Implementing a SYCL Backend for Kokkos

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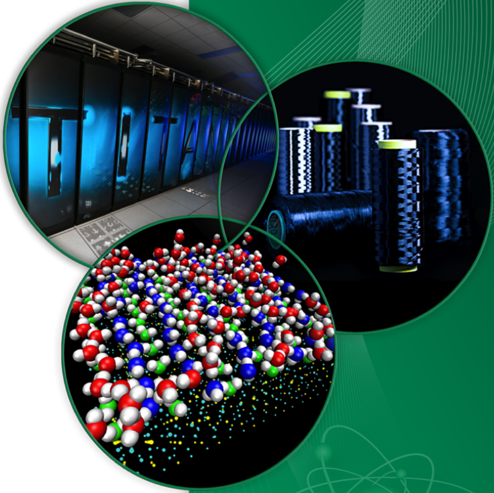

What is Kokkos?

- A C++ Programming Model for Performance Portability
  - Template library on top CUDA, HIP, OpenMP, SYCL, ...
  - Aligns with developments in the C++ standard, e.g., `mdspan`, `atomic_ref`
- Expanding solution for common needs of modern science and engineering codes
  - Math libraries based on Kokkos
  - Tools for debugging, profiling and tuning
  - Interoperability with Fortran and Python
- Open Source project with a growing community
  - Maintained and developed at `https://github.com/kokkos`
  - Hundreds of users at many large institutions

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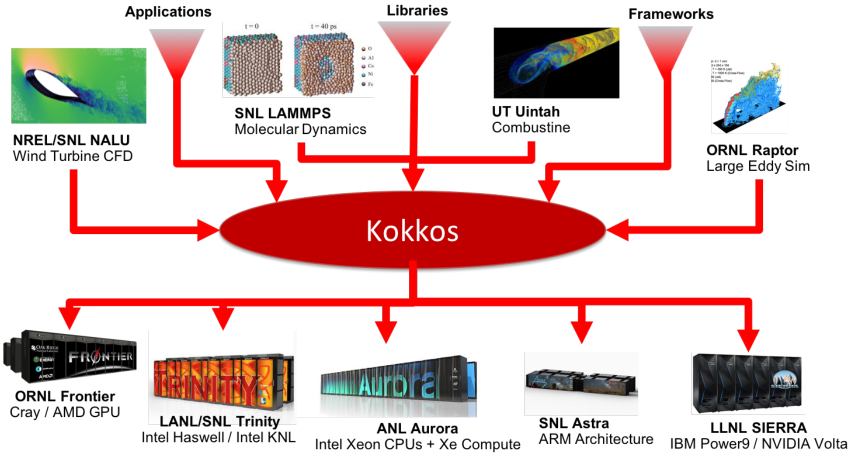
Kokkos as Portability Layer



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kokkos

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Kokkos Tools	C.R. Trott, V. Kale, D. Lebrun-Grandie, D. Ibanez, S. Moore, A. Powell

Kokkos - Applications

More than 50% of C++ Codes in the Exascale Computing Project use Kokkos.

Example of Applications:

- Trilinos (Linear Algebra)
- PETSc (Linear Algebra)
- deal.II (Finite Element Library)
- LAMMPS (Molecular Dynamics)
- XGC (Fusion Reactor Simulation)
- ArborX (Geometry Search)
- Uintah (Chemical Reactions)
- VTK-m (Visualization)
- ...

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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 KokkosKernels math library

Feature Status Kokkos+SYCL

Near feature-complete since release 3.4.00 (April 2021).

Unsupported

- ~~atomic operations for big types~~ (since Kokkos 4.0.00)
- `WorkGraphPolicy`
- `Tasks`
- `Graphs`
- Virtual functions/function pointer

Kokkos Core Functionalities, Mapping to SYCL

Constructs

- parallel_for ⟶ sycl::parallel_for
- parallel_reduce ⟶ sycl::parallel_for
- parallel_scan ⟶ sycl::parallel_for

Policies

- RangePolicy ⟶ sycl::range
- MDRangePolicy ⟶ sycl::nd_range
- TeamPolicy ⟶ sycl::nd_range

Memory

- View ⟶ sycl::malloc/sycl::free

Translate Kokkos to SYCL

```
#include <Kokkos_Core.hpp>
int main() {
  Kokkos::ScopeGuard scope_guard;
  auto do_work = KOKKOS_LAMBDA(int) {};
  Kokkos::parallel_for(100, do_work);
}
```

is loosely translated to

```
#include <sycl/sycl.hpp>
int main()
{
  sycl::queue q;
  auto do_work = [](int) {};
  q.parallel_for(sycl::range<1>(100),
    [=](sycl::item<1> item){
      do_work(item.get_id());
  });
}
```

Kokkos Hello World

```
#include <Kokkos_Core.hpp>
int main() {
  Kokkos::ScopeGuard scope_guard;
  Kokkos::parallel_for(1, KOKKOS_LAMBDA(int){
    printf("Hello World!\n");
  });
}
```

Problem:

- `printf` doesn't work in SYCL kernels.
- Can't pass `sycl::stream` anywhere.

