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# Kokkos Tutorial

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**Compilers and Libraries for your Compute Node**

- **CPU**: GCC 4.7.2 (or newer) *OR* Intel 14 (or newer) *OR* Clang 3.5.2 (or newer)
- **GPU**: CUDA nvcc 6.5.14 (or newer) *AND* NVIDIA compute capability 3.0 (or newer)

**Install Kokkos and Exercises on your Compute Node**

- **Kokkos**: github.com/kokkos/kokkos,
  *clone in ${HOME}/kokkos*
- **Tutorial**: github.com/kokkos/kokkos-tutorials/SC15
  *makefiles look for ${HOME}/kokkos*

**Knowledge of C++**: class constructors, member variables, member functions, member operators, template arguments

**Understand Kokkos Programming Model Abstractions**

- What, how and why of *performance portability*
- Productivity and hope for future-proofing

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**Part One:**

- Simple data parallel computations
- Deciding where code is run and where data is placed

**Understand Kokkos Programming Model Abstractions**

- What, how and why of *performance portability*
- Productivity and hope for future-proofing

**Part One:**

- Simple data parallel computations
- Deciding where code is run and where data is placed

**Part Two:**

- Managing data access pattens for performance portability
- Thread safety and *thread scalability*
- Thread-teams for maximizing parallelism

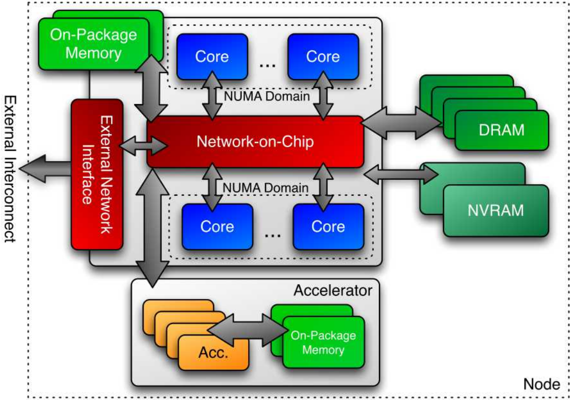
- High performance computers are increasingly **heterogenous**
  *MPI-only is no longer sufficient.*
- For **portability**: OpenMP, OpenACC, ... or Kokkos.
- Only Kokkos obtains performant memory access patterns via **architecture-aware** arrays and work mapping.
  *i.e.*, not just portable, *performance portable*.
- With Kokkos, **simple things stay simple** (parallel-for, etc.).
  *i.e.*, it's *no more difficult* than OpenMP.
- **Advanced performance-optimizing patterns are simpler** with Kokkos than with native versions.
  *i.e.*, you're *not missing out* on advanced features.

# Kokkos and the HPC Landscape

**Learning objectives:**

- How Kokkos fits in the context of modern HPC.
- Kokkos scope, goals, and philosophy.
- Difference between Kokkos and `#pragma` methods.

Compute nodes will be **heterogeneous** in cores *and* memory:



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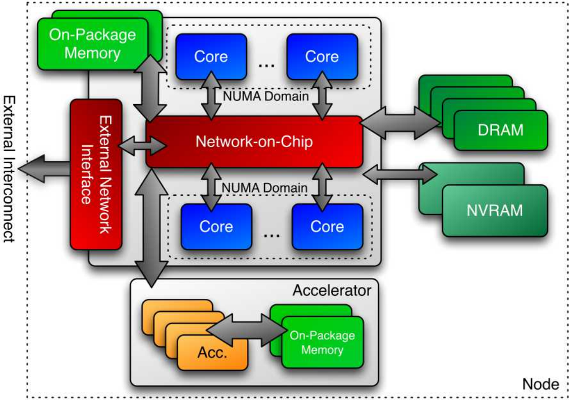


**Many-core revolution**: 20-year "just recompile" **free ride is over**.

**How much** do I have to **learn and change** to use these nodes?

**Key Considerations** for GPUs:

- GPUs support **thousands** of simultaneously-executing threads.
- You need **O(10,000) threads** to use a GPU effectively.
- Cores are "**simple**" - no transistors are dedicated to branch prediction, out of order execution, etc. Instead, more cores.
- Current GPUs can't *performantly* access CPU memory, you have to **move data**
- *GPU cores* **cannot run MPI's** *heavy processes*.

**Operating assumptions:**

- Compute nodes have ˜50 complex cores, ˜5000 simple cores, *and* heterogenous memory.
- Separate inter-node and intra-node programming models *e.g.*, message passing + threading)

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**Solutions**:

- Maintain **separate versions** for each target architecture (Xeon, Xeon Phi, GPU, GPU with NVLink, etc.)

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  - Note: not all alternatives support heterogenous memory

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## Important Point

There's a difference between *portability* and *performance portability*.

**Example**: implementations may target particular architectures and may not be *thread scalable*.

(e.g., locks on CPU won't scale to 100,000 threads on GPU)

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- compiles and **runs on multiple architectures**,
- obtains **performant memory access patterns** across architectures,
- can leverage **architecture-specific features** where possible.

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**Kokkos**: performance portability across manycore architectures.

# Threaded (intra-node) data parallelism

**Learning objectives:**

- Terminology of pattern, policy, and body.
- The data layout problem.

Loop bodies are prime candidates for **data parallelism**.

**Test**: Same answer if the loop iterates backwards? random order?

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**Test**: Same answer if the loop iterates backwards? random order?

**Examples:**

- Thermodynamic quantities at quadrature points in FEA:

```
for (element = 0; element < numElements; ++element) {
  total = 0;
  for (qp = 0; qp < numQPs; ++qp) {
    total += dot(left[element][qp], right[element][qp]);
  }
  elementValues[element] = total;
}
```

```
for (element = 0; element < numElements; ++element) {
  total = 0;
  for (qp = 0; qp < numQPs; ++qp) {
    total += dot(left[element][qp], right[element][qp]);
  }
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}
```

Pattern Policy

```
for (element = 0; element < numElements; ++element) {
  total = 0;
  for (qp = 0; qp < numQPs; ++qp) {
    total += dot(left[element][qp], right[element][qp]);
  }
  elementValues[element] = total;
}
```

Body

Terminology:

- **Pattern**: structure of the computations
  for, reduction, scan, task-graph, ...
- **Execution Policy**: how computations are executed
  static scheduling, dynamic scheduling, thread teams, ...
- **Computational Body**: code which performs each unit of work; *e.g.*, the loop body

⇒ The **pattern** and **policy** drive the computational **body**.

What if we want to **thread** the FEA algorithm?

```
for (element = 0; element < numElements; ++element) {
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What if we want to **thread** the FEA algorithm?

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#pragma omp parallel for
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(Change the *execution policy* from "serial" to "parallel.")

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```

(Change the *execution policy* from "serial" to "parallel.")

OpenMP is simple for parallelizing loops on multi-core CPUs, but what if we then want to do this on **other architectures**?

Intel MIC *and* NVIDIA GPU *and* AMD Fusion *and* ...

## Option 1: OpenMP 4.0

```
#pragma omp target data map(...)
#pragma omp teams num_teams(...) num_threads(...) private(...)
#pragma omp distribute
for (element = 0; element < numElements; ++element) {
  total = 0
#pragma omp parallel for
  for (qp = 0; qp < numQPs; ++qp)
    total += dot(left[element][qp], right[element][qp]);
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  for (qp = 0; qp < numQPs; ++qp)
    total += dot(left[element][qp], right[element][qp]);
  elementValues[element] = total;
}
```

## Option 2: OpenACC

```
#pragma acc parallel copy(...) num_gangs(...) vector_length(...)
#pragma acc loop gang vector
for (element = 0; element < numElements; ++element) {
  total = 0;
  for (qp = 0; qp < numQPs; ++qp)
    total += dot(left[element][qp], right[element][qp]);
  elementValues[element] = total;
}
```

A standard thread parallel programming model
*may* give you portable parallel execution
*if* it is supported on the target architecture.

But what about performance?

A standard thread parallel programming model
*may* give you portable parallel execution
*if* it is supported on the target architecture.

But what about performance?

Performance depends upon the computation's **memory access pattern**.

## Problem: memory access pattern

```
#pragma something, opencl, etc.
for (element = 0; element < numElements; ++element) {
  total = 0;
  for (qp = 0; qp < numQPs; ++qp) {
    for (i = 0; i < vectorSize; ++i) {
      total +=
        left[element * numQPs * vectorSize +
             qp * vectorSize + i] *
        right[element * numQPs * vectorSize +
              qp * vectorSize + i];
    }
  }
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**Memory access pattern problem:** CPU data layout reduces GPU performance by more than 10X.

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```

**Memory access pattern problem:** CPU data layout reduces GPU performance by more than 10X.

## Important Point

For performance, the memory access pattern *must* depend on the architecture.

How does Kokkos address performance portability?

