

The Kokkos Lectures

Module 1: Introduction and Parallel Dispatch

April 24, 2024

Kokkos is C++ Performance Portability

- ▶ Write a *single source* implementation using C++
- ▶ Use a *descriptive* Programming Model
- ▶ Compile for GPUs and CPUs

Kokkos is Ready for Use

- ▶ Well established project since 2012
- ▶ Major buy-in by DOE National Labs
- ▶ Well over 100 projects with over 500 developers use Kokkos
- ▶ Dedicated developer staff at 5 National Labs
- ▶ Robust support for software stacks: GCC 8+, Clang 8+, NVCC 11+, ROCM 5.2, Intel 19+

- ▶ 07/17 Module 1: Introduction, Building and Parallel Dispatch
- ▶ 07/24 Module 2: Views and Spaces
- ▶ 07/31 Module 3: Data Structures + MultiDimensional Loops
- ▶ 08/07 Module 4: Hierarchical Parallelism
- ▶ 08/14 Module 5: Tasking, Streams and SIMD
- ▶ 08/21 Module 6: Internode: MPI and PGAS
- ▶ 08/28 Module 7: Tools: Profiling, Tuning and Debugging
- ▶ 09/04 Module 8: Kernels: Sparse and Dense Linear Algebra
- ▶ 09/11 Reserve Day

Exercises

- ▶ Exercises are small codes with places to do modifications.
- ▶ Access to GPUs helpful for most of them, but most can be done on pure CPU systems.
- ▶ Only dependent on standard compilers (e.g. Clang, NVCC)

Introduction

What is Kokkos? Who is behind it? Why should you use it?

Parallel Dispatch

Pattern, Policy and Body: how to parallelize simple code with Kokkos.

Introduction

Learning objectives:

- ▶ Why do we need Kokkos
- ▶ The Kokkos EcoSystem

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



LANL/SNL Trinity
Intel Haswell / Intel KNL
OpenMP 3



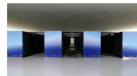
LLNL SIERRA
IBM Power9 / NVIDIA Volta
CUDA / OpenMP^(a)



ORNL Summit
IBM Power9 / NVIDIA Volta
CUDA / OpenACC / OpenMP^(a)



SNL Astra
ARM CPUs
OpenMP 3



Riken Fugaku
ARM CPUs with SVE
OpenMP 3 / OpenACC^(b)

Upcoming Generation: Programming Models OpenMP 5, CUDA, HIP and DPC++ depending on machine



NERSC Perlmutter
AMD CPU / NVIDIA GPU
CUDA / OpenMP 5^(c)



ORNL Frontier
AMD CPU / AMD GPU
HIP / OpenMP 5^(d)



ANL Aurora
Xeon CPUs / Intel GPUs
DPC++ / OpenMP 5^(e)



LLNL El Capitan
AMD CPU / AMD GPU
HIP / OpenMP 5^(d)

- (a) Initially not working. Now more robust for Fortran than C++, but getting better.
- (b) Research effort.
- (c) OpenMP 5 by NVIDIA.
- (d) OpenMP 5 by AMD.
- (e) OpenMP 5 by Intel.
- (f) OpenMP 5 by HPE.

Industry Estimate

A full time software engineer writes 10 lines of production code per hour: 20k LOC/year.

Conservative estimate: need to rewrite 10% of an app to switch Programming Model

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Software Cost Switching Vendors

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

- ▶ A C++ Programming Model for Performance Portability
 - ▶ Implemented as a template library on top CUDA, HIP, OpenMP, ...
 - ▶ Aims to be descriptive not prescriptive
 - ▶ Aligns with developments in the C++ standard
- ▶ Expanding solution for common needs of modern science and engineering codes
 - ▶ Math libraries based on Kokkos
 - ▶ Tools for debugging, profiling and tuning
 - ▶ Utilities for integration with Fortran and Python
- ▶ It is an Open Source project with a growing community
 - ▶ Maintained and developed at <https://github.com/kokkos>
 - ▶ Hundreds of users at many large institutions

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

Using your own `${HOME}`

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

Slides are in

`${HOME}/Kokkos/kokkos-tutorials/LectureSeries`

Exercises are in

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

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

Online Resources:

- ▶ <https://github.com/kokkos>: Primary Kokkos GitHub Organization
- ▶ <https://kokkos.github.io/kokkos-core-wiki>: Wiki including API reference
- ▶ <https://github.com/kokkos/kokkos-tutorials>: Tutorial exercises
- ▶ <https://kokkosteam.slack.com>: Slack channel for Kokkos. Join the **doe-portability-training** channel.

