SAND2020-7263PE

The Kokkos Lectures

Module 1: Introduction, Building and Parallel Dispatch

July 16, 2020

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 5+, Clang 4+, NVCC 9+, ROCM 3.5, XL16

Online Resources:

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

Lecture Series Outline

- 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 7: Internode: MPI and PGAS
- 08/28 Module 8: Tools: Profiling, Tuning and Debugging
- 09/04 Module 9: Kernels: Sparse and Dense Linear Algebra
- 09/11 Reserve Day

What to Expect

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)
- Office hours on Tuesdays (potentially with AWS access).
- 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

The HPC Hardware Landscape

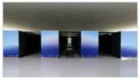
Current Generation: Programming Models OpenMP 3, CUDA and OpenACC depending on machine

LANL/SNL Trinity
Intel Haswell / Intel KNL
OpenMP 3

LLNL SIERRA
IBM Power9 / NVIDIA Volta
*CUDA / OpenMP**

ORNL Summit
IBM Power9 / NVIDIA Volta
*CUDA / OpenACC / OpenMP**

SNL Astra
ARM CPUs
OpenMP 3



Riken Fugaku
ARM CPUs with SVE
*OpenMP 3 / OpenACC***

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

NERSC Perlmutter
AMD CPU / NVIDIA GPU
*CUDA / OpenMP 5****

ORNL Frontier
AMD CPU / AMD GPU
*HIP / OpenMP 5*****

ANL Aurora
Xeon CPUs / Intel GPUs
*DPC++ / OpenMP 5******

LLNL El Capitan
AMD CPU / AMD GPU
*HIP / OpenMP 5*****

* Initially not working. Now more robust for Fortran than C++, but getting better.
** Research effort.
*** OpenMP 5 by NVIDIA.
**** OpenMP 5 by HPE.
***** OpenMP 5 by Intel.

Industry Estimate

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

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

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

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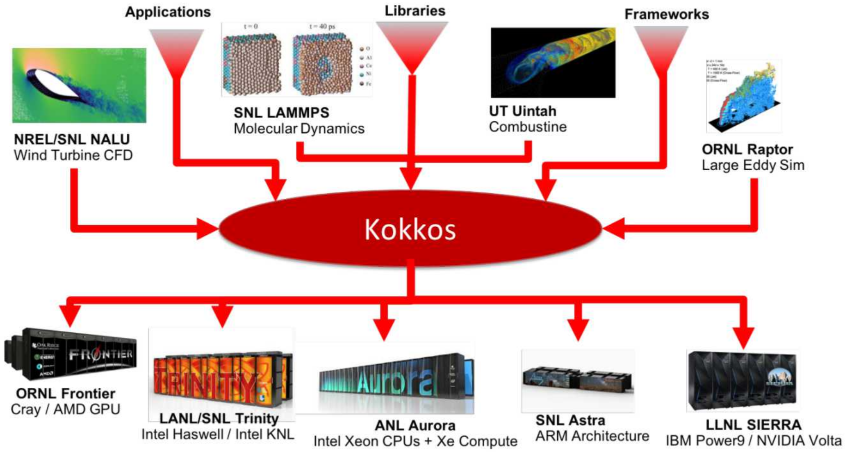
Software Cost Switching Vendors

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

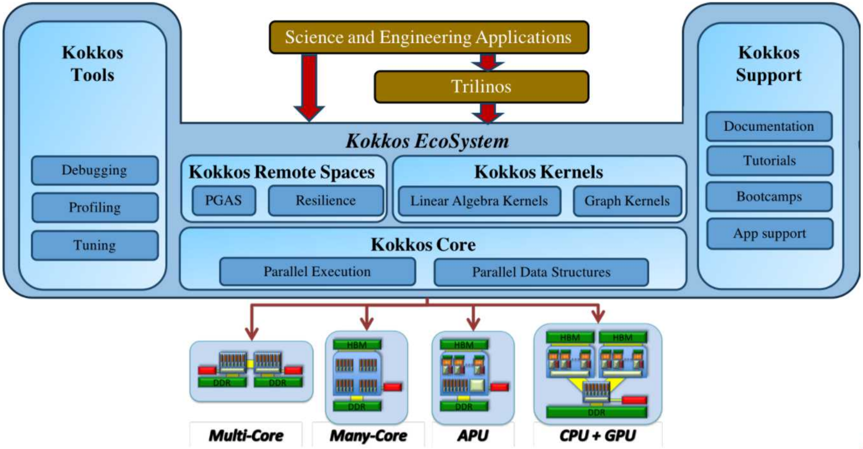
What is Kokkos?