**Kokkos** is a *productive*, *portable*, *performant*, shared-memory programming model.

- is a C++ **library**, not a new language or language extension.
- supports **clear, concise, thread-scalable** parallel patterns.
- lets you write algorithms once and run on **many architectures**
  e.g. multi-core CPU, Nvidia GPGPU, Xeon Phi, ...
- **minimizes** the amount of architecture-specific **implementation details** users must know.
- *solves the data layout problem* by using multi-dimensional arrays with architecture-dependent **layouts**

# Data parallel patterns

**Learning objectives:**

- How computational bodies are passed to the Kokkos runtime.
- How work is mapped to cores.
- The difference between `parallel_for` and `parallel_reduce`.
- Start parallelizing a simple example.

## Data parallel patterns and work

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

Kokkos maps **work** to cores

## Data parallel patterns and work

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

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

## Data parallel patterns and work

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- 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, Kokkos maps iteration indices to cores and then runs the computational body on those cores.

**How are computational bodies given to Kokkos?**

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

## How are computational bodies given to Kokkos?

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

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

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

**How is work assigned to functor operators?**

## 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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struct Functor {
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struct Functor {
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}
```

### Warning: concurrency and order

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

## How is data passed to computational bodies?

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

```
struct AtomForceFunctor {
  ...
  void operator()(const size_t atomIndex) const {
    atomForces[atomIndex] = calculateForce(...data...);
  }
  ...
}
```

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struct AtomForceFunctor {
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  }
  ...
}
```

How does the body access the data?

**Important concept**

A parallel functor body must have access to all the data it needs through the functor's **data members**.

**Putting it all together: the complete functor**:

```
struct AtomForceFunctor {
  ForceType _atomForces;
  AtomDataType _atomData;
  void operator()(const size_t atomIndex) const {
    _atomForces[atomIndex] = calculateForce(_atomData);
  }
}
```

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**Q/** How would we **reproduce serial execution** with this functor?

**Serial**

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for (atomIndex = 0; atomIndex < numberOfAtoms; ++atomIndex){
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**Serial**

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

**Functor**

```
AtomForceFunctor functor(atomForces, data);
for (atomIndex = 0; atomIndex < numberOfAtoms; ++atomIndex){
  functor(atomIndex);
}
```

**The complete picture** (using functors):

1. Defining the functor (operator+data):

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

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

  void operator()(const size_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 verbose ⇒ **C++11 Lambda** are concise

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

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

**Warning: Lambda capture and C++ containers**

For portability (*e.g.*, to GPU) a lambda must capture by value [=]. Don't capture containers (*e.g.*, std::vector) by value because this copies the container's entire contents.

## How does this compare to OpenMP?

**Serial**

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

**OpenMP**

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

**Kokkos**

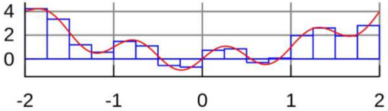
```
parallel_for(N, [=] (const size_t i) {
  /* loop body */
});
```

### Important concept

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

**Riemann-sum-style numerical integration**:

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




*wikipedia*

## Riemann-sum-style numerical integration:

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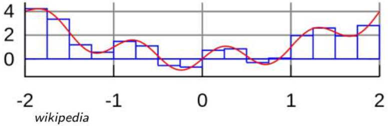


```
double totalIntegral = 0;
for (size_t i = 0; i < numberOfIntervals; ++i) {
  const double x =
    lower + (i/numberOfIntervals) * (upper - lower);
  const double thisIntervalsContribution = function(x);
  totalIntegral += thisIntervalsContribution;
}
totalIntegral *= dx;
```

## Riemann-sum-style numerical integration:

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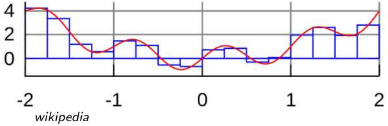


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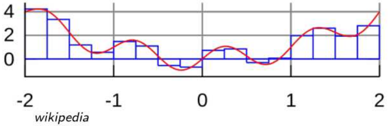


Pattern?

Policy?

Body?

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```

How would we **parallelize** it?

## An (incorrect) attempt:

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

Second problem: race condition

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

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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 (size_t i = 0; i < N; ++i) {
  finalReducedValue += ...
}
```

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for (size_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 (size_t i = 0; i < numberOfIntervals; ++i) {
  totalIntegral += function(...);
}
```

Kokkos

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

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

**Warning: Parallelism is NOT free**

Dispatching (launching) parallel work has non-negligible cost.

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Dispatching (launching) parallel work has non-negligible cost.

Simplistic data-parallel performance model: Time $= \alpha + \frac{\beta * N}{P}$

- $\alpha =$ dispatch overhead
- $\beta =$ time for a unit of work
- $N =$ number of units of work
- $P =$ available concurrency

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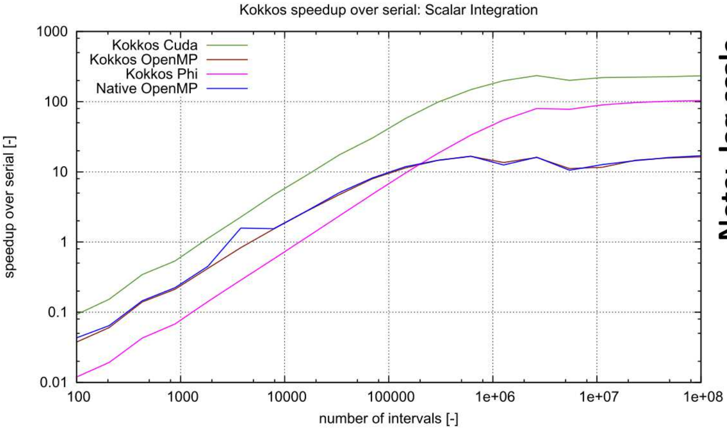
Simplistic data-parallel performance model: Time $= \alpha + \frac{\beta * N}{P}$

- $\alpha =$ dispatch overhead
- $\beta =$ time for a unit of work
- $N =$ number of units of work
- $P =$ available concurrency

Speedup $= P \div \left(1 + \frac{\alpha * P}{\beta * N}\right)$

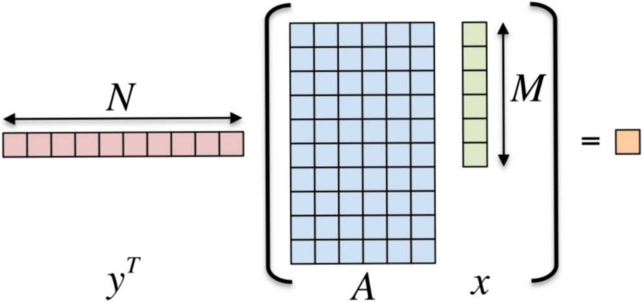
- Should have $\alpha * P \ll \beta * N$
- *All* runtimes strive to minimize launch overhead $\alpha$
- Find more parallelism to increase $N$
- Merge (fuse) parallel operations to increase $\beta$

**Results**: illustrates simple speedup model $= P \div \left(1 + \frac{\alpha * P}{\beta * N}\right)$




**Note: log scale**

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




**Details**:

- $y$ is $N$x1, $A$ is $N$x$M$, $x$ is $M$x1
- We'll use this exercise throughout the tutorial

## Exercise #1: include, initialize, finalize Kokkos

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

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

(Optional) Command-line arguments:

| | |
|---|---|
| `--kokkos-threads=INT` | total number of threads (or threads within NUMA region) |
| `--kokkos-numa=INT` | number of NUMA regions |
| `--kokkos-device=INT` | device (GPU) ID to use |

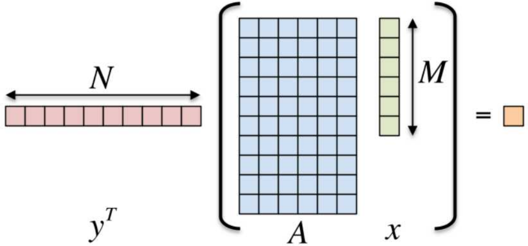
## Compiling for CPU

```
cd ~/kokkos-tutorial/SC15/Exercises/01/
# gcc using OpenMP (default) and Serial back-ends
make -j 4 [KOKKOS_DEVICES=OpenMP,Serial]
# Intel using OpenMP (default) and Serial back-ends
make -j 4 CXX=icpc [KOKKOS_DEVICES=OpenMP,Serial]
# Intel using OpenMP for Xeon Phi Knights Corner cross-compile
# For execution natively on the KNC. NOT for offload.
make -j CXX=icpc [KOKKOS_DEVICES=OpenMP,Serial] KOKKOS_ARCH=KNC
```

## Running on CPU with OpenMP back-end

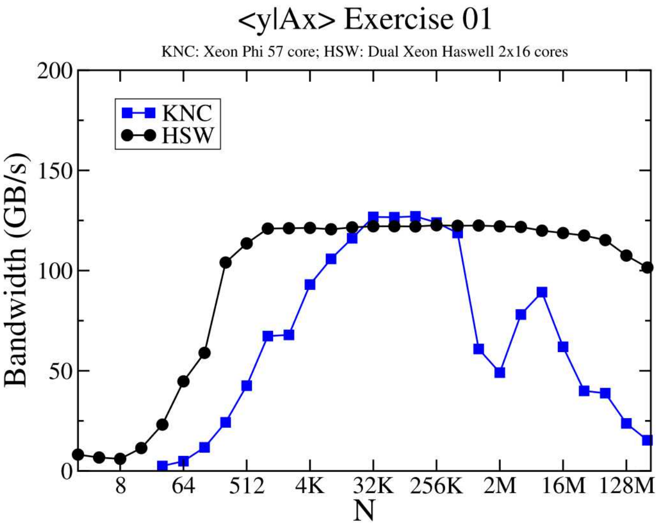
```
# Set OpenMP affinity
export GOMP_CPU_AFFINITY=0-NumberOfCoresOnASingleSocket
# Print example command line options:
./exercise.host -h
# Run with defaults on CPU
./exercise.host
```

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




**Details**:

- Location: `~/kokkos-tutorials/SC15/Exercises/01/`
- See `~/kokkos-tutorials/SC15/Exercises/HOW_TO_COMPILE_AND_RUN`
- Look for comments labeled with "EXERCISE"
- Parallelize loops with `parallel_for` or `parallel_reduce`
- Use lambdas instead of functors for computational bodies.
- For now, this will only use the CPU.


