The Kokkos Lectures

Kokkos Execution Space Instances

May 5, 2022

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This is NOT a general tutorial!

Today: three topics with exercises.

- Three Short Lectures
  - Execution Space Instances
  - PyKokkos
  - New KokkosKernels Capabilities
- Hands-On Exercise
  - Split Into Breakout Rooms
  - One per topic: Choose which one you want to attend

Tuesday 2022-05-10: Community BOF Days with presentations on more new capabilities.

https://www.exascaleproject.org/event/ecp-community-bof-days-2022

Online Resources:

- https://github.com/kokkos:
  - Primary Kokkos GitHub Organization
- https://github.com/kokkos/kokkos-tutorials/wiki/Kokkos-Lecture-Series:
  - Slides, recording and Q&A for the Lectures
- 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.

Instructions for joining the exercises can be found here:
`https://github.com/kokkos/kokkos-tutorials/issues/60`

Issue: ECP Annualmeeting 2022 - Kokkos Tutorial AWS Instances

Claim an instance in the Google spreadsheet.

SSH to the instance.

The slides are available at:
`https://github.com/kokkos/kokkos-tutorials`
under `Other/ECP-Annualmeeting/2022`

Asynchronicity and ExecutionSpace Instances

The (non-)blocking behavior of Kokkos operations.

Learning objectives:

- What are blocking and non-blocking operations in Kokkos.
- What kind of work can overlap.
- How to wait for completion.
- How to run kernels simultaneously on a GPU.

Most operations in Kokkos are non-blocking

- The caller returns before the operation is finished
- The caller can do other things, while operations are executing

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So what is the ordering behavior?

- Execution Spaces have an ordered execution queue
- The queue is first-in/first-out (FIFO)

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So what is the ordering behavior?

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Important Point

Execution Spaces execute operations in dispatch order.

Execution Space Instances

- Each unique **Instance** of an execution space has its own queue
- Execution Policies can take an instance as the first argument
- deep_copy can take an instance as a first argument
- For every **Execution Space Type** there is a **default instance**
  - It is a singleton
  - The **default instance** is returned by the default constructor
  - Used if no specific instance is provided

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  - Used if no specific instance is provided

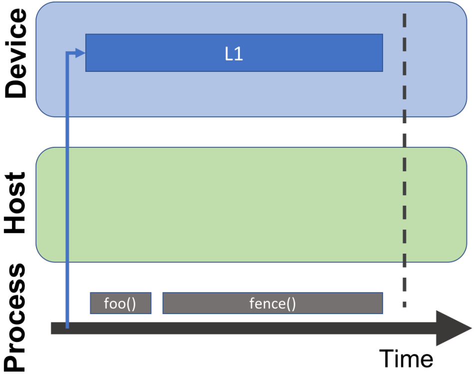
```
// This is equivalent:
RangePolicy<ExecSpace>
  policy_1(0, N);
RangePolicy<ExecSpace>
  policy_2(ExecSpace(), 0, N);
```

We use the following conventions in subsequent slides

```
// Execution Space types
using device = Kokkos::DefaultExecutionSpace;
using host = Kokkos::DefaultHostExecutionSpace;

// Execution Space instances
device dev1(..), dev2(..)
device host1(..), host2(..);

// Execution Policies
RangePolicy<device> policy_d(0,N), policy_device(0,N);
RangePolicy<host> policy_h(0,K), policy_host(0,K);
RangePolicy<device> policy_d1(dev1, 0,N), policy_d2(dev2, 0,N);
RangePolicy<host> policy_h1(host1, 0,N), policy_h2(host2, 0,N);

// Functors/Lambda for parallel_for
auto L1 = KOKKOS_LAMBDA(int i) {...};
auto L2 = ...; auto L3 = ...; auto L4 = ...; auto L5 = ...;
// Functors/Lambda for parallel_reduce
auto R1 = KOKKOS_LAMBDA(int i, double& lsum) {...};
```

Most Kokkos Operations are Asynchronous

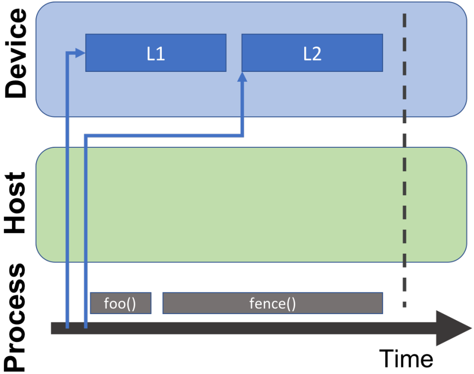
- Best to assume all of them are asynchronous
- They overlap with work in the process thread
- Use `Kokkos::fence()` to wait for completion




```
RangePolicy<>
  policy_device(0,N)
FunctorL1 L1(...);

parallel_for("L1",
  policy_device, L1);
foo();
fence();
```

