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deal.II and GPUs

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U.S. DEPARTMENT OF ENERGY

deal.II and GPUs

Places in `deal.II` that (can) use GPUs

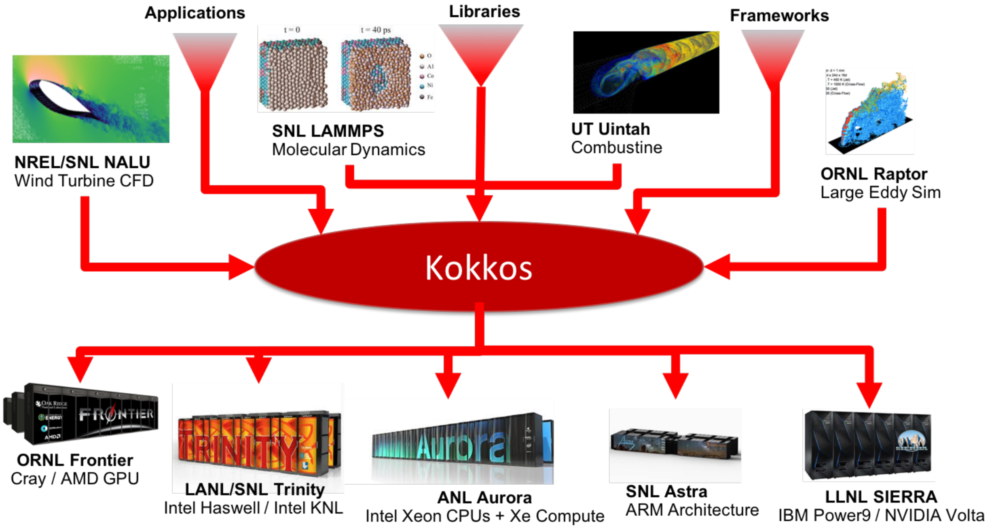
- `PETSc` (TBD)
- `Trilinos`
- `Portable::MatrixFree`
- `LinearAlgebra::distributed::Vector`
- `CUDAWrappers` (to be removed in the next release)

Most of these (except the latter two) use `Kokkos` under the hood!

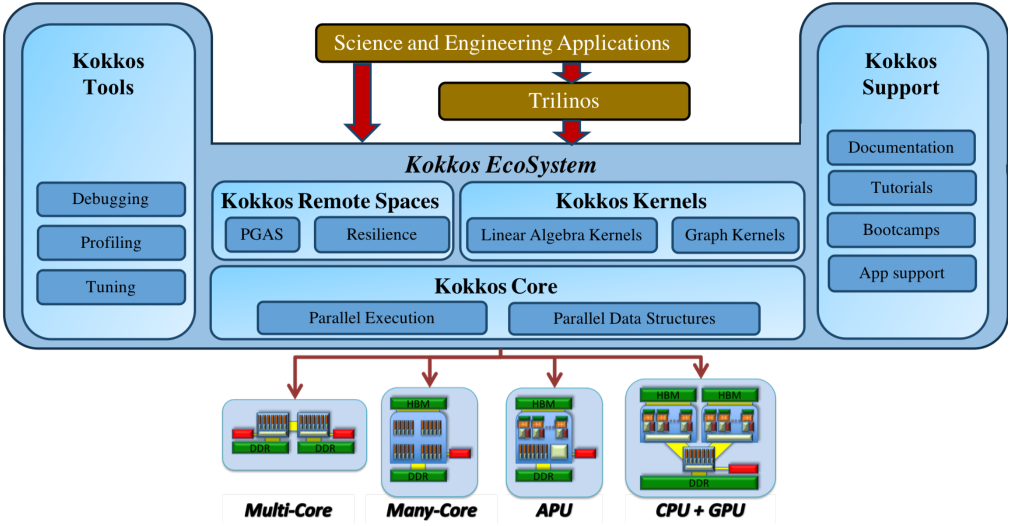
What is Kokkos?

- 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 communixty
  - Maintained and developed at `https://github.com/kokkos`
  - Hundreds of users at many large institutions

Kokkos as Portability Layer



Kokkos EcoSystem



kokkos

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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

Kokkos Resources

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://kokkos.github.io/kokkos-core-wiki`:
  - Kokkos Core Wiki with API documentation
- `https://kokkosteam.slack.com`:
  - Slack channel for Kokkos.
  - Please join: fastest way to get your questions answered.
  - Can whitelist domains, or invite individual people.

