etc.).
4. **Deep copy** `hostView`'s array to `view`'s array.
   ```
   Kokkos::deep_copy(view, hostView);
   ```

Mirroring pattern

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

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.
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view_type::HostMirror 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 });
```
6. If needed, **deep copy** the `view`'s updated array back to the `hostView`'s array to write file, etc.
```
Kokkos::deep_copy(hostView, view);
```

Mirrors of Views in HostSpace

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

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

- `create_mirror_view` allocates data only if the host process cannot access view's data, otherwise hostView references the same data.
- `create_mirror` **always** allocates data.
- Reminder: Kokkos *never* performs a **hidden deep copy**.

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

Details:

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

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

Things to try:

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

View and Spaces Section Summary

- Data is stored in `Views` that are “pointers” to **multi-dimensional arrays** residing in **memory spaces**.
- `Views` **abstract away** platform-dependent allocation, (automatic) deallocation, and access.
- **Heterogeneous nodes** have one or more memory spaces.
- **Mirroring** is used for performant access to views in host and device memory.
- Heterogeneous nodes have one or more **execution spaces**.
- You **control where** parallel code is run by a template parameter on the execution policy, or by compile-time selection of the default execution space.

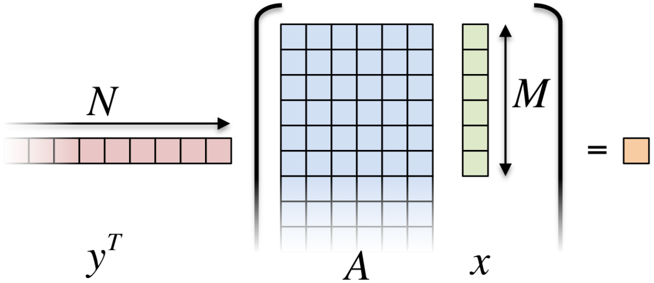
Managing memory access patterns for performance portability

Learning objectives:

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

Example: inner product (0)

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



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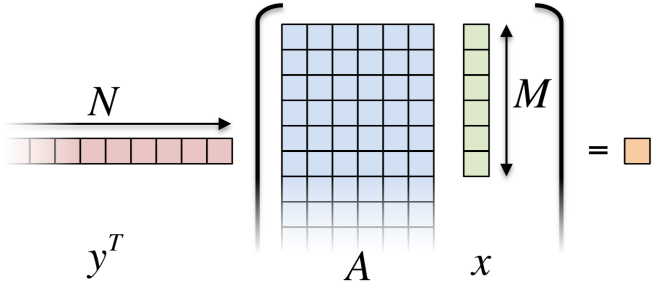
    for (size_t entry = 0; entry < M; ++entry) {
      thisRowsSum += A(row, entry) * x(entry);
    }
    valueToUpdate += y(row) * thisRowsSum;
  }, result);
```



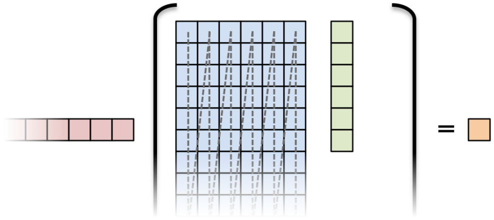
Driving question: How should A be laid out in memory?

Example: inner product (1)

Layout is the mapping of multi-index to memory:

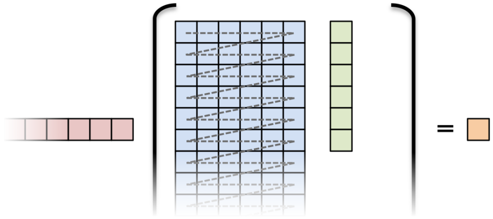
LayoutLeft

in 2D, "column-major"



LayoutRight

in 2D, "row-major"



Important concept: Layout

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

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

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

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```

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

Exercise #4: Inner Product, Flat Parallelism

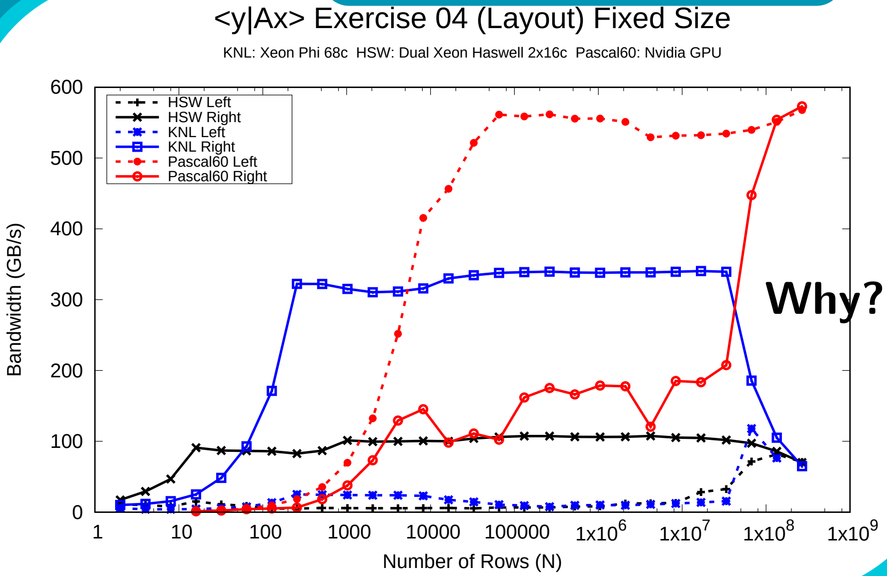
Details:

- 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



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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operator()(int index, double & valueToUpdate) const {
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- **CPU** threads are independent.
  - i.e., threads may execute at any rate.