Kokkos Hello World - SYCL

```cpp
#include <Kokkos_Core.hpp>
int main() {
  Kokkos::ScopeGuard scope_guard;
  Kokkos::parallel_for(1, KOKKOS_LAMBDA(int){
    KOKKOS_IMPL_DO_NOT_USE_PRINTF("Hello␣World!\n");
    // sycl::ext::oneapi::experimental::printf(
    //   "Hello World!\n");
  });
}
```

Kokkos iota

```
#include <Kokkos_Core.hpp>
int main() {
  Kokkos::ScopeGuard scope_guard;
  const int N = 100;
  Kokkos::View<int*> view("view", N);
  Kokkos::parallel_for(N, KOKKOS_LAMBDA(int i){
    view(i) = i;
  });
}
```

Problem:

- `Kokkos::View` is not trivially copyable.
- `sycl::is_device_copyable`?

sycl::is_device_copyable

> *It is unspecified whether the implementation actually calls the copy constructor, move constructor, copy assignment operator, or move assignment operator of a class declared as `is_device_copyable_v` when doing an inter-device copy.*
> *[...]*
> *Likewise, it is unspecified whether the implementation actually calls the destructor for such a class on the device since the destructor must have no effect on the device.*

Issue:

- Implementations actually call special member functions[1]
- We need another workaround!

[1] `https://github.com/intel/llvm/issues/5320`

sycl::is_device_copyable - Workaround I

```
union TrivialWrapper {
  TrivialWrapper(){};
  TrivialWrapper(const Functor& f) {
    std::memcpy(&m_f, &f, sizeof(m_f)); }
  TrivialWrapper(const TrivialWrapper& other) {
    std::memcpy(&m_f, &other.m_f, sizeof(m_f));
  }
  TrivialWrapper(TrivialWrapper&& other) {
    std::memcpy(&m_f, &other.m_f, sizeof(m_f));
  }
  TrivialWrapper& operator=(const TrivialWrapper& other) {
    std::memcpy(&m_f, &other.m_f, sizeof(m_f));
    return *this;
  }
  TrivialWrapper& operator=(TrivialWrapper&& other) {
    std::memcpy(&m_f, &other.m_f, sizeof(m_f));
    return *this;
  }
  ~TrivialWrapper(){};
  Functor m_f;
};
```

sycl::is_device_copyable - Workaround II

```
template <typename Functor>
class SYCLFunctionWrapper {
  union TrivialWrapper m_functor;

 public:
  SYCLFunctionWrapper(const Functor& functor, Storage&)
    : m_functor(functor) {}
  const Functor& get_functor() const {
    return m_functor.m_f;
  }
};

template <typename Functor>
struct sycl::is_device_copyable<
    SYCLFunctionWrapper<Functor, Storage, false>>
    : std::true_type {};
```

Minor annoyances compared with CUDA/HIP

- `sycl::group_barrier(sycl::sub_group)` doesn't allow masking for active threads, yet.[2]
- Address space annotations (`sycl::multi_ptr`) important, also for `sycl::atomic_ref`.
- Backend-specific information limited on Intel GPUs; difficult to choose good group sizes, e.g., according to occupancy, register usage.
- Status of SYCL standard implementation unclear, CUDA and HIP just tell what they have.
- Important features are only `oneAPI` extensions.
- Compile time for `Kokkos` unit tests (Release)
  - SYCL+Cuda: 100 min
  - CUDA/HIP: 45 min

[2] `https://github.com/intel/llvm/pull/6169`

Used Extensions

- `sycl::ext::oneapi::experimental::this_nd_item`
- `sycl::ext::oneapi::experimental::printf`
- `sycl::ext::oneapi::experimental::device_global`
- `sycl::ext::oneapi::experimental::properties`
- `sycl::ext::oneapi::experimental::device_image_scope`
- `sycl::ext::oneapi::experimental::this_sub_group`
- `sycl::ext::oneapi::group_ballot`
- `sycl::ext::oneapi::sub_group_mask`

Summary

A lot of complaints but `SYCL/DPC++`

- integration was otherwise pretty smooth
- works well on Intel GPUs (Aurora)
- works much better than `OpenMPTarget`
- has better support for newer C++ features than `nvcc`
- is a real portability solution with an interface close to `Kokkos`

Questions?

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