Fast CUDA-Aware MPI Datatypes without Platform Support

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MPI Derived Datatypes are an abstraction that simplifies handling of non-contiguous data in MPI applications. These datatypes are recursively constructed at runtime from primitive Named Types defined in the MPI standard. More recently, the development and deployment of CUDA-aware MPI implementations has encouraged the transition of distributed high-performance MPI codes to use GPUs. These implementations allow MPI functions to directly operate on GPU buffers, easing integration of GPU compute into MPI codes. Despite substantial attention to CUDA-aware MPI implementations, they continue to offer cripplingly poor GPU performance when manipulating derived datatypes on GPUs. This work presents an approach to integrating fast derived datatype handling into existing MPI deployments through an interposed library. This library can be used regardless of MPI deployment and without modifying application code. Furthermore, this work presents a performance model of GPU derived datatype handling, demonstrating that "one-shot" methods are not always fastest. Ultimately, the interposed-library model of this work demonstrates MPI_Pack speedup of up to 724,000× and MPI_Send speedup of up to 59,000× compared to the MPI implementation deployed on a leadership-class supercomputer. This yields speedup of more than 20,000× in a 3D halo exchange.

CCS Concepts: • **Software and its engineering → Software libraries and repositories**; • **Computing methodologies → Massively parallel algorithms**.

Additional Key Words and Phrases: MPI, CUDA, derived datatype, pack

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1 INTRODUCTION

MPI derived datatypes [12, p. 83] are a useful abstraction for describing the layout of non-contiguous data in memory. They allow MPI functions to operate on such data without intermediate handling by the user application, especially packing the data into a contiguous buffer before transfer. As GPUs have become a dominant high-performance computing accelerator, MPI implementations such as OpenMPI [3], MVAPICH [9], Spectrum MPI [6] and MPICH [4] have become "CUDA-aware". In such implementations MPI can directly operate on CUDA device allocations, again simplifying application development and with the potential of accelerating inter-rank transfers of GPU-resident data.

Operating on non-contiguous datatypes has been recognized as a challenge in its own right, orthogonal to the details of high-performance GPU-to-GPU communication. Previous works have contributed solutions to handling arbitrary

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datatypes on GPUs, noted that GPU latency is a significant contribution to end-to-end time, and integrated datatype handling with the communication layer. Despite broad GPU deployment in distributed computing and years of work in datatype handling, no widely-deployed MPI implementation has high-performance handling of derived datatypes on GPUs.

Therefore, the challenge of deployment unaddressed in previous work may be a fundamental one. Consequently, one contribution of this work is to demonstrate that a library-interposed approach can work in practice and yield large performance improvements for MPI applications that use derived datatypes. These contributions are implemented in the Topology Experiments for MPI (TEMPI) library, which has been tested with OpenMPI 4.0.5, MVAICH 2.3.4, and Spectrum MPI 10.3.1.2. TEMPI is available at https://github.com/cwpearson/tempi.

Secondarily, this work presents a new approach for handling strided MPI datatypes. Prior work recognizes that all MPI datatypes can be generalized to a list of contiguous blocks defined by offsets and sizes. Further, certain types are more structured than that and can be individually specialized. This work extends that approach by observing that compositions of contiguous, vector, hvector, and subarray types are all the same class of objects suitable for a compact representation. Instead of a specialized kernel to handle different derived datatypes, this work proposes a canonicalization phase to transform strided datatypes into a common representation, then chooses optimized datatype handling approach based on that representation.

Thirdly, this work presents the first published performance model of derived datatype operations on GPU. The model is simple, but yields an insight about when prior "one-shot" methods not desirable. The model is evaluated in the context of the OLCF Summit system.

Combined, these contributions yield a speedup of up to 724,000× for MPI_Pack and MPI_Unpack, 59,000× for MPI_Send, and 20,000× for a 3D stencil halo exchange on the OLCF Summit system, which does not natively support fast datatype operations on GPU.

This paper is organized in the following way: Section 2 introduces MPI derived datatypes and how they may be composed to describe strided objects. Section 3 describes the library-interposer method that makes the derived type modifications available without application modification. Section 4 describes how TEMPI transfoms datatypes and selects the kernel. Section 5 describes the microbenchmark and 3D stencil results. Section 6 describes future work for the library. Section 7 describes related work. Finally, Section 8 concludes.

2 BACKGROUND

MPI datatypes can be composed to describe multi-dimensional strided objects. This work considers the following subset due to their direct application to describing such objects.

- "predefined" or "named"[12, §3.2.2]: these are the base MPI datatypes (MPI_BYTE, MPI_FLOAT, etc) that correspond to various C or Fortran types.
- "contiguous"[12, §4.1.2]: describing "replication of a datatype in contiguous locations."
- "vector/hvector"[12, §4.1.2]: "replication of a datatype into...equally spaced blocks."
- "subarray"[12, §4.1.3]: describing "n-dimensional subarray of an n-dimensional array."