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

Kokkos at the Center



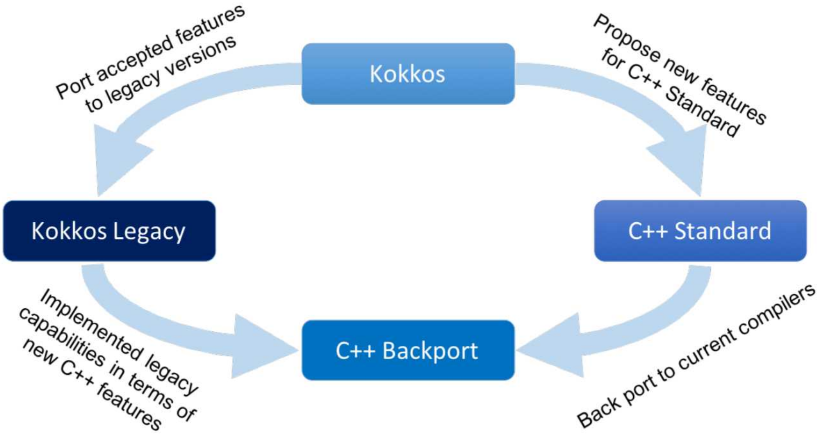
The Kokkos EcoSystem



The Kokkos Team

Kokkos Core:	**C.R.Trott**, J. Ciesko, V. Dang, N. Ellingwood, D.S. Hollman, D. Ibanez, J. Miles, J. Wilke, , H. Finkel, N. Liber, D. Lebrun-Grandie, D. Arndt, B. Turcksin, J. Madsen, R. Gayatri `former:` H.C. Edwards, D. Labreche, G. Mackey, S. Bova, D. Sunderland
Kokkos Kernels:	**S. Rajamanickam**, L. Berger, V. Dang, N. Ellingwood, E. Harvey, B. Kelley, K. Kim, C.R. Trott, J. Wilke, S. Acer
Kokkos Tools	**D. Poliakoff**, C. Lewis, S. Hammond, D. Ibanez, J. Madsen, S. Moore, C.R. Trott
Kokkos Support	**C.R. Trott**, G. Shipmann, G. Womeldorff, and all of the above `former:` H.C. Edwards, G. Lopez, F. Foertter

Kokkos helps improve ISO C++


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

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

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<int**[5], LayoutLeft> a("A",10,12); a(3,5,1) = 5;

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

Prerequisites for Tutorial Exercises

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

Using your own ${HOME}

- Git
- GCC 4.8.4 (or newer) *OR* Intel 15 (or newer) *OR* Clang 3.5.2 (or newer)
- CUDA nvcc 9.0 (or newer) *AND* NVIDIA compute capability 3.0 (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/Intro-Full/Slides`

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

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

Lecture Series Objectives

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

Tutorial Takeaways

- 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

Operating assumptions (0)

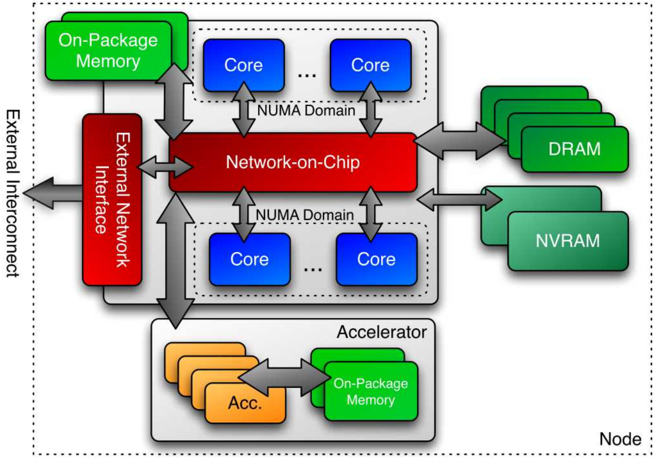
Assume you are here because:

- 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: Performance Portability

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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- obtains **performant memory access patterns** across architectures,
- 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.