<y|Ax> Exercise 01
KNC: Xeon Phi 57 core; HSW: Dual Xeon Haswell 2x16 cores
KNC
HSW
Bandwidth (GB/s)
0
50
100
150
200
8
64
512
4K
32K
256K
2M
16M
128M
N

Review: Simple parallel reduce using a lambda:

```
ReductionType reducedValue; // initial value irrelevant
Kokkos::parallel_reduce(numberOfIterations,
  [=] (const size_t index,
       ReductionType & valueToUpdate) {
    valueToUpdate += // ... contribution for index
  },
  reducedValue);
```

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Limitation of using defaults: the reduced value is (re-)initialized to zero and is reduced with `operator+=`.

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  reducedValue);
```

Limitation of using defaults: the reduced value is (re-)initialized to zero and is reduced with `operator+=`.

For non-trival reductions you need to use a **general reduction** functor.

How do you do **arbitrary reductions**?

## Example: finding index of closest point

```
Point searchLocation = ...;
size_t indexOfClosest = 0;
for (size_t i = 1; i < numberOfPoints; ++i) {
  if (magnitude(searchLocation - points[i]) <
      magnitude(searchLocation - points[indexOfClosest])) {
    indexOfClosest = i;
  }
}
```

How do you do **arbitrary reductions**?

## Example: finding index of closest point

```
Point searchLocation = ...;
size_t indexOfClosest = 0;
for (size_t i = 1; i < numberOfPoints; ++i) {
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      magnitude(searchLocation - points[indexOfClosest])) {
    indexOfClosest = i;
  }
}
```

- This **isn't possible** with openmp's reduction clause
- Manual threading versions must avoid **false sharing**
- Parallel programming models should support **robust, arbitrary, performant** reductions **tuned to the architecture**.

**General reductions**:

**What information** must we provide to do a reduction?

- The **type** of the value to reduce ("value_type")
- How to combine ("**join**") two value_types
- How to **initialize** a value_type

```
struct ParallelFunctor {
  typedef double value_type;
  void operator()(const size_t index,
                  value_type & valueToUpdate) const {...}

  void join(volatile value_type & destination,
            const volatile value_type & source) const {...}

  void init(value_type & initialValue) const {...}
}
```

- Exclusive and inclusive **prefix scan** with the `parallel_scan` pattern.
- Using *tag dispatch* interface to allow non-trivial functors to have multiple "`operator()`" functions.
- Directed acyclic graph (DAG) of tasks pattern (experimental).
- **Concurrently** executing parallel kernels on CPU and GPU (experimental).
- Hierarchical parallelism with **team policies**, covered later.

- **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**, **space**, and **body**.
- User provides **computational bodies** as functors or lambdas which handle a single work item.

# Views

**Learning objectives:**

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

View motivation

## Example: running daxpy on the GPU:

Lambda

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

Functor

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

View motivation

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**Problem**: x and y reside in CPU memory.

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struct Functor {
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  }
};
```

**Problem**: x and y reside in CPU memory.

**Solution:** We need a way of storing data (multidimensional arrays) which can be communicated to 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(N, [=] (const size_t i) {
    // Views x and y are captured by value (copy)
    y(i) = a * x(i) + y(i);
  });
```

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

### Important point

Views are **like pointers** so copy them.

**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.

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

**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
```

Note: runtime-sized dimensions must come first.

**View** life cycle:

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

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**Example**:

```
void assignValueInView(View<double*> data) { data(0) = 3; }

View<double*> a("a", N0), b("b", N0);
a(0) = 1;
b(0) = 2;
a = b;
View<double*> c(b);
assignValueInView(c);
print a(0)
```

What gets printed?

**View** life cycle:

- Allocations only happen when *explicitly* specified.
  i.e., there are **no hidden allocations**.
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View<double*> c(b);
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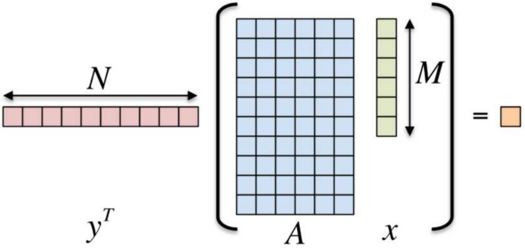
print a(0)
```

What gets printed?
`3.0`

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

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




**Details**:

- Location: `~/kokkos-tutorials/SC15/Exercises/02/`
- Change data storage from arrays to Views.
- Use lambdas instead of functors for computational bodies.
- For now, this will only use the CPU.

- **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; *will not be covered today*.

# 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 memory movement.
- The need for `Kokkos::initialize` and `finalize`.
- Where to use Kokkos annotation macros for portability.

**Thought experiment**: Consider this code:

section 1

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

section 2

**Thought experiment**: Consider this code:

section 1

section 2

```
MPI_Reduce(...);
FILE * file = fopen(...);
runANormalFunction(...data...);
Kokkos::parallel_for(numberOfSomethings,
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                       const double y = ...;
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                     );
```

- Where will section 1 be run? CPU? GPU?
- Where will section 2 be run? CPU? GPU?
- How do I **control** where code is executed?

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MPI_Reduce(...);
FILE * file = fopen(...);
runANormalFunction(...data...);
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                       const double y = ...;
                       // do something interesting
                     }
                     );
```

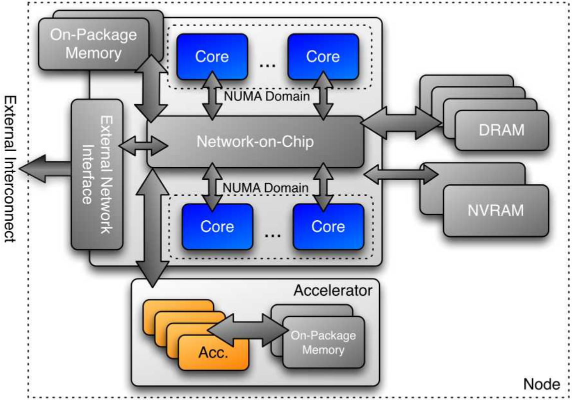
section 2

- Where will section 1 be run? CPU? GPU?
- Where will section 2 be run? CPU? GPU?
- How do I **control** where code is executed?

$\Rightarrow$ **Execution spaces**

**Execution Space**

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




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

## Execution spaces (2)

Host

Parallel

```
MPI_Reduce(...);
FILE * file = fopen(...);
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```

Parallel

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

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

# Execution spaces (2)

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```

Parallel

- 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**

Host

Parallel

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MPI_Reduce(...);
FILE * file = fopen(...);
runANormalFunction(...data...);
Kokkos::parallel_for(numberOfSomethings,
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                       // 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(
  RangePolicy< ExecutionSpace >(0,numberOfIntervals),
  [=] (const size_t i) {
    /* ... body ... */
  });
```

Default

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

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Default

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  numberOfIntervals, // == RangePolicy<>(0,numberOfIntervals)
  [=] (const size_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 size_t s) const {...}
  KOKKOS_INLINE_FUNCTION
  void operator()(const size_t index) const {
    helperFunction(index);
  }
}
// Where kokkos defines:
#define KOKKOS_INLINE_FUNCTION inline                     /* #if CPU-only */
#define KOKKOS_INLINE_FUNCTION inline __device__ __host__ /* #if CPU+Cuda */
```

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Lambda annotation with KOKKOS_LAMBDA macro (CUDA requires v 7.5)

```
Kokkos::parallel_for(numberOfIterations,
  KOKKOS_LAMBDA (const size_t index) {...});

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

## **Memory space motivating example:** summing an array

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

double sum = 0;
Kokkos::parallel_reduce(
  RangePolicy<ExecutionSpace>(0, size),
  KOKKOS_LAMBDA (const size_t index, double & valueToUpdate) {
    valueToUpdate += data(index);
  },
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Question: Where is the data stored? GPU memory? CPU memory? Both?