Kokkos' basic capabilities:

- ▶ Simple 1D data parallel computational patterns
- ▶ Deciding where code is run and where data is placed
- ▶ Managing data access patterns for performance portability
- ▶ Multidimensional data parallelism

Kokkos' advanced capabilities:

- ▶ Thread safety, thread scalability, and atomic operations
- ▶ Hierarchical patterns for maximizing parallelism
- ▶ Task based programming with Kokkos

Kokkos' tools and Kernels:

- ▶ How to profile, tune and debug Kokkos code
- ▶ Interacting with Python and Fortran
- ▶ Using Kokkos Kernels math library

- ▶ Kokkos enables **Single Source Performance Portable Codes**
- ▶ **Simple things stay simple** - it is not much more complicated than OpenMP
- ▶ **Advanced performance optimizing capabilities** easier to use with Kokkos than e.g. CUDA or HIP
- ▶ Kokkos provides data abstractions critical for performance portability not available in other programming models
Controlling data access patterns is key for obtaining performance
- ▶ The **Kokkos Ecosystem** comes with tools (profiling, debugging, tuning, math libraries, etc.) needed for application development in professional settings

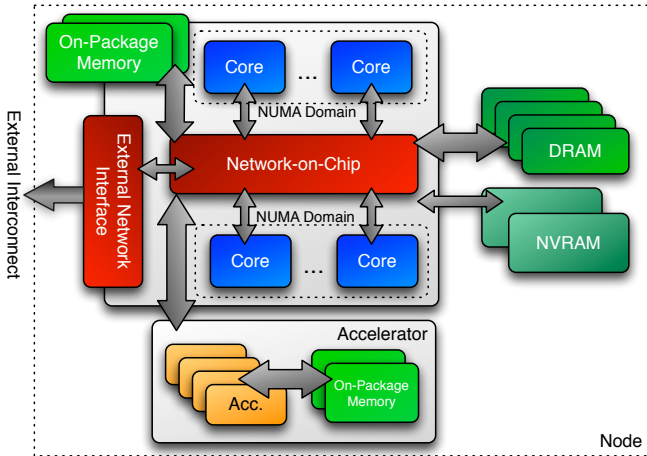
Assume you are here because:

- ▶ Want to use **all** HPC node architectures; including GPUs
- ▶ Are familiar with **C++**
- ▶ Want GPU programming to be **easier**
- ▶ Would like **portability**, as long as it doesn't hurt performance

Helpful for understanding nuances:

- ▶ Are familiar with **data parallelism**
- ▶ Are familiar with **OpenMP**
- ▶ Are familiar with **GPU architecture** and **CUDA**

Target machine:



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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Goal: write **one implementation** which:

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

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- ▶ can leverage **architecture-specific features** where possible.

Kokkos: performance portability across manycore architectures.

Concepts for Data Parallelism

Learning objectives:

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

```
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;  
}
```

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 loop?

```
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What if we want to **thread** the loop?

```
#pragma omp parallel for
for (element = 0; element < numElements; ++element) {
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```

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

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    elementValues[element] = total;
}
```

(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 PHI *and* NVIDIA GPU *and* AMD GPU *and* ...

Option 1: OpenMP 4.5

```
#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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        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?

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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.

Data parallel patterns

Learning objectives:

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

Data parallel patterns and work

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

Kokkos maps **work** to execution resources

Data parallel patterns and work

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

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

Data parallel patterns and work

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

Important concept: Work mapping

You give an **iteration range** and **computational body** (kernel) to Kokkos, and Kokkos decides how to map that work to execution resources.

How are computational bodies given to Kokkos?

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

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

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

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

How is work assigned to functor operators?

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

```
ParallelFunctor functor;  
Kokkos::parallel_for(numberOfIterations, functor);
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struct Functor {  
    void operator()(const int64_t index) const {...}  
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struct Functor {  
    void operator()(const int64_t index) const {...}  
}
```

Warning: concurrency and order

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

How is data passed to computational bodies?