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

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

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- **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?

Caching and coalescing (2)

Important point

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

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

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

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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)

Mapping indices to cores (2)

Rule of Thumb

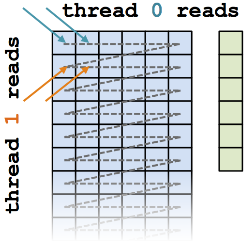
Kokkos index mapping and default layouts provide efficient access if **iteration indices** correspond to the **first index** of array.

Example:

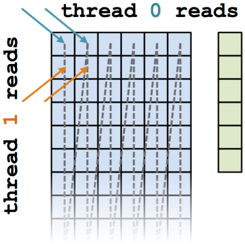
```
View<double***, ...> view(...);
...
Kokkos::parallel_for("Label", ... ,
  KOKKOS_LAMBDA (int workIndex) {
    ...
    view(..., ... , workIndex ) = ...;
    view(... , workIndex, ... ) = ...;
    view(workIndex, ... , ... ) = ...;
  });
...
```

Analysis: Kokkos architecture-dependent

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



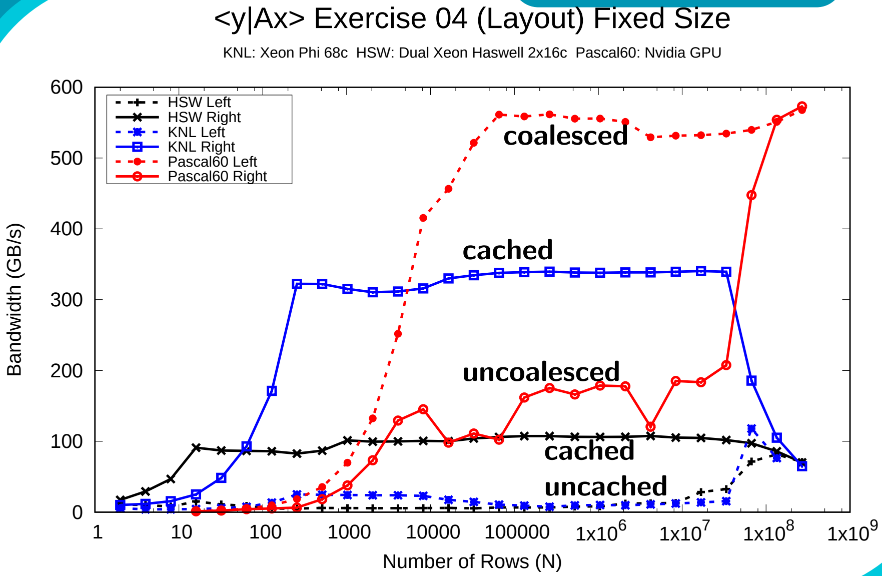
(a) OpenMP



(b) Cuda

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

Example: inner product (5)



Memory Access Pattern Summary

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

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

MDRangePolicy (0)

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 */
    }
  }
}
```

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    }
  }
}
```

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

MDRangePolicy (1)

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      /* 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 1 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 $Rank < DIM >$.

MDRangePolicy (2)

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

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      /* 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);
```

MDRangePolicy (3)

You can also do Reductions:

```
double result;
parallel_reduce("Label",
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- The Policy doesn't change the rules for ‘parallel_reduce‘.

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- Additional Thread Local Argument.

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- Can use ‘View‘s as reduction argument.

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}, 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);
```

MDRangePolicy (5)

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;
});
```

MDRangePolicy (5)

Initializing a Matrix:

```
View<double**,LayoutLeft> A("A",N0,N1);
parallel_for("Label",
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  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

MDRangePolicy (7)

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

Common Policy Arguments

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.

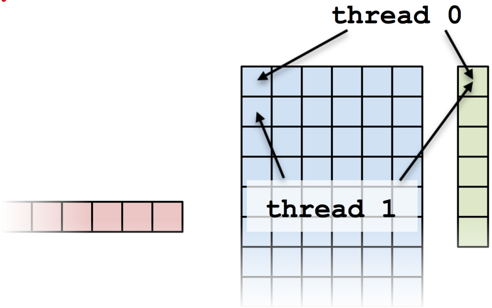
Learning objectives:

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

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);
```