These types may be composed in many ways to describe the same non-contiguous bytes. For example, consider the 3D object in Fig. 1, which can be visualized as a three-dimensional sub-object of an enclosing three-dimensional object, where the sub-region shares an origin with the enclosing object. Each element of the object be a single-precision floating-point number (an MPI_FLOAT), consuming four bytes.

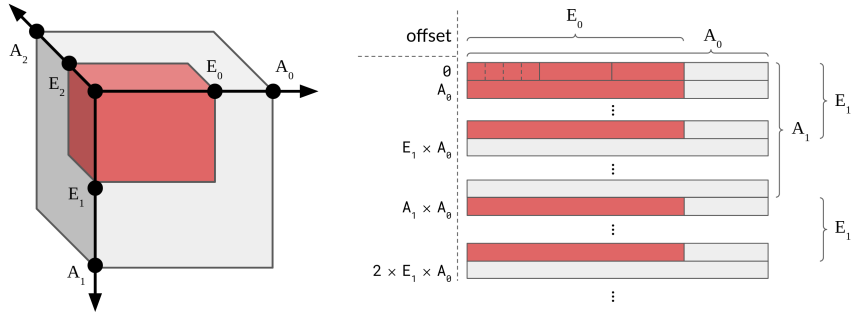


Fig. 1. A 3D object with extent $E_0 \times E_1 \times E_2$ in an allocation $A_0 \times A_1 \times A_2$ bytes, and the memory layout.

The flexibility of the MPI derived datatype system allows each 1D row of the object ($E_0 \times 4$ contiguous bytes) to be described in many ways. A non-exhaustive list follows:

- MPI_Type_contiguous(E_0, MPI_FLOAT, &row)
- MPI_Type_contiguous($E_0 \times 4$, MPI_BYTE, &row)
- MPI_Type_vector(E_0, 1, 1, MPI_FLOAT, &row)
- MPI_Type_vector(1, E_0, 1, MPI_FLOAT, &row)
- MPI_Type_vector(E_0, 4, 4, MPI_BYTE, &row)
- MPI_Type_vector(1, E_0, $E_0 \times 4$, MPI_BYTE, &row)
- MPI_Type_vector(E_0, 1, 1, MPI_FLOAT, &row)
- MPI_Type_create_hvector($E_0 \times 4$, 1, 1, MPI_BYTE, &row)
- MPI_Type_create_subarray(1, A_0, E_0, 0 ,MPI_ORDER_C, MPI_FLOAT, &row)
- MPI_Type_create_subarray(1, $A_0 \times 4$, $E_0 \times 4$, 0, MPI_ORDER_C, MPI_BYTE, &row)

These types are not completely interchangable – the vector's extent[1] is the distance between the first byte and the last byte, while a subarray's extent is instead the product of its sizes. This distinction is relevant for certain compositions of these types (e.g., below), or when multiple types are manipulated at once. Nonetheless, they are equivalent for describing a single such object.

A 2D plane (E_1 rows, offset by A_0 bytes between the beginning of each row) can be constructed directly from named types:

- MPI_Type_vector(E_1, E_0, A_0, MPI_FLOAT, &plane)
- MPI_Type_vector(E_1, $E_0 \times 4$, A_0, MPI_BYTE, &plane)
- MPI_Type_create_subarray(2, A_0, A_1, E_0, E_1, 0, 0, MPI_ORDER_C, MPI_FLOAT, &plane)
- MPI_Type_create_subarray(2, $A_0 \times 4, A_1$, $E_0 \times 4, E_1$, 0, 0, MPI_ORDER_C, MPI_BYTE, &plane)

alternatively, as an hvector of rows:

- MPI_Type_create_hvector(E_1, 1, A_0, row, &plane)

and for the subarray types (that have the proper extent):

- MPI_Type_vector(E_1, 1, 1, row, &plane)
- MPI_Type_create_subarray(1, A_1, E_1, 0, MPI_ORDER_C, row, &plane)

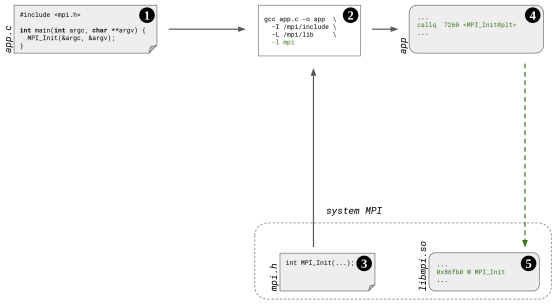
[1] MPI_Type_get_extent()

Similarly planes comprise a cuboid (E_2 planes, offset by $A_0 \times A_1$ bytes between the beginning of each plane). For example,