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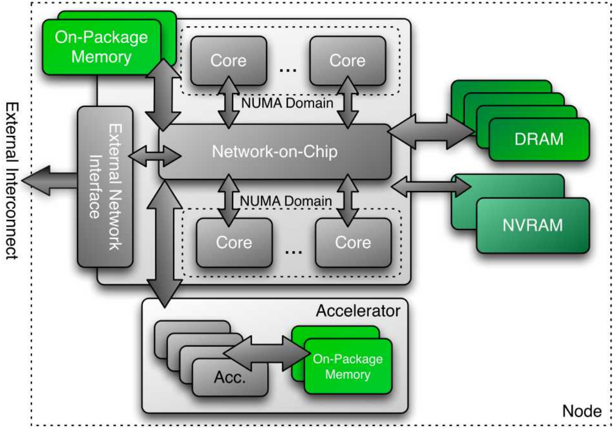
```

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

$\Rightarrow$ **Memory Spaces**

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



## Important concept: Memory spaces

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

# Memory spaces (1)

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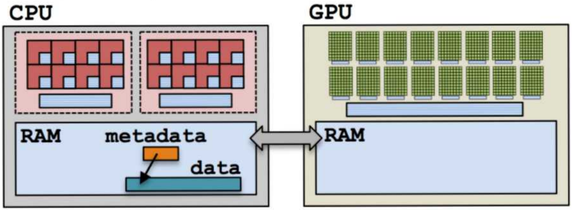
- Available **memory spaces**:
  `HostSpace, CudaSpace, CudaUVMSpace, ...` more
- Each **execution space** has a default memory space, which is used if **Space** provided is actually an execution space
- If no `Space` is provided, the view's data resides in the **default memory space** of the **default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

## Example: HostSpace

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



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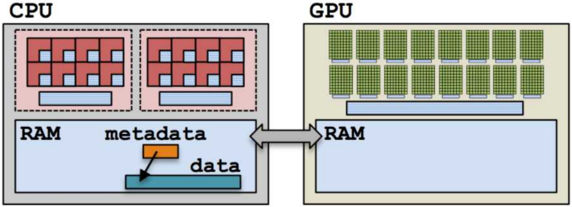
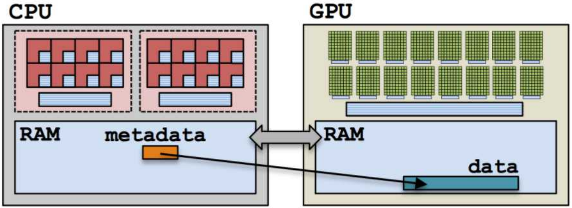



## Example: CudaSpace

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



## Anatomy of a kernel launch:

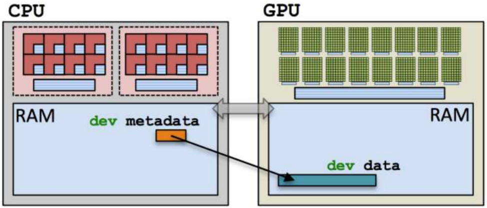
1. User declares views, allocating.
2. User instantiates a functor with views.
3. User launches `parallel_***`:
   - Functor is copied to the device.
   - Kernel is run.
   - Copy of functor on the device is released.

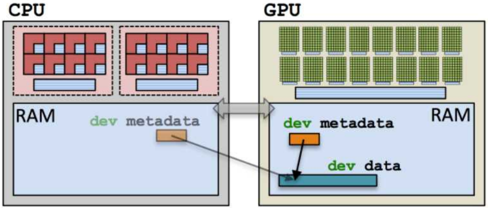
```
View<int*, Cuda> dev;
parallel_for(N,
  [=] (int i) {
    dev(i) = ...;
  });
```

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

## Example: one view

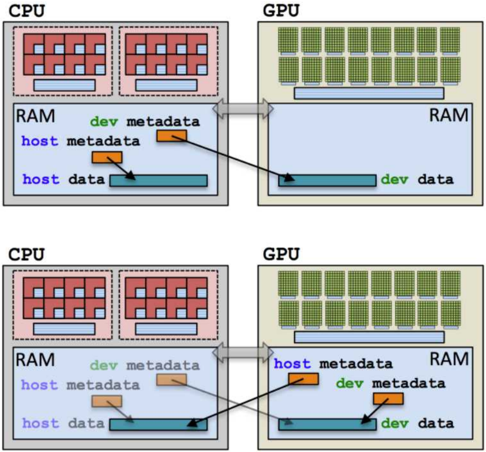
```
View<int*, Cuda> dev;
parallel_for(N,
  [=] (int i) {
    dev(i) = ...;
  });
```



## Example: two views

```
View<int*, Cuda> dev;
View<int*, Host> host;
parallel_for(N,
  [=] (int i) {
    dev(i)  = ...;
    host(i) = ...;
  });
```



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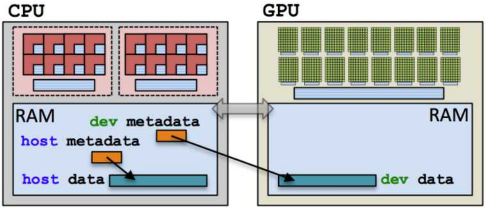


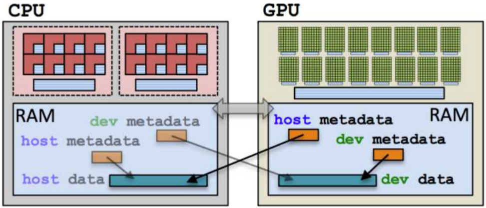

## Example (redux): summing an array with the GPU

(failed) Attempt 1:

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

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

## Example (redux): summing an array with the GPU

(failed) Attempt 2:

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

double sum = 0;
Kokkos::parallel_reduce(
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  KOKKOS_LAMBDA (const size_t index, double & valueToUpdate) {
    valueToUpdate += array(index);
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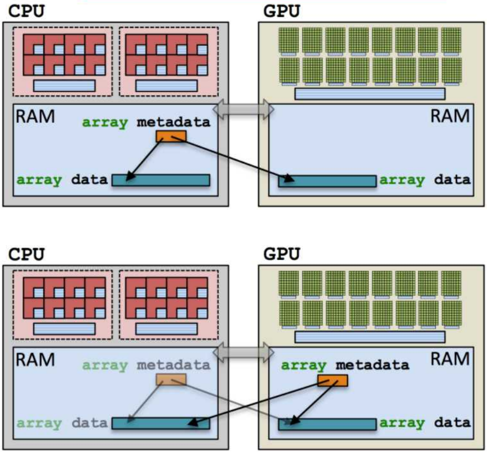
```

What's the solution?

- CudaUVMSpace
- CudaHostPinnedSpace
- Mirroring

## CudaUVMSpace

```
View<double*,
     CudaUVMSpace> array
array = ...from file...
double sum = 0;
parallel_reduce(N,
  [=] (int i,
       double & d) {
     d += array(i);
  },
  sum);
```

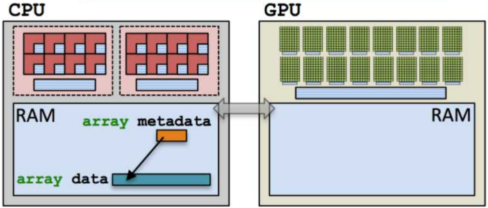


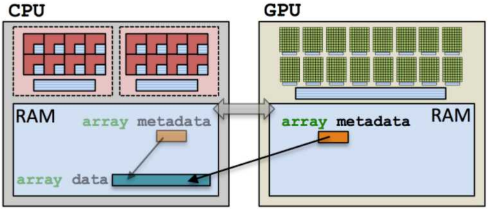

Cuda runtime automatically handles data movement, at **performance hit**.

## Execution and Memory spaces (6)

CudaHostPinnedSpace

```
View<double*,
     CudaHost...> array;
array = ...from file...
double sum = 0;
parallel_reduce(N,
  [=] (int i,
       double & d) {
    d += array(i);
  },
  sum);
```




Cuda runtime allows cuda-code access to CPU memory, at a **performance hit**.

## Important concept: Mirrors

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

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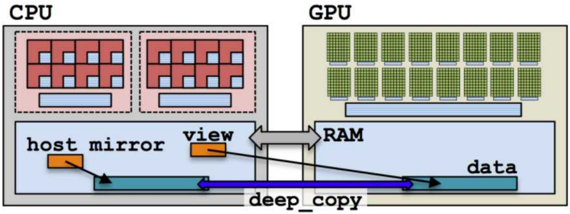
### Mirroring schematic

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



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```
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Kokkos::parallel_for(
  RangePolicy< Space>(0, size),
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```

