

Module 2: Views and Spaces

April 25, 2024

Kokkos View

What are Views? How to create them? Why should you use it?

Memory and Execution Spaces

How to control where data lives and code executes.

Memory Access Patterns

The importance of access patterns for performance portability and how to control it.

Module 2

Views

Learning objectives:

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



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];
    }
};
```



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Problem: x and y reside in CPU memory.

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	<pre>void operator()(const int64_t i) const {</pre>
Ĕ	_y[i] = _a * _x[i] + _y[i];
Ξ	}
]};

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

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View abstraction

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

High-level example of Views for daxpy using lambda:

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



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    // Views x and y are captured by value (shallow copy)
    y(i) = a * x(i) + y(i);
});
```

Important point

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

View overview:

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

Views (1)

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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.
```

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Views (1)

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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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) );
```

Views (2)

View life cycle:

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c(0,2) = 3;
print_value( a(0,2) );
What gets printed?
```

Views (2)

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",NO);
assert(a.extent(0) == NO);
assert(a.extent(1) == 5);
static_assert(a.static_extent(1) == 5);
assert(a.data() != nullptr);
assert(a.label() == "A");
```

Views (3)

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

```
# CPU-only using OpenMP
cmake -B build-openmp -DKokkos_ENABLE_OPENMP=ON
cmake --build build-openmp
# GPU - note UVM in Makefile
cmake -B build-cuda -DKokkos_ENABLE_CUDA=ON
cmake --build build-cuda
# Run exercise
./build-openmp/02_Exercise -S 26
./build-cuda/02_Exercise -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

- Memory space in which view's data resides; covered next.
- deep_copy view's data; covered later.
 Note: Kokkos never hides a deep_copy of data.
- **Layout** of multidimensional array; *covered later*.
- **Memory traits**; covered later.
- Subview: Generating a view that is a "slice" of other multidimensional array view; covered later.

Execution and Memory Spaces

Learning objectives:

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

Execution Space

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



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 \Rightarrow Always in the **host process**





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



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- ► 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:

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

	<pre>parallel_for("Label",</pre>
Ħ	<pre>numberOfIntervals, // => RangePolicy<>(0,numberOfIntervals)</pre>
a	[=] (const int64_t i) {
ē	/* body */
	});

Changing the parallel execution space:

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e	/* body */
וכ	});

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 */
```

Execution spaces (5)

Kokkos function and lambda portability annotation macros:

Function annotation with KOKKOS_INLINE_FUNCTION macro



Lambda annotation with KOKKOS_LAMBDA macro

```
Kokkos::parallel_for("Label",numberOfIterations,
KOKKOSLAMBDA (const int64_t index) {...});
// Where Kokkos defines:
#define KOKKOSLAMBDA [=] /* #if CPU-only */
#define KOKKOSLAMBDA [=] __device____host__ /* #if CPU+Cuda */
```

Execution spaces (5)

```
View<double*> data("data", size);
for (int64_t i = 0; i < size; ++i) {
   data(i) = ...read from file...
}
double sum = 0;
Kokkos::parallel_reduce("Label",
   RangePolicy<SomeExampleExecutionSpace>(0, size),
   KOKKOS_LAMBDA (const int64_t index, double & valueToUpdate) {
    valueToUpdate += data(index);
   },
   sum);
```

```
View<double*> data("data", size);
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Question: Where is the data stored? GPU memory? CPU memory? Both?

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\Rightarrow Memory Spaces





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

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- Available memory spaces:

HostSpace, CudaSpace, CudaUVMSpace, ... more Portable: SharedSpace, SharedHostPinnedSpace

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

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- Available memory spaces:

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

Memory spaces (1)

Example: HostSpace

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



Memory spaces (2)

Example: HostSpace

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

Example: CudaSpace

View<double**, CudaSpace> view(...constructor arguments...); CPU RAM metadata RAM metadata data

Memory spaces (2)

Anatomy of a kernel launch:

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

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

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

Execution and Memory spaces (1)



Example: two views

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



host data

🖌 dev data

Example: two views

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





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);

Execution and Memory spaces (3) Example (redux): summing an array with the GPU (failed) Attempt 1: View lives in CudaSpace View<double*, CudaSpace> array("array", size); for (int64_t i = 0; i < size; ++i) { array(i) = ...read from file... fault }</pre>

