View-aware Message Passing Through the Integration of Kokkos and ExaMPI

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Introduction

- Advanced C++ libraries/code are rapidly being adopted in HPC, but many are constrained by their use with C libraries not designed for interacting with them.
- Message Passing Interface (MPI) standard specifies a programming model for passing messages between processes.
- ExaMPI is a modern C++ focused implementation of the MPI Standard.
- Kokkos is a programming model for C++ that provides data structures, concurrency features, and algorithms to support advanced C++ parallel programming across different memory spaces.
- MPI is an inter-process/node parallel programming model while Kokkos is an intra-process/node parallel programming model.
- However, parallel applications want to use both.

Goals

- To improve the general programming experience when using MPI with Kokkos.
- To minimize the possibility of bugs from MPI+Kokkos programs
- To enable optimizations for MPI+Kokkos at the language binding level or below.

ExaMPI is focused on principles-first design, highlighting the principles below:

- • Enable rapid new development of new features, identify ways to increase performance, and improve understanding of the MPI standard
- • Support the research interests and experiments of developers, such as effective overlap of communication and computation

Goals cont.

- Create an MPI Extension composed of a series of function bindings within ExaMPI to handle a Kokkos View as input or output in a similar way to buffers in MPI.
- Interface should not require the user to touch the .data() method.
- Ensure the MPI+Kokkos extension with comparable performance to traditional methods
- Due to additional handling cost, performance may be slightly worse, but has the benefit of functionality.
- Gather ideas for what further work can be done, and how feasible it is to create a larger extension

Objectives

Our objectives are as follows:

- To create a series of function bindings within ExaMPI whose syntax utilizes Kokkos objects in the same manner as standard MPI buffers
- These function bindings should have at least comparable performance to existing practices for the majority of use cases
- Allow for easier building of MPI applications using Kokkos alongside ExaMPI

Objectives cont.

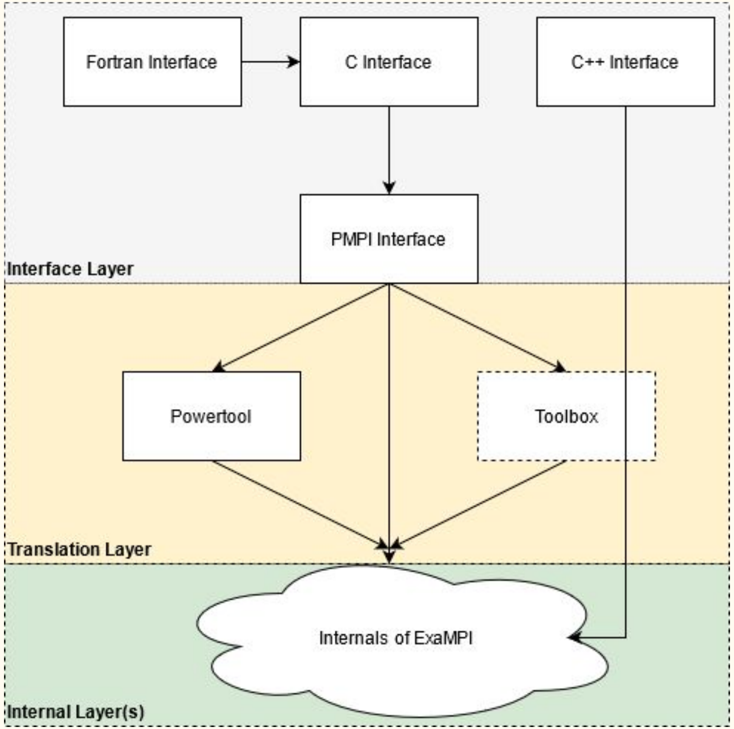
These objectives are accompanied by the following questions:

- How useful are these new bindings for users?
- What are the long term opportunities created by these bindings?
- Should these bindings follow the more traditional C-style MPI bindings or experiment with new parameters?
- Do these bindings increase or decrease performance?