## Mirroring pattern

1. **Create** a `view`'s array in some memory space.
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ViewType view(...);
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Kokkos::parallel_for(
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```
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);
```

- 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.
- **Heterogenous nodes** have one or more memory spaces.
- **Mirroring** is used for performant access to views in host and device memory.
- Heterogenous 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.

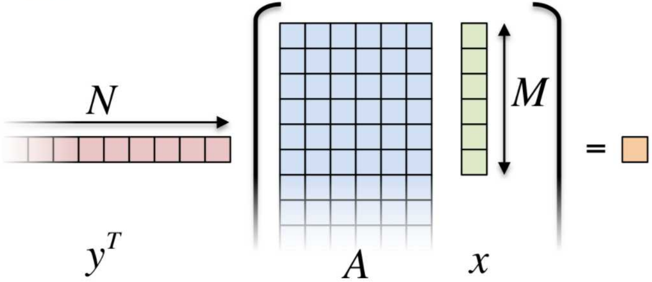
# Managing memory access patterns for performance portability

**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(
  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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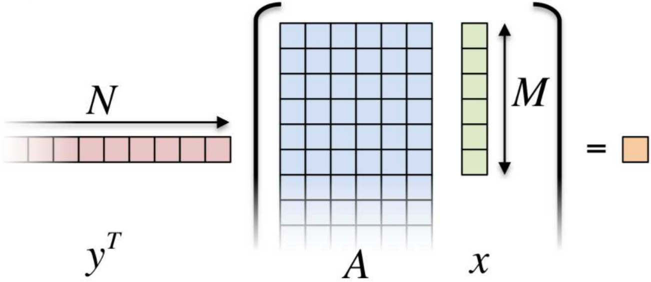


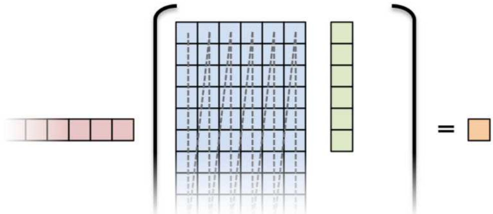

How should A be laid out in memory?

# Example: inner product (1)

Layout is the mapping of multi-index to memory:

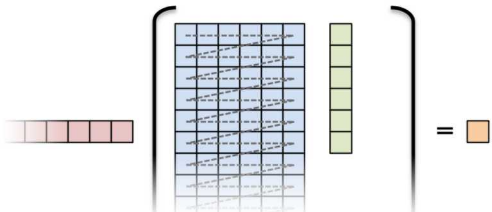
**LayoutLeft**

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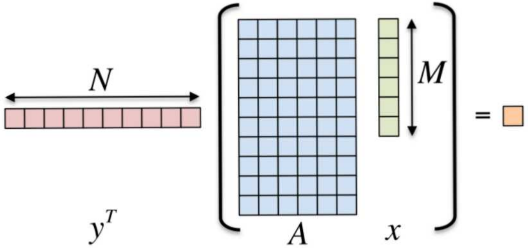
- Most-common layouts are `LayoutLeft` and `LayoutRight`.
  `LayoutLeft`: left-most index is stride 1.
  `LayoutRight`: right-most index is stride 1.
- If no layout specified, default for that memory space is used.
  `LayoutLeft` for `CudaSpace`, `LayoutRight` for `HostSpace`.
- Layouts are extensible: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

## Exercise #3: Inner Product, Flat Parallelism

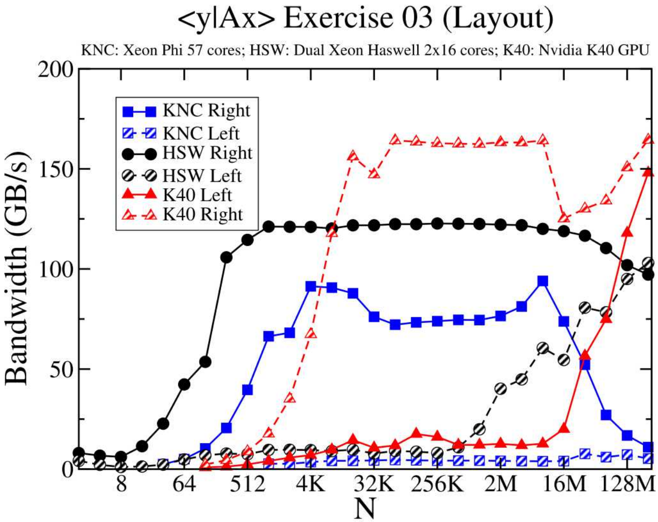
**Exercise**: Inner product $< y, A * x >$




**Details**:

- Location: `~/kokkos-tutorials/SC15/Exercises/03/`
- Use lambdas instead of functors for computational bodies.
- Replace ``N'' in parallel dispatch with `RangePolicy<Space>`
- Add `Space` to all `Views` and `Layout` to `A`
- Experiment with the combinations of `Space`, `Layout` to view performance

# Exercise #3: Inner Product, Flat Parallelism




**Why?**

## Thread independence:

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

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

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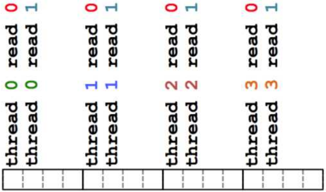
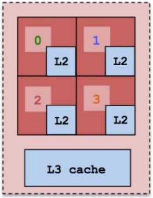
  i.e., threads may execute at any rate.
- **GPU** threads are synchronized in groups (of 32).
  i.e., threads in groups must execute instructions together.

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

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

**CPUs**: few (independent) cores with separate caches:



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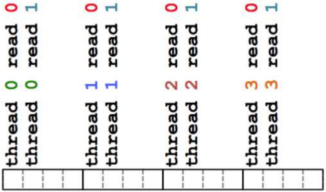
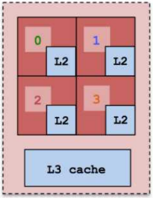
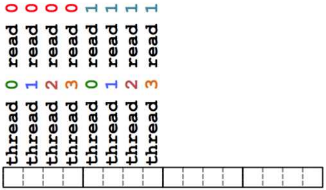
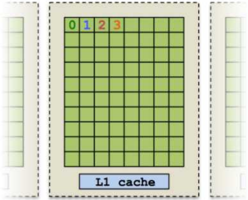



**GPUs**: many (synchronized) cores with a shared cache:



## Important point

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

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

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Uncoalesced access in `CudaSpace` *greatly* reduces performance (more than 10X)

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### Warning

Uncoalesced access in `CudaSpace` *greatly* reduces performance (more than 10X)

Note: uncoalesced *read-only, random* access in `CudaSpace` is okay through Kokkos `const RandomAccess` views (more later).

Consider the array summation example:

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

double sum = 0;
Kokkos::parallel_reduce(
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Given `P` threads, **which indices** do we want thread 0 to handle?

| Contiguous: | Strided: |
|---|---|
| `0, 1, 2, ..., N/P` | `0, N/P, 2*N/P, ...` |

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| **CPU** | **GPU** |

**Why?**

## Iterating for the execution space:

```
operator()(const size_t index, double & valueToUpdate) {
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As users we don't control how indices are mapped to threads, so how do we achieve good memory access?

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

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

### Important point

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

## Important point

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

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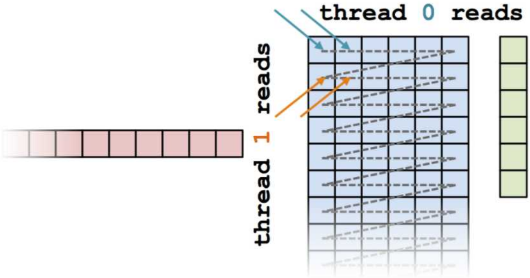
**Analysis: row-major** (`LayoutRight`)



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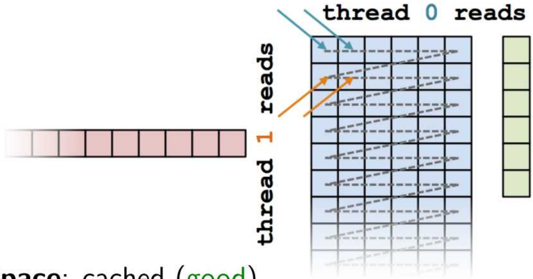
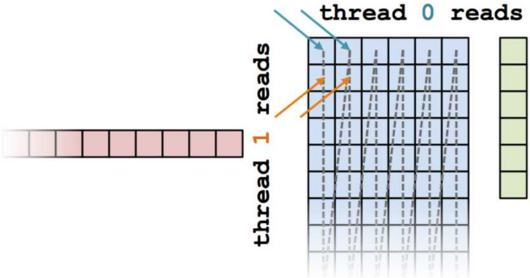



- **HostSpace**: cached (good)
- **CudaSpace**: uncoalesced (bad)

## Important point

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

**Analysis: column-major** (`LayoutLeft`)



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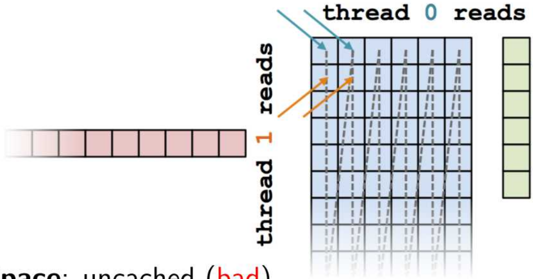
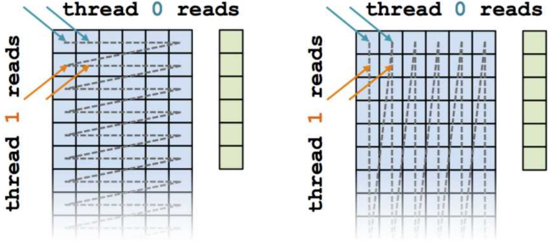



- **HostSpace**: uncached (bad)
- **CudaSpace**: coalesced (good)