Execution Spaces execute in dispatch order

- Dispatches to the same space instance will never overlap
- Executed in order FIFO
- Use `Kokkos::fence()` to wait for completion




```
RangePolicy<>
  policy_device(0,N)
FunctorL1 L1(...);
FunctorL2 L2(...);

parallel_for("L1",
  policy_device, L1);
parallel_for("L2",
  policy_device, L2);
foo();
fence();
```

Execution Spaces execute in dispatch order

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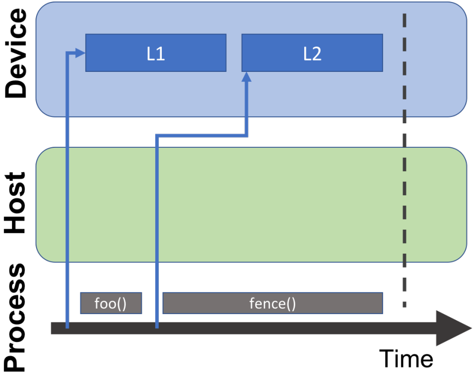
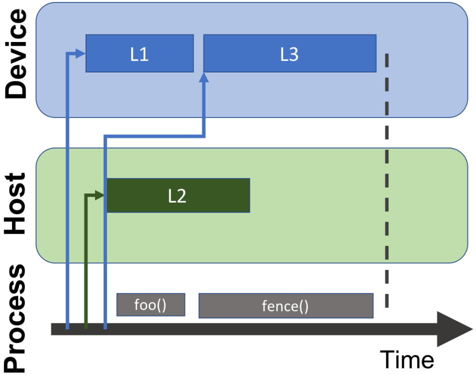



```
RangePolicy<>
  policy_device(0,N)
FunctorL1 L1(...);
FunctorL2 L2(...);

parallel_for("L1",
  policy_device, L1);
foo();
parallel_for("L2",
  policy_device, L2);
fence();
```

ExecutionSpaces are Independent

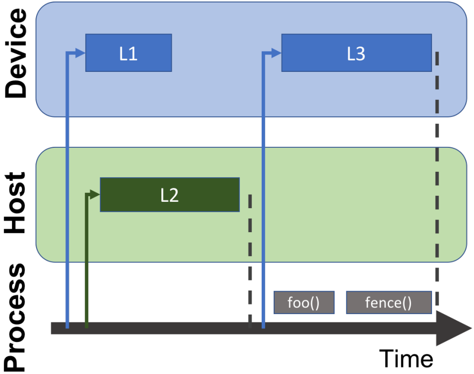
- Dispatches into different ExecutionSpaces may overlap.
- Overlap with process thread functions and each other
- Use `Kokkos::fence()` to wait for completion of all




```
RangePolicy<>
  policy_d(0,N)
RangePolicy<Host>
  policy_host(0,N)
FunctorL1 L1(...);
FunctorL2 L2(...);
FunctorL3 L3(...);
parallel_for("L1",
  policy_d, L1);
parallel_for("L2",
  policy_host, L2);
parallel_for("L3",
  policy_d, L3);
foo();
fence();
```

Reality: Some Host Backends Block

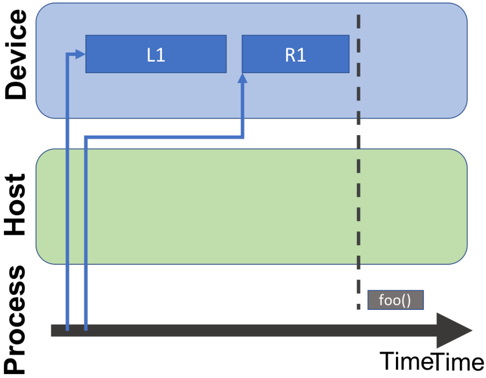
- Most host backends are blocking dispatches (except HPX)
- They never overlap with process thread functions
- But: **Do NOT rely on blocking behavior!!**




```
RangePolicy<>
  policy_d(0,N)
RangePolicy<Host>
  policy_host(0,N)
FunctorL1 L1(...);
FunctorL2 L2(...);
FunctorL3 L3(...);
parallel_for("L1",
  policy_d, L1);
parallel_for("L2",
  policy_host, L2);
parallel_for("L3",
  policy_d, L3);
foo();
fence();
```

