The Kokkos Lectures

Module 1: Introduction, Building and Parallel Dispatch

November 25, 2025

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SAND2020-7263 PE

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
- Part of the Linux Foundation's HPSF
- Major buy-in by US DOE National Labs and the French CEA
- Well over 300 projects with over 1500 developers use Kokkos
- Robust support for software stacks: GCC 11+, Clang 14+, NVCC 12+, ROCM 6.2, Intel 2022+, MSVC

Online Resources:

- https://github.com/kokkos:
  - Primary Kokkos GitHub Organization
- https://github.com/kokkos/kokkos-tutorials/LectureSeries:
  - Find these slides
- https://kokkos.org:
  - Project website including API reference
- https://kokkosteam.slack.com:
  - Slack channel for Kokkos.
  - Please join: fastest way to get your questions answered.
  - Can whitelist domains, or invite individual people. Email: crtrott@sandia.gov lebrungrandt@ornl.gov

- Module 1: Introduction, Building and Parallel Dispatch
- Module 2: Views and Spaces
- Module 3: Data Structures + MultiDimensional Loops
- Module 4: Hierarchical Parallelism
- Module 5: Tasking, Streams and SIMD
- Module 6: Internode: MPI and PGAS
- Module 7: Tools: Profiling, Tuning and Debugging
- Module 8: Kernels: Sparse and Dense Linear Algebra
- Module 9: Fortran inter-op

Lectures

- Typically 90 minutes of lecture
- Submodules have associated exercise as homework
- Typically 2-3 Exercises per lecture
- Exercises will be talked through at next meeting.

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)
- Ongoing support at `https://kokkosteam.slack.com`

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.

Building

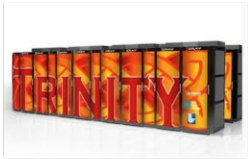
What do you need to build Kokkos and Apps? How to integrate into your build system?

Introduction

Learning objectives:

- Why do we need Kokkos
- The Kokkos Ecosystem
- The Kokkos Team

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



LANL/SNL Trinity
Intel Haswell / Intel KNL
OpenMP 3

LLNL SIERRA
IBM Power9 / NVIDIA Volta
CUDA / *OpenMP*[(a)]

ORNL Summit
IBM Power9 / NVIDIA Volta
CUDA / *OpenACC* / *OpenMP*[(a)]

SNL Astra
ARM CPUs
OpenMP 3

Riken Fugaku
ARM CPUs with SVE
OpenMP 3 / *OpenACC*[(b)]

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

NERSC Perlmutter
AMD CPU / NVIDIA GPU
CUDA / *OpenMP 5*[(c)]

ORNL Frontier
AMD CPU / AMD GPU
HIP / *OpenMP 5*[(d)]

ANL Aurora
Xeon CPUs / Intel GPUs
DPC++ / *OpenMP 5*[(e)]

LLNL El Capitan
AMD CPU / AMD GPU
HIP / *OpenMP 5*[(d)]

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

Industry Estimate

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

- Typical HPC production app: 300k-600k lines
  - Sandia alone maintains a few dozen
- Large Scientific Libraries:
  - E3SM: 1,000k lines
  - Trilinos: 4,000k lines