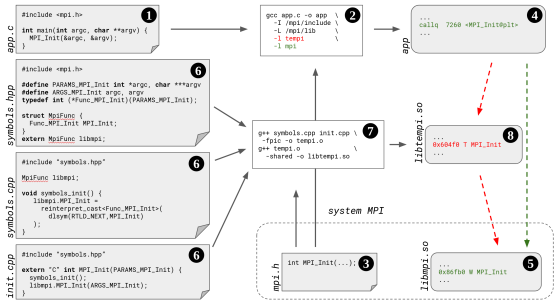
- MPI_Type_create_hvector(E_2, 1, $A_0 \times A_1$, plane, &cuboid)
- MPI_Type_create_subarray(2, A_0, A_1, A_2, E_0, E_1, E_2, 0, 0, 0, MPI_ORDER_C, MPI_FLOAT, &cuboid)
- MPI_Type_create_subarray(2, $A_0 \times 4, A_1, A_2$, $E_0 \times 4, E_1, E_2$, 0, 0, 0, MPI_ORDER_C, MPI_BYTE, &cuboid)

There are additional alternate constructions that are equally valid, especially if we allow MPI datatypes excluded from this discussion (hindexed, etc.) and special cases (A_0 is a multiple of MPI_FLOAT, etc.). The challenge, therefore, is to treat all these different constructions equally when being handled in MPI operations.

3 LIBRARY ARCHITECTURE



(a) MPI application compilation. The application source file (❶) includes the MPI header file provided by the system (❸). It is compiled (❷) and linked with the system MPI implementation. When the binary (❹) is executed, symbols are resolved and the MPI code from the system MPI library is executed.



(b) Using TEMPI. The TEMPI source files (❻) are compiled (❼) into a dynamic library (❽) using the system MPI header. The application is compiled as normal except for TEMPI being inserted into the link order (❶), or an unmodified application can be used with the LD_PRELOAD mechanism. When the application is executed, any symbols defined by the TEMPI library will be resolved there (❽), allowing the TEMPI code to be executed. Any others will be resolved in the system implementation.

Fig. 2. Integration of TEMPI with an existing MPI application. The application is unmodified. TEMPI is compiled using the same MPI implementation as the application, and then the TEMPI shared library (❽) is introduced into the link order (❷) before the system MPI library.

The Topology Experiments for MPI library is designed to make MPI modifications available to research and production code without relying on updates to the system MPI implementation. Fig. 2 shows an overview of the usual MPI compilation flow and how TEMPI interposes alternate implementations into existing MPI functions. For reference, Fig. 2a shows a standard MPI compilation flow on Linux. The application source (❶) includes the system MPI headers (❹) and is compiled (❷) to produce a binary (❸). At run time, the operating system will resolve the symbols in the application binary according to the order of linked libraries, and MPI_Init is found in the system MPI implementation (❺).

Fig. 2b shows how TEMPI provides new MPI functionality for unmodified applications by exporting a partial implementation for the MPI interface. For example, init.cpp (❻) implements the MPI_Init function. The TEMPI source includes the system MPI header, and must be compiled (❼) with the same MPI as the target application so that the ABI matches. If the original application can be recompiled, the TEMPI library (❽) may be inserted into the link order before

the system MPI library (2b, ❷). If not, the TEMPI library can be injected using LD_PRELOAD or similar mechanism (not shown).

Either way, the perating system will search for the MPI_Init symbol in the TEMPI library. As it is found there, that function will be called instead of the system MPI. Internally, TEMPI may ultimately call some system MPI function after introducing its own functionality. This is achieved through the dlsym function. Any parts of the MPI interface that TEMPI does not cover will fall back to the system MPI library automatically.

4 MPI DERIVED TYPE HANDLING

To facilitate handling of equivalent datatypes, we introduce a two phase translation and transformation approach to convert the MPI datatype to a common format describing all N-dimensional strided patterns. The standard advises that "the system may compile at commit time an internal representation for the datatype...and select the most convenient transfer mechanism." [12, p. 110]. In line with that advice, TEMPI's translation and transformation is implemented within the MPI_Type_commit function and cached for later use in pack and send operations.

Two operations occur once for each unique type constructed using MPI_Type_commit():

(1) Translation to an internal representation (IR)
(2) Transformation to a common representation to facilitate kernel selection.

The IR is a tree of *Type* modeled after the graph of MPI derived types. Each *Type* represents a (possibly non-contiguous) set of bytes from a memory region. Each *Type* has a field *data* of *TypeData*, which represents information about the node and is also used to discriminate the kind of node. Each *Type* also tracks zero or more of its children. The root of the *Type* tree and its children describe the MPI datatype, the structure of the tree matches the pattern of the constructed MPI datatype. The IR currently includes two kinds of TypeData; *DenseData* for contiguous bytes, and *StreamData* for strided patterns of a single child Type. *DenseData* plays the same role as a named type in MPI: it represents a sequence of contiguous bytes and has no children.

(1) *DenseData*
  (a) offset *integer*, the number of bytes between the lower bound and the first byte of the Type
  (b) extent *integer*, the number of contiguous bytes in the Type
(2) *StreamData*, a strided sequence of elements of the child type
  (a) offset *integer*, as DenseData
  (b) integer *stride*, the number of bytes between elements
  (c) integer *count*, the number of elements in the stream

4.1 Conversion

The first phase of the datatype handling process is to convert the MPI derived datatype into a *Type*. This is done by converting each MPI datatype to a corresponding DenseData or StreamData node, and then recursively doing the same to its children before attaching them to the converted node. The recursive base case is when an MPI Named type is reached, which by definition have no children. Algorithm 1 shows the `from_mpi_type` procedure, which delegates based on the incoming MPI type.

