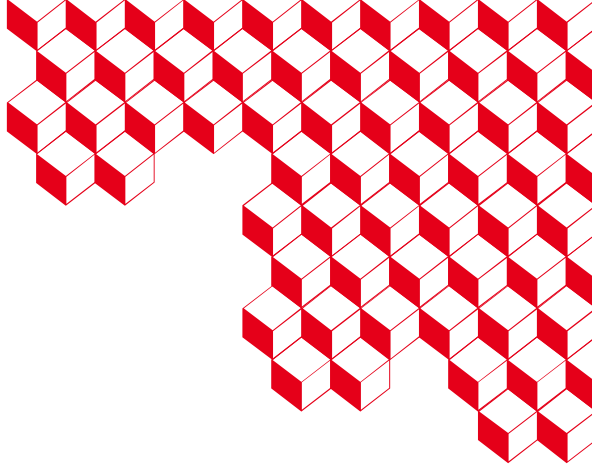

KokkosComm

A Communication Layer for Distributed Kokkos Applications

EuroMPI 2024, September 25-27 , Perth, Australia

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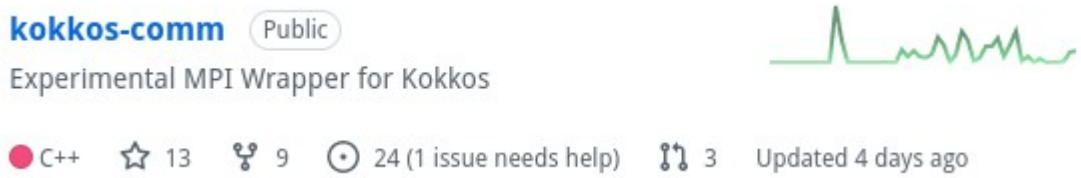

The Kokkos C++ Performance Portability Programming ecosystem

- Kokkos Core implements a programming model in C++ for writing performance portable applications targeting all major HPC platforms
- Kokkos is a basic building block for various applications
  - Trilinos
  - PETSc
  - LAMMPS
  - Cabana
  - ...
- Kokkos is OpenSource
- Kokkos is a High Performance Sofware Foundation project

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The Kokkos C++ Performance Portability Programming ecosystem

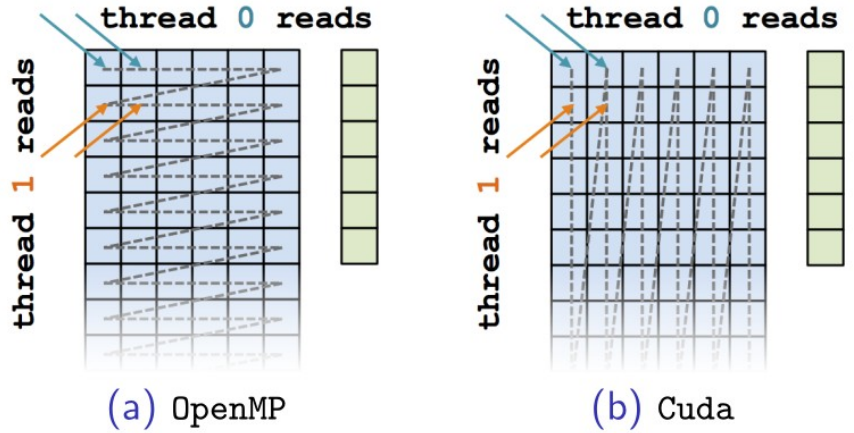
How it works?