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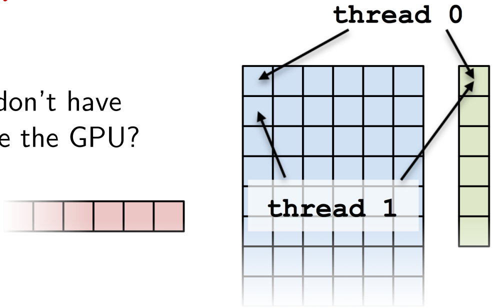
  }, result);
```

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



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```

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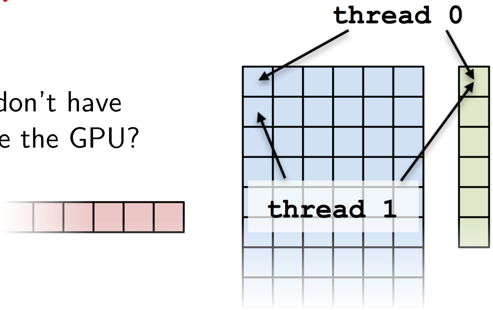
Solutions?



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    double thisRowsSum = 0;
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      thisRowsSum += A(row,col) * x(col);
    }
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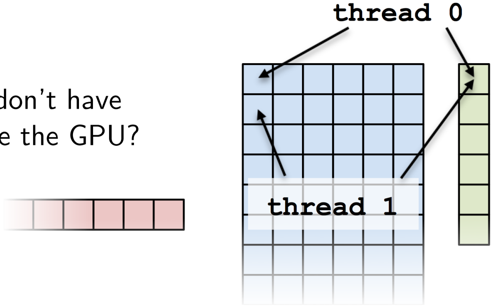
  }, result);
```

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

Solutions?

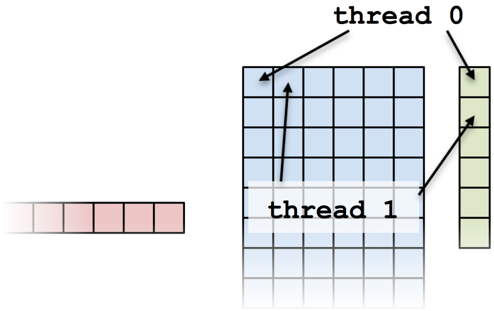
- Atomics
- Thread teams



Example: inner product (1)

Atomics kernel:

```
Kokkos::parallel_for("yAx", N*M,
  KOKKOS_LAMBDA (const size_t index) {
    const int row = extractRow(index);
    const int col = extractCol(index);
    atomic_add(&result, y(row) * A(row,col) * x(col));
  });
```



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    const int row = extractRow(index);
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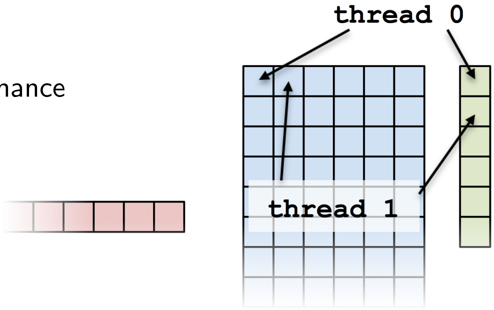
    atomic_add(&result, y(row) * A(row,col) * x(col));
  });
```

Problem: Poor performance



Example: inner product (2)

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);
}
```

Example: inner product (2)

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**.

Example: inner product (3)

Important concept: Thread team

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

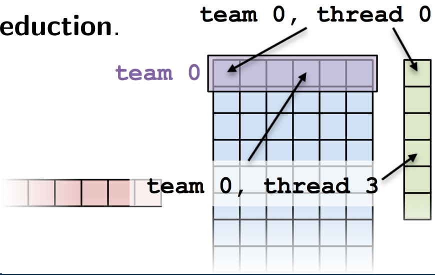
Example: inner product (3)

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**.



Example: inner product (4)

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);
```

TeamPolicy (0)

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);
```

TeamPolicy (0)

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();

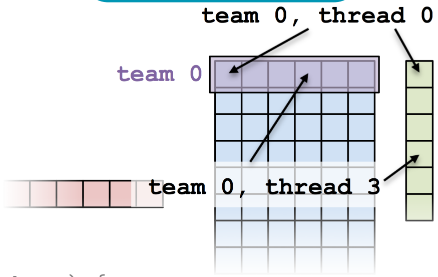
  // Which team am I on?
  const unsigned int league_rank = teamMember.league_rank();

  // 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();
}
```

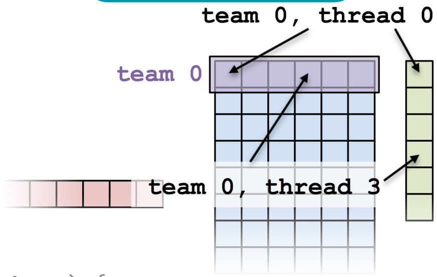
TeamThreadRange (0)



First attempt at exercise:

```
operator() (member_type & teamMember ) {
  const size_t row = teamMember.league_rank();
  const size_t col = teamMember.team_rank();
  atomic_add(&result,y(row) * A(row,col) * x(entry));
}
```

TeamThreadRange (0)



First attempt at exercise:

```
operator() (member_type & teamMember ) {
  const size_t row = teamMember.league_rank();
  const size_t col = teamMember.team_rank();
  atomic_add(&result,y(row) * A(row,col) * x(entry));
}
```

- When team size $\neq$ number of columns, how are units of work mapped to team's member threads? Is the mapping architecture-dependent?

Second attempt at exercise:

Divide row length among team members.