Reductions to Scalars are Blocking

- The call only returns after result is available.
- FIFO implies, every other kernel in the same ExecutionSpace instance will be done too

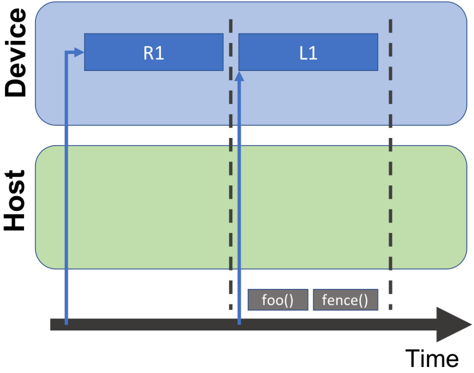



```
RangePolicy<>
  policy_d(0,N)
FunctorL1 L1(...);
FunctorR1 R1(...);

double result;
parallel_for("L1",
  policy_d, L1);
parallel_reduce("R1",
  policy_d, R1, result);
foo();
```

Reductions to Scalars are Blocking

- The call only returns after result is available.
- For subsequent dispatches previous rules apply

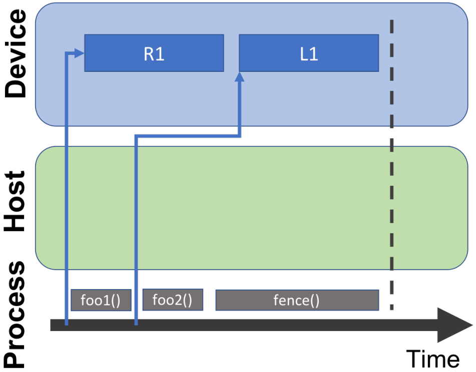



```
RangePolicy<>
  policy_d(0,N)
FunctorL1 L1(...);
FunctorR1 R1(...);

double result;
parallel_reduce("R1",
  policy_d, R1, result);
parallel_for("L1",
  policy_d, L1);
foo();
fence();
```

Reductions to Views are Non-blocking

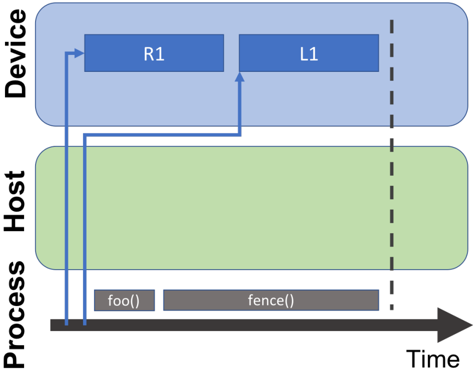
- Behave like a `parallel_for`
- Results are only available after a `Kokkos::fence()`
- Even true for unmanaged `Views` of host variables!




```
...
double result;
View<double, HostSpace>
  v_result(&result);
parallel_reduce("R1",
  policy_d,R1,v_result);
foo1();
parallel_for("L1",
  policy_d, L1);
foo2();
fence();
```

Simple Parallel Loop

- Asynchronous
- Overlaps with host functions
- Use `Kokkos::fence()` to wait for completion

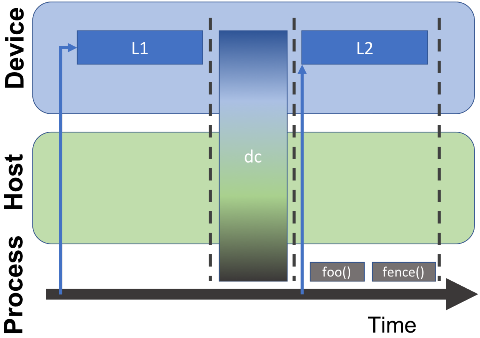



```
RangePolicy<>
  policy_device(0,N)
FunctorL1 L1(...);
FunctorL2 L2(...);

parallel_for("L1",
  policy_device, L1);
parallel_for("L2",
  policy_device, L2);
foo();
fence();
```