Kokkos iota

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

`Kokkos::View`

- managed, multi-dimensional, reference-counted data container, or
- unmanaged, multi-dimensional accessor for external data
- motivated C++23 `std::mdspan`

parallel_reduce

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

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_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;
 });
```

MDRangePolicy

`MDRangePolicy` allows using up to a 6-dimensional index space with tiling

```
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 */
  });
```

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Trilinos - Tpetra

Added support for Tpetra in this release (Jan-Philip Thiele and Sebastian Kinnewig)

- `Trilinos::TpetraWrappers::Vector<Number, MemorySpace>`
- `Trilinos::TpetraWrappers::SparseMatrix<Number, MemorySpace>`
- `Trilinos::TpetraWrappers::Solver*<Number, MemorySpace>`

Uses `DualView`: Memory is duplicated for `MemorySpace::Default`. All operations happen under the hood.

Standalone linear algebra

`LinearAlgebra::distributed::Vector`

- `LinearAlgebra::distributed::Vector<Number, MemorySpace>`

Memory allocation only for the requested memory space, `MemorySpace::Host` (default) and `MemorySpace::Default`. Requires moving memory to and from the device explicitly.

Assembly in deal.II

Assembly approaches in `deal.II`

- Manually write the assembly of the matrix
- `MatrixCreator`
- `MeshWorker/MeshLoop`
- `MatrixFree`
- `MatrixFreeOperators` Idea:
  - Only overload write (cell) operator (`apply_add`),
  - `MatrixFreeOperators` takes care of the rest

  Similar to `MeshWorker`.

All of them only use CPUs

SPMV matrix-based vs. matrix-free

matrix-based

$$A = \sum_k P_k^T A_k P_k$$

$$v = Au$$

Separate steps for

- Assembly
- matrix-vector product

bandwidth limited: <1 Flop/Byte

matrix-free

$$v = A(u) = \sum_k^{ncells} P_k^T A_k P_k u$$

- Extract local elements: $u_k = P_k u$
- Compute the matrix-vector product on the fly: $v_k = A_k u_k$
- Add to global vector: $v += P_k^T v_k$

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Matrix-vector product on cell, Laplacian

$$(A_K u_K)_j = \int_K \nabla_x \phi \cdot \nabla_x u^h \, dx \approx \sum_q w_q \det J_q \nabla \phi_j \cdot \nabla u^h \Big|_{x=x_q}$$

$$= \sum_q \nabla_\eta \phi_j J_q^{-1} (w_q \det J_q) J_q^{-T} \sum_i \nabla_\eta \phi_i u_{K,i} \Big|_{x=x_q}$$

- Compute unit cell gradients $\sum_i \nabla_\eta \phi_i u_{K,i}$ at all quadrature points
- At each quadrature point, apply geometry J_q^{-T}, multiply by quadrature weight and Jacobian determinant $w_q \det J_q$, and apply geometry for test function J_q^{-1}
- Test by unit cell gradients of all basis functions and sum over quadrature points

Sum factorization

$$\sum_i \phi_i(x_q) u_{K,i} = \sum_{i_z} \phi_{i_z}(x_{q_z}) \sum_{i_y} \phi_{i_y}(x_{q_y}) \sum_{i_x} \phi_{i_x}(x_{q_x}) u_{K,i}$$

Take advantage of the tensor product structure of shape functions and quadrature points since $\xi_q = \xi_{q_x}, \xi_{q_y}, \xi_{q_z}$ and $\phi_{x,y,z} = \phi_x \phi_y \phi_z$

$$S = \nabla_\eta \phi_i \big|_{\xi_q} = \begin{bmatrix} D_z \otimes D_y \otimes S_x \\ D_z \otimes S_y \otimes D_x \\ S_z \otimes D_y \otimes D_x \end{bmatrix}$$

with

$$D_x = \phi_x(\xi_{q_x})$$
$$S_x = \nabla_\eta \phi_x(\xi_{q_x})$$

Evaluation costs reduce from $\mathcal{O}((p+1)^{2d})$ to $\mathcal{O}(d(p+1)^{d+1})$.

History of Portable MatrixFree in deal.II

- introduced to deal.II with `https://github.com/dealii/dealii/pull/4293` (deal.II 9.0.0)
- decided to switch to Kokkos in `https://github.com/dealii/dealii/pull/15200` last year
- renamed in `https://github.com/dealii/dealii/pull/16497` this year

Portable MatrixFree limitations

- Only `FE_Q` elements, continuous Galerkin
- no face terms
- only one component
- limited optimizations, even-odd, cartesian meshes
- degree coupled with # quadrature points

Portable MatrixFree implementation

Kokkos implementation

- Uses TeamPolicy for looping over the cells (coloring possible), every team gets a cell batch
- scratch memory for working values and gradients buffers
- TeamThreadRange for tensor contractions on every cell, parallelize over quadrature points
- TeamThreadMDRange for newer Kokkos

deal.II tutorial: step-64

In this example, we consider the Helmholtz problem

$$-\nabla \cdot \nabla u + a(\mathbf{x})u = 1,$$
$$u = 0 \quad \text{on } \partial\Omega$$

where $a(\mathbf{x})$ is a variable coefficient.

We choose as domain $\Omega = [0,1]^3$ and $a(\mathbf{x}) = \frac{10}{0.05+2\|\mathbf{x}\|^2}$. Since the coefficient is symmetric around the origin but the domain is not, we will end up with a non-symmetric solution.

step-64