- Simple parallel primitives:
  - `for`
  - `reduce`
  - `scan`

- Multi-dimensional data structure: Views
  - Data representation changes to optimize memory access performance on the target hardware
    - *LayoutRight* (row-major) on CPU
    - *LayoutLeft* (col-major) on GPU
  - Can express non-contiguous slices of data: subviews

```
View<double**, LayoutRight> A(N, M);
auto first_col_of_A = subview(A, Kokkos::ALL, 0);
assert(not first_col_of_A.span_is_contiguous());
```

```
View<double**, ExecutionSpace> A(N, M);
parallel_for(RangePolicy< ExecutionSpace>(0, N),
  ... thisRowsSum += A(j, i) * x(i);
```



- **HostSpace**: cached (good)
- **CudaSpace**: coalesced (good)

From Kokkos' tutorial

Extending Kokkos to distributed computing

No primitives for distributed computing

- HPC applications based on Kokkos must rely on external frameworks for distributed computing
  - Generally message-passing based: MPI, NCCL, RCCL, etc.
  - Also an official remote memory access library: kokkos-remote-spaces

- Challenges for programmers
  - Must handle implementation-defined specificities
    - Is the MPI GPU-aware?
    - Explicitly copy Views from CPU ⟺ GPU?
  - Must handle non-contiguous Views
    - Send as multiple "small" contiguous chunks
    - Pack/unpack as one "big" contiguous chunk

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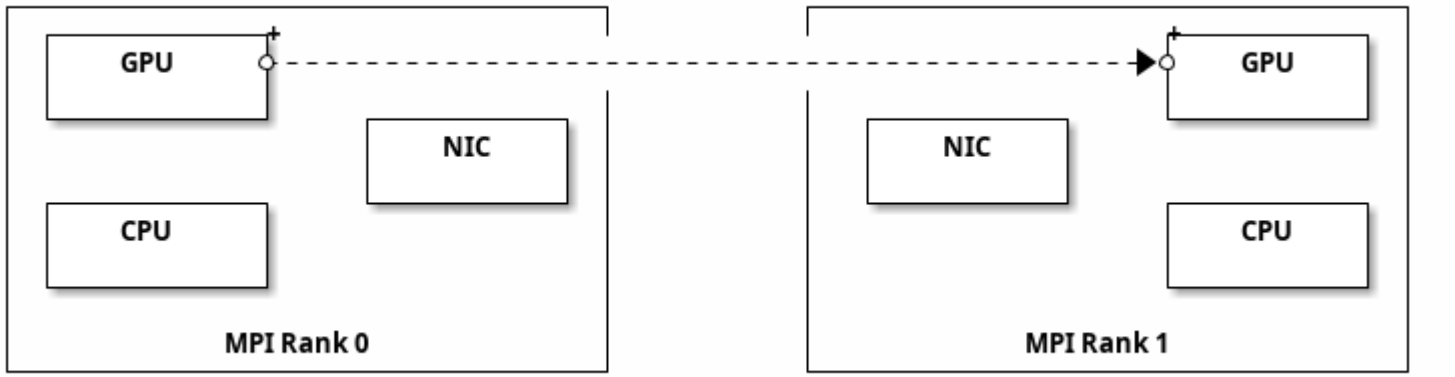
⟹ Lots of code duplication across Kokkos projects

Motivations

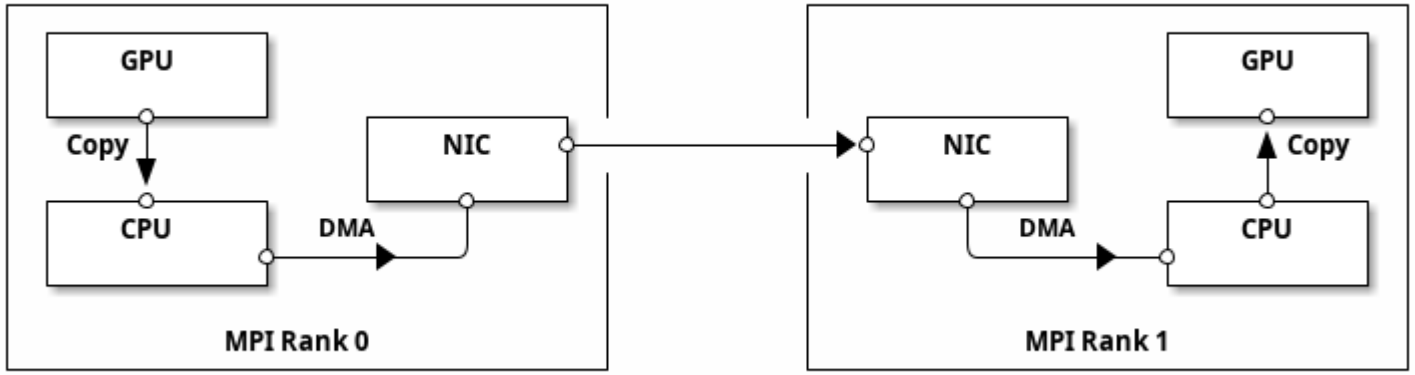
How do we communicate a Kokkos::View between the two MPI processes?