2-Argument deep_copy is fully blocking

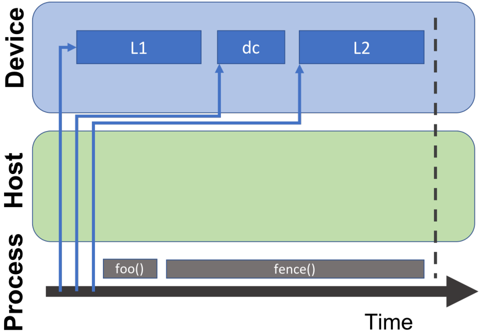
- Implies a full `fence` before the copy
- Copy is done by the time call returns.
- Even if it is a no-op due to `src == dst`!




```
parallel_for("L1",
  policy_device, L1);
deep_copy(dest,src);
parallel_for("L2",
  policy_device, L2);
foo();
fence();
```

deep_copy with space argument are non-blocking

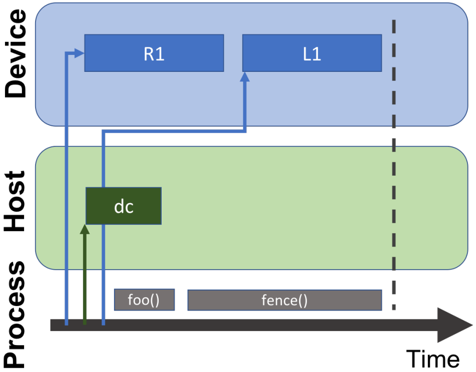
- Execute in dispatch order in the queue of the space
- Overlap with host process functions
- Use `Kokkos::fence()` to wait for completion




```
parallel_for("L1",
  policy_device, L1);
deep_copy(device,
  dest,src);
parallel_for("L2",
  policy_device, L2);
foo();
fence();
```

deep_copy with space argument are non-blocking

- Execute in dispatch order in the queue of the space
- Overlap with other execution spaces
- Use `Kokkos::fence()` to wait for completion




```
parallel_for("L1",
  policy_device, L1);
deep_copy(host(),
  dest,src);
parallel_for("L2",
  policy_device, L2);
foo();
fence();
```

So what about CUDA/HIP streams and SYCL queues?
Up to now we only used default execution space instances, but what if you want to have concurrent kernels on the GPU?

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Execution Space Instances

Execution Space instances behave largely like CUDA/HIP streams

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Execution Space Instances

Execution Space instances behave largely like CUDA/HIP streams

You can create different instances:

```
ExecSpace space;
std::vector<ExecSpace> instances =
  Kokkos::Experimental::partition_space(space, w1, ..., wN);
```

- Creates a vector of N new instances of ExecSpace

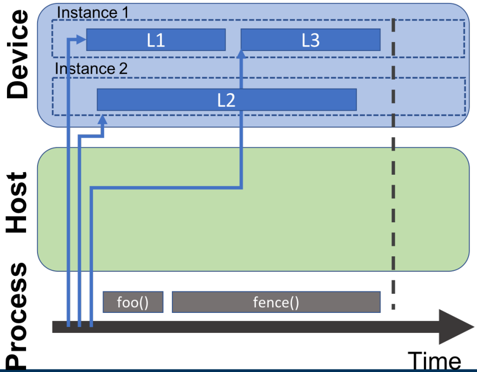
So what about CUDA/HIP streams and SYCL queues?

```
ExecSpace space;
std::vector<ExecSpace> instances =
  Kokkos::Experimental::partition_space(space, w1, ..., wN);
```

- The new instances will submit to a subset of the resources associated with `space`.
- The weights are hints as to the fraction of resources these instances are allowed to dispatch too.
  - Use integers or floating point numbers
  - Number of instances created is equal to number of weights
  - Note weights are hints, and might be ignored.
- Returns a `std::vector` of execution space instances
- The function may return just N copies of `space`
- all the created instances are independent of each other and from the original instance

Instances of Execution Spaces own an exec queue

- Work dispatched to different instances overlaps with each other
- Overlaps with host process functions
- Use `Kokkos::fence()` to wait for completion of all