```
template <int dim, int fe_degree>
  void HelmholtzOperator<dim, fe_degree>::vmult(
    LinearAlgebra::distributed::Vector<double, MemorySpace::Default>       &dst,
    const LinearAlgebra::distributed::Vector<double, MemorySpace::Default> &src)
    const
  {
    dst = 0.;
    LocalHelmholtzOperator<dim, fe_degree> helmholtz_operator(
      coef.get_values());
    mf_data.cell_loop(helmholtz_operator, src, dst);
    mf_data.copy_constrained_values(src, dst);
  }
```

step-64

```
template <int dim, int fe_degree>
DEAL_II_HOST_DEVICE void LocalHelmholtzOperator<dim, fe_degree>::operator()(
  const unsigned int                                         cell,
  const typename Portable::MatrixFree<dim, double>::Data   *gpu_data,
  Portable::SharedData<dim, double>                        *shared_data,
  const double                                             *src,
  double                                                   *dst) const
{
  Portable::FEEvaluation<dim, fe_degree, fe_degree + 1, 1, double> fe_eval(
    gpu_data, shared_data);
  fe_eval.read_dof_values(src);
  fe_eval.evaluate(EvaluationFlags::values | EvaluationFlags::gradients);
  fe_eval.apply_for_each_quad_point(
    HelmholtzOperatorQuad<dim, fe_degree>(gpu_data, coef, cell));
  fe_eval.integrate(EvaluationFlags::values | EvaluationFlags::gradients);
  fe_eval.distribute_local_to_global(dst);
}
```

step-64

```
template <int dim, int fe_degree, int n_q_points_1d, int n_components_, typename Number
DEAL_II_HOST_DEVICE void
FEEvaluation<dim, fe_degree, n_q_points_1d, n_components_, Number>::
  read_dof_values(const Number *src)
{
  Kokkos::parallel_for(
    Kokkos::TeamThreadRange(shared_data->team_member, n_q_points),
      [&](const int &i) {
        shared_data->values(i) = src[data->local_to_global(cell_id, i)];
      });
  shared_data->team_member.team_barrier();

  internal::resolve_hanging_nodes<dim, fe_degree, false>(
    shared_data->team_member,
    data->constraint_weights,
    data->constraint_mask(cell_id),
    shared_data->values);
}
```

Generic - evaluate values and gradients in 3D

```
template <int direction, bool dof_to_quad, bool add, bool in_place,
          typename ViewTypeIn, typename ViewTypeOut>
DEAL_II_HOST_DEVICE void values(const ViewTypeIn in, ViewTypeOut out) const; //apply

values<0, true, false, true>(u, u);
team_member.team_barrier();
values<1, true, false, true>(u, u);
team_member.team_barrier();
values<2, true, false, true>(u, u);
team_member.team_barrier();

gradients<0, true, false, false>(u, Kokkos::subview(grad_u, Kokkos::ALL, 0));
gradients<1, true, false, false>(u, Kokkos::subview(grad_u, Kokkos::ALL, 1));
gradients<2, true, false, false>(u, Kokkos::subview(grad_u, Kokkos::ALL, 2));
```

Generic