Concepts: Patterns, Policies, and Bodies

```
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;
}
```

Concepts: Patterns, Policies, and Bodies

Pattern Policy

Body

```
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;
}
```

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

$\Rightarrow$ The **pattern** and **policy** drive the computational **body**.

Threading “Parallel for”

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

```
for (element = 0; element < numElements; ++element) {
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Threading "Parallel for"

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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```

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

"Parallel for" on a GPU via pragmas

Option 1: OpenMP 4.5

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

Portable, but not performance portable

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

But what about performance?

Portable, but not performance portable

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

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             qp * vectorSize + i] *
        right[element * numQPs * vectorSize +
              qp * vectorSize + i];
    }
  }
  elementValues[element] = total;
}
```

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 cores.
- The difference between `parallel_for` and `parallel_reduce`.
- Start parallelizing a simple example.

Using Kokkos for data parallel patterns (0)

Data parallel patterns and work

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

Kokkos maps **work** to execution resources

Using Kokkos for data parallel patterns (0)

Data parallel patterns and work

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

Kokkos maps **work** to execution resources

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

Using Kokkos for data parallel patterns (0)

Data parallel patterns and work

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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.

Using Kokkos for data parallel patterns (2)

How are computational bodies given to Kokkos?

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How are computational bodies given to Kokkos?

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

Using Kokkos for data parallel patterns (2)

How are computational bodies given to Kokkos?

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

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

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

Using Kokkos for data parallel patterns (3)

How is work assigned to functor operators?

Using Kokkos for data parallel patterns (3)

How is work assigned to functor operators?

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

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

Using Kokkos for data parallel patterns (3)

How is work assigned to functor operators?

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

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

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

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

Using Kokkos for data parallel patterns (3)

How is work assigned to functor operators?

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

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

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.

Using Kokkos for data parallel patterns (4)

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

Using Kokkos for data parallel patterns (4)

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 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**.

Using Kokkos for data parallel patterns (5)

Putting it all together: the complete functor:

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

Using Kokkos for data parallel patterns (5)

Putting it all together: the complete functor:

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

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

Serial

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

Using Kokkos for data parallel patterns (5)

Putting it all together: the complete functor:

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

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);
}
```

Using Kokkos for data parallel patterns (6)

The complete picture (using functors):

1. Defining the functor (operator+data):

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

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

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

2. **Executing** in parallel with Kokkos pattern:

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

Using Kokkos for data parallel patterns (7)

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

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

Using Kokkos for data parallel patterns (7)

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atomForces already exists
data already exists
Kokkos::parallel_for(numberOfAtoms,
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  }
);
```

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

Using Kokkos for data parallel patterns (7)

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```
atomForces already exists
data already exists
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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

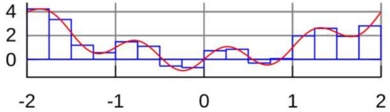
```
parallel_for(N, [=] (const int64_t i) {
  /* loop body */
});
```

Important concept

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

Riemann-sum-style numerical integration:

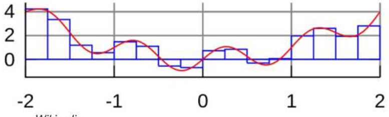
$$y = \int_{lower}^{upper} function(x)\, dx$$



Wikipedia

Riemann-sum-style numerical integration:

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

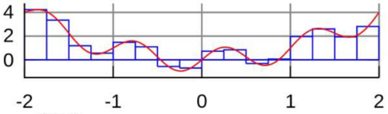


Wikipedia

```
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:

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



Wikipedia

```
double totalIntegral = 0;
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```

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

Riemann-sum-style numerical integration:

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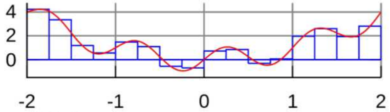

Wikipedia

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

Scalar integration (3)

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

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Important concept: Reduction

Reductions combine the results contributed by parallel work.