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

```
struct AtomForceFunctor {  
    ...  
    void operator()(const int64_t atomIndex) const {  
        atomForces[atomIndex] = calculateForce(...data...);  
    }  
    ...  
}
```

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    ...  
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        atomForces[atomIndex] = calculateForce(...data...);  
    }  
    ...  
}
```

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;
    DataType _atomData;
    AtomForceFunctor(/* args */) {...}
    void operator()(const int64_t atomIndex) const {
        _atomForces[atomIndex] = calculateForce(_atomData);
    }
};
```

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};
```

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

Serial

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

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```

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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;
    DataType _atomData;

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

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

2. Executing in parallel with Kokkos pattern:

```
AtomForceFunctor functor(atomForces, data);
Kokkos::parallel_for(numberOfAtoms, functor);
```

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

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

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

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

Warning: Lambda capture and C++ containers

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

How does this compare to OpenMP?

Serial

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

OpenMP

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

Kokkos

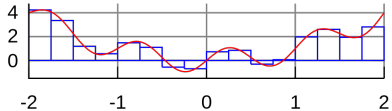
```
parallel_for(N, [=] (const int64_t i) {  
    /* loop body */  
});
```

Important concept

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

Riemann-sum-style numerical integration:

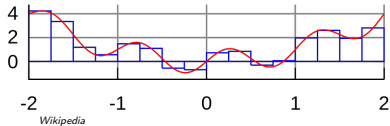
$$y = \int_{\text{lower}}^{\text{upper}} \text{function}(x) dx$$



Wikipedia

Riemann-sum-style numerical integration:

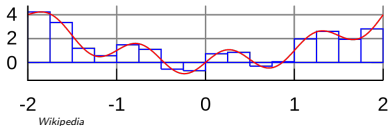
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```
double totalIntegral = 0;
for (int64_t i = 0; i < numberOfIntervals; ++i) {
    const double x =
        lower + (i/numberOfIntervals) * (upper - lower);
    const double thisIntervalsContribution = function(x);
    totalIntegral += thisIntervalsContribution;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

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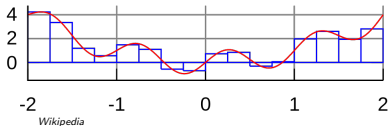


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Riemann-sum-style numerical integration:

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Pattern?

```

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```

Body?

Policy?

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

An (incorrect) attempt:

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

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

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

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

Reductions combine the results contributed by parallel work.

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

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

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

Important concept: Reduction

Reductions combine the results contributed by parallel work.

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

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

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

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


Example: Scalar integration

OpenMP

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

Kokkos

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

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

Warning: Parallelism is NOT free

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

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- ▶ α = dispatch overhead
- ▶ β = time for a unit of work
- ▶ N = number of units of work
- ▶ P = available concurrency

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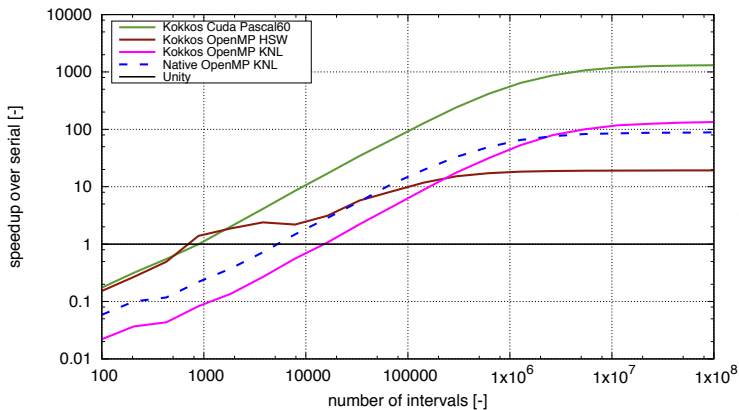
- ▶ α = dispatch overhead
- ▶ β = time for a unit of work
- ▶ N = number of units of work
- ▶ P = available concurrency

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

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

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

Kokkos speedup over serial: Scalar Integration



Note: log scale

Always name your kernels!