```
operator() (member_type & teamMember ) {
  const size_t row = teamMember.league_rank();

  int begin = teamMember.team_rank();
  for(int col = begin; col < M; col += teamMember.team_size()) {
    atomic_add(&result, y(row) * A(row,col) * x(entry));
  }
}
```

TeamThreadRange (1)

Second attempt at exercise:

Divide row length among team members.

```
operator() (member_type & teamMember ) {
  const size_t row = teamMember.league_rank();

  int begin = teamMember.team_rank();
  for(int col = begin; col < M; col += teamMember.team_size()) {
    atomic_add(&result, y(row) * A(row,col) * x(entry));
  }
}
```

- Still bad because `atomic_add` performs badly under high contention, how can team's member threads performantly cooperate for a nested reduction?
- On CPUs you get a bad data access pattern: this hardcodes coalesced access, but not caching.

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;
  }
}
```

TeamThreadRange (2)

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

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

If this were a parallel execution,

we'd use `Kokkos::parallel_reduce`.

TeamThreadRange (2)

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If this were a parallel execution,

we'd use `Kokkos::parallel_reduce`.

Key idea: this *is* a parallel execution.

TeamThreadRange (2)

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

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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 (3)

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 (3)

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:

```
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.

What should the team size be?

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

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

What should the team size be?

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

```
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**

What should the team size be?

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

```
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

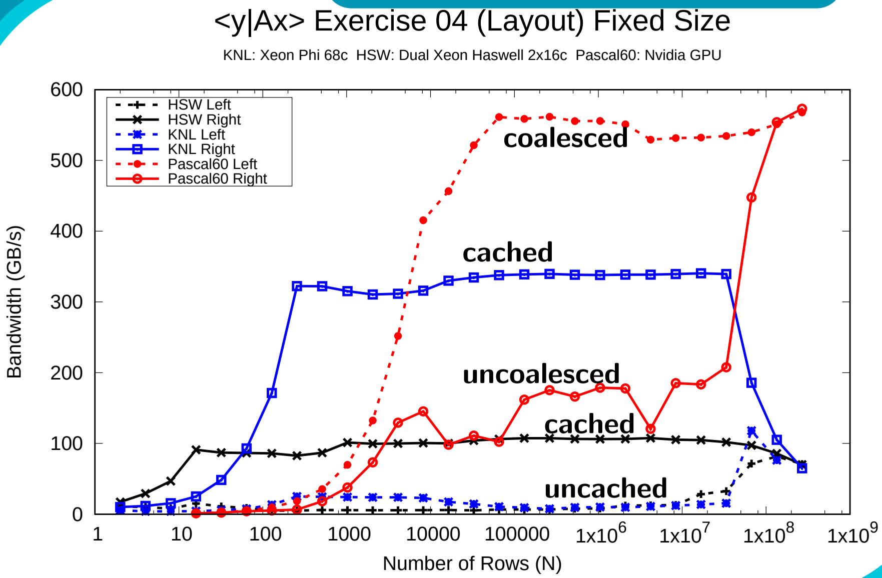
Details:

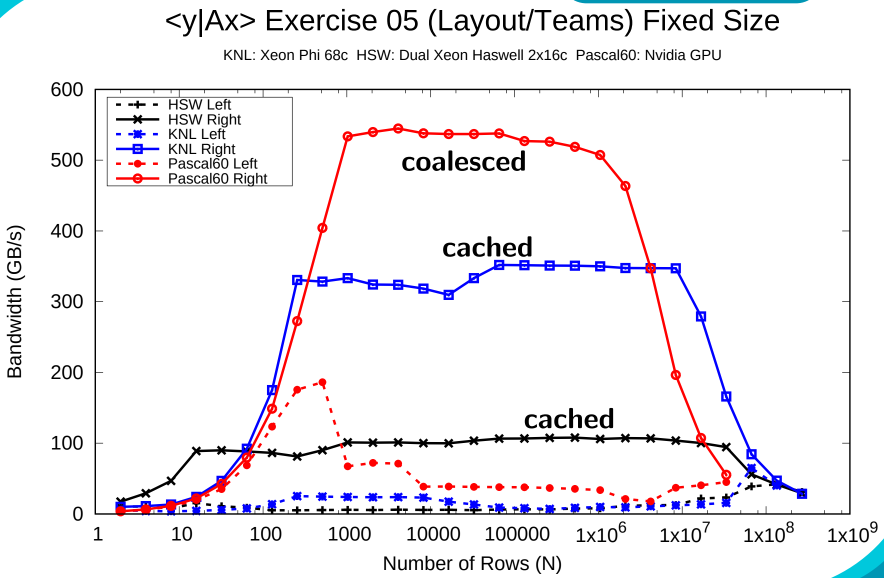
- Location: `Exercises/team_policy/`
- Replace `RangePolicy<Space>` with `TeamPolicy<Space>`
- Use `AUTO` for `team_size`
- Make the inner loop a `parallel_reduce` with `TeamThreadRange` policy
- Experiment with the combinations of `Layout`, `Space`, `N` to view performance
- Hint: what should the layout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

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
HSW Left
HSW Right
KNL Left
KNL Right
Pascal60 Left
Pascal60 Right
coalesced
cached
cached
Bandwidth (GB/s)
Number of Rows (N)
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 */
  }[, ...]);
```

Sum sanity checks (0)