## Analysis: Kokkos architecture-dependent

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




(a) OpenMP (b) Cuda

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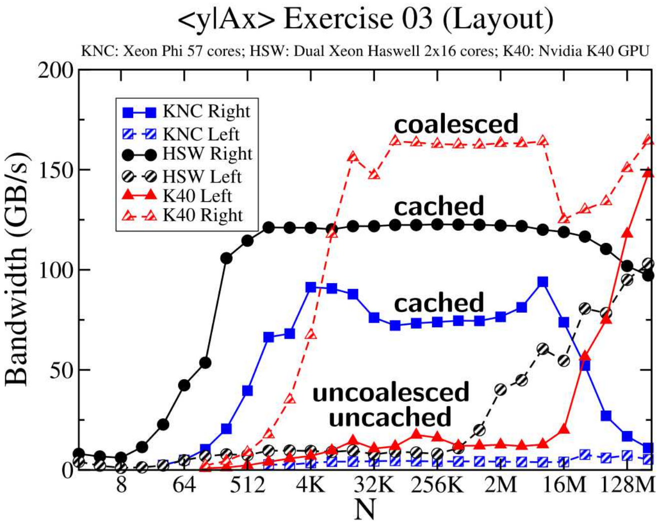
- **CudaSpace**: coalesced (good)

## **Layout performance**, revisited



# Memory Access Pattern Summary

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

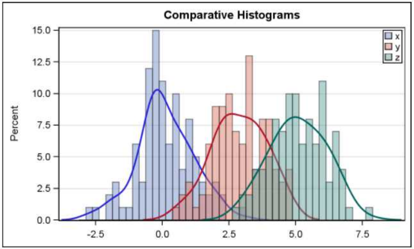
# Thread safety and atomic operations

**Learning objectives:**

- Understand that coordination techniques for low-count CPU threading are not scalable.
- Understand how atomics can parallelize the **scatter-add** pattern.
- Gain **performance intuition** for atomics on the CPU and GPU, for different data types and contention rates.

## Histogram kernel:

```
parallel_for(N, KOKKOS_LAMBDA(const size_t index) {
    const int value = ...;
    const int bucketIndex = computeBucketIndex(value);
    ++_histogram(bucketIndex);
  });
```




http://www.farmaceuticas.com.br/tag/graficos/

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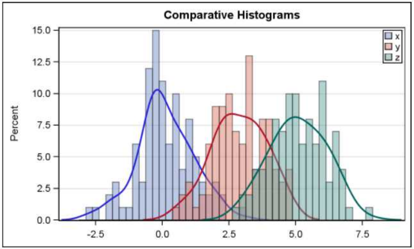
**Problem**: Multiple threads may try to write to the same location.

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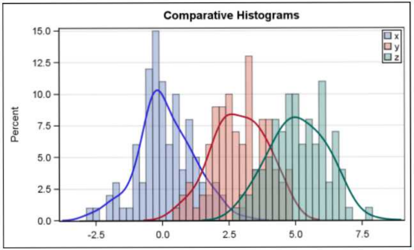
```

**Problem**: Multiple threads may try to write to the same location.

**Solution strategies**:

- Locks
- Thread-private copies
- Atomics

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## Thread safety solution: Locks

```
parallel_for(N, KOKKOS_LAMBDA(const size_t index) {
    const int value = ...;
    const int bucketIndex = computeBucketIndex(value);
    // LOCK   the lock that protects bucket bucketIndex
    ++_histogram(bucketIndex);
    // UNLOCK the lock that protects bucket bucketIndex
  });
```

## Thread safety solution: Locks

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parallel_for(N, KOKKOS_LAMBDA(const size_t index) {
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    const int bucketIndex = computeBucketIndex(value);
    // LOCK   the lock that protects bucket bucketIndex
    ++_histogram(bucketIndex);
    // UNLOCK the lock that protects bucket bucketIndex
  });
```

**Problem**: contention is too high at O(10,000) threads.

## Thread safety solution: Thread-private copies

```
#pragma omp parallel shared(histogram)
{
  HistogramType thisThreadsHistogram(histogram.size())
#pragma omp for nowait
  for each input {
    ...
    const int value = ...;
    const int bucketIndex = computeBucketIndex(value);
    ++thisThreadsHistogram(bucketIndex);
  }
#pragma omp critical
  for each bucket {
    histogram[bucketIndex] += thisThreadsHistogram[bucketIndex];
  }
}
```

## Thread safety solution: Thread-private copies

```
#pragma omp parallel shared(histogram)
{
  HistogramType thisThreadsHistogram(histogram.size())
#pragma omp for nowait
  for each input {
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    const int value = ...;
    const int bucketIndex = computeBucketIndex(value);
    ++thisThreadsHistogram(bucketIndex);
  }
#pragma omp critical
  for each bucket {
    histogram[bucketIndex] += thisThreadsHistogram[bucketIndex];
  }
}
```

**Problems**: insufficient memory for `thisThreadsHistogram`
ratio of parallel/serial work too low.

## Thread safety solution: Atomics

```
parallel_for(N, KOKKOS_LAMBDA(const size_t index) {
    const int value = ...;
    const int bucketIndex = computeBucketIndex(value);
    Kokkos::atomic_add(&_histogram(bucketIndex), 1);
  });
```

## Thread safety solution: Atomics

```
parallel_for(N, KOKKOS_LAMBDA(const size_t index) {
    const int value = ...;
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```

- Atomics are the **only scalable** solution to thread safety.
- Locks or data replication are **strongly discouraged**.

## How expensive are atomics?

Thought experiment: scalar integration

```
operator()(const unsigned int intervalIndex,
           double & valueToUpdate) const {
  double contribution = function(...);
  valueToUpdate += contribution;
}
```

## How expensive are atomics?

Thought experiment: scalar integration

```
operator()(const unsigned int intervalIndex,
           double & valueToUpdate) const {
  double contribution = function(...);
  valueToUpdate += contribution;
}
```

Idea: what if we instead do this with `parallel_for` and atomics?

```
operator()(const unsigned int intervalIndex) const {
  const double contribution = function(...);
  Kokkos::atomic_add(&globalSum, contribution);
}
```

How much of a performance penalty is incurred?

**Two costs:** (independent) work and coordination.

```
parallel_reduce(numberOfIntervals,
  KOKKOS_LAMBDA (const unsigned int intervalIndex,
                 double & valueToUpdate) {
    valueToUpdate += function(...);
  }, totalIntegral);
```

**Two costs:** (independent) work and coordination.

```
parallel_reduce(numberOfIntervals,
  KOKKOS_LAMBDA (const unsigned int intervalIndex,
                 double & valueToUpdate) {
    valueToUpdate += function(...);
  }, totalIntegral);
```

## Experimental setup