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

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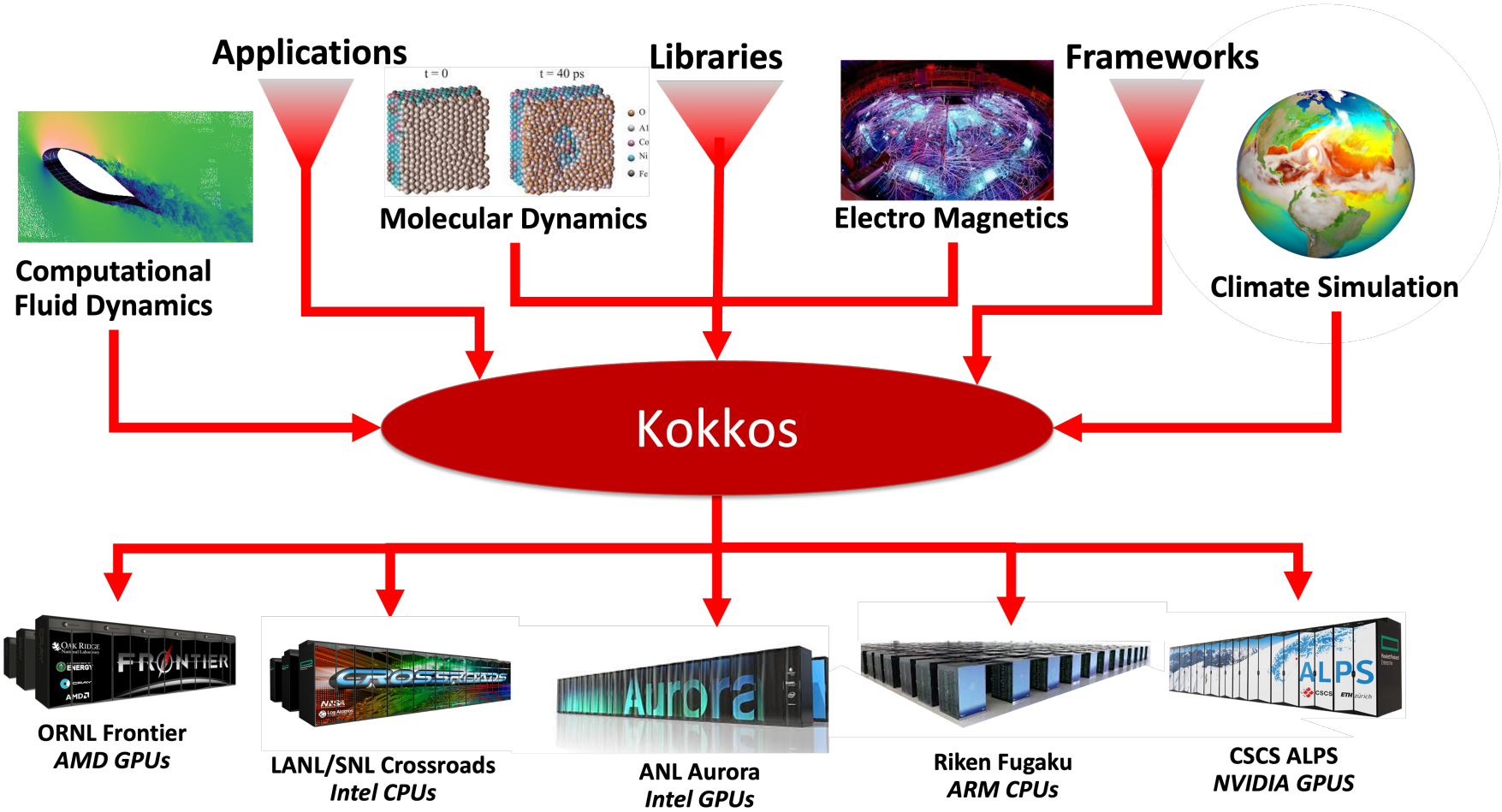
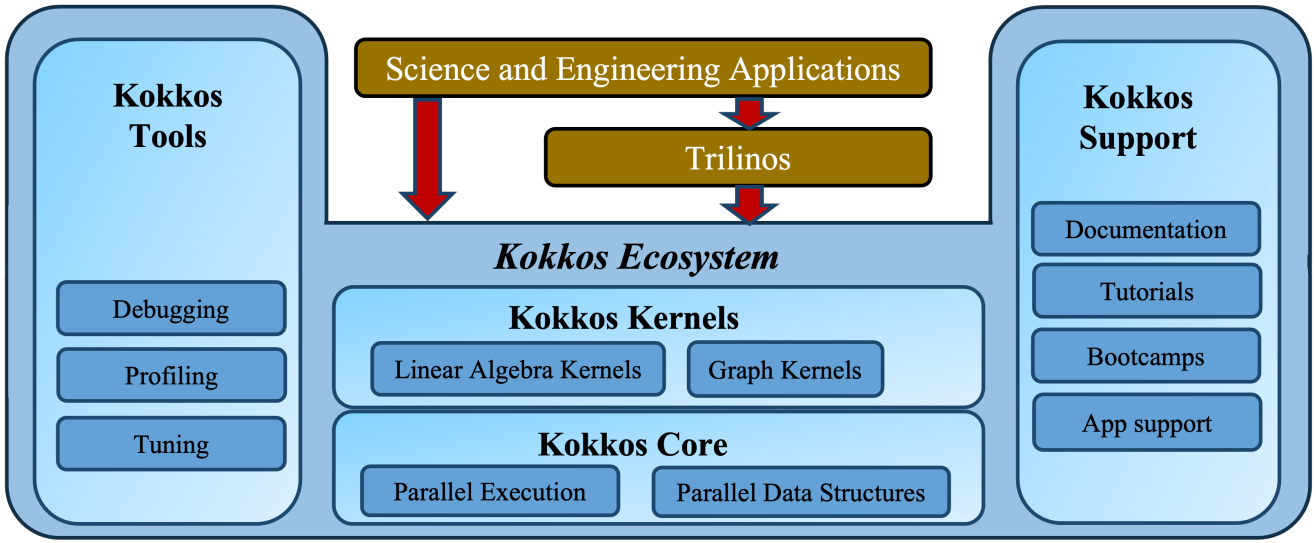
Software Cost Switching Vendors

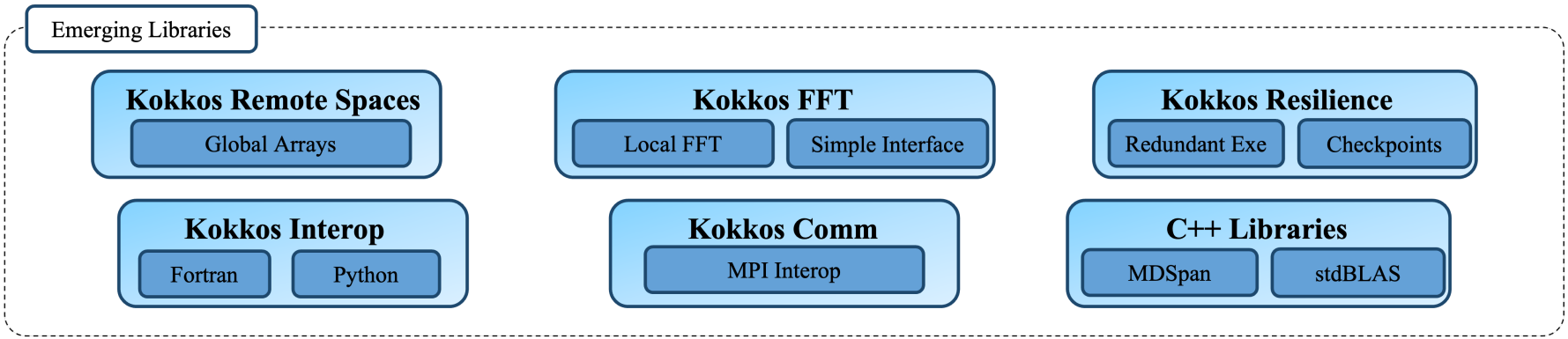
Just switching Programming Models costs multiple person-years per app!

- 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


Applications
Libraries
Frameworks
Computational Fluid Dynamics
t = 0
t = 40 ps
Molecular Dynamics
Electro Magnetics
Climate Simulation
Kokkos
FRONTIER
ORNL Frontier
AMD GPUs
CROSSROADS
LANL/SNL Crossroads
Intel CPUs
Aurora
ANL Aurora
Intel GPUs
Riken Fugaku
ARM CPUs
ALPS
CSCS ALPS
NVIDIA GPUS