```
typename ViewTypeOut>
DEAL_II_HOST_DEVICE void apply_3d(
  const Kokkos::TeamPolicy<...>::member_type &team_member,
  const Kokkos::View<Number *, ...> shape_data, const ViewTypeIn in, ViewTypeOut out)
    { [...]
      Number t[n_q_points] = {};
      auto thread_policy = Kokkos::TeamThreadMDRange<Kokkos::Rank<3>, TeamType>(
        team_member, n_q_points_1d, n_q_points_1d, n_q_points_1d);
      Kokkos::parallel_for(
        thread_policy, [&](const int i, const int j, const int q) {
          const int q_point = ...;
          for (int k = 0; k < n_q_points_1d; ++k) {
              const unsigned int shape_idx  = ...;
              const unsigned int source_idx = ...;
              t[q_point] += shape_data[shape_idx] * in(source_idx);
            }
        }); [...]
    }
```

step-64

```
template <int dim, int fe_degree>
DEAL_II_HOST_DEVICE void HelmholtzOperatorQuad<dim, fe_degree>::operator()(
  Portable::FEEvaluation<dim, fe_degree, fe_degree + 1, 1, double> *fe_eval,
  const int q_point) const
{
  const unsigned int pos =
    gpu_data->local_q_point_id(cell, n_q_points, q_point);

  fe_eval->submit_value(coef[pos] * fe_eval->get_value(q_point), q_point);
  fe_eval->submit_gradient(fe_eval->get_gradient(q_point), q_point);
}
```

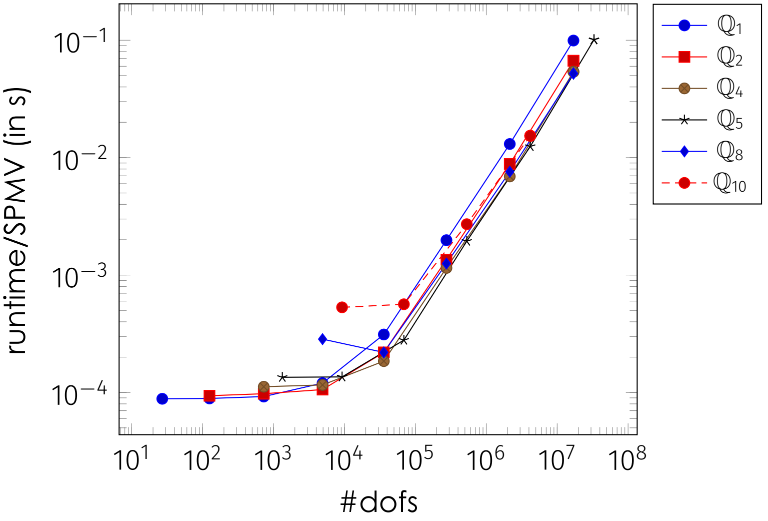
Generic integrate values and gradients in 3D

```
template <int direction, bool dof_to_quad, bool add, bool in_place,
          typename ViewTypeIn, typename ViewTypeOut>
DEAL_II_HOST_DEVICE void values(const ViewTypeIn in, ViewTypeOut out) const; // apply

gradients<2, false, true, false>(Kokkos::subview(grad_u, Kokkos::ALL, 2), u);
team_member.team_barrier();
gradients<1, false, true, false>(Kokkos::subview(grad_u, Kokkos::ALL, 1), u);
team_member.team_barrier();
gradients<0, false, true, false>(Kokkos::subview(grad_u, Kokkos::ALL, 0), u);
team_member.team_barrier();

values<2, false, false, true>(u, u);
team_member.team_barrier();
values<1, false, false, true>(u, u);
team_member.team_barrier();
values<0, false, false, true>(u, u);
team_member.team_barrier();
```

step-64

```
template <int dim, int fe_degree, int n_q_points_1d, int n_components_, typename Number>
 DEAL_II_HOST_DEVICE void
 FEEvaluation<dim, fe_degree, n_q_points_1d, n_components_, Number>::
   distribute_local_to_global(Number *dst) const
 {
   internal::resolve_hanging_nodes<dim, fe_degree, true>(
     shared_data->team_member, data->constraint_weights,
     data->constraint_mask(cell_id), shared_data->values);