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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 += ...
}
```

Scalar integration (3)

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

Important concept: Reduction

Reductions combine the results contributed by parallel work.

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.

Amdahl's Law (1)

Warning: Parallelism is NOT free

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

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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

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- $\alpha =$ dispatch overhead
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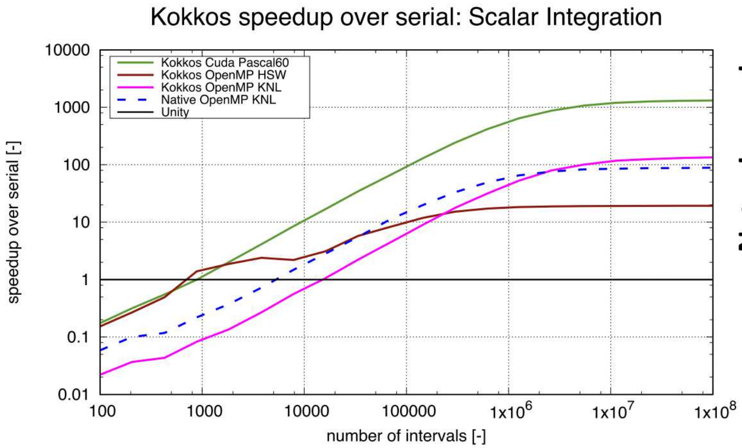
- $P =$ available concurrency

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

Amdahl's Law (2)

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



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!

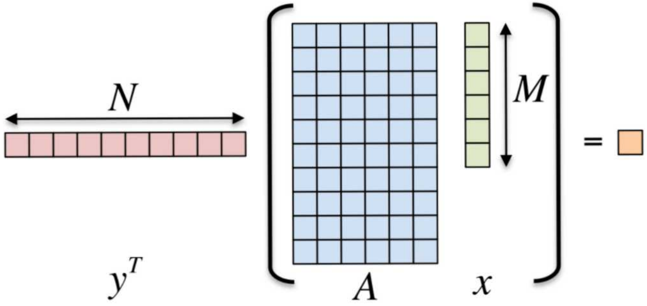
- Non-nested parallel patterns can take an optional string argument.
- The label doesn't need to be unique, but it is helpful.
- Anything convertible to "std::string"
- Used by profiling and debugging tools (see Profiling Tutorial)

Example:

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

Recurring Exercise: Inner Product

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



Details:

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

Exercise #1: include, initialize, finalize Kokkos

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

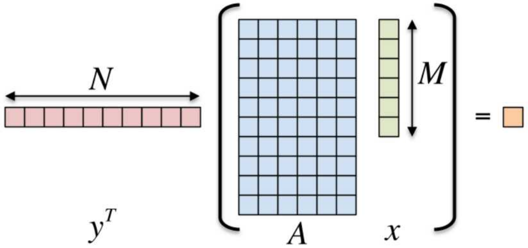
```
#include <Kokkos_Core.hpp>
int main(int argc, char** argv) {
  /* ... do any necessary setup (e.g., initialize MPI) ... */
  Kokkos::initialize(argc, argv);
  {
  /* ... do computations ... */
  }
  Kokkos::finalize();
  return 0;
}
```

(Optional) Command-line arguments or environment variables:

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

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

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



Details:

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

Compiling for CPU