The Kokkos Ecosystem

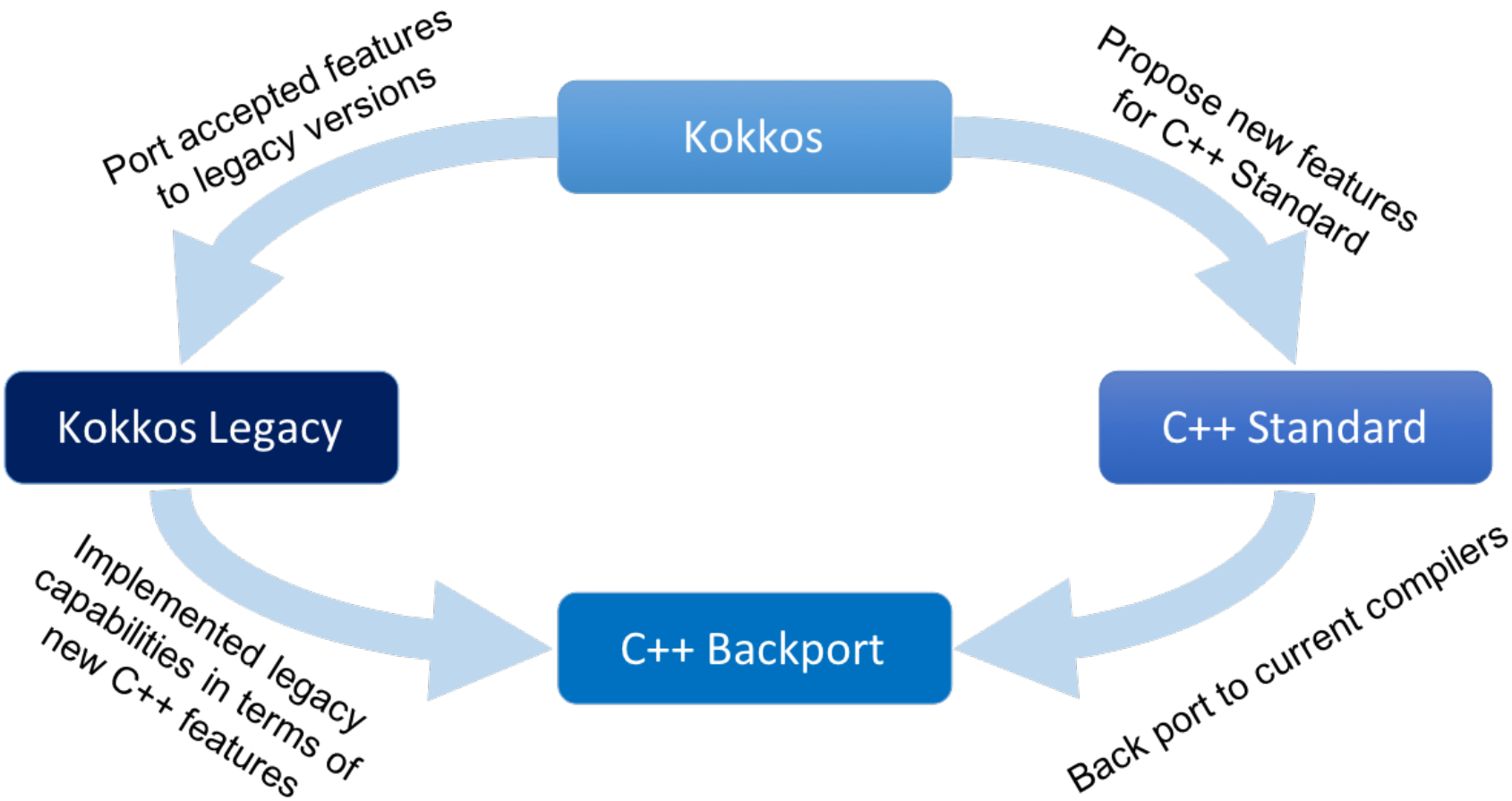




Primary Teams

Support Efforts

Kokkos helps improve ISO C++



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

C++11 std::atomic insufficient for HPC

- Objects, not functions, with only atomic access
- Can't use non-atomic access in one operation, and then atomic access in the next

C++20 std::atomic_ref adds atomic capabilites as in Kokkos

- Can wrap standard allocations.
- Works also for sizes which can't be done lock-free (e.g. `complex<double>`)
- Atomic operations on reasonably arbitrary types

```
// Kokkos today
Kokkos::atomic_add(&a[i],5.0);

// atomic_ref in ISO C++20
std::atomic_ref(a[i]) += 5.0;
```

C++ does not provide multi dimensional arrays

- Every scientific programming language has them: Fortran, Matlab, Python, ...

C++23 std::mdspan adds Kokkos::View like arrays

- Reference semantics.
- Compile time and runtime extents (also mixed)
- Data layouts to allow for adapting hardware specific access patterns.
- Subviews!

```
// Kokkos today
View<float**[5],LayoutLeft> a("A",10,12); a(3,5,1) = 5;

// mdspan in ISO C++23
using ext = extents<int,dynamic_extent,dynamic_extent,5>;
mdspan<float,ext,layout_left> a(ptr,10,12); a[3,5,1]+=5;
```

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

Using your own ${HOME}

- Git
- CMake 3.16 (or newer)
- GCC 8.2 (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-tutorials
  into `${HOME}/Kokkos/kokkos-tutorials`

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

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

Online Resources:

- https://kokkos.org: Project website with documentation
- https://github.com/kokkos: GitHub organization
- https://github.com/kokkos/kokkos-tutorials: Tutorial exercises
- https://kokkosteam.slack.com: Slack channel for Kokkos

