Experiences with Implementing Kokkos’ SYCL Backend

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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
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)
- ...
Feature Status Kokkos+SYCL targeting Aurora/Intel GPUs

Feature complete apart from
- 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`
parallel_for RangePolicy

Kokkos::parallel_for(
    Kokkos::RangePolicy(execution_space, start, end)),
    KOKKOS_LAMBDA(int i) { /*...*/});

is mapped to SYCL code as

Functor functor;
q.parallel_for(sycl::range<1>(end - begin),
    [=](sycl::id<1> idx) {
        int i = idx + begin;
        functor(i);
    });
#include <Kokkos_Core.hpp>

```cpp
int main() {
    Kokkos::ScopeGuard scope_guard;
    Kokkos::View<int*> view("view", 100);
    Kokkos::parallel_for(100, KOKKOS_LAMBDA(int i){view(i) = i;});
}
```

⇒ Using `sycl::buffer` for `Kokkos::View` not feasible.

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

sycl::is_device_copyable - Workaround I
```cpp
sycl::is_device_copyable - Workaround II

```cpp
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;
    }
};

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

MDRangePolicy maps up to 6 dimensions with tiling to three dimensions in `sycl::nd_range`

```cpp
struct Functor{
    KOKKOS_FUNCTION void operator(
        int i, int j, int k, int l, int m) const { /*...*/
    };
Kokkos::parallel_for(
    Kokkos::MDRangePolicy(execution_space,
        {s0,s1,s2,s3,s4}, {e0,e1,e2,e3,e4}),
    Functor{});
```
TeamPolicy

```
parallel_for("Label", TeamPolicy<>(numberOfTeams, teamSize, vectorLength),
    KOKKOS_LAMBDA (const member_type & teamMember) {
        /* beginning of outer body */
        parallel_for(TeamThreadRange(teamMember, thisTeamsRangeSize),
            [=] (const int indexWithinBatch [, ...]) {
            /* begin middle body */
            parallel_for(ThreadVectorRange(teamMember, thisVectorRangeSize),
                [=] (const int indexVectorRange) /* inner body */);
            /* end middle body */
        });
        parallel_for(TeamVectorRange(teamMember, someSize),
            [=] (const int indexTeamVector) /* nested body */;
        /* end of outer body */
    });
```
TeamPolicy

Only policy to allow scratch allocations.

Mappings:

• team $\rightarrow$ sycl::group
• multiple threads $\rightarrow$ sycl::subgroup

Problem:

• thread synchronization requires a barrier on part of a subgroup $\rightarrow$ tangle_group or similar
• communicating address space information for scratch allocations
parallel_reduce

double result;
Kokkos::parallel_reduce(
    Kokkos::RangePolicy(execution_space, start, end)),
KOKKOS_LAMBDA(int i, double& partial_sum) {
    partial_sum += i;
}, result);

doesn’t use SYCL’s reduction variables. Features:
• simple reductions (sum)
• multiple reductions per parallel construct
• custom reductions with arbitrary value types and reduction operations
• runtime sized array reductions
• pre- and post-callbacks for reductions (init, final)
parallel_reduce

per_thread:
  value& tmp=init(local_tmp);
  for (i in local range)
    functor(i, tmp)
call join for merging values between threads
  in the same workgroup
let one (the last) workgroup merge all results
  from all workgroups
call final(result) on one thread

Shuffle-based implementation gives worse results than using local memory on Intel GPUs.
parallel_scan

Kokkos::parallel_scan(
    Kokkos::RangePolicy(execution_space, start, end),
    KOKKOS_LAMBDA (const int index, value_type& update,
        const bool is_final) {
        const value_type local_value = in_data(i);
        // exclusive scan
        if (is_final)
            out_data_exclusive(i) = update;
        update += local_value;
        // inclusive scan
        if (is_final)
            out_data_inclusive(i) = update;
    });
**parallel_scan**

**first kernel:**

**per_thread:**
- `value & tmp = init(local_tmp);`
- `for (i in local range)`
  - `functor(i, tmp, /*is_final*/ false)`
- call join for implementing a prefix sum
  - in the same workgroup
- let the last workgroup compute the prefix sum for the totals of all workgroups and store the result
- store intermediate results on each thread

**second kernel:**
- combine workgroup totals with thread intermediate results
- call the functor again for final result (with `final=true`)

As opposed to `parallel_reduce`, a shuffle-based implementation is used.
Performance comparisons

AXPBY - parallel_for
DOT - parallel_reduce
SPMV - TeamPolicy
Conjugate Gradient

One node of Sunspot with Intel® Data Center GPU Max 1550 GPUs
peak memory bandwidth 3276.8 GB/s (2 tiles)
AXPBY benchmark

// Kokkos
for (int r = 0; r < R; r++) {
    Kokkos::parallel_for("axpby", N, KOKKOS_LAMBDA(int i) {
        z(i) = alpha*x(i) + beta*y(i);
    });
}

// SYCL
sycl::queue q{sycl::property::queue::in_order()} ;
for (int r = 0; r < R; r++) {
    q.parallel_for(sycl::range<1>(N), [=](sycl::id<1> idx){
        int i = idx;
        z[i] = alpha*x[i] + beta*y[i];
    });
}
Achieved effective bandwidth for the AXPBY benchmark