```
# gcc using OpenMP (default) and Serial back-ends,
# (optional) change non-default arch with KOKKOS_ARCH
  make -j KOKKOS_DEVICES=OpenMP,Serial KOKKOS_ARCH=...
```

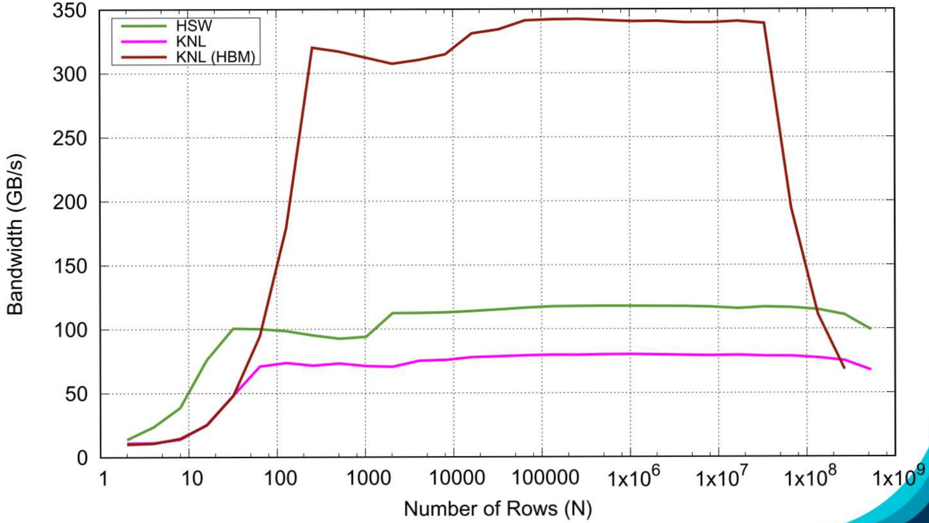
Running on CPU with OpenMP back-end

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

Things to try:

- Vary problem size with cline arg -S *s*
- Vary number of rows with cline arg -N *n*
- Num rows = 2^n, num cols = 2^m, total size = $2^s == 2^{n+m}$

<y,Ax> Exercise 01, Fixed Size



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::dealloc` 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

```
# provide KOKKOS_ARCH below
# common values include Kepler35, Pascal60, Volta70, etc.
  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

Section Summary

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

Building Applications with Kokkos

Learning objectives:

- Install Kokkos via CMake
- Build Kokkos inline via CMake
- Using Spack
- Build Kokkos inline via GNU Makefiles

Options for Building Kokkos

- **Install Kokkos via CMake:** For large projects with multiple dependencies installing Kokkos via CMake and then building against it is the best option.
- **Build Kokkos inline via CMake:** This is an option suited for projects which have few dependencies and want to build Kokkos inline.
- **Using Spack:** For projects which largely rely on components provided by Spack.
- **Build Kokkos inline via GNU Makefiles:** The option for projects which don't want to use CMake. Only inline builds are supported via Makefiles though. Often this works well for small codes.

Kokkos CMake Basics

- In the spirit of C++ for *code* performance portability, modern CMake aims for *build system* performance 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!
- Single build system call in your project should configure all compiler/linker flags:

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

- Kokkos configure options are enabled/disabled via CMake as:

```
cmake -DKokkos_XYZ=ON
```

CMake Backend Options

- Numerous backends can be activated
  - Only one GPU, one parallel CPU, and Serial at the same time!
- `-DKokkos_ENABLE_CUDA=ON`
- `-DKokkos_ENABLE_HIP=ON`
- `-DKokkos_ENABLE_OPENMP=ON`
- `-DKokkos_ENABLE_OPENMPTARGET=ON`

CMake Backend Options

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- `-DKokkos_ENABLE_CUDA=ON`
- `-DKokkos_ENABLE_HIP=ON`
- `-DKokkos_ENABLE_OPENMP=ON`
- `-DKokkos_ENABLE_OPENMPTARGET=ON`
- Verify execution spaces in CMake Output, e.g. CUDA

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

CMake Architecture Options

- Device backends *require* architecture be specified (CUDA , OpenMPTarget, and HIP)
  - `-DKokkos_ARCH_VOLTA70=ON`
  - `-DKokkos_ARCH_VEGA906=ON`: MI50/MI60
- Host backends *recommend* architecture be specified to enable architecture-specific optimizations
  - `-DKokkos_ARCH_HSW=ON`: Haswell
  - `-DKokkos_ARCH_ZEN2=ON`: Ryzen (2nd gen)
- Architecture flags will automatically propagate to your project via transitive CMake properties

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  - `-DKokkos_ARCH_VOLTA70=ON`
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  - `-DKokkos_ARCH_ZEN2=ON`: Ryzen (2nd gen)
- Architecture flags will automatically propagate to your project via transitive CMake properties
- Verify architectures in CMake Output, e.g. Volta 7.0

```
-- The project name is: Kokkos
...
-- Architectures:
--  VOLTA70
```