   if (data->use_coloring) {
       Kokkos::parallel_for(
         Kokkos::TeamThreadRange(shared_data->team_member, n_q_points),
           [&](const int &i) {
             dst[data->local_to_global(cell_id, i)] += shared_data->values(i);
           });
     }
   else { [...] }
 }
```

Performance results on Polaris - NVIDIA A100



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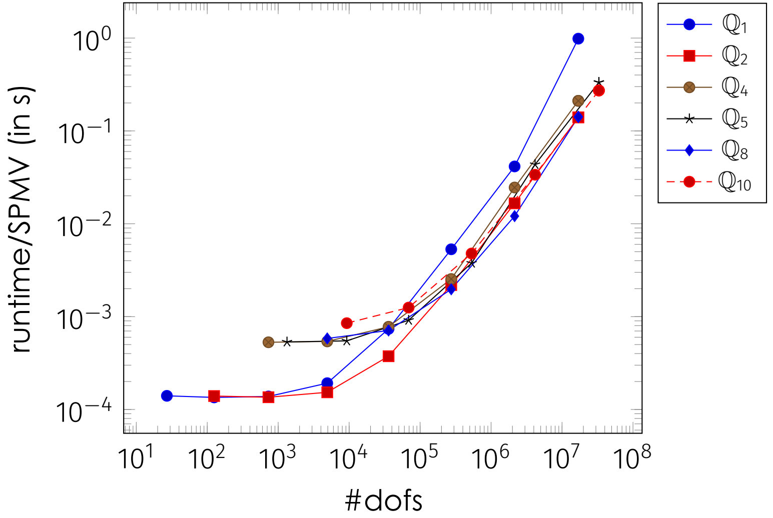
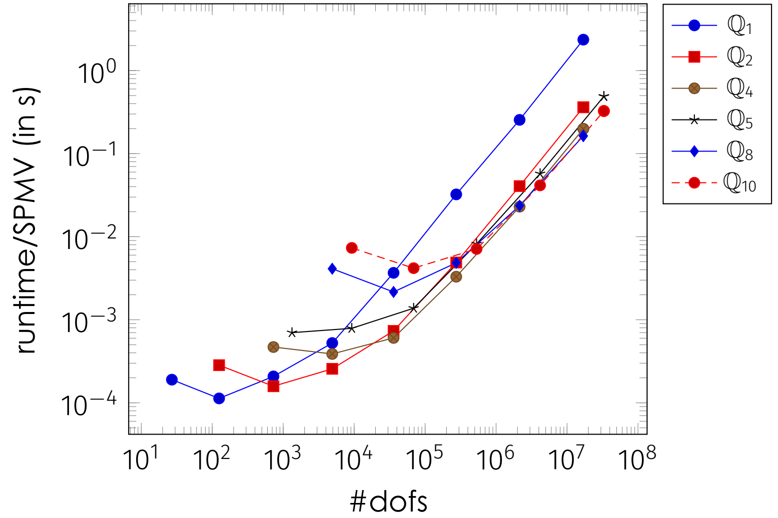
Performance results on Frontier - AMD MI 250X, 1 GCD



Performance results on Sunspot - Intel GPU Max 1550, 1 tile



Summary

- GPUs can be used without changing code using `Tpetra`.
- Portable matrix-free implementation: we can run on CPUs, NVIDIA, AMD, and Intel GPUs using the same code
- Performance tuning needed, in particular for Intel GPUs
- Need to add more capabilities that the CPU version provides

Questions?

Acknowledgments

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Cuda: Performance, A100

Results from `bytes_and_flops(TeamPolicy)`

scalar	Bandwidth	Compute	Cache
`float`	1251 GiB/s	14280 GFlop/s	3762 GiB/s
`double`	1267 GiB/s	7592 GFlop/s	6938 GiB/s
`int32_t`	1222 GiB/s	18457 GFlop/s	4684 GiB/s
`int64_t`	1267 GiB/s	3778 GFlop/s	6895 GiB/s