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);
```

Sum sanity checks (0)

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

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

`totalSum = numberOfThreads * 10`

Sum sanity checks (1)

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

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

`totalSum = numberOfTeams * team_size * 10`

Sum sanity checks (2)

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);
```

Sum sanity checks (2)

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);
```

`totalSum = numberOfTeams * team_size * team_size * 10`

Restricting Execution: single pattern

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
```

Exercise: TeamVectorLoop

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

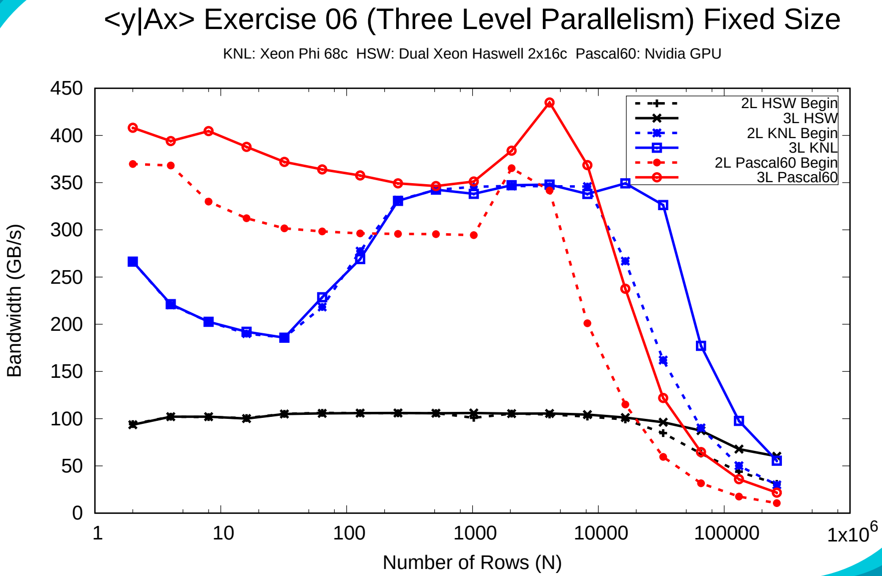
Details:

- 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



Section Summary

- **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.

Scratch memory

Learning objectives:

- Understand concept of **team** and **thread** private **scratch pads**
- Understand how scratch memory can **reduce global memory accesses**
- Recognize **when to use** scratch memory
- Understand **how to use** scratch memory and when barriers are necessary

Types of Scratch Space Uses

Two Levels of Scratch Space

- Level 0 is limited in size but fast.
- Level 1 allows larger allocations but is equivalent to High Bandwidth Memory in latency and bandwidth.

Team or Thread private memory

- Typically used for per work-item temporary storage.
- Advantage over pre-allocated memory is aggregate size scales with number of threads, not number of work-items.

Manually Managed Cache

- Explicitly cache frequently used data.
- Exposes hardware specific on-core scratch space (e.g. NVIDIA GPU Shared Memory).

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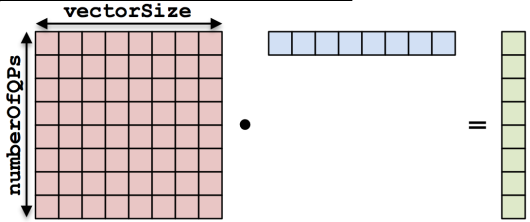
Now: Discuss Manually Managed Cache Usecase.

Example: contractDataFieldScalar (1)

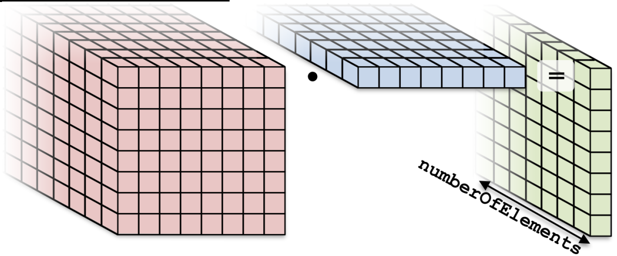
One slice of contractDataFieldScalar:



```
for (qp = 0; qp < numberOfQPs; ++qp) {
  total = 0;
  for (i = 0; i < vectorSize; ++i) {
    total += A(qp, i) * B(i);
  }
  result(qp) = total;
}
```

Example: contractDataFieldScalar (2)