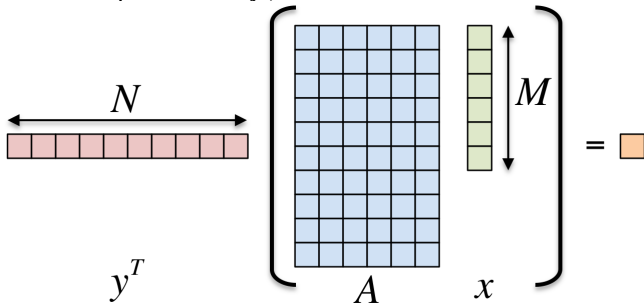
Giving unique names to each kernel is immensely helpful for debugging and profiling. You will regret it if you don't!

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

Example:

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

Exercise: Inner product $\langle y, A * x \rangle$



Details:

- ▶ y is $N \times 1$, A is $N \times M$, x is $M \times 1$
- ▶ We'll use this exercise throughout the tutorial

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

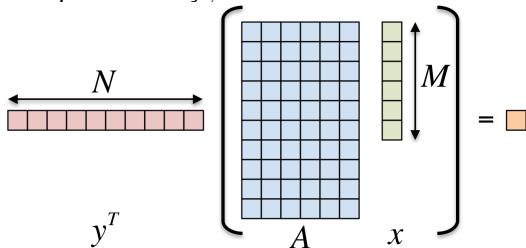
```
#include <Kokkos_Core.hpp>
int main(int argc, char* argv[]) {
    /* ... do any necessary setup (e.g., initialize MPI) ... */
    Kokkos::initialize(argc, argv);
    {
        /* ... do computations ... */
    }
    Kokkos::finalize();
    return 0;
}
```

(Optional) Command-line arguments or environment variables:

<code>--kokkos-num-threads=INT</code> or <code>KOKKOS_NUM_THREADS</code>	total number of threads
<code>--kokkos-device-id=INT</code> or <code>KOKKOS_DEVICE_ID</code>	device (GPU) ID to use

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

Exercise: Inner product $\langle y, A * x \rangle$



Details:

- ▶ Location: Exercises/01/Begin/
- ▶ Look for comments labeled with “EXERCISE”
- ▶ Need to include, initialize, and finalize Kokkos library
- ▶ Parallelize loops with `parallel_for` or `parallel_reduce`
- ▶ Use lambdas instead of functors for computational bodies.
- ▶ For now, this will only use the CPU.

Compiling for CPU

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

Running on CPU with OpenMP backend

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

Things to try:

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

- ▶ Customizing `parallel_reduce` data type and reduction operator
e.g., minimum, maximum, ...
- ▶ `parallel_scan` pattern for exclusive and inclusive prefix sum
- ▶ Using *tag dispatch* interface to allow non-trivial functors to have multiple “operator()” functions.
very useful in large, complex applications

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

Building Applications with Kokkos

Learning objectives:

- ▶ Kokkos-docs : <https://kokkos.org/kokkos-core-wiki/building.html>
- ▶ NERSC-docs : <https://docs.nersc.gov/development/programming-models/kokkos/>

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Ignore This For Tutorial Only

The following details on options to integrate Kokkos into your build process are NOT necessary to know if you just want to do the tutorial.

Kokkos EcoSystem:

- ▶ C++ Performance Portability Programming Model.
- ▶ The Kokkos Ecosystem provides capabilities needed for serious code development.
- ▶ Kokkos is supported by multiple National Laboratories with a sizeable dedicated team.

Data Parallelism:

- ▶ Simple things stay simple!
- ▶ You use **parallel patterns** and **execution policies** to execute **computational bodies**
- ▶ Simple parallel loops use the `parallel_for` pattern:

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

- ▶ Reductions combine contributions from loop iterations

```
int result;  
parallel_reduce("Label", N, [=] (int64_t i, int& lres) {  
    /* loop body */  
    lres += /* something */  
}, result);
```


Kokkos::View:

- ▶ Solving the data-layout issue.
- ▶ Controlling data life-time.

Execution and Memory Spaces:

- ▶ How to control where data lives.
- ▶ How to control where code executes.
- ▶ How to manage data transfers.

Don't Forget: Join our Slack Channel and drop into our office hours on Tuesday.

Updates at:

<https://github.com/kokkos/kokkos-tutorials/issues/38>