Algorithm 2 shows how an MPI named type (MPI_INT, etc), is converted into a *Type*. A named type is not a derived type, so it has no children. All MPI named types are dense, so the *extent* field of the DenseData is set to the extent of the MPI type, and the bytes start at offset 0.

Algorithm 1: from_mpi_type

```
input  : MPI datatype d
output : Type ty
if d is vector then
    return from_vector(d);
end
else if d is contiguous then
    return from_contiguous(d);
end
else if d is named then
    return from_named(d);
end
else if d is subarray then
    return from_subarray(d);
end
```

Algorithm 2: from_named

```
input  : MPI named type t
output : Type ty
DenseData tyData;
data.offset ← 0;
data.extent ← extent(t);
ty.data ← data;
```

Algorithm 3 shows how an MPI Contiguous type (MPI_Type_contiguous, etc), is converted into a *Type*. This is a special case of a strided layout where the stride matches the size of the element. The first element is at offset 0.

Algorithm 3: from_contiguous

```
input  : MPI contiguous type c
output : Type ty
StreamData data;
data.offset ← 0 data.stride ← extent(c.oldtype);
data.count ← c.count;
ty.data ← data;
ty.child ← from_mpi_type(v.oldtype);                    ▷ recursive descent
```

Algorithm 4 shows how an MPI vector type (MPI_Type_vector), is converted into a *Type*. A Vector generally represents a nested pair of strided patterns. The inner pattern is the set of elements that make up a block, and the outer pattern is the stride between blocks. For the inner type, *count* is the number of elements in the block, and *stride* is the MPI extent of each element. For the outer type, *count* is the number of blocks, and *stride* is computed as the MPI extent of each element times the stride provided to the vector constructor. The child of the inner stride is a Type constructed from the MPI vector element. Both Types have offset 0.

Algorithm 5 shows how an MPI hvector type (MPI_Type_create_hvector), is converted into a Type. It matches the conversion from MPI vector, except the outer stride is explicitly provided in the MPI hvector constructor and does not need to be derived from other fields.

Algorithm 4: from_vector

```
input  : MPI vector v
output : Type ty
Type child;
StreamData tyData;
StreamData chData;                                              ▷ child data
tyData.offset ← 0;
tyData.count ← v.count;                                         ▷ outer stream
tyData.stride ← extent(v.oldtype) × v.stride;
cdData.offset ← 0;
chData.count ← v.blocklength;                                   ▷ inner stream
chData.stride ← extent(v.oldtype);
ty.data ← tyData;
child.data ← chData;
Type gchild ← from_mpi_type(v.oldtype);                         ▷ type tree
child.child ← gchild;
ty.child ← child;
```

Algorithm 5: from_hvector

```
input  : MPI hvector v
output : Type ty
Type child;
StreamData tyData;
StreamData chData;                                              ▷ child data
tyData.offset ← 0;
tyData.count ← v.count;                                         ▷ outer stream
tyData.stride ← v.stride;                          ▷ hvector stride provided in bytes
chData.offset ← 0;
chData.count ← v.blocklength;                                   ▷ inner stream
chData.stride ← extent(v.oldtype);
ty.data ← tyData;
child.data ← chData;
Type gchild ← from_mpi_type(v.oldtype);                         ▷ type tree
child.child ← gchild;
ty.child ← child;
```

Algorithm 6 shows how an MPI subarray type (MPI_Type_create_subarray, etc), is converted into a *Type*. Each dimension of the subarray is represented as a nested stride, with dimension 0 being lowest in the *Type* tree. The count of dimension is provided by the corresponding subarray *subsize*. The stride of dimension i is the product of the MPI extent of the element and the $i-1$ subarray sizes. The offset of each dimension is given in terms of elements and is converted to bytes for the *TypeData*.

Algorithm 6: from_subarray

```
input  : MPI subarray s
output : Type ty
datas ← [];
extent ← extent(s.oldtype);
for i ← 0 to s.ndims do
    StreamData data;
    data.stride ← extent;
    data.off ← s.size[i] × extent;
    for j ← i + 1 to s.ndims do
        data.stride ← data.stride × s.size[j];
        data.off ← data.off × s.size[j];
    end
    data.count ← s.subsize[i];
    datas.prepend(data);
end
ty ← from_mpi_type(v.oldtype);                          ▷ build type tree
for i ← 0 to s.ndims do
    Type parent;
    parent.data ← datas[i];
    parent.child ← child;
    ty ← parent;
end
```

4.2 Simplification

The construction of the Type tree described in Section 4.1 yields trees of StreamData with a leaf node of DenseData. In order to provide fast handling of equivalent types, these various representations need to be canonicalized and optimized.

We introduce two transformations are used to canonicalize the Type tree. *Dense Folding* collapses DenseData into a parent StreamData. *Stream Elision* removes a StreamData representing a stream of one element. The optimizations are applied repeatedly in turn, only terminating when neither optimization modifies the *Type*. Algorithm 7 shows the overall simplification process.