- If MPI is not GPU-aware
- If MPI is GPU aware



Motivations (non) GPU awareness

Message have to be copied on the CPU memory.

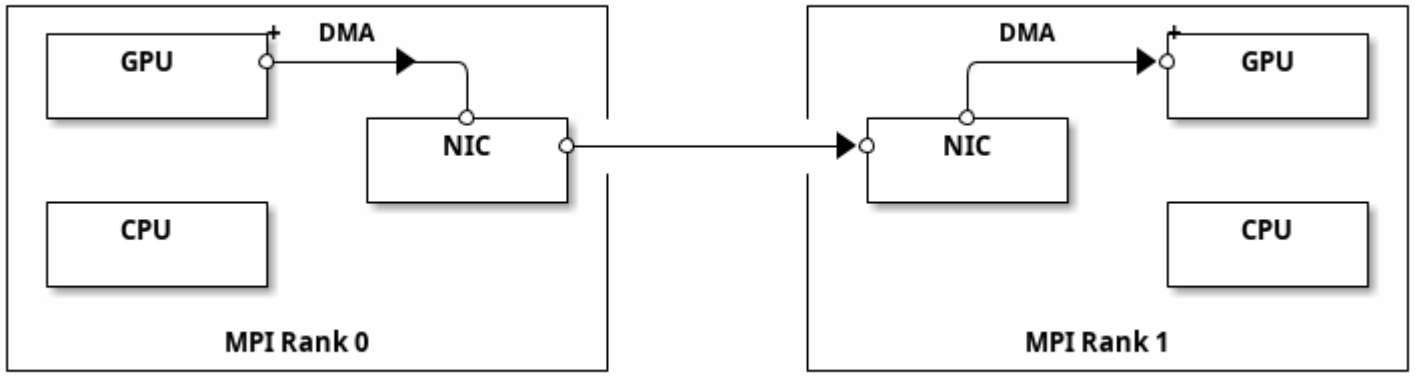



```
// Kokkos::View<double*, Kokkos::CudaSpace>
↪  to_send;
auto host_buffer =
  create_mirror_view_and_copy(to_send);
MPI_Send(host_buffer.span(),
  host_buffer.extent(0),
  MPI_DOUBLE, 1, TAG, MPI_COMM_WORLD);
```

```
// Kokkos::View<double*, Kokkos::CudaSpace>
↪  to_recv;
auto host_buffer =
  create_mirror_view(to_recv);
MPI_Recv(host_buffer.span(),
  host_buffer.extent(0),
  MPI_DOUBLE, 0, TAG, MPI_COMM_WORLD);
// Copy back to GPU
deep_copy(to_recv, host_buffer);
```

Motivations GPU-awareness

Message does not need to be copied on CPU memory!




```
// Kokkos::View<double*, Kokkos::CudaSpace>
↪  to_send;
MPI_Send(to_send.span(), to_send.extent(0),
  MPI_DOUBLE, 1, TAG, MPI_COMM_WORLD);
```

```
// Kokkos::View<double*, Kokkos::CudaSpace>
↪  to_recv;
MPI_Recv(to_recv.span(), to_recv.extent(0),
  MPI_DOUBLE, 0, TAG, MPI_COMM_WORLD);
```

Motivation : Kokkos specifics

Kokkos::Views are multi-dimentional arrays that can be stored in various ways:

- LayoutRight, LayoutLeft, LayoutStride, etc.
- Contiguous or non-contiguous (sub-views?)