```
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) {</pre>
  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):
```

Execution and Memory spaces (4)

Example (redux): summing an array with the GPU

(failed) Attempt 2: View lives in HostSpace

```
View<double*, HostSpace> array("array", size);
for (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

```
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for (int64_t i = 0; i < size; ++i) {</pre>
  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):
                          CudaUVMSpace
What's the solution?
                          CudaHostPinnedSpace (skipping)
                          Mirroring
```

Execution and Memory spaces (5)



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

Important concept: Mirrors

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

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Mirroring schematic

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





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

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

2. Create hostView, a mirror of the view's array residing in the host memory space. view_type::HostMirror hostView =

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

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

- 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.).
- 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 });

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

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

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

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

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

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

```
# Compile for CPU
cmake -B build-openmp -DKokkos_ENABLE_OPENMP=ON
cmake --build build-openmp
# Compile for GPU (we do not need UVM anymore)
cmake -B build-cuda -DKokkos_ENABLE_CUDA=ON
cmake --build build-cuda
# Run on GPU
./build-cuda/03_Exercise -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) {</pre>
      thisRowsSum += A(row, entry) * x(entry);
    }
    valueToUpdate += y(row) * thisRowsSum;
  }. result).
                                              M
            Ν
                                          х
```

```
Kokkos::parallel_reduce("Label",
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    }
    valueToUpdate += y(row) * thisRowsSum;
  }, result).
            N
                                          х
```

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

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Layout is the mapping of multi-index to memory:



Important concept: Layout

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

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

Layout

Important concept: Layout

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

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, ...

Layout

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



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

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

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

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

CPUs: few (independent) cores with separate caches:

0 1	0 H	0 H	0 H
read read	read read	read read	read read
00	H H	NN	ოო
thread thread	thread thread	thread thread	thread thread



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CPUs: few (independent) cores with separate caches:





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

000	0 +	<u> </u>	ч		
read read read	read read	read read	read		
0 H 0	m O		ო		
thread thread thread	thread thread	thread thread	thread		
			l		



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

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

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

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Warning

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

```
Consider the array summation example:
```

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

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

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

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

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

Iterating for the execution space:

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

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

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Important point

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

Rule of Thumb

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

Example:

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

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

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Analysis: Kokkos architecture-dependent

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



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

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



April 25, 2024

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

 \Rightarrow You'll need multiple versions of code or pay the performance penalty.

Kokkos View

- Multi Dimensional Array.
- Compile and Runtime Dimensions.
- Reference counted like a std::shared_ptr to an array.

```
Kokkos::View<int*[5]> a("A", N);
a(3,2) = 7;
```

Execution Spaces

- Parallel operations execute in a specified Execution Space
- Can be controlled via template argument to Execution Policy
- If no Execution Space is provided use DefaultExecutionSpace

```
// Equivalent:
parallel_for("L", N, functor);
parallel_for("L",
    RangePolicy<DefaultExecutionSpace>(0, N), functor);
```

Memory Spaces

- Kokkos Views store data in Memory Spaces.
- Provided as template parameter.
- If no Memory Space is given, use Kokkos::DefaultExecutionSpace::memory_space.
- deep_copy is used to transfer data: no hidden memory copies by Kokkos.

```
View<int*, CudaSpace> a("A", M);
// View in host memory to load from file
auto h_a = create_mirror_view(a);
load_from_file(h_a);
// Copy
deep_copy(a,h_a);
```

Layouts

- Kokkos Views use an index mapping to memory determined by a Layout.
- Provided as template parameter.
- If no Layout is given, derived from the execution space associated with the memory space.
- Defaults are good if you parallelize over left most index!

```
View<int**, LayoutLeft> a("A", N, M);
View<int**, LayoutRight> b("B", N, M);
parallel_for("Fill", N, KOKKOS_LAMBDA(int i) {
  for(int j = 0; j < M; j++) {
    a(i,j) = i * 1000 + j; // coalesced
    b(i,j) = i * 1000 + j; // cached
  }
});
```