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

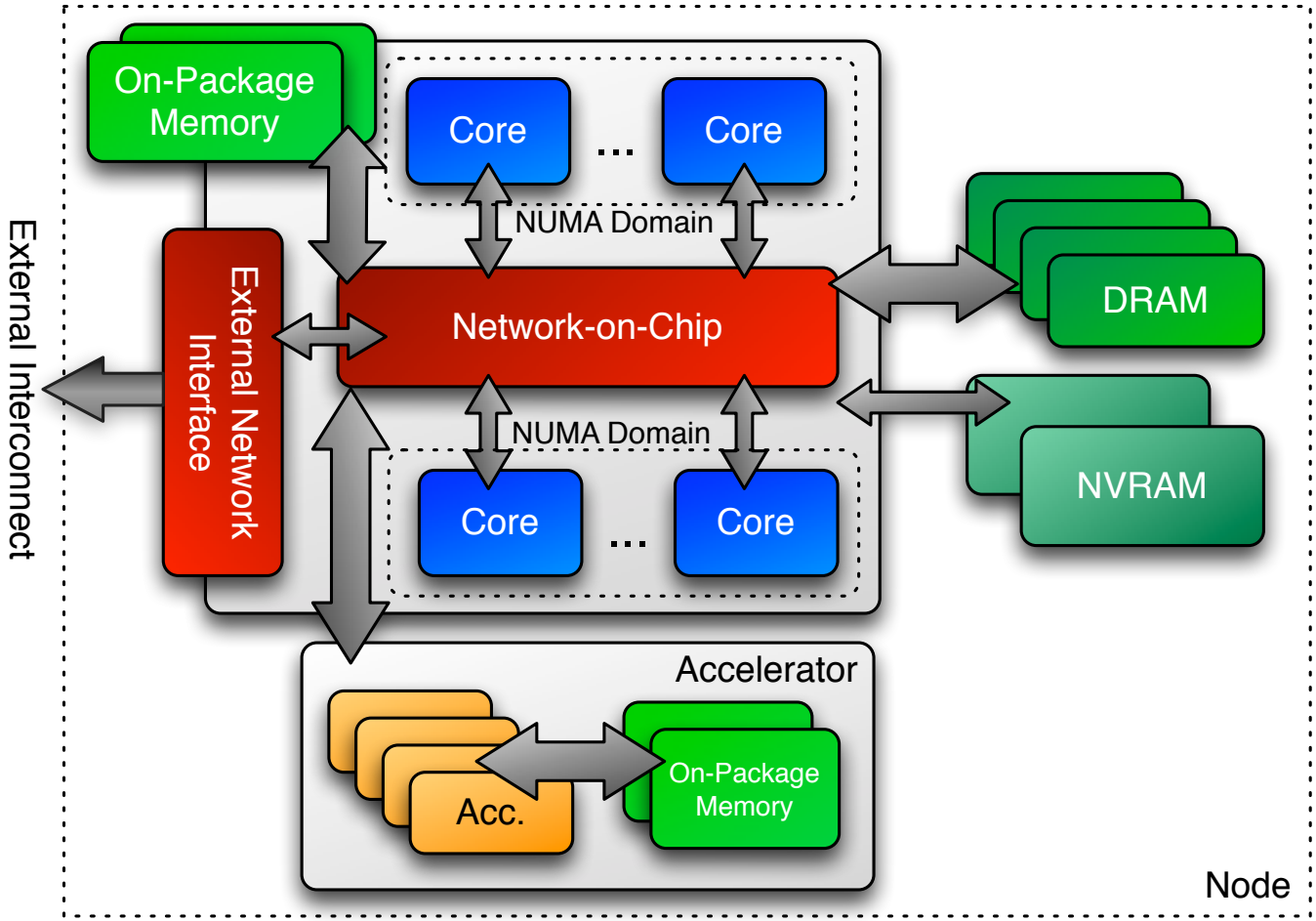
Assume you are here because:

- 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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Goal: write **one implementation** which:

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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]);
  }
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```

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?

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

```
#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 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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}
```

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];
    }
  }
  elementValues[element] = total;
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```

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

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  }
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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.
- provides **clear, concise, scalable** parallel patterns.
- lets you write algorithms once and run on **many architectures**
  e.g. multi-core CPU, GPUs, 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 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

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

Kokkos maps **work** to execution resources

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

Data parallel patterns and work

```
for (atomIndex = 0; atomIndex < numberOfAtoms; ++atomIndex) {
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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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```

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

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

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

```
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...);
  }
  ...
}
```

How is data passed to computational bodies?

```
for (atomIndex = 0; atomIndex < numberOfAtoms; ++atomIndex) {
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}
```

```
struct AtomForceFunctor {
  ...
  void operator()(const int64_t atomIndex) const {
    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);
}
```

Putting it all together: the complete functor:

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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);
}
```

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 ⇒ **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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Kokkos::parallel_for(numberOfAtoms,
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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

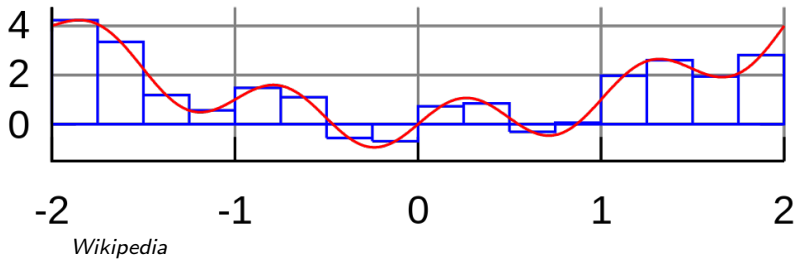
```
parallel_for(N, [=] (const int64_t i) {
  /* loop body */
});
```

Important concept

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

Riemann-sum-style numerical integration:

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



Wikipedia

Riemann-sum-style numerical integration:

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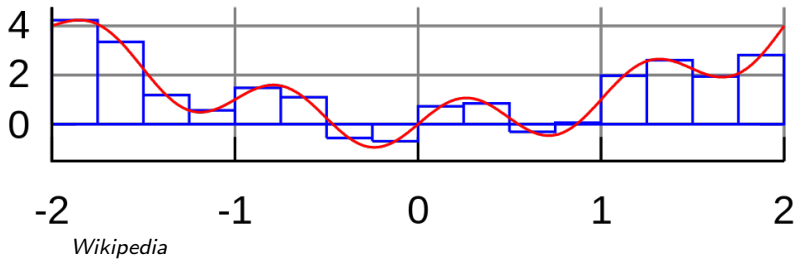
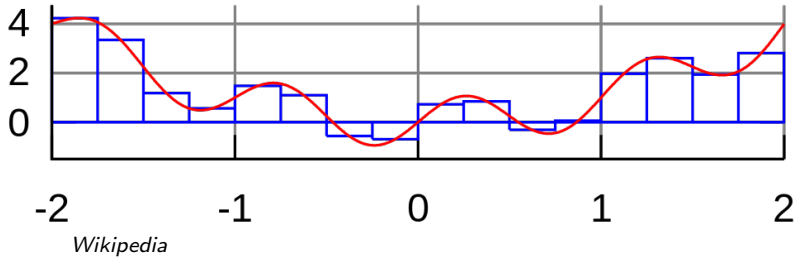


Wikipedia

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

Riemann-sum-style numerical integration:

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

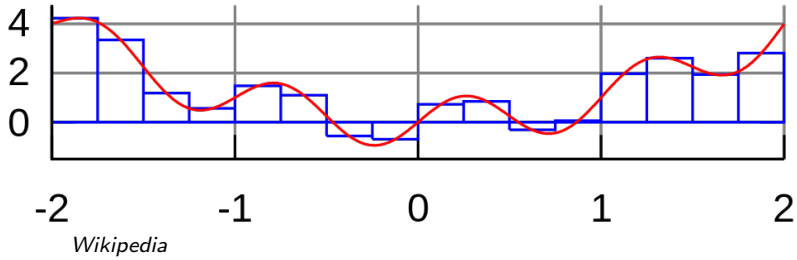



```
double totalIntegral = 0;
for (int64_t i = 0; i < numberOfIntervals; ++i) {
  const double x =
    lower + (i/numberOfIntervals) * (upper - lower);
  const double thisIntervalsContribution = function(x);
  totalIntegral += thisIntervalsContribution;
}
totalIntegral *= dx;
```

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

Riemann-sum-style numerical integration:

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



Pattern?