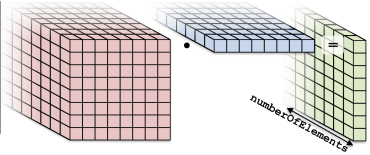
contractDataFieldScalar:



```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```

Example: contractDataFieldScalar (3)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```



Parallelization approaches:

- Each thread handles an `element`.

  Threads: `numberOfElements`

Example: contractDataFieldScalar (3)

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for (element = 0; element < numberOfElements; ++element) {
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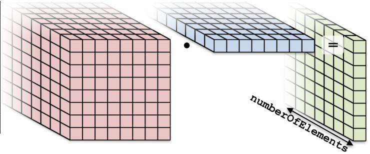
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```



Parallelization approaches:

- Each thread handles an `element`.
  Threads: `numberOfElements`
- Each thread handles a `qp`.
  Threads: `numberOfElements * numberOfQPs`

Example: contractDataFieldScalar (3)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
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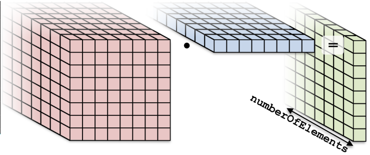
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```

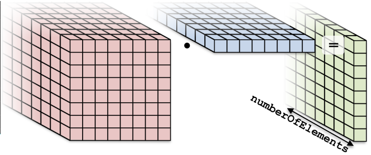


Parallelization approaches:

- Each thread handles an `element`.
  Threads: `numberOfElements`
- Each thread handles a `qp`.
  Threads: `numberOfElements * numberOfQPs`
- Each thread handles an `i`.
  Threads: `numElements * numQPs * vectorSize`
  Requires a `parallel_reduce`.

Example: contractDataFieldScalar (3)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```



Parallelization approaches:

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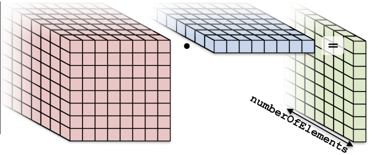
  Threads: `numberOfElements`
- Each thread handles a `qp`.
  Threads: `numberOfElements * numberOfQPs`
- Each thread handles an `i`.
  Threads: `numElements * numQPs * vectorSize`
  Requires a `parallel_reduce`.

Example: contractDataFieldScalar (4)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```

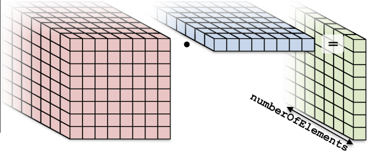


Flat kernel: Each thread handles a quadrature point

```
parallel_for("L",MDRangePolicy<Rank<2>>({0,0},{numE,numQP}),
  KOKKOS_LAMBDA(int element, int qp) {
  double total = 0;
  for (int i = 0; i < vectorSize; ++i) {
    total += A(element, qp, i) * B(element, i);
  }
  result(element, qp) = total;
}
```

Example: contractDataFieldScalar (6)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```

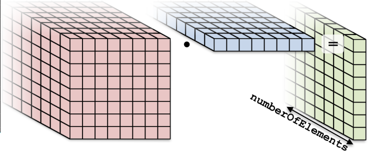


Teams kernel: Each team handles an element

```
operator()(member_type teamMember) {
  int element = teamMember.league_rank();
  parallel_for(
    TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * B(element, i);
      }
      result(element, qp) = total;
    });
}
```

Example: contractDataFieldScalar (6)

```
for (element = 0; element < numberOfElements; ++element) {
  for (qp = 0; qp < numberOfQPs; ++qp) {
    total = 0;
    for (i = 0; i < vectorSize; ++i) {
      total += A(element, qp, i) * B(element, i);
    }
    result(element, qp) = total;
  }
}
```



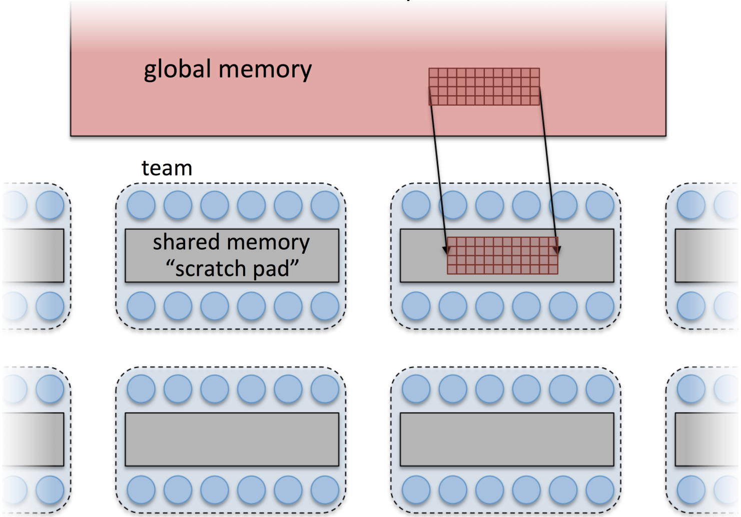
Teams kernel: Each team handles an element

```
operator()(member_type teamMember) {
  int element = teamMember.league_rank();
  parallel_for(
    TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * B(element, i);
      }
      result(element, qp) = total;
    });
}
```

No real advantage (yet)

Scratch memory (0)

Each team has access to a "scratch pad".



Scratch memory (1)

Scratch memory (scratch pad) as manual cache:

- Accessing data in (level 0) scratch memory is (usually) **much faster** than global memory.
- **GPUs** have separate, dedicated, small, low-latency scratch memories (*NOT subject to coalescing requirements*).
- **CPUs** don't have special hardware, but programming with scratch memory results in cache-aware memory access patterns.
- Roughly, it's like a *user-managed* L1 cache.

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- **CPUs** don't have special hardware, but programming with scratch memory results in cache-aware memory access patterns.
- Roughly, it's like a *user-managed* L1 cache.

Important concept

When members of a team read the same data multiple times, it's better to load the data into scratch memory and read from there.

Scratch memory (2)

Scratch memory for temporary per work-item storage:

- Scenario: Algorithm requires temporary workspace of size W.
- **Without scratch memory:** pre-allocate space for N work-items of size N x W.
- **With scratch memory:** Kokkos pre-allocates space for each Team or Thread of size T x W.
- `PerThread` and `PerTeam` scratch can be used concurrently.
- Level 0 and Level 1 scratch memory can be used concurrently.

Scratch memory (2)

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- `PerThread` and `PerTeam` scratch can be used concurrently.
- Level 0 and Level 1 scratch memory can be used concurrently.

Important concept

If an algorithm requires temporary workspace for each work-item, then use Kokkos' scratch memory.

Scratch memory (3)

To use scratch memory, you need to:

1. **Tell Kokkos how much** scratch memory you'll need.
2. **Make** scratch memory **views** inside your kernels.

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To use scratch memory, you need to:

1. **Tell Kokkos how much** scratch memory you'll need.
2. **Make** scratch memory **views** inside your kernels.