- Peak FP64 Vector: 19.5 TFLOPS
- Memory Bandwidth: 1.6 TB/sec
- Cache Size: 192KB (per SM)/40 MB

HIP: Performance MI250, one GCD

Results from `bytes_and_flops` (`TeamPolicy`)

scalar	Bandwidth	Compute	Cache
`float`	1160 GiB/s	20544 GFlop/s	2756 GiB/s
`double`	1140 GiB/s	19320 GFlop/s	2883 GiB/s
`int32_t`	1150 GiB/s	20194 GFlop/s	2757 GiB/s
`int64_t`	1140 GiB/s	4979 GFlop/s	2865 GiB/s

- Peak FP64 Vector: 23.95 TFLOPS
- Memory Bandwidth: 1.6 TB/sec
- Cache Size: 16KB (per CU)/16 MB

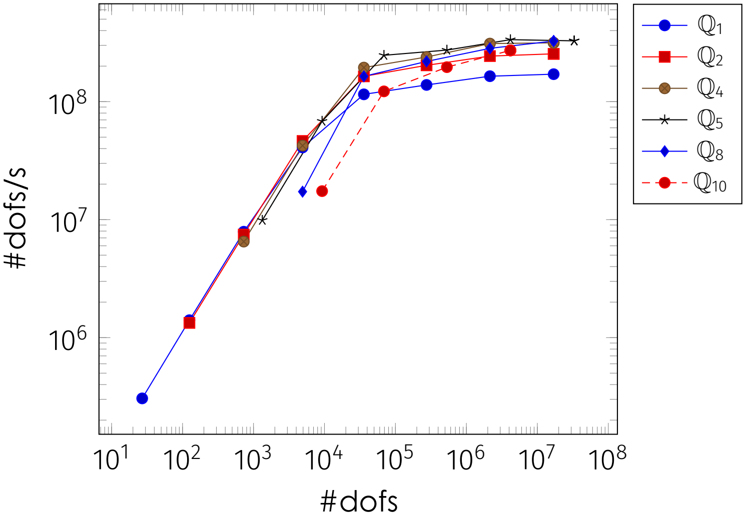
SYCL: Performance Intel Data Center GPU Max 1550, one tile

Results from `bytes_and_flops(TeamPolicy)`

scalar	Bandwidth	Compute	Cache
`float`	1002 GiB/s	17484 GFlop/s	4973 GiB/s
`double`	960 GiB/s	8746 GFlop/s	6928 GiB/s
`int32_t`	1007 GiB/s	6108 GFlop/s	4714 GiB/s
`int64_t`	958 GiB/s	982 GFlop/s	4715 GiB/s

- Peak FP64 Vector: 22.9 TFLOPS/tile
- Memory Bandwidth: 1.6 TB/sec/tile
- Cache Size: 128KB (per work group)/408 MB

Performance results on Polaris - NVIDIA A100



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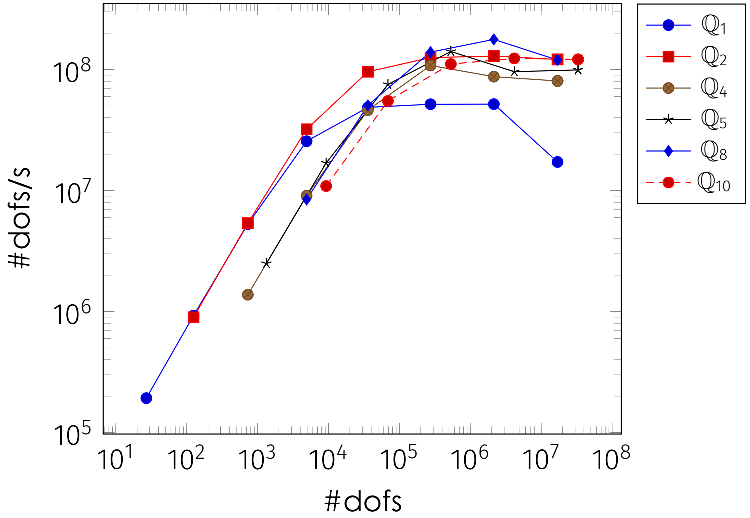

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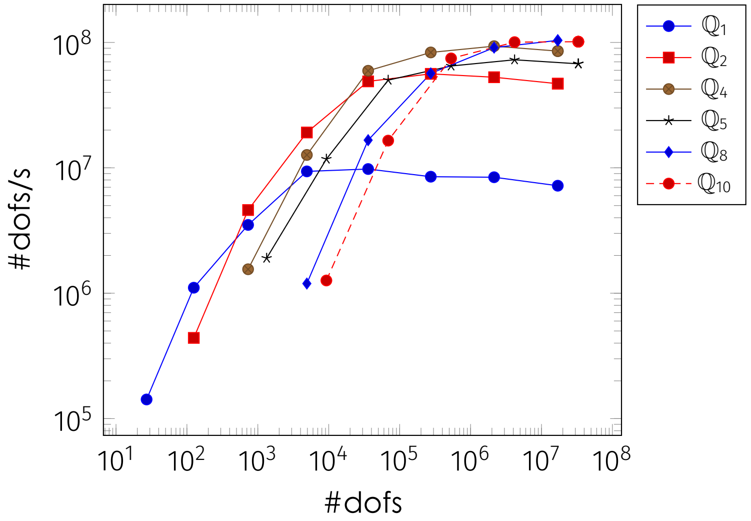
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