Policy?

Body?

```
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;
```

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);}
  );
totalIntegral *= dx;
```

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

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

Second problem: race condition

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

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

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Important concept: Reduction

Reductions combine the results contributed by parallel work.

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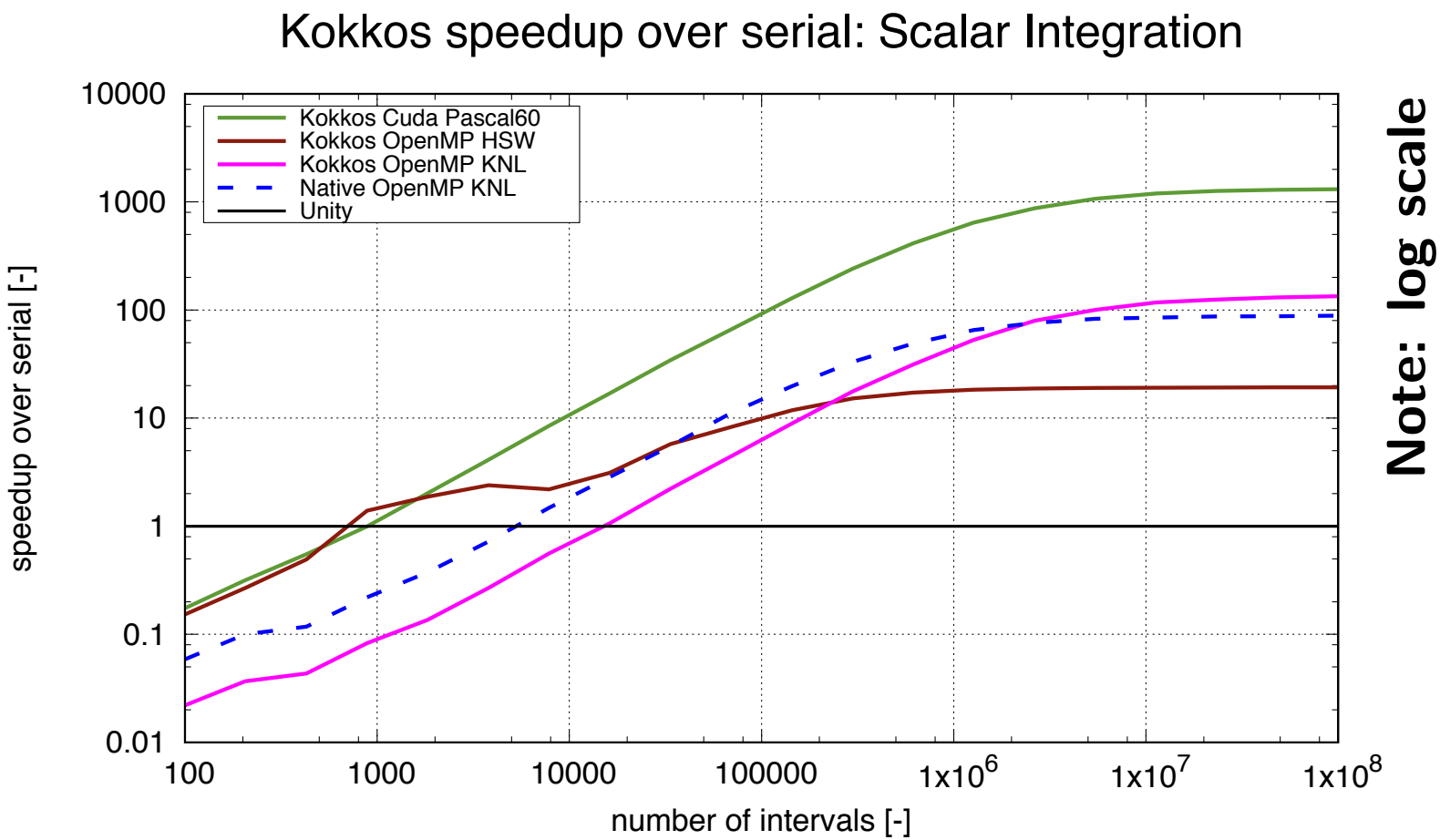
Simplistic data-parallel performance model: Time $= \alpha + \frac{\beta * N}{P}$

- α = dispatch overhead
- β = 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 α
- Find more parallelism to increase N
- Merge (fuse) parallel operations to increase β

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



Always name your kernels!

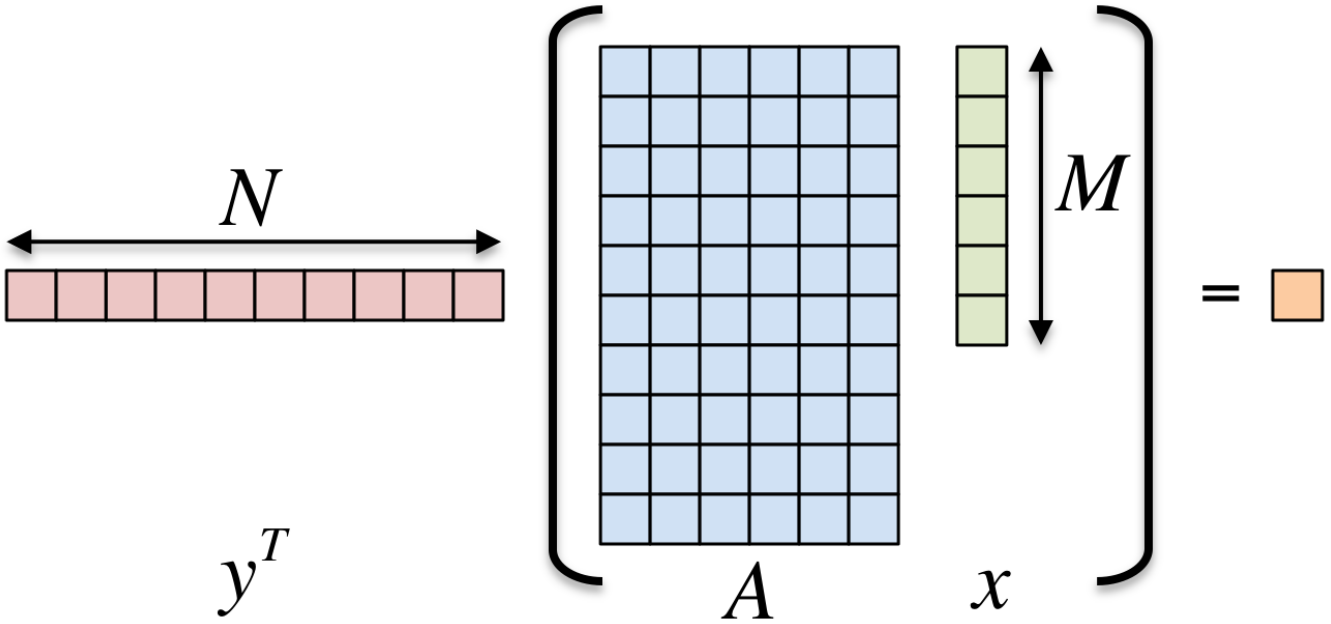
Giving unique names to each kernel is immensely helpful for debugging and profiling. You will regret it if you don't!

- 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 $< y, A * x >$



Details:

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

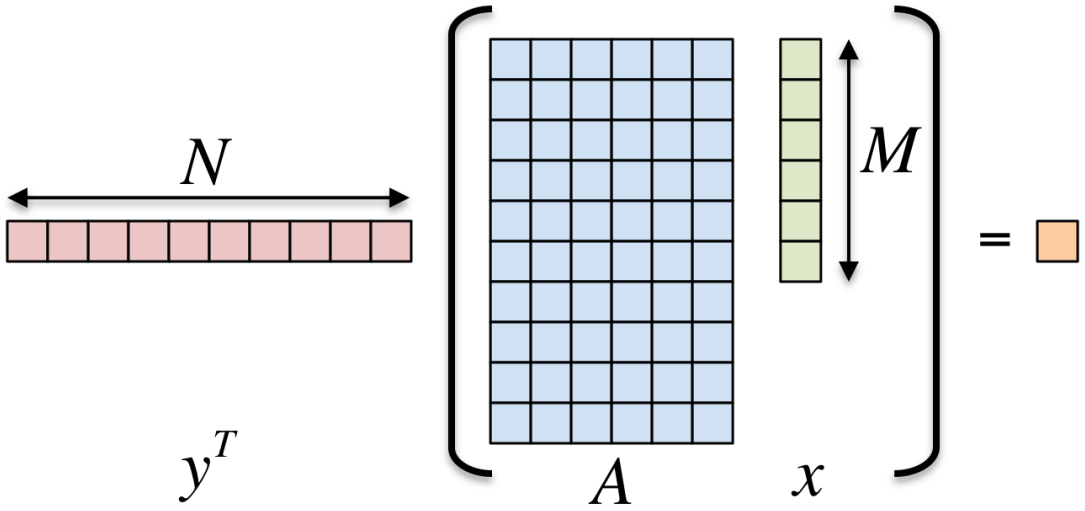
The **first step** in using Kokkos is to include, initialize, and finalize:

```
#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:

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

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



Details:

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

Compiling for CPU

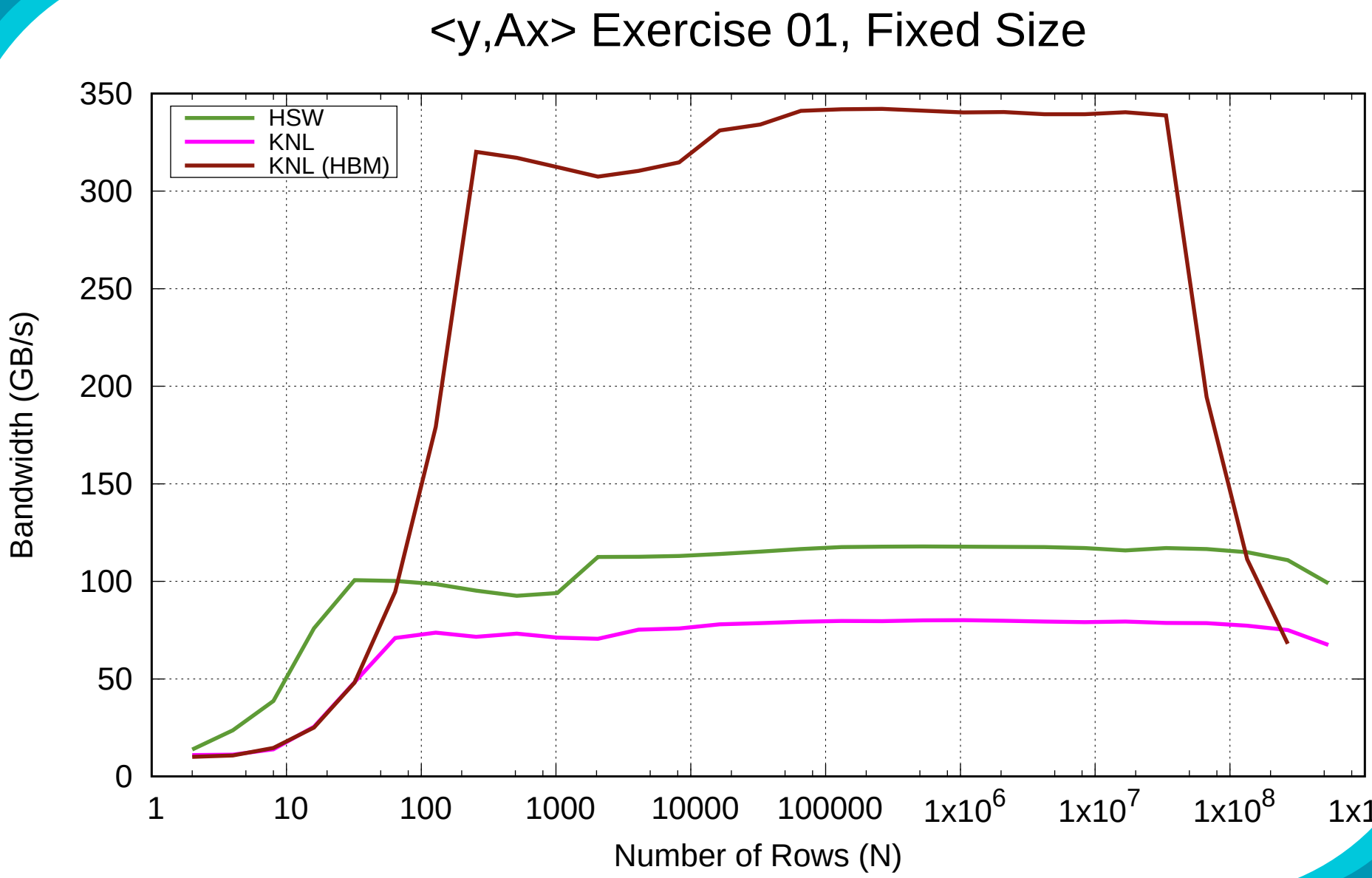
```
cmake -B build_openmp -DKokkos_ENABLE_OPENMP=ON \
    -DCMAKE_BUILD_TYPE=Release
cmake --build build_openmp
```