```
TeamPolicy<ExecutionSpace> policy(numberOfTeams, teamSize);

// Define a scratch memory view type
using ScratchPadView =
    View<double*,ExecutionSpace::scratch_memory_space>;
// Compute how much scratch memory (in bytes) is needed
size_t bytes = ScratchPadView::shmem_size(vectorSize);

// Tell the policy how much scratch memory is needed
int level = 0;
parallel_for(policy.set_scratch_size(level, PerTeam(bytes)),
  KOKKOS_LAMBDA (const member_type& teamMember) {

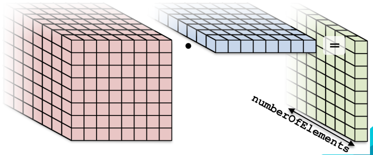
    // Create a view from the pre-existing scratch memory
    ScratchPadView scratch(teamMember.team_scratch(level),
                           vectorSize);
});
```

Example: contractDataFieldScalar (7)

Kernel outline for teams with scratch memory:

```
operator()(member_type teamMember) {
  ScratchPadView scratch(teamMember.team_scratch(0),
                         vectorSize);
  // TODO: load slice of B into scratch

  parallel_for(
    TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        // total += A(element, qp, i) * B(element, i);
        total += A(element, qp, i) * scratch(i);
      }
      result(element, qp) = total;
    });
}
```

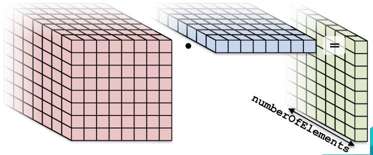


Example: contractDataFieldScalar (8)

How to populate the scratch memory?

- One thread loads it all?

```
if (teamMember.team_rank() == 0) {
  for (int i = 0; i < vectorSize; ++i) {
    scratch(i) = B(element, i);
  }
}
```



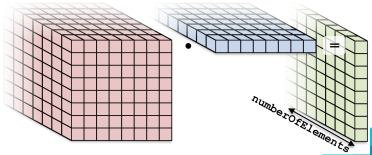
How to populate the scratch memory?

- ~~One thread loads it all?~~ Serial

```
if (teamMember.team_rank() == 0) {
  for (int i = 0; i < vectorSize; ++i) {
    scratch(i) = B(element, i);
  }
}
```

- Each thread loads one entry?

```
scratch(team_rank) = B(element, team_rank);
```



How to populate the scratch memory?

- ~~One thread loads it all?~~ Serial

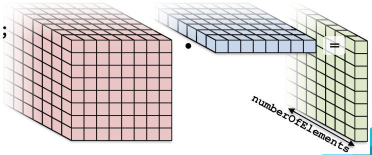
```
if (teamMember.team_rank() == 0) {
  for (int i = 0; i < vectorSize; ++i) {
    scratch(i) = B(element, i);
  }
}
```

- ~~Each thread loads one entry?~~ teamSize $\neq$ vectorSize

```
scratch(team_rank) = B(element, team_rank);
```

- TeamVectorRange

```
parallel_for(
  TeamVectorRange(teamMember, vectorSize),
  [=] (int i) {
    scratch(i) = B(element, i);
  });
```



How to populate the scratch memory?

- ~~One thread loads it all?~~ Serial

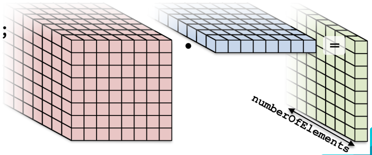
```
if (teamMember.team_rank() == 0) {
  for (int i = 0; i < vectorSize; ++i) {
    scratch(i) = B(element, i);
  }
}
```

- ~~Each thread loads one entry?~~ teamSize $\neq$ vectorSize

```
scratch(team_rank) = B(element, team_rank);
```

- TeamVectorRange

```
parallel_for(
  TeamVectorRange(teamMember, vectorSize),
  [=] (int i) {
    scratch(i) = B(element, i);
  });
```



(incomplete) Kernel for teams with scratch memory:

```
operator()(member_type teamMember) {
  ScratchPadView scratch(...);

  parallel_for(TeamVectorRange(teamMember, vectorSize),
    [=] (int i) {
      scratch(i) = B(element, i);
    });
  // TODO: fix a problem at this location

  parallel_for(TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * scratch(i);
      }
      result(element, qp) = total;
    });
}
```

(incomplete) Kernel for teams with scratch memory:

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operator()(member_type teamMember) {
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  parallel_for(TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * scratch(i);
      }
      result(element, qp) = total;
    });
}
```

Problem: threads may start to use `scratch` before all threads are done loading.