Literature Review

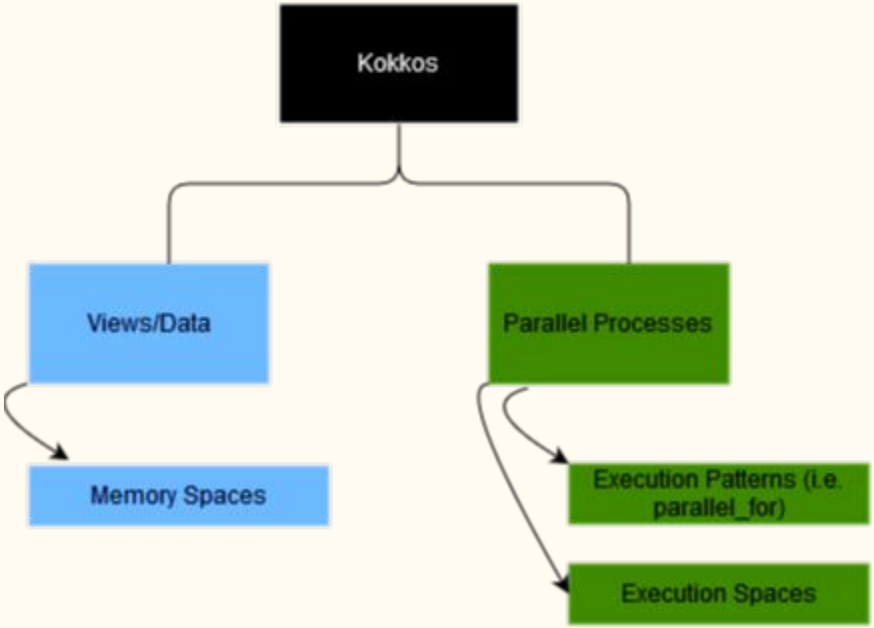
MPI and ExaMPI

- The Message Passing Interface (MPI) standard specifies a programming model interface for passing messages between peer processes.
- MPI offers a wide range of functions, but the most common are the point-to-point functions, MPI_Send and MPI_Recv.
- Buffers in MPI are often a contiguous array of a single type of data primitive.
- ExaMPI is a modern C++ implementation of MPI, which enabled this paper to put C++ features, such as templates, into the work.
- ExaMPI is focused on being a tool for rapid research, implementing a subset of MPI functions rather than the full standard.



Kokkos

- Kokkos is a programming model and library that provides data structures, concurrency features and algorithms to support advanced C++ parallel programming across different memory spaces.
- Kokkos is centered around its primary data structure, the View, a smart pointer class wrapping primitive datatypes arrays
- Kokkos has a few parallel dispatch operations similar to those used in OpenMP: `parallel_for`, `parallel_reduce`, and `parallel_scan`.



Kokkos

- Coding example below shows initialization of a Kokkos View.

```
Kokkos::View<double*>check( ”check”, n );
Kokkos::parallel_for(check.extent(0), KOKKOS LAMBDA(int i) {
   check(i) = i*i;
});
```

Related Work

- There exist a few previous attempts unite MPI or MPI alternatives with Kokkos
- Khuvis et al. have a shown a speedup of General Matrix Multiplication (GEMM) code and the Graph500 benchmark using MPI+Kokkos.
- The GEMM code uses Kokkos for parallelism of matrix multiplication alongside MPI to distribute the matrices, this code has noticeable improvement with each additional process for up to 64 processes.
- The Graph500 results show a speed-up with the locking implementation over the MPI-only one up to forty processes, and continued speed-up with the non-locking implementation of up to 5x on 64 processes.

Related Work

- The Uintah framework for modeling chemical reactions uses MPI + Kokkos to consolidate the use of both MPI + Pthreads and MPI + CUDA into a single approach that also enables added portability.
- The UPC++ framework replaces MPI in simulating heat conduction without radical changes in performance compared to the IBM version of MPI.
- Con et al. demonstrated use of the distributed many-task MPI alternative Legion with Kokkos to offload "boiler-plate code" away from the user.
- The primary innovation that distinguishes this project from previous forms of MPI+Kokkos interaction is the ability to take Kokkos Views directly.

Methodology and Implementation

Further Requirements

- Able to handle Views with up to 3 dimensions
- Able to handle any contiguous View regardless of layout
- The interface should not require the user to create new derived datatypes for Views
- Retain datatype compatibility with Kokkos
- Avoid reliance on the MPI Datatype by using template parameters

MPI_Kokkos_Send & Recv Implementation

MPI_Kokkos_Send⟨View_t, Datatype⟩(

View_t * buf, int count, MPI Datatype datatype, int dest, int tag, MPI Comm comm)

MPI_Kokkos_Recv⟨View_t, Datatype⟩(

View_t * buf, int count, MPI Datatype datatype, int source, int tag, MPI Comm comm)

- The template parameters decide the datatype information for View operations
- MPI_Kokkos_Send's counterpart, MPI_Kokkos_Recv receives the Payload send in MPI_Kokkos_Send, then wraps that in a View object and sends that to the pointer passed as a parameter.

```
Kokkos::View<int*>check( ”check”, n );
MPI_Kokkos_Send<Kokkos::View<int*>, int>(&check, n, MPI_INT, 0, 0, MPI_COMM_WORLD);
int* check_arr = check.data();
MPI_Send(check_arr, n, MPI_INT, 0, 0, MPI_COMM_WORLD);
```

Further Implementations

- MPI_Kokkos_ISend⟨View_t, Datatype⟩(View_t * buf, int count, MPI Datatype datatype, int dest, int tag, MPI Comm comm, MPI Request *request)
- MPI_Kokkos_Irecv⟨View_t, Datatype⟩(View_t * buf, int count, MPI Datatype datatype, int dest, int tag, MPI Comm comm, MPI Request *request)
  - Synchronizes with standard functions (i.e. MPI_Wait)
- MPI_Kokkos_Bcast⟨View_t, Datatype⟩(View_t * buf, int count, MPI Datatype datatype, int root, MPI Comm comm)
- MPI_Kokkos_Allgather⟨View_t, Datatype⟩(View_t * buf, int count, MPI Datatype datatype, View_t * recv buf, int recv_count, MPI_Datatype recv_type, MPI_Comm comm, MPI_Request *request)
  - MPI Kokkos Allgather takes (gathers) an input View from all processes.
  - Then, these are compiled into a View ordered by their sending process's index ranking.
- MPI_Kokkos_Allreduce⟨View_t, Datatype⟩(View_t * buf, View_t * recv_buf, int count, MPI Datatype datatype, MPI_Op op, MPI_Comm comm)
  - The key design choice is whether this extension should return the resulting buffer from the reduce operation as a View or as a data primitive.
  - To be more consistent with the previously covered functions, this function uses Views for both the send and receive buffers

MPI_Kokkos_Bcast Implementation

MPI_Kokkos_Bcast⟨View_t, Datatype⟩(View_t * buf, int count, MPI Datatype datatype, int root, MPI Comm comm)

- MPI_Kokkos_Bcast (short for Broadcast) resembles the functionality of Send and Receive combined into one function.
- The root process sends (Broadcasts) its View to all the other process ranks in the given communicator group, enabling a process to send to any number of other processes.
- Broadcast functions are a form of collective communication as it handles several processes.
- In communicator groups, only one process rank is identified as the root process.

MPI_Kokkos_Allgather Implementation

MPI_Kokkos_Allgather⟨View_t, Datatype⟩(View_t * buf, int count, MPI Datatype datatype, View_t * recv buf, int recv_count, MPI_Datatype recv_type, MPI_Comm comm, MPI_Request *request)

- MPI Kokkos Allgather takes (gathers) an input View from all processes.
- Then, these are compiled into a View ordered by their sending process's index ranking.
- MPI_Allgather functions are classified as a form of collective communication as it handles several processes.

MPI_Kokkos_Allreduce Implementation

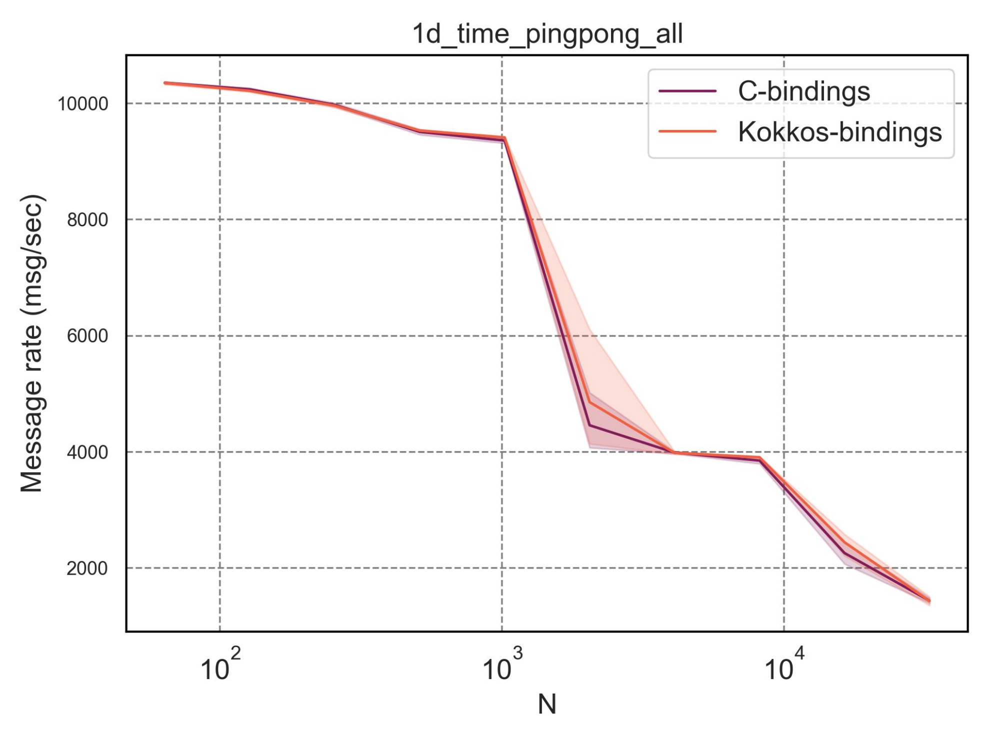
MPI_Kokkos_Allreduce⟨View_t, Datatype⟩(View_t * buf, View_t * recv_buf, int count, MPI Datatype datatype, MPI_Op op, MPI_Comm comm)

- MPI_Kokkos_Allreduce is a collective function that collects values from several processes, performs an operation on them (MPI_Op) and broadcasts the result to all processes involved.
- The MPI_Op can be any of a number of operations such as sum, max, etc. This function required more conceptual work than previous function.
- The key design choice is whether this extension should return the resulting buffer from the reduce operation as a View or as a data primitive.
- To be more consistent with the previously covered functions, this function uses Views for both the send and receive buffers

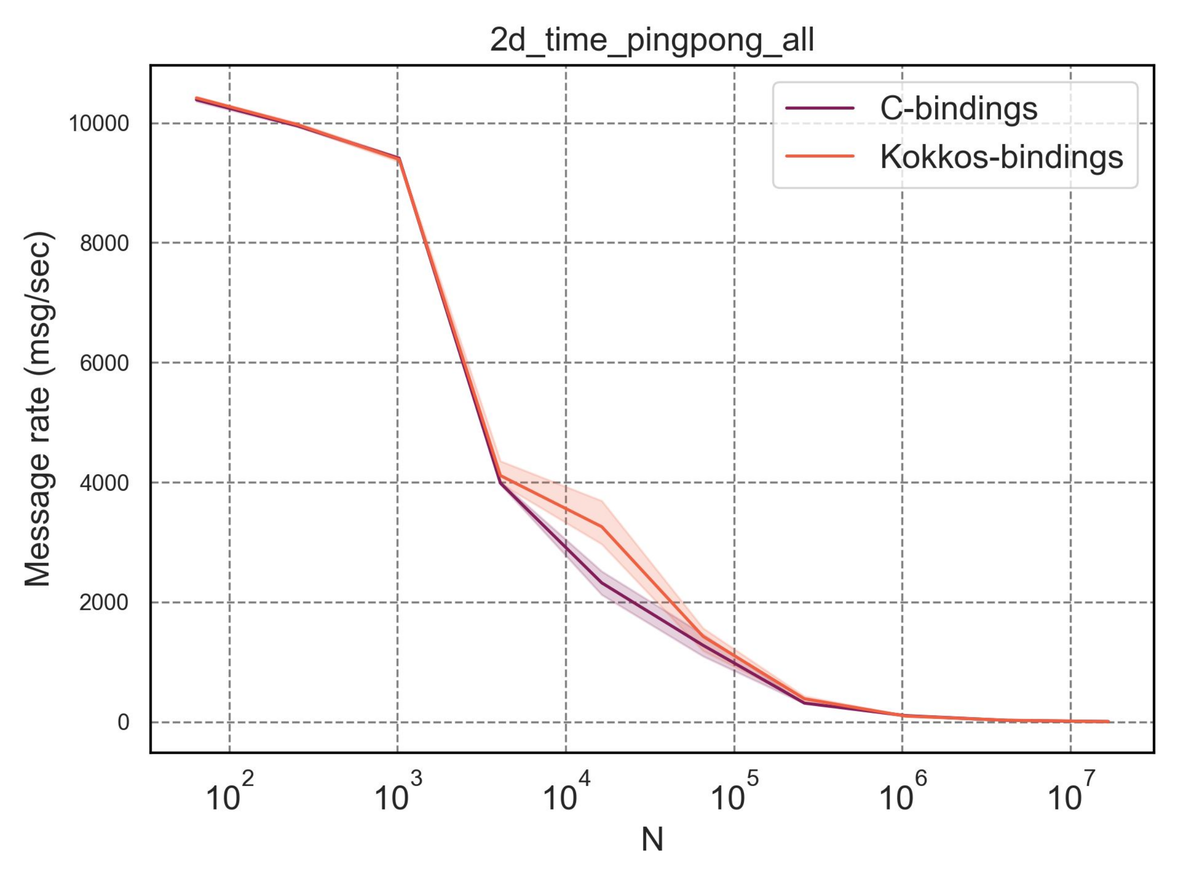
Test Results

Single-Dimension Ping-Pong Tests

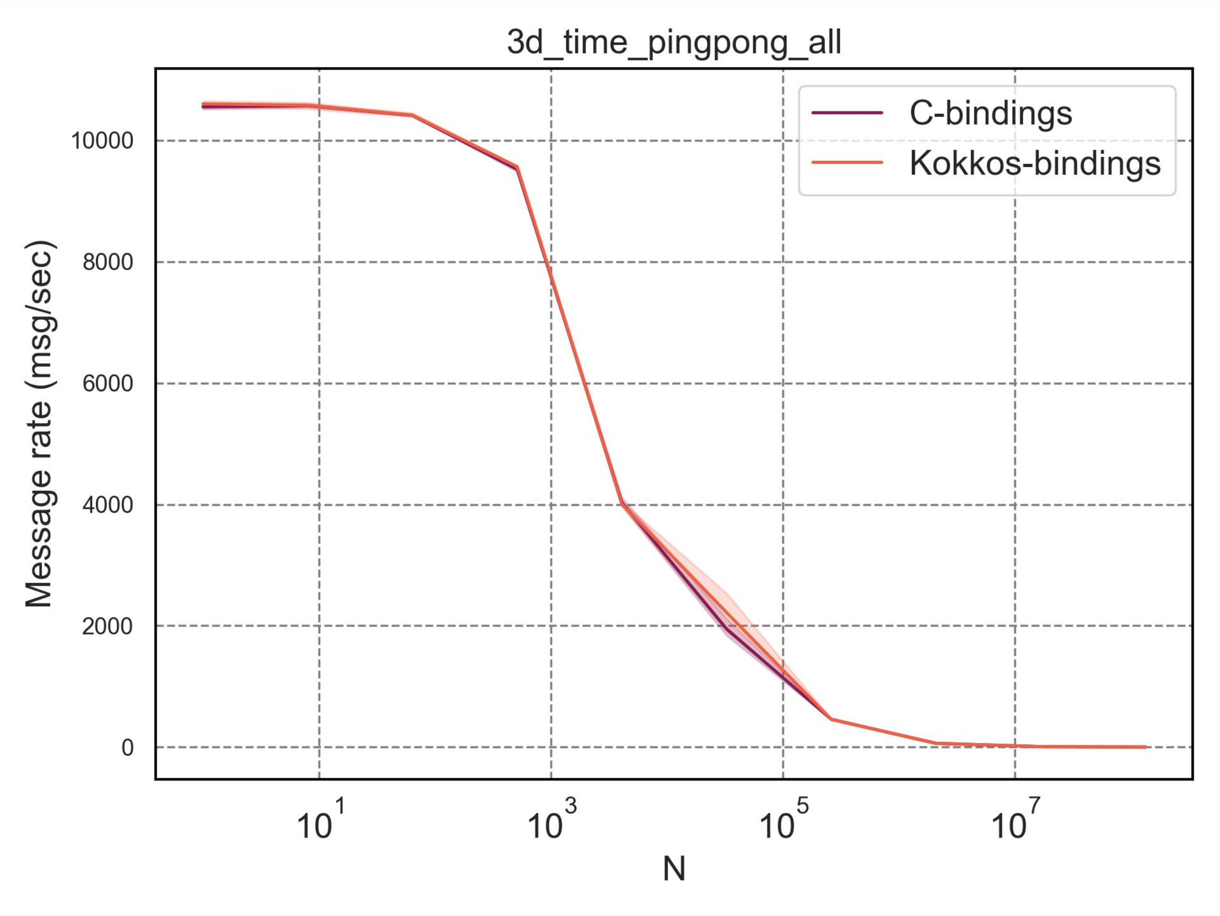
- 500 runs were averaged on Views with from 64 to 32768 elements
- The primary goal was not a significant change in performance, but roughly equal performance for both bindings
- Both types of bindings are better at different times, with very low standard deviation of the mean



Two-Dimensional Tests

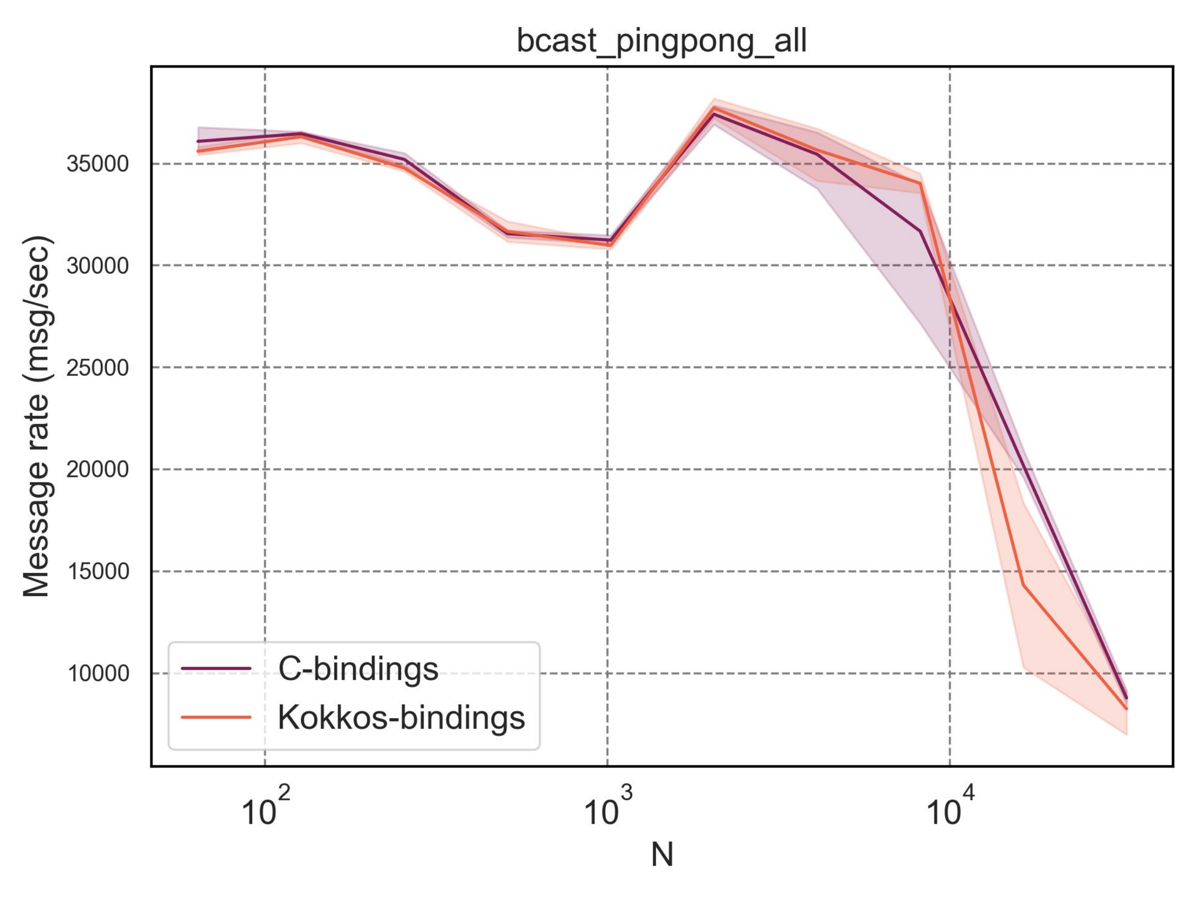


Three-Dimensional Tests



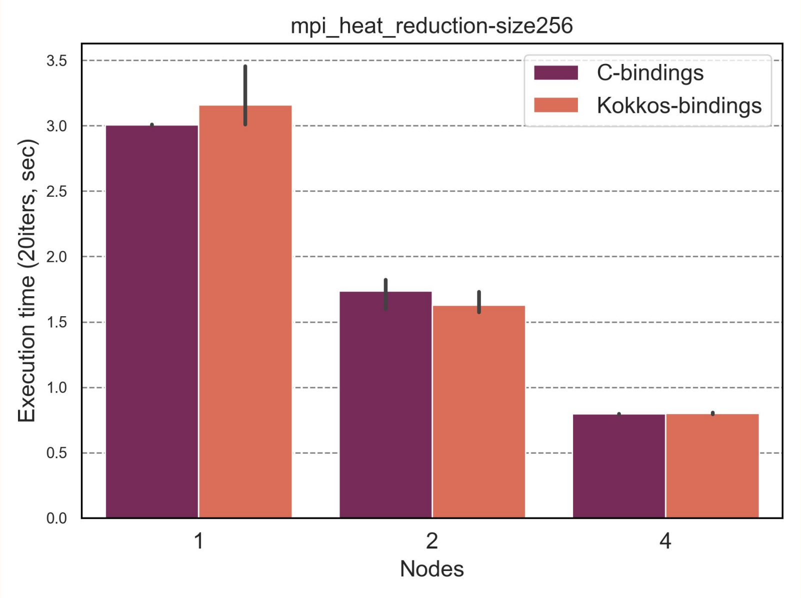
Broadcast Tests

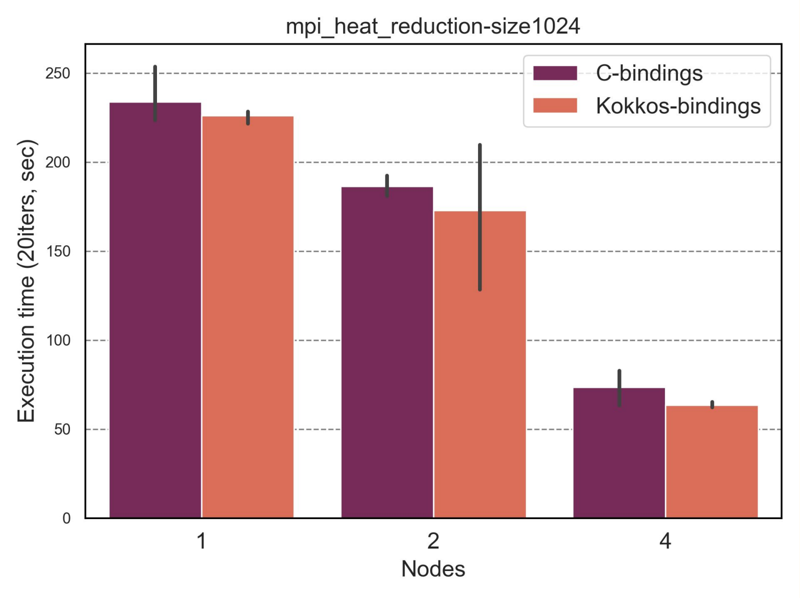
- Each test is run 100 times, then the first warm-up time is discarded.
- While the new bindings may look generally better here, all of this is more dependent on non-deterministic portions of timing and transports rather than simpler sends.



Heat Reduction Tests

- This test uses the heat reduction code in Kokkos tutorials which uses Views with MPI, with only the bindings altered for the our version.
- The Kokkos-bindings have a slightly better execution time, especially for the increased 1024 size





Conclusion

- This paper set about to integrate two programming models, MPI and Kokkos.
- Implemented several MPI bindings with Kokkos View objects as their primary buffers without sacrificing the C++ nature of the Kokkos View.
- Using ExaMPI benefitted the project, as it enables the use of templates to better interact with Kokkos.
- After implementing the bindings for this project, we found that the new bindings' performed similarly to the old bindings's.

Future Work

- Wider range of MPI functions such as All-To-All, Scatter, and Gather.
- Change from MPI_Kokkos_X to overloading existing MPI functions.
- More device-specific support (i.e., MPI_Send<View, class, Device>).
- Testbed for new functions, such as byte-mapping-based transports, rather than traditional datatype-based transports.
- Reconciling the differences between MPI and Kokkos methods of dealing with non-contiguous data, and add non-contiguous View support.
- A creation of new backends to increase speed for specific types of Views (i.e., Views on GPUs, non-contiguous, etc.).

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Questions