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_openmp/01_Exercise -h
# Run with defaults on CPU
./build_openmp/01_Exercise
# Run larger problem
./build_openmp/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 $= 2^s == 2^{n+m}$


<y,Ax> Exercise 01, Fixed Size
HSW
KNL
KNL (HBM)
Bandwidth (GB/s)
0
50
100
150
200
250
300
350
1
10
100
1000
10000
100000
1x10^6
1x10^7
1x10^8
1x10^9
Number of Rows (N)

More things to try: port your solution to work on the device

- You will need to update the dynamic memory allocation.
- Replace `std::malloc` and `std::free` with `Kokkos::kokkos_malloc` and `Kokkos::kokkos_free`.
- Bonus question: Why does this perform so poorly? (hint: the answer is in this slide deck somewhere)
- Note that this is just for learning purposes and by no mean a recommended way to manage the lifetime of your arrays. We will see a better way to do this soon.

Compiling for GPU

```
# if the architecture autodetection fails configure with
# -DKokkos_ARCH_VOLTA70=ON for V100
# refer to the documentation for the complete list of supported
# architectures and corresponding flags, or use ccmake to disco
  cmake -B build-cuda -DKokkos_ENABLE_CUDA=ON
  cmake --build build-cuda
  make -j KOKKOS_DEVICES=Cuda KOKKOS_ARCH=...
```

Basic capabilities we haven't covered

- 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:

- Integrate Kokkos into your project
- Build from source
- Package managers

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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.

- **Install Kokkos and find it as external package:** For large projects with multiple dependencies installing Kokkos via CMake and then building against it is the best option.
- **Build Kokkos embedded in your project:** This is an option suited for applications which have few dependencies (and no one depending on them) and want to build Kokkos inline with their application.
- **Using Spack:** For projects which largely rely on components provided by the Spack package manager.

- In the spirit of C++ for *code* performance portability, modern CMake aims for *build system* portability
- Projects that depend on Kokkos should be agnostic to the exact build configuration of Kokkos
- No CUDA details in C++! No CUDA details in CMake!
- Kokkos provides a `Kokkos::kokkos` target.
  - Include directories
  - Link libraries
  - Compiler options
  - Etc
- Single command in your project should configure all compiler/linker flags:

```
add_library(myLib goTeamVenture.cpp)
target_link_libraries(myLib PUBLIC Kokkos::kokkos)
```

```
cmake_minimum_required(VERSION 3.22)
project(MyProject CXX)

find_package(Kokkos 4.2 REQUIRED CONFIG) # Find Kokkos version 4.2 or later

add_executable(HelloKokkos HelloKokkos.cpp)
target_link_libraries(HelloKokkos PRIVATE Kokkos::kokkos)
```

How do I control cmake's search procedure?

```
cmake -DKokkos_ROOT=/path/to/kokkos
```

Option 1: via Git Submodules and `add_subdirectory()`

```
git submodule add -b 4.5.01 https://github.com/kokkos/kokkos.git tpls/kokkos
git commit -m 'Adding Kokkos v4.5.1 as a submodule'
```

```
add_subdirectory(tpls/kokkos)
target_link_libraries(MyTarget PRIVATE Kokkos::kokkos)
```

Option 2: via `FetchContent`

```
include(FetchContent)
FetchContent_Declare(
    Kokkos
    URL      https://github.com/kokkos/kokkos/releases/download/4.5.01/kokkos-4.5.01.tar.gz
    URL_HASH SHA256=52d003ffbbe05f30c89966e4009c017efb1662b02b2b73190670d3418719564c
)
FetchContent_MakeAvailable(Kokkos)
target_link_libraries(MyTarget PRIVATE Kokkos::kokkos)
```

Supporting Both External and Embedded Kokkos

```
find_package(Kokkos CONFIG) # Try to find Kokkos externally
if(Kokkos_FOUND)
    message(STATUS "Found external Kokkos")
else()
    message(STATUS "Kokkos not found. Using embedded Kokkos.")
    # or FetchContent if you prefer
    add_subdirectory(tpls/kokkos)
endif()
target_link_libraries(MyTarget PRIVATE Kokkos::kokkos)
```

```
find_package(Kokkos CONFIG) # Try to find Kokkos externally
if(Kokkos_FOUND)
    message(STATUS "Found external Kokkos")
else()
    message(STATUS "Kokkos not found. Using embedded Kokkos.")
    # or FetchContent if you prefer
    add_subdirectory(tpls/kokkos)
endif()
target_link_libraries(MyTarget PRIVATE Kokkos::kokkos)
```

How do I control the Kokkos integration?

```
find_package(Kokkos CONFIG) # Try to find Kokkos externally
if(Kokkos_FOUND)
    message(STATUS "Found external Kokkos")
else()
    message(STATUS "Kokkos not found. Using embedded Kokkos.")
    # or FetchContent if you prefer
    add_subdirectory(tpls/kokkos)
endif()
target_link_libraries(MyTarget PRIVATE Kokkos::kokkos)
```

How do I control the Kokkos integration?