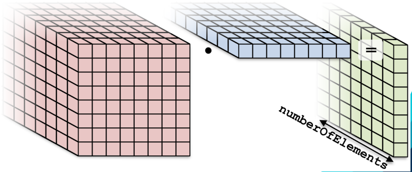
Example: contractDataFieldScalar (10)

Kernel for teams with scratch memory:

```
operator()(member_type teamMember) {
  ScratchPadView scratch(...);

  parallel_for(ThreadVectorRange(teamMember, vectorSize),
    [=] (int i) {
      scratch(i) = B(element, i);
    });
  teamMember.team_barrier();

  parallel_for(TeamThreadRange(teamMember, numberOfQPs),
    [=] (int qp) {
      double total = 0;
      for (int i = 0; i < vectorSize; ++i) {
        total += A(element, qp, i) * scratch(i);
      }
      result(element, qp) = total;
    });
}
```



Exercise: Scratch Memory

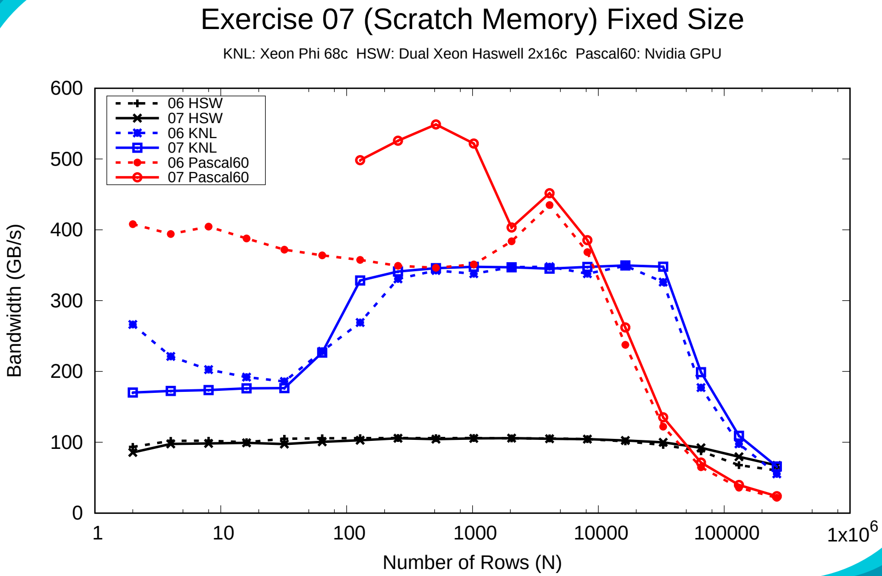
Use Scratch Memory to explicitly cache the x-vector for each element.

Details:

- Location: `Exercises/team_scratch_memory/`
- Create a scratch view
- Fill the scratch view in parallel using a TeamVectorRange

Things to try:

- Vary problem size and number of rows (-S ...; -N ...)
- Compare behavior with Exercise 6
- Compare behavior of CPU vs GPU


Exercise 07 (Scratch Memory) Fixed Size
KNL: Xeon Phi 68c HSW: Dual Xeon Haswell 2x16c Pascal60: Nvidia GPU
Bandwidth (GB/s)
Number of Rows (N)
06 HSW
07 HSW
06 KNL
07 KNL
06 Pascal60
07 Pascal60
0
100
200
300
400
500
600
1
10
100
1000
10000
100000
1x10^6

Scratch Memory: API Details

Allocating scratch in different levels:

```
int level = 1; // valid values 0,1
policy.set_scratch_size(level,PerTeam(bytes));
```

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```
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Using PerThread, PerTeam or both:

```
policy.set_scratch_size(level,PerTeam(bytes));
policy.set_scratch_size(level,PerThread(bytes));
policy.set_scratch_size(level,PerTeam(bytes1),
                              PerThread(bytes2));
```

Scratch Memory: API Details

Allocating scratch in different levels:

```
int level = 1; // valid values 0,1
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Using PerThread, PerTeam or both:

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policy.set_scratch_size(level,PerThread(bytes));
policy.set_scratch_size(level,PerTeam(bytes1),
                              PerThread(bytes2));
```

Using both levels of scratch:

```
policy.set_scratch_size(0,PerTeam(bytes0))
      .set_scratch_size(1,PerThread(bytes1));
```

Note: `set_scratch_size()` returns a new policy instance, it doesn't modify the existing one.

Section Summary

- **Scratch Memory** can be use with the `TeamPolicy` to provide thread or team **private** memory.
- Usecase: per work-item temporary storage or manual caching.
- Scratch memory exposes on-chip user managed caches (e.g. on NVIDIA GPUs)
- The size must be determined before launching a kernel.
- Two levels are available: large/slow and small/fast.

What we didn't cover

This was a short introduction
Didn't cover many things:

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- Full BuildSystem integration.

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- Tools for Profiling, Debugging and Tuning.
- Math Kernels (KokkosKernels).

The Kokkos Lectures

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

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

`https://kokkos.link/the-lectures`

Find More

Online Resources:

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

Acknowledgments

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