Contiguous vs non-contiguous

```
if constexpr (to_send.span_is_contiguous()) {
  MPI_Send(to_send.span(), to_send.extent(0), MPI_DOUBLE,
           1, TAG, MPI_COMM_WORLD);
} else {
  Kokkos::View<...> send_buffer;
  Kokkos::deep_copy(send_buffer, to_send);
  MPI_Send(send_buffer.span(), send_buffer.extent(0), MPI_DOUBLE,
           1, TAG, MPI_COMM_WORLD);
}
```

- Kokkos execution contexts: interactions with asynchronous execution
  - When to fence() and where?

Related work

Kokkos + MPI interoperability interfaces

- Teuchos: MPI toolkit from Trilinos
  - MPI abstraction but no Kokkos::View abstraction

- Custom implementation in user applications
  - Cabana
  - LAMMPS
  - ...

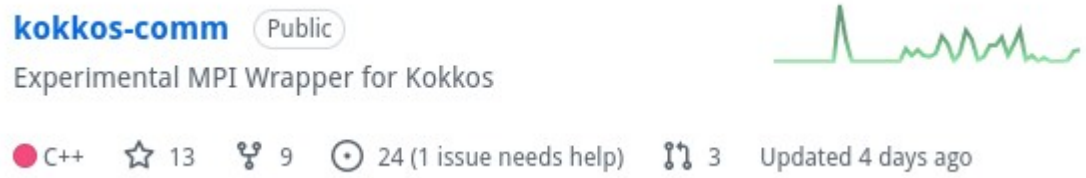
- ExaMPI: View-aware Message Passing
  - C++ implementation of MPI
  - Extends MPI API to deal with Kokkos Views
    - Still C-like interface: exposes counts, datatypes, etc.
    - Non-standard implementation that is harder to integrate into existing projects

Introducing KokkosComm

An official Kokkos organization project

- Collaborative development from CEA, SNL, Tenessee Technical University, etc.
- Provide a unified interface for distributed computing with Kokkos
- Launched on March 2024 !

Project goals (short term)



- Primarily address Kokkos + MPI interoperability
  - Simplify usage of both frameworks
  - Handle error-prone cases: non-contiguous data, GPU-aware support, etc.
  - Built on top of classical MPI implementation
- Guarantee performance portability across heterogeneous hardware
  - Automatically choose the best strategy for exchanging Views
- Make it hard to misuse
  - Simplify the API (so cannot follow stricly all the MPI semantics)
  - Leverage modern C++ features to make compile-time guarantees

Introducing KokkosComm

Project goals ("longer" term)

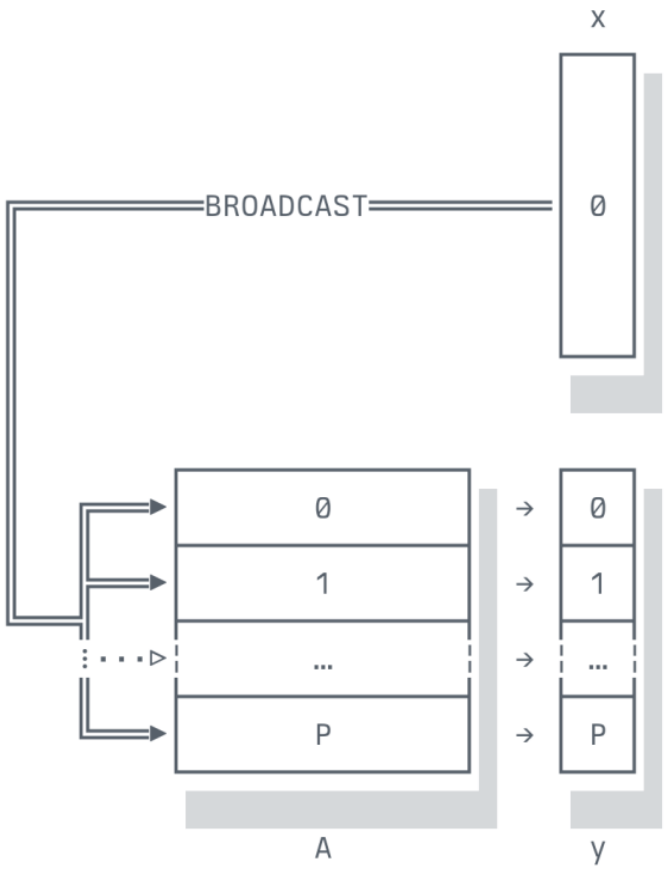
- Design a high-level, extensible and composable API
  - Abstract away concepts from underlying message-passing libraries
    - MPI, NCCL/RCCL, Portals, etc.
    - Communicators, requests, etc.
  - Provide a sensible subset of P2P & collective operations
    - Only non-blocking/asynchronous functions
    - P2P: **`send`** and **`recv`**
    - Collectives: **`broadcast`**, **`reduce`**, **`all_reduce`**, **`all_gather`** and **`all_to_all`**