Algorithm 7: simplify

```
input  : Type ty
output : Type simplified
simplified ← ty
changed ← TRUE
while changed do
    changed ← FALSE
    changed ← changed ∨ dense_fold(simplified)
    changed ← changed ∨ stream_elision(simplified)
end
```

4.2.1 Dense Folding. The first optimization is driven by the observation that stride of a StreamData may match the extent of a child DenseData. Such a configuration represents a stream of repeated contiguous dense elements. In that

```
MPI_Type_vector(copyExt.x, 1, 1, MPI_BYTE, &row);
MPI_Type_create_hvector(copyExt.y, 1,
   allocExt.x, row, &plane);
MPI_Type_create_hvector(copyExt.z, 1,
   allocExt.x * allocExt.y, plane, &cube);
```

```
StreamData{count:47,stride:131072}
 StreamData{count:1,stride:3172}
  StreamData{count:13,stride:256}
   StreamData{count:1,stride:100}
    StreamData{count:100,stride:1}
     StreamData{count:1,stride:1}
      DenseData{extent: 1}
```

```
int array_of_sizes[3]
    {allocExt[0], allocExt[1], allocExt[2]};
int array_of_subsizes[3]
    {copyExt[0], copyExt[1], copyExt[2]};
int array_of_starts[3]{0, 0, 0};
MPI_Type_create_subarray(
    3, array_of_sizes, array_of_subsizes,
   array_of_starts, MPI_ORDER_C, MPI_BYTE, &cube);
```

```
StreamData{count:47,stride:131072}
 StreamData{count:13,stride:256}
  StreamData{count:100,stride:1}
   DenseData{extent: 1}
```

```
int array_of_sizes[2]{allocExt[0], allocExt[1]};
int array_of_subsizes[2]{copyExt[0], copyExt[1]};
int array_of_starts[2]{0, 0};
MPI_Type_create_subarray(
    2, array_of_sizes, array_of_subsizes,
   array_of_starts, MPI_ORDER_C, MPI_BYTE, &plane);
MPI_Type_vector(copyExt[2], 1, 1, plane, &cube);
```

```
StreamData{count:47,stride:131072}
 StreamData{count:1,stride:131072}
  StreamData{count:13,stride:256}
   StreamData{count:100,stride:1}
    DenseData{extent: 1}
```

Fig. 3. C MPI code to generate equivalent subarrays, and the corresponding nested Type structure. Note that the C code constructs from the bottom up, but the nested type structure is shown with the root at the top.

case, the DenseData extent can be "folded" up into the StreamData, and the pair can be represented as a single DenseData node. This scenario may arise when an MPI vector, subarray, or contiguous type is used to describe a contiguous region larger than any MPI named type.

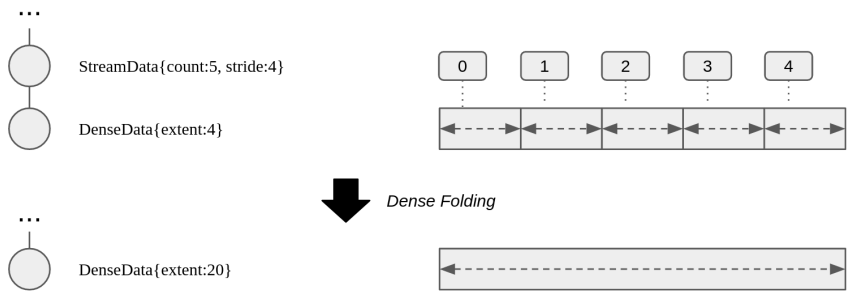


Fig. 4. Example of Dense Folding. When the extent of a DenseData matches the stride of a parent StreamData, the parent/child combination can be replaced with a single larger DenseData.

Algorithm 8 shows how the transformation is applied to a *Type*, and Fig. 4 shows an example. The transformation is applied to each Type node of the Type tree in a depth-first order. At each node, the transformation only applies if the node (*ty*) is a StreamData kind and the node's child (*child*) is a DenseData. If the parent's *stride* matches the child's *extent*, the parent is replaced with a larger DenseData node that represents the entire contiguous stream. The child's offset is increased to include any offset the parent had.

Algorithm 8: dense folding

```
in/out : Type ty
output : changed
changed ← FALSE;
for child of ty do
    dense_folding(child);                                   ▷ fold from bottom up
end
if ty.data is not StreamData then
    return changed;
end
Type child = ty.children[0];
if child.data is not DenseData then
    return changed;
end
StreamData cData ← child.data;
StreamData pData ← ty.data;
if cData.extent == pData.stride then
    changed ← TRUE;
    cData.off ← cData.off + pData.off;
    cData.extent ← pData.count × pData.stride;
    ty ← child;                                             ▷ replace ty with child
end
return changed
```

4.2.2 Stream Elision. Consider *ty*, a StreamData with a child StreamData whose count is one. In such a case, *child* is a single element and can be elided. This construction arises in the case of an MPI vector with *blocklength* one, or a subarray dimension with *subsize* one.