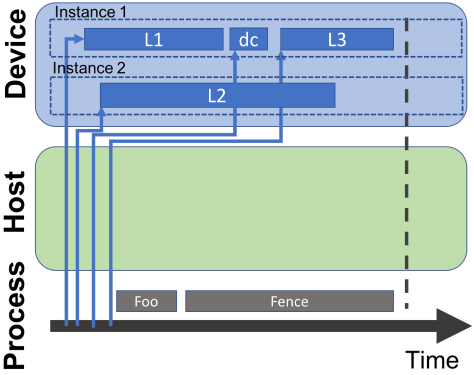



```
auto instances = partiti
Device dev1 = instances[
Device dev2 = instances[
RangePolicy<Device>
  policy_d1(dev1,0,N);
RangePolicy<Device>
  policy_d2(dev2,0,N);

parallel_for("L1",
  policy_d1, L1);
parallel_for("L2",
  policy_d2, L2);
parallel_for("L3",
  policy_d1, L3);
foo();
fence();
```

deep_copy with an instance argument also overlap

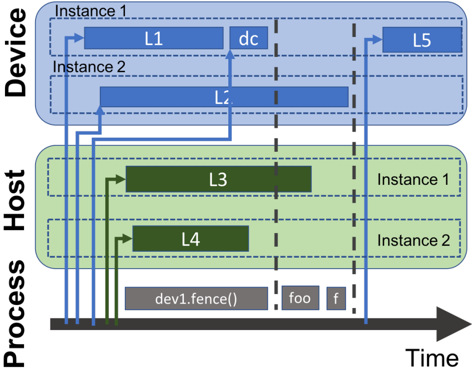
- deep_copy with an instance argument are like any other parallel operation
- Overlaps with parallel operations in other instance




```
parallel_for("L1",
  policy_d1, L1);
parallel_for("L2",
  policy_d2, L2);
deep_copy(dev1,
  dest, src);
parallel_for("L3",
  policy_d1, L3);
foo();
fence();
```

There are instance fences

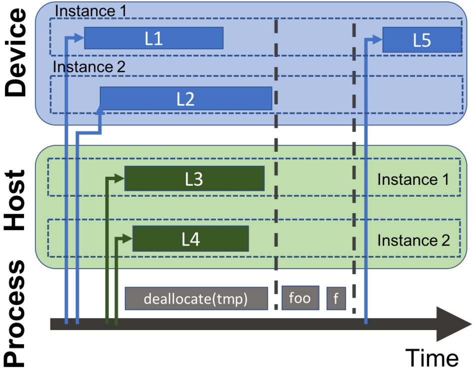
- Use instance specific fence to only wait on that instance
- Operations in other instances can overlap with that fence
- Use `Kokkos::fence()` to wait for all outstanding ops




```
parallel_for("L1",
  policy_d1, L1);
parallel_for("L2",
  policy_d2, L2);
deep_copy(dev1,
  dest, src);
parallel_for("L3",
  policy_h1, L3);
parallel_for("L4",
  policy_h2, L4);
dev1.fence();
foo();
fence();
parallel_for("L5",
  policy_d1, L5);
```

Reality Check: Kokkos Views deallocation implies fence!

- Due to limitations of reference counting, deallocations fence!
- **Important:** this is implementation limitation not semantic!
- **Do NOT rely on deallocations fencing!**




```
{
View<..> tmp(...);
parallel_for("L1",
  policy_d1, L1);
parallel_for("L2",
  policy_d2, L2);
parallel_for("L3",
  policy_h1, L3);
parallel_for("L4",
  policy_h2, L4);
}
foo();
fence();
parallel_for("L5",
  policy_d1, L5);
```

- Execution Space Instances execute work in order of dispatch.
- Operations dispatched to different Execution Space Instances can overlap.
- Each Execution Space type has a default instance as a singleton.
- Use `Kokkos::fence()` to wait for completion of ALL outstanding work.
- Use `exec_space_instance.fence()` to wait for completion of outstanding work dispatched to a specific execution space instance.

Exercise: Explore impact of using instances for concurrent execution.

Getting set up in your home directory:

```
mkdir Kokkos
cd Kokkos
git clone https://github.com/kokkos/kokkos
git clone https://github.com/kokkos/kokkos-tutorials
```

Find the exercise in the kokkos-tutorials/Exercises/instances folder.

The Begin subdirectory contains the code. Only instances_begin.cpp needs modifications.

Simply type `make -j 8` to build the exercise.

Look for EXERCISE comments to find places to modify.

Tasks:

- Create ExecutionSpace instances
- Use the instances to dispatch the kernels and `deep_copy`
- Remember to use device and host accessible views as results for reductions!

Things to try:

- Compare using the same instance for both data sets, and different ones.
- Compare performance for small (e.g. -N 5000) and large (e.g. -N 30000) problems.
- What happens if you create the result Views inside the repeat loop?