```
operator()(const unsigned int index) const {
  Kokkos::atomic_add(&globalSums[index % atomicStride], 1);
}
```

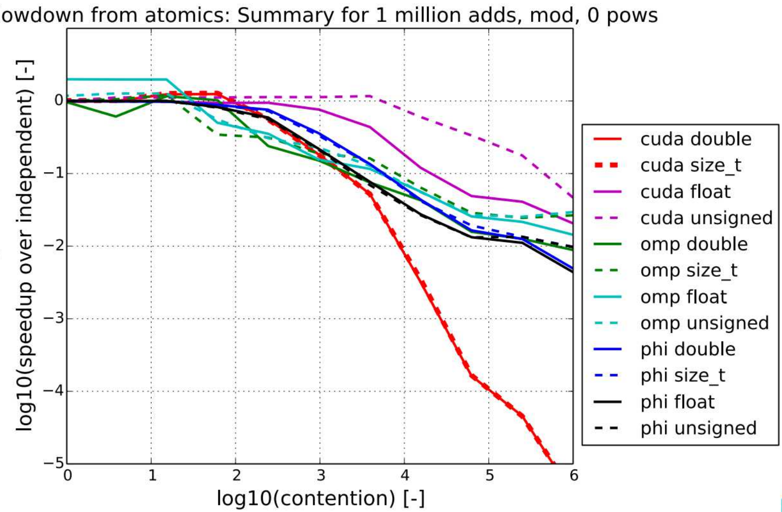
- This is the most extreme case: all coordination and no work.
- Contention is captured by the `atomicStride`.

  `atomicStride` $\rightarrow$ 1 $\Rightarrow$ Scalar integration

  `atomicStride` $\rightarrow$ large $\Rightarrow$ Independent

## **Atomics performance:** 1 million adds, **no** work per kernel

Note: **log scale**



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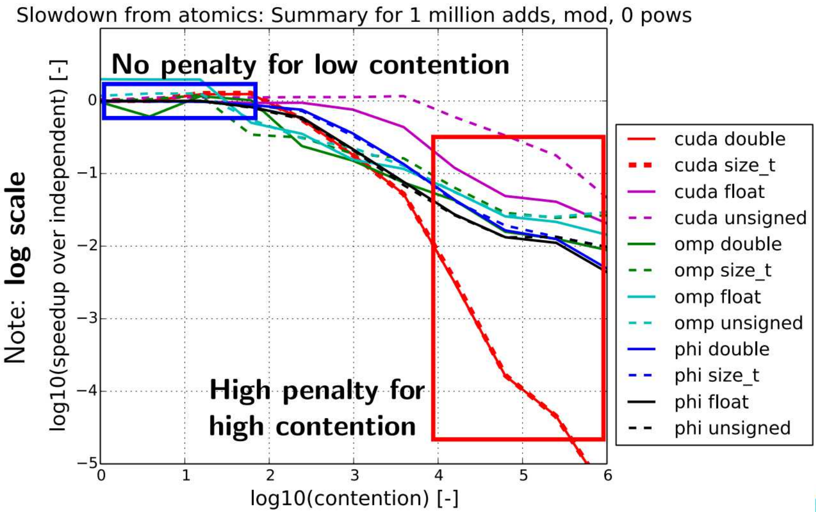
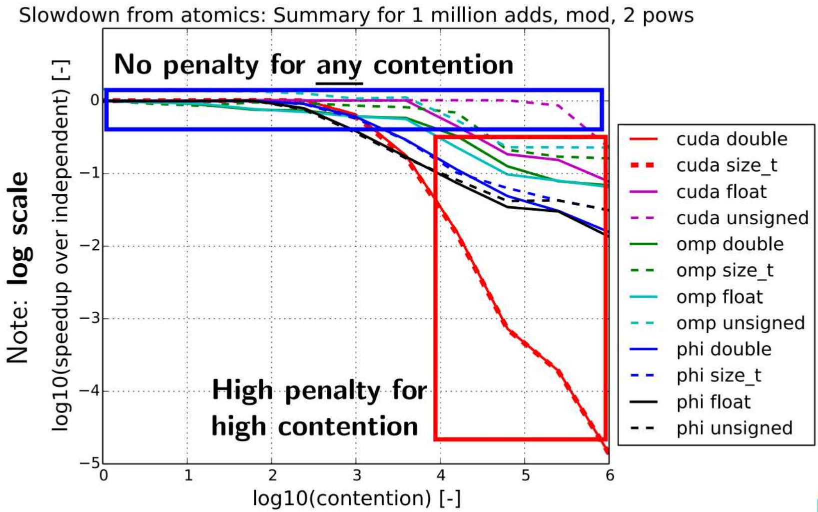
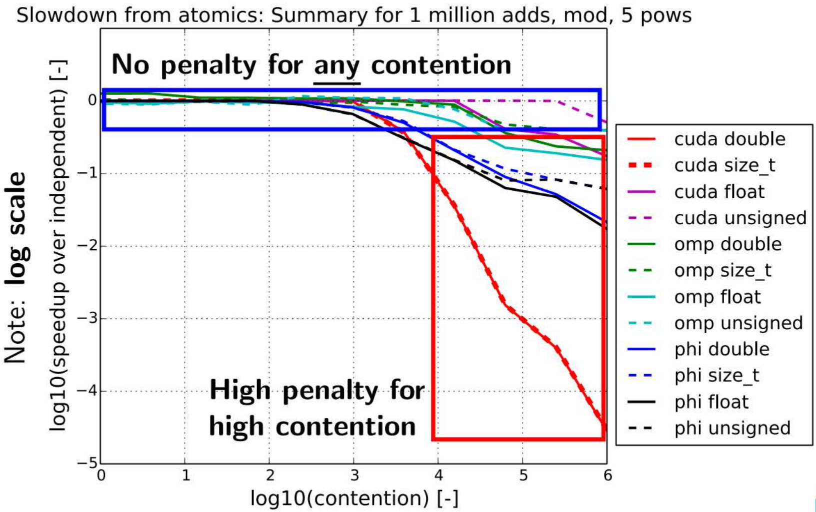


## **Atomics performance:** 1 million adds, **some** work per kernel



## **Atomics performance:** 1 million adds, **lots of** work per kernel



## Atomics on arbitrary types:

- Atomic operations work if the corresponding operator exists , i.e., `atomic_add` works on any data type with "+".
- Atomic exchange works on any data type.

```
// Assign *dest to val, return former value of *dest
template<typename T>
T atomic_exchange(T * dest, T val);
// If *dest == comp then assign *dest to val
// Return true if succeeds.
template<typename T>
bool atomic_compare_exchange_strong(T * dest, T comp, T val);
```

## `View` memory traits:

- Beyond a `Layout` and `Space`, `Views` can have memory traits.
- Memory traits either provide **convenience** or allow for certain **hardware-specific optimizations** to be performed.

Example: If all accesses to a `View` will be atomic, use the `Atomic` memory trait:

```
View<double**, Layout, Space,
     MemoryTraits<Atomic> > forces(...);
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View<double**, Layout, Space,
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```

Many memory traits exist or are experimental, including `Read`, `Write`, `ReadWrite`, `ReadOnce` (non-temporal), `Contiguous`, and `RandomAccess`.

**Example:** `RandomAccess` **memory trait:**

On **GPUs**, there is a special pathway for fast **read-only**, **random** access, originally designed for textures.

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How to access texture memory via **CUDA**:

```
cudaResourceDesc resDesc;
memset(&resDesc, 0, sizeof(resDesc));
resDesc.resType = cudaResourceTypeLinear;
resDesc.res.linear.devPtr = buffer;
resDesc.res.linear.desc.f = cudaChannelFormatKindFloat;
resDesc.res.linear.desc.x = 32; // bits per channel
resDesc.res.linear.sizeInBytes = N*sizeof(float);

cudaTextureDesc texDesc;
memset(&texDesc, 0, sizeof(texDesc));
texDesc.readMode = cudaReadModeElementType;

cudaTextureObject_t tex=0;
cudaCreateTextureObject(&tex, &resDesc, &texDesc, NULL);
```

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resDesc.res.linear.desc.x = 32; // bits per channel
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cudaTextureDesc texDesc;
memset(&texDesc, 0, sizeof(texDesc));
texDesc.readMode = cudaReadModeElementType;

cudaTextureObject_t tex=0;
cudaCreateTextureObject(&tex, &resDesc, &texDesc, NULL);
```

How to access texture memory via **Kokkos**:

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

- Atomics are the only thread-scalable solution to thread safety.
  - Locks or data replication are **strongly discouraged**
- Atomic performance **depends on ratio** of independent work and atomic operations.
  - With more work, there is a lower performance penalty, because of increased opportunity to interleave work and atomic.
- The `Atomic` **memory trait** can be used to make all accesses to a view atomic.
- The cost of atomics can be negligible:
  - **CPU** ideal: contiguous access, integer types
  - **GPU** ideal: scattered access, 32-bit types
- Many programs with the **scatter-add** pattern can be thread-scalably parallelized using atomics without much modification.

# Hierarchical parallelism

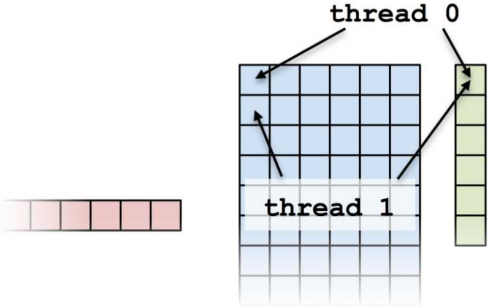
Finding and exploiting more parallelism in your computations.

**Learning objectives:**

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

## (Flat parallel) Kernel:

```
Kokkos::parallel_reduce(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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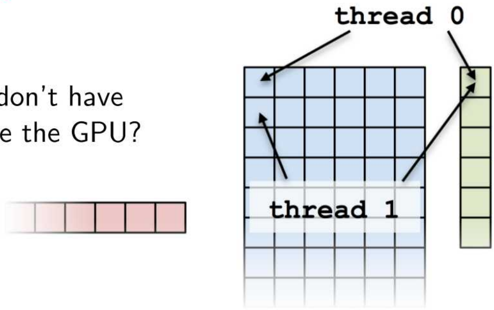
```

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



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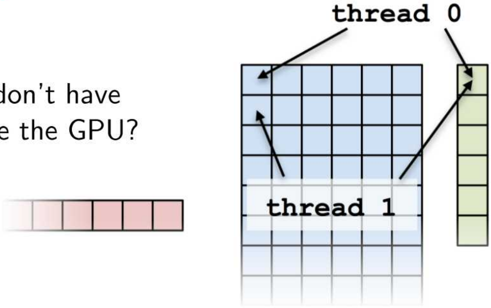


**Problem:** What if we don't have enough rows to saturate the GPU?

**Solutions?**

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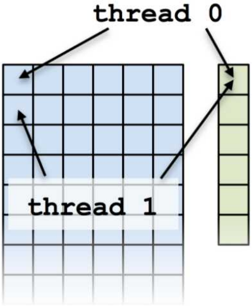


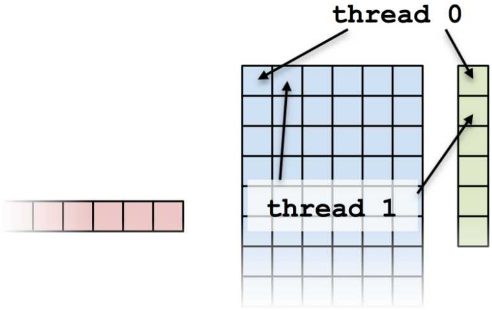

**Problem:** What if we don't have enough rows to saturate the GPU?

**Solutions?**

- Atomics
- Thread teams

## Atomics kernel:

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



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  });
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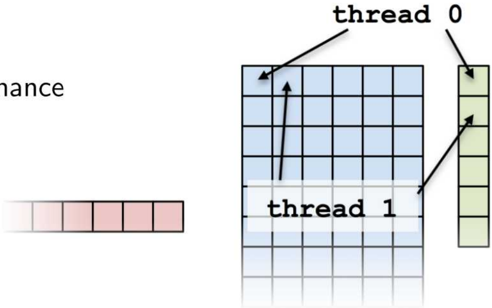
**Problem:** Poor performance



Doing each individual row with atomics is like doing scalar integration with atomics.

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

```
for each row
  Functor functor(row, ...);
  parallel_reduce(M, functor);
}
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Instead, you could envision doing a large number of `parallel_reduce` kernels.