Algorithm 9 shows how the transformation is applied to a *Type*, and Fig. 5 shows an example. Like with dense folding, stream elision is applied separately to each Type node in a depth-first order. After that, if both the type *ty* and its child *child* are StreamData, then if the child has count of 1, the child is replaced with its own children.

4.3 Kernel Selection

Once the type is canonicalized, it is converted into a StridedBlock structure. The StridedBlock structure is semantically similar to an MPI subarray.

(1) *StridedBlock*
   (a) integer *start*: byte offset between the lower bound and the first element
   (b) integer[] *counts*: number of elements in the dimension

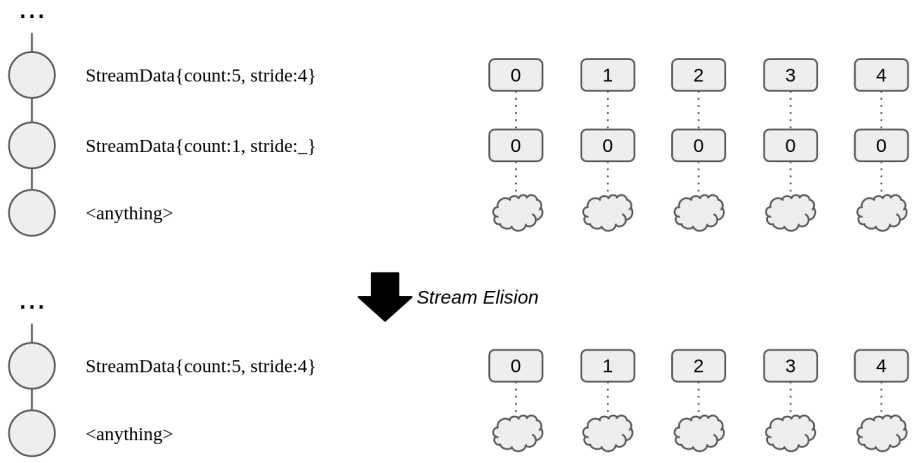


Fig. 5. Example of Stream Elision

Algorithm 9: stream_elision procedure

```
in/out : Type ty
output : changed
changed ← FALSE;
for child of ty do
    changed ← changed ∨ stream_elision(child);          ▷ elide from the bottom up
end
if ty.data is not StreamData then
    return changed;
end
Type child = ty.child;
if child.data is not StreamData then
    return changed;
end
StreamData cData ← child.data;
if 1 == cData.count then
    changed ← TRUE;
    ty.child ← child.children;                  ▷ replace child with its own children
end
return changed
```

(c) integer[] *strides*: bytes between the start of each element in the dimension

The first byte is *start* bytes from some arbitrary starting point. Each dimension describes *count* repetitions of the previous dimension, separated by *stride* bytes.

Algorithm 10 describes the conversion from *Type* to *StridedBlock*. This is only possible if the bottom is a DenseData and every other object is a StreamData. The process in Section 4.2 will apply the conversion if it is possible. The DenseData describes the first dimension, which will have stride 1 and count equal to the extent of the DenseData. Each

higher dimension directly corresponds to the StreamData. The offset of each dimension is accumulated into the single offset of the StridedBlock.

Algorithm 10: stream_elision procedure

```
in/out : Type ty
output: StridedBlock sb
datas ← [];
cur ← ty;                                                    ▷ Add all datas to an array
while true do
    datas.append(cur);
    if cur.children().size() == 0 then
        break;
    end
    else if cur.children().size() == 2 then
        return NULL;                                                    ▷ Not strided
    end
    else
        cur ← cur.children()[0];
    end
end
for i = 0 to datas.size() do
    if i == 0 then
        if data is DenseData then
            sb.off ← data.off;
            sb.counts.append(data.extent);
            sb.strides.append(1);                                ▷ DenseData stride is 1
        end
        else
            return NULL;                                                ▷ Not strided
        end
    end
    else
        if data is StreamData then
            sb.off ← sb.off + data.off;
            sb.counts.append(data.count);
            sb.strides.append(data.stride);
        end
        else
            return NULL;                                                ▷ Not strided
        end
    end
end
return sb;
```

Once the *Type* is converted into a *StridedBlock*, the next task is to choose a method for fast packing and unpacking on the GPU. If the StridedBlock is 1D (contiguous), we issue a single cudaMemcpyAsync to move the data into the destination buffer, followed by a cudaStreamSynchronize. This is similar to the implementation in MVAPICH, OpenMPI,

and Spectrum MPI. If the StridedBlock is 2D we select a kernel that maps the X-dimension of the thread index into the blockLength and the Y-dimension to the number of blocks. If the StridedBlock is 3D, we map the X dimension to the block length, Y dimension to the inner count, and Z dimension to the outer count. Higher dimensional objects can follow the same general pattern, with additional outer loops for each dimension.

Each kernel is specialized to a "word size" W, which is the largest GPU-native type that is both aligned to the object and is a factor of the blockLength. Each thread loads and stores elements of size W. At type-commit time, the appropriate W is chosen for each type.

In addition to a datatype, Pack and Unpack accept an incount/outcount parameter, which specify how many of the datatype are present in the input buffer. This could be viewed as an additional nested stride on the type, except that it is not known until the Pack/Unpack call and therefore is not included in the type optimization. Therefore, the kernels all handle this value dynamically.

Each kernel dimension is filled from X to Z by the largest power of two that encompasses the structure described above, ultimately limited by a block limit of 1024 threads. The grid is sized to cover the entire input object once the block size is chosen.

5 RESULTS

SpecturmMPI 10.3.1.2, MVAPICH2 2.3.4 and OpenMPI 4.0.5 all support a derived datatype handling approach, where each contiguous portion of the derived datatype are copied into a contiguous buffer through cudaMemcpyAsync (or similar function). These baselines are compared against the combined type optimization and kernel selection method described here, and implemented in the TEMPI library.

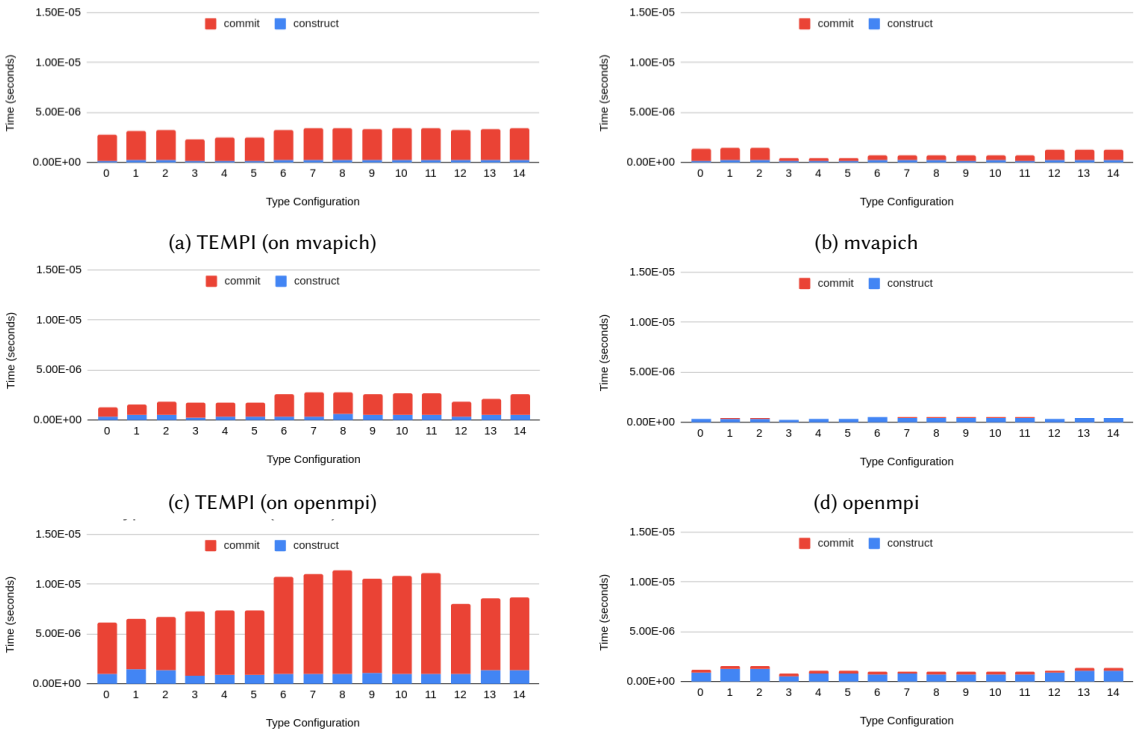
5.1 Experimental Environments

The experiments are carried out on three MPI implementations spanning two hardware platforms. All multi-node performance is evaluated on OLCF Summit, where only a single MPI implementation is suported. Pack performance is evaluated on the single-node *openmpi* and *mvapich* platforms.

	OLCF Summit	**openmpi**	**mvapich**
MPI	Spectrum MPI 10.3.1.2	OpenMPI 4.0.5	Mvapich 2.3.4
CPU	IBM POWER 9	AMD Ryzen 7 3700x	
GPU	Nvidia V100	Nvidia GTX 1070	
nvcc	11.0.221	11.1.105	
gcc	9.3.0	10.2	
Nvidia Driver	418.116.00	455.32.00	

5.2 MPI_Type_commit

The type transformation and kernel selection process is executed when the application calls MPI_Type_commit. Fig. 6 shows the run-time impact of creating MPI derived types, broken down into two phases. Construction refers to using the MPI_Type and MPI_Type_create functions to assemble the type description. Commit refers to calling MPI_Type_commit on that description. TEMPI does the same operations in each instance; however, it relies on the performance of the MPI_Type_get_envelope, MPI_Type_get_extent, MPI_Type_size, and MPI_Type_get_contents functions. The different implementations will have different performance for those routines, and therefore the "commit" component takes variable amounts of time. Within a particular implementation, different type configurations have different commit



(a) TEMPI (on mvapich)

(b) mvapich

(c) TEMPI (on openmpi)

(d) openmpi

(e) TEMPI on Summit

(f) Summit

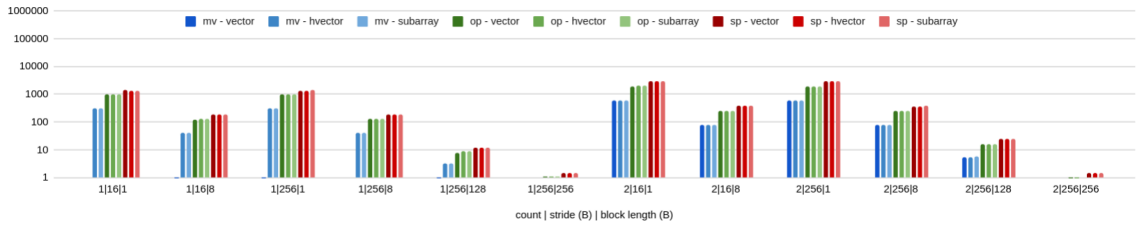
Fig. 6. Breakdown of MPI derived type construction and commit time for a variety of strided objects. The "construction" component is uses MPI_Type* and MPI_Type_create* family of MPI functions to describe the type. The "commit" component is how much time is consumed in MPI_Type_commit. The trimean of 30000 executions of each phase is reported. Though TEMPI does the same operations regardless of the MPI implementation, it uses MPI function calls, which have different performance characteristics in different implementations. Within an implementation, the commit time varies as different configurations require different transformations to arrive at the canonical form.

times as a different sequence of optimizations is run to arrive at the canonical form. Overall, the transformation and kernel selection process slows down the create+commit process by 2.1× to 5.5× vs mvapich, 3.5× to 6.8× vs openmpi, and 4.2× to 11, 6× vs Summit. This slowdown is a one-time cost during program startup and is small in magnitude.

5.3 MPI_Pack and MPI_Unpack

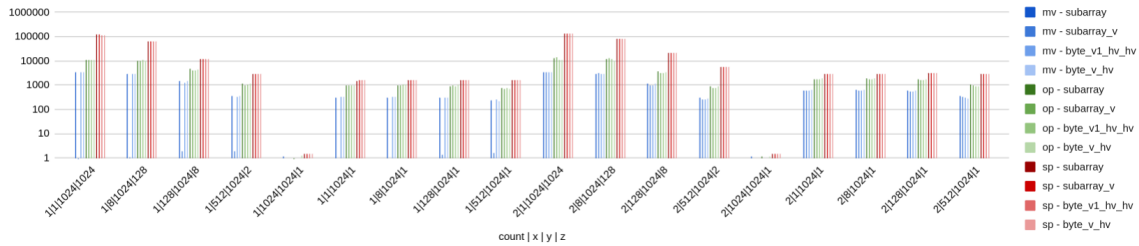
Once a type has been committed, it can be used in a communication routine. The simplest examination of such a routine is MPI_Pack, where a buffer is "sent" into another buffer in the same process. When GPU buffers are passed to the *inbuf* and *outbuf* parameters of MPI_Pack/Unpack, TEMPI uses the selected GPU kernel to complete the packing.

Fig. 7 shows the pack bandwidth achieved for various objects. First, for Vector types, MVAPICH2 achieves slightly better performance thanks to specialized kernel implementations for different named types. For equivalent datatypes represented as an Hvector or Subarray, MVAPICH falls back to a baseline implementation, where each separate contiguous region of the datatype is transferred with a cudaMemcpyAsync (or equivalent). The single-kernel of TEMPI greatly surpasses the achieved bandwidth, from 3× to 22, 000× faster. Generally, the kernel performance is relatively



(a) Speedup for 1 KiB 2D objects equivalently represented through a vector, hvector, and subarray. Mvapich has specialized single-vector handling, yielding a speedup 1 for those cases. All implementations achieve similar results for contiguous data, with speedups $< 1.5\times$. Overall, speedup ranges from $0.9\times$ in contiguous blocks to $2850\times$ for multiple objects of small blocks with large strides.

(b) Speedup for 1 MiB 2D objects equivalently represented through a vector, hvector, and subarray. Mvapich has specialized single-vector handling, yielding a speedup 1 for those cases. All other implementations and types are handled with one copy per contiguous block. All implementations achieve similar results for contiguous data, with speedups $< 1.5\times$. Overall, speedup ranges from $0.98\times$ in contiguous blocks to $720,400\times$ for multiple objects of small blocks with large strides.



(c) Speedup for 3D objects vs mvapich (mv), openmpi (op), and Summit (sp). Each object is equivalently represented in a variety of ways. x, y, z represent the size of a $1024B^3$ allocation that is packed. MVAPICH has specialize handling of a single vector of subarray (but not a subarray), yielding speedup close to 1. All other implementations and types are handled with one copy per contiguous block. Overall, speedup ranges from $0.89\