External

```
cmake -DCMAKE_REQUIRE_FIND_PACKAGE_Kokkos=ON -DKokkos_ROOT=/path/to/kokkos
```

Embedded

```
cmake -DCMAKE_DISABLE_FIND_PACKAGE_Kokkos=ON
```

Assert that the (experimental) relaxed constexpr support is enabled

```
if(Kokkos_ENABLE_CUDA)
    kokkos_check(OPTIONS CUDA_CONSTEXPR)
    # fatal error if not enabled
endif()
```

Query whether generation of relocatable device code is enabled

```
kokkos_check(
    OPTIONS CUDA_RELOCATABLE_DEVICE_CODE
    RESULT_VARIABLE KOKKOS_HAS_CUDA_RDC
)
if(NOT KOKKOS_HAS_CUDA_RDC)
    # ...
```

Getting the Kokkos Source Code

Option 1: Downloading a Release Archive (Recommended)

Go to the Kokkos releases page and find the latest release (or a specific version you need).

```
curl -sLO https://github.com/kokkos/kokkos/releases/download/4.6.01/kokkos-4.6.01.tar.gz
curl -sLO https://github.com/kokkos/kokkos/releases/download/4.6.01/kokkos-4.6.01-SHA-256.txt
grep kokkos-4.6.01.tar.gz kokkos-4.6.01-SHA-256.txt | shasum -c
# the output should be "kokkos-4.6.01.tar.gz: OK" or similar
# if the checksum doesn't match, do not use the archive
tar -xzvf kokkos-4.6.01.tar.gz
```

Option 2: Cloning the Git Repository (For Development Versions)

If you need the latest features or want to contribute to Kokkos, you can clone the Git repository.

```
git clone https://github.com/kokkos/kokkos.git
cd kokkos
# checkout a release tag
git checkout 4.6.01
```

Configuring Kokkos

`cmake -B builddir [<options...>]`

Common CMake options:

- `-DCMAKE_CXX_COMPILER=<compiler>` for example `hipcc` for AMD GPUs, `icpx` for Intel GPUs, `nvcc_wrapper` for NVIDIA GPUs
- `-DCMAKE_CXX_STANDARD=<standard>` default is 17 for Kokkos 4.X, 20 in 5.0
- `-DCMAKE_BUILD_TYPE=<type>` choose from `Debug`, `Release`, `RelWithDebInfo` (default), and `MinSizeRel`
- `-DCMAKE_INSTALL_PREFIX=<prefix>`

Important Kokkos-specific options:

- `-DKokkos_ENABLE_<BACKEND>=ON`
- `-DKokkos_ARCH_<ARCHITECTURE>=ON`
- `-DKokkos_ENABLE_DEPRECATED_CODE_4=ON`
- `-DKokkos_ENABLE_DEPRECATION_WARNINGS=ON`

Refer to https://kokkos.org >Documentation>Get Started>Configuration Guide

Backends

- You can only enable one "device" backend at a time (e.g., `CUDA`, `HIP`, or `SYCL`)
- Only one "host parallel" backend at a time (e.g., `OPENMP` or `THREADS`)
- A host backend is always required
- If no host backend is explicitly enabled, the `SERIAL` backend will be used.

```
-- The project name is: Kokkos
...
-- Execution Spaces:
--     Device Parallel: CUDA
--     Host Parallel: NONE
--       Host Serial: SERIAL
```

Architectures

- Device architecture is required, Kokkos will try to autodetect it at configuration time if you don't specify anything
- Host architecture is optional, none by default, you may be able to use `-DKokkos_ARCH_NATIVE=ON`

```
-- The project name is: Kokkos
...
-- Architectures:
--  HOPPER90
```

Build

After configuring, build Kokkos using:

```
cmake --build builddir [-j<N>]
```

This compiles Kokkos. You can add `-j<N>` to use multiple cores for faster compilation (replace `<N>` with the number of cores).

Install

To install Kokkos (header files and libraries), use:

```
cmake --install builddir [--prefix <prefix>]
```

The `--prefix <prefix>` option specifies the installation directory. If omitted, Kokkos will be installed to a default location, often `/usr/local` (not recommended).

Kokkos via Spack: Command Line

- Spack provides a package manager that automatically downloads, configures, and installs package dependencies
- Kokkos itself can be easily installed with specific variants (+) and compilers (%)

```
spack install kokkos@develop +openmp %gcc@8.3.0
```

- Good practice is to define "best variant" in your packages.yaml directory, e.g. for Volta system

```
packages:
   kokkos:
    variants: +cuda +openmp \
              ^cuda@12.0 cuda_arch=70
    compiler: [gcc@8.3.0]
```

- Build rules in `package.py` automatically map Spack variants to correct CMake options
- Run `spack info kokkos` to see full list of variants

- Build rules created in a `package.py` file
- Step 1: Declare dependency on specific version of kokkos (4.x or develop)

```
class myLib(CMakePackage):
  depends_on('kokkos@4.2')
```

- Step 2: Add build rule pointing to Spack-installed Kokkos and same C++ compiler Kokkos uses

```
def cmake_args(self):
  options = []
  ...
  options.append('-DCMAKE_CXX_COMPILER={}'.format(
      self['kokkos'].kokkos_cxx)
  return options
```

- More details on https://kokkos.org >Documentation>Get Started>Package Managers>Spack

- Kokkos' primary build system is CMAKE.
- Kokkos options are transitively passed on, including many necessary compiler options.
- The Spack package manager does support Kokkos.
- If you write an application, and have few if any dependencies, building Kokkos as part of your code is an option.

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.

Building Kokkos

- Kokkos' build system is generated using CMake.
- Kokkos options are transitively passed on, including many necessary compiler options.
- The Spack package manager does support Kokkos.

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.

Slack channel: https://kokkosteam.slack.com/

Recordings/Slides:

https://kokkos.org/kokkos-core-wiki/videolectures.html