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}
```

This is an example of *hierarchical work*.

**Important concept: Hierarchical parallelism**

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

## Important concept: Thread team

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

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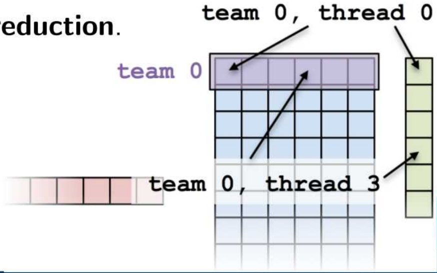
A collection of threads which are guaranteed to be executing **concurrently** and **can synchronize**.

High-level **strategy**:

1. Do **one parallel launch** of `N` teams of `M` threads.
2. Each thread performs **one** entry in the row.
3. The threads within **teams perform a reduction**.
4. The thread teams **perform a reduction**.



## The final hierarchical parallel kernel:

```
parallel_reduce(
  team_policy(N, Kokkos::AUTO),
  KOKKOS_LAMBDA (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);
```

The **performance** and **flexibility** of teams is *naturally* and *concisely* expressed under the Kokkos model.

Let's walk through how we got to this *final* answer.

## 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(
  RangePolicy<ExecutionSpace>(0,N), functor);
```

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We specify a *total amount of work*.

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

## Important point

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

```
typedef typename TeamPolicy<ExecSpace>::member_type member_type;

void operator()(const member_type & teamMember) {
  // Which team am I on?
  const unsigned int leagueRank = teamMember.league_rank();
  // Which thread am I on this team?
  const unsigned int teamRank = teamMember.team_rank();
}
```

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void operator()(const member_type & teamMember) {
  // Which team am I on?
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}
```

**Warning**

There may be more (or fewer) team members than pieces of your algorithm's work per team

First attempt at inner product exercise:

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

First attempt at inner product exercise:

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operator() (const member_type & teamMember ) {
  const unsigned int row = teamMember.league_rank();
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}
```

- When team size $\neq$ number of columns, how are units of work mapped to team's member threads? Is the mapping architecture-dependent?
- `atomic_add` performs badly under high contention, how can team's member threads performantly cooperate for a nested reduction?

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

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

we'd use `Kokkos::parallel_reduce`.

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

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  }
}
```

If this were a parallel execution,

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

$\Rightarrow$ **Nested parallel patterns**

## TeamThreadRange:

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

## 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 & rowUpdate ) {
      rowUpdate += 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`.
- Intra-team reduction handled for you.

## **Anatomy** of nested parallelism:

```
parallel_outer(
  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`, `reduce`, or `scan`.
- The inner lambda may capture by reference, but capture-by-value is recommended.
- The policy of the inner lambda is always a `TeamThreadRange`.
- `TeamThreadRange` cannot be nested.

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

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

- Special hardware available for coordination within a team.
- Within a team 32 threads (*warp*) execute "lock step."
- Maximum team size: **1024**; Recommended team size: **256**

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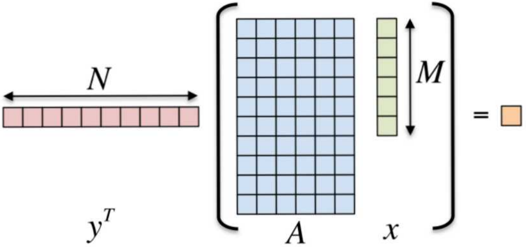
**Intel Xeon Phi**:

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

## Exercise #4: Inner Product, Hierarchical Parallelism

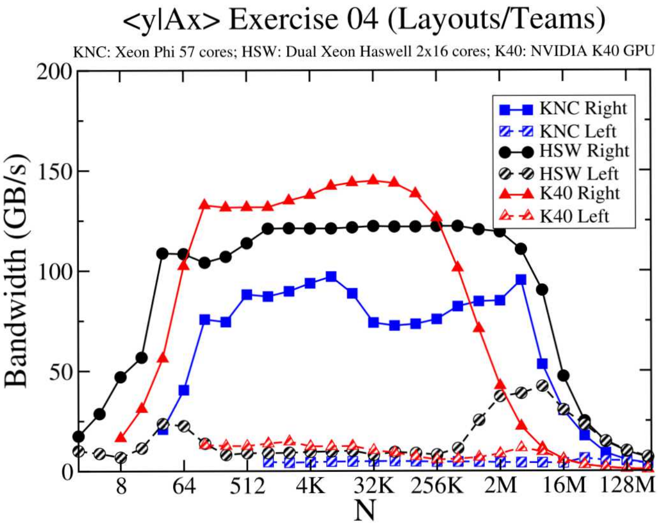
**Exercise**: Inner product $< y, A * x >$




**Details**:

- Location: `~/kokkos-tutorials/SC15/Exercises/03/`
- Use lambdas instead of functors for computational bodies.
- Replace `RangePolicy<Space>` with `TeamPolicy<Space>`
- Experiment with the combinations of `Layout`, `Space`, `N` to view performance
- Hint: what should the layout of `A` be?

## Exercise #4: Inner Product, Hierarchical Parallelism

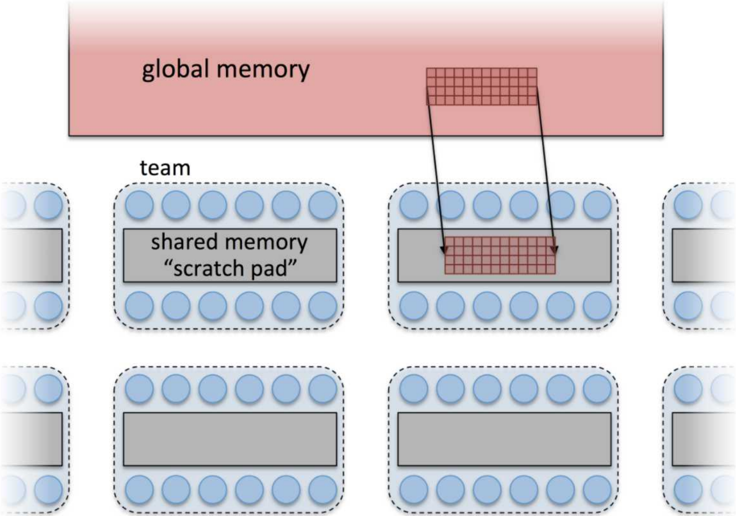


# Shared memory

**Learning objectives:**

- Understand how shared memory can reduce global memory accesses
- Recognize when to use shared memory
- Understand how to use shared memory and why barriers are necessary

Each team has access to a "scratch pad".



Shared memory (scratch pad) **details**:

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

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**Important concept**

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

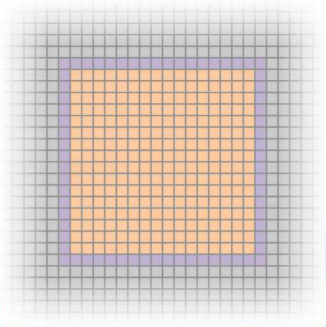
**Main idea**: Load global data into shared memory and reuse

```
operator()(member_type teamMember) const {
  // Declare team-shared tile of memory
  View< double***
      , execution_space::scratch_memory_space
      > tile( teamMember.team_shared(), ... );

  // copy subgrid data into tile

  teamMember.team_barrier();

  // Compute stencil using tile
}
```



- There is **a third level** in the hierarchy below `TeamThreadRange`: `ThreadVectorRange`
  - Just like for `TeamThreadRange`, you can perform `parallel_for`, `parallel_reduce`, or `parallel_scan`.
  - Important for full performance of Xeon Phi and GPUs
- Restricting execution to a **single member**:

  `PerTeam`: one thread per team

  `PerThread`: one vector lane per thread
- **Multiple shared views** can be made in shared memory.

- **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` policy.
- Teams can be used to **reduce contention** for global resources even in "flat" algorithms.
- Teams have access to "scratch pad" **shared memory**.

- High performance computers are increasingly **heterogenous**
  *MPI-only is no longer sufficient.*
- For **portability**: OpenMP, OpenACC, ... or Kokkos.
- Only Kokkos obtains performant memory access patterns via **architecture-aware** arrays and work mapping.
  *i.e.*, not just portable, *performance portable*.
- With Kokkos, **simple things stay simple** (parallel-for, etc.).
  *i.e.*, it's *no more difficult* than OpenMP.
- **Advanced performance-optimizing patterns are simpler** with Kokkos than with native versions.
  *i.e.*, you're *not missing out* on advanced features.