- Kokkos is a *C++* performance portability layer, but CUDA is usually built as a separate language with `nvcc`.
- `nvcc` doesn't accept all C++ compiler flags
- Kokkos' solution for now is to provide `nvcc_wrapper` that converts `nvcc` into a full C++ compiler.[1]

[1] This may change significantly with nvc++ and/or build system changes

CMake And CUDA

- Kokkos is a *C++* performance portability layer, but CUDA is usually built as a separate language with `nvcc`.
- `nvcc` doesn't accept all C++ compiler flags
- Kokkos' solution for now is to provide `nvcc_wrapper` that converts `nvcc` into a full C++ compiler.[1]
- Set CMake C++ compiler to `nvcc_wrapper`

```
> cmake ${KOKKOS_SRC}
  -DCMAKE_CXX_COMPILER=${KOKKOS_SRC}/bin/nvcc_wrapper
  -DKokkos_ENABLE_CUDA=ON
```

[1] This may change significantly with nvc++ and/or build system changes

- Kokkos is a *C++* performance portability layer, but CUDA is usually built as a separate language with `nvcc`.
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- Set CMake C++ compiler to `nvcc_wrapper`
- CMake will report compiler as host C++ compiler

```
> cmake ${KOKKOS_SRC}
  -DCMAKE_CXX_COMPILER=${KOKKOS_SRC}/bin/nvcc_wrapper
  -DKokkos_ENABLE_CUDA=ON
-- The CXX compiler identification is GNU 7.2.0
-- Check for working CXX compiler: bin/nvcc_wrapper
```

[1] This may change significantly with nvc++ and/or build system changes

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  -DKokkos_ENABLE_CUDA=ON
-- The CXX compiler identification is GNU 7.2.0
-- Check for working CXX compiler: bin/nvcc_wrapper
```

- Or simply use clang++ as your compiler...

[1] This may change significantly with nvc++ and/or build system changes

Enable experimental HIP backend Configure with:

```
-D Kokkos_ENABLE_HIP=ON
```

Compiler Starting from ROCm v3.5 release, HCC is deprecated and replaced with HIP-Clang. Transition is transparent when using `hipcc`:

```
-D CMAKE_CXX_COMPILER=hipcc
```

Architecture flags Chose one from:

```
-D Kokkos_ARCH_VEGA900=ON # for AMD Radeon Instinct MI25
-D Kokkos_ARCH_VEGA906=ON # for AMD Radeon Instinct MI50 or MI60
```

CMake And OpenMPTarget

- Similar configuration as CUDA/HIP backends, but use:
  `cmake -DKokkos_ENABLE_OPENMPTARGET=ON`
- Still requires target device architecture to be given:
  `cmake -DKokkos_ARCH_VOLTA70=ON`
- Currently very sensitive to exact compiler/STL combination
  - Clang9+
  - GCC6 Toolchain
  - See `scripts/docker/Dockerfile.openmptarget` for recipe
- C++17 is required
- Working on Spack packages to handle complex version dependencies

Building Against an Installed Kokkos (i)

Find exported Kokkos configuration (include dirs, libraries to link against, compile options, etc.) and generate my project's build system accordingly.

Basic starting point Create a `CMakeLists.txt` file.

```
cmake_minimum_required(VERSION 3.12)
project(myProject CXX) # C++ needed to build my project

find_package(Kokkos REQUIRED) # fail if Kokkos not found

# build my executable from the specified source code
add_executable(myExe source.cpp)
# declare dependency on Kokkos
target_link_libraries(myExe PRIVATE Kokkos::kokkos)
```

Working with a library

```
find_package(Kokkos 3.1 REQUIRED) # request Kokkos minimum versio
add_library(myLib ${SOURCES})
target_link_libraries(myLib PUBLIC Kokkos::kokkos)
```

Building Against an Installed Kokkos (ii)

Finding Kokkos Add Kokkos installation prefix to the list of directories searched by CMake:

```
cmake .. -DCMAKE_PREFIX_PATH=<prefix> -DCMAKE_CXX_COMPILER=<...>
```

or via `-DKokkos_ROOT=<prefix>` if you explicitly set policy `CMP0074` to `NEW` in your project.

Kokkos package introspection Assert that support for `__host__`, `__device__` annotations in lambdas declaration is enabled

```
# (optional) assume my project uses lambdas
if(Kokkos_ENABLE_CUDA)
  # fatal error if not enabled
  kokkos_check(OPTIONS CUDA_ENABLE_LAMBDA)
endif()
```

or query that generation of relocatable device code is enabled

```
kokkos_check(DEVICES CUDA OPTIONS CUDA_RELOCATABLE_DEVICE_CODE
  RESULT_VARIABLE KOKKOS_HAS_CUDA_RDC)
if(KOKKOS_HAS_CUDA_RDC)
  ...
```

CMake Building Kokkos Inline

Build Kokkos as part of your own project (as opposed to finding a pre-installed Kokkos) [2]

```
add_subdirectory(<kokkos source dir>)

# identical as when finding an installed Kokkos package
add_library(myLib ${SOURCES})
target_link_libraries(myLib PUBLIC Kokkos::kokkos)
```

Pass Kokkos options along with app-specific options at configuration time

```
cmake .. -DCMAKE_CXX_COMPILER=<kokkos dir>/bin/nvcc_wrapper \
  -DKokkos_ENABLE_CUDA=ON -DKokkos_ENABLE_CUDA_LAMBDA=ON \
  -DmyApp_ENABLE_FOO=ON -DmyApp_ENABLE_BAR=ON
```

[2] Special steps required for projects using FetchContent/ExternalProject and nvcc_wrapper

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_lambda +wrapper \
              ^cuda@10.1 cuda_arch=70
    compiler: [gcc@7.2.0]
```

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

Kokkos via Spack: Package Files

- Build rules created in a `package.py` file
- Step 1: Declare dependency on specific version of kokkos (3.x, master, or develop)

```
class myLib(CMakePackage):
  depends_on('kokkos@3.2')
```

- 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.spec['kokkos'].kokkos_cxx)
  options.ppend('-DKokkos_ROOT={}'.format(
     self.spec['kokkos'].prefix)
  return options
```

- Full details can be found in Spack.md in Kokkos repo.

Building Kokkos Inline via GNU Makefiles

Building Kokkos inline with GNU Makefiles in three steps:

- Set Kokkos Options e.g. `KOKKOS_DEVICES`, `KOKKOS_ARCH`
- Include `Makefile.kokkos`
- Add `KOKKOS_CXXFLAGS`, `KOKKOS_LDFLAGS` etc. to build rules

Most Important Settings:

- `KOKKOS_DEVICES`: What backends to enabled. Comma separated list: `Serial,OpenMP,Cuda,HIP,OpenMPTarget`
- `KOKKOS_ARCH`: Set architectures. Comma separated list: `HSW,Volta70,Power9,...`

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Most Important Settings:

- `KOKKOS_DEVICES`: What backends to enabled. Comma separated list: `Serial,OpenMP,Cuda,HIP,OpenMPTarget`
- `KOKKOS_ARCH`: Set architectures. Comma separated list: `HSW,Volta70,Power9,...`

Order Matters!

Add default target, Kokkos settings, and CXXFLAGS before including Makefile.kokkos!

Example Makefile

```
KOKKOS_PATH = ${HOME}/Kokkos/kokkos
SRC = $(wildcard *.cpp)
KOKKOS_DEVICES=OpenMP,Cuda
KOKKOS_ARCH = SKX,Volta70

default: test
  echo "Start Build"

CXX = clang++
CXXFLAGS = -O3 -g
LINK = ${CXX}

OBJ = $(SRC:.cpp=.o)

include $(KOKKOS_PATH)/Makefile.kokkos

test: $(OBJ) $(KOKKOS_LINK_DEPENDS)
  $(LINK) $(KOKKOS_LDFLAGS) $(OBJ) $(KOKKOS_LIBS) -o test

%.o:%.cpp $(KOKKOS_CPP_DEPENDS)
  $(CXX) $(KOKKOS_CPPFLAGS) $(KOKKOS_CXXFLAGS) $(CXXFLAGS)
      -c $<
```