<table>
<thead>
<tr>
<th>#elements</th>
<th>Kokkos 1-tile</th>
<th>SYCL 1-tile</th>
<th>Kokkos 2-tile</th>
<th>SYCL 2-tile</th>
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DOT benchmark

// Kokkos
for (int r = 0; r < R; r++) {
    Kokkos::parallel_reduce("dot", N,
        KOKKOS_LAMBDA(int i, double& sum) {sum += x(i) * y(i);},
        result);
}

// SYCL
sycl::queue q{sycl::property::queue::in_order()};
for (int r = 0; r < R; r++) {
    q.parallel_for(sycl::range<1>(N_),
        sycl::reduction(result_ptr, 0., sycl::plus<
            double>()) ,
        [=](sycl::id<1> idx, auto&sum) {sum += x[idx] * y[idx];});
    q.memcpy(&result, result_ptr, sizeof(double));
    q.wait();
}
Achieved effective bandwidth for the DOT benchmark

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<th>Bandwidth GB/s</th>
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- Kokkos 1-tile
- SYCL 1-tile
- Kokkos 2-tile
- SYCL 2-tile
Run time ratio for DOT between Kokkos and SYCL

#elements

- 1-tile
- 2-tile
SPMV benchmark - Kokkos I

```cpp
int rows_per_team = 32; // optimized for GPU
int team_size = 16; // optimized for GPU
int vector_size = 4; // optimized for GPU
int n_teams = (nrows + rows_per_team - 1)/rows_per_team;
using TeamMember = Kokkos::TeamPolicy<>::member_type;
// parallelize over the row blocks
Kokkos::parallel_for("SPMV",
    Kokkos::TeamPolicy<>(n_teams, team_size, vector_size),
    KOKKOS_LAMBDA(const TeamMember &team) {
        int64_t first_row=team.league_rank()*rows_per_team;
        int64_t last_row=first_row + rows_per_team < nrows
            ? first_row + rows_per_team : nrows;
```
SPMV benchmark - Kokkos II

// parallelize over rows owned by the team
Kokkos::parallel_for(
    Kokkos::TeamThreadRange(team, first_row, last_row),
    [&](const int64_t row) {
        const int64_t row_start = A.row_ptr(row);
        const int64_t row_length = A.row_ptr(row + 1) - row_start;
        // perform the dot-product of a matrix row with vector
        Kokkos::parallel_reduce(
            Kokkos::ThreadVectorRange(team, row_length),
            [=](const int64_t i, double &sum) {
                sum += A.values(i + row_start) * x(A.col_idx(i + row_start));
                }, y(row));
    });
int rows_per_team = 32; //optimized for GPU
int team_size = 16; //optimized for GPU
int n_teams = (nrows + rows_per_team - 1)/rows_per_team;
q.submit([&] (sycl::handler& cgh) {
    // parallelize over the row blocks
    cgh.parallel_for_work_group(sycl::range<1>(n),
                                sycl::range<1>(team_size), [=](sycl::group<1> g) {
        int64_t first_row= g.get_group_id(0)*rows_per_team;
        int64_t last_row=first_row + rows_per_team < nrows
                          ? first_row + rows_per_team : nrows;
    });
});
// parallelize over rows owned by the team

g.parallel_for_work_item(
    sycl::range<1>(last_row-first_row),
    [&](sycl::h_item<1> item) {
        int64_t row = item.get_local_id(0)+first_row;
        int64_t row_start = row_ptr[row];
        int64_t row_length = row_ptr[row+1]-row_start;
        double y_row = 0.;
        for (int64_t i = 0; i < row_length; ++i)
            y_row += values[i + row_start] * xp[col_idx[i + row_start]];
        yp[row] = y_row;
    });
Achieved effective bandwidth for the SPMV benchmark on the GPU

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Bandwidth GB/s vs. #rows graph.
CG benchmark I

```cpp
for (int64_t k = 1; k <= max_iter && normr > tolerance; ++k) {
    if (k == 1) {
        axpby(p, one, r, zero, r);
    } else {
        oldrtrans = rtrans;
        rtrans = dot(r, r);
        double beta = rtrans / oldrtrans;
        axpby(p, one, r, beta, p);
    }
    normr = std::sqrt(rtrans);
    double alpha = 0;
    double p_ap_dot = 0;
    spmv(Ap, A, p);
}  
```
CG benchmark II

```c
p_ap_dot = dot(Ap, p);
if (p_ap_dot < brkdown_tol) {
    if (p_ap_dot < 0) {
        std::cerr << "numerical breakdown!\n";
        return num_iters;
    } else {
        brkdown_tol = 0.1 * p_ap_dot;
    }
}
alpha = rtrans / p_ap_dot;
axpby(x, one, x, alpha, p);
axpby(r, one, r, −alpha, Ap);
num_iters = k;
```
Achieved effective bandwidth for the CG benchmark on the GPU

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Summary

Despite some hiccups, SYCL/DPC++
  • integration was pretty smooth
  • works well on Intel GPUs (Aurora)
  • works much better than OpenMPTarget
  • has better support for newer C++ features than nvcc

We still rely on many extensions, though.
Questions?
Acknowledgments

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• This work was done on a pre-production supercomputer with early versions of the Aurora software development kit.
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`
- `sycl::ext::oneapi::experimental::bfloat16`
- `sycl::ext::oneapi::group_local_memory_for_overwrite`