- Overlap communication and data transformation
  - on-the-fly layout transformation of multi-dimensional data
  - e.g. transpose a 2D view in the correct layout (depending on comm target)

- Explore modern approaches for a new MPI API for C++
  - Deal with multi-dimensional data with `std::mdspan` (C++23)
  - Express dependencies between operations with `std::execution`'s sender/receiver model (C++26)

Distributed matrix-vector product (1D row-wise partitioning)

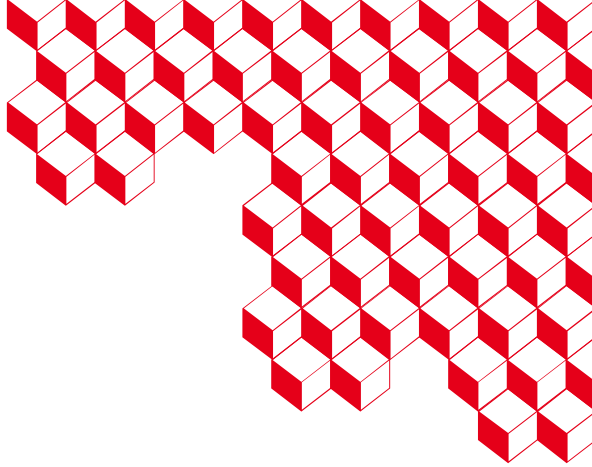
```cpp
// Initialize vector `x` from the root process, and broadcast it
Vector x("x", global_n);
if (rank == 0) {
  Kokkos::parallel_for("init_x", global_n, KOKKOS_LAMBDA(int i) { x(i) = 3.0; });
}
auto bcast_req = KokkosComm::broadcast(space, handle, x, 0);
// Local Matrix `A` and result vector `y`
Matrix A_local("local_A", local_m, global_n);
Vector y_local("local_y", local_m);
// Initialize local `A` on each process
Kokkos::parallel_for("init_local_A",
  Kokkos::MDRangePolicy<Kokkos::Rank<2>>({0, 0}, {local_m, global_n}),
  KOKKOS_LAMBDA(int i, int j) { A_local(i, j) = 1.0; }
);
// Wait for broadcast of `x` to finish
KokkosComm::wait(bcast_req);

// Perform local matrix-vector multiplication
KokkosBlas::gemv("N", alpha, A_local, x, beta, y_local);

// Gather results (if needed)
Vector y("y", global_m);
auto gather_req = KokkosComm::all_gather(space, handle, y_local, y);
KokkosComm::wait(gather_req);
```



Summary & Take away

- Basic MPI wrapper for Kokkos::Views by the end of the year
  - To be tested on Trilinos and PETSc
  - Looking for different communication patterns (LAMMPS, Cabana, your app?)

- Open development
  - https://github.com/kokkos/kokkos-comm
  - #mpi-interop on Kokkos' Slack
  - Bi-weekly telecom, open to all (you are welcome!)



Thank you for your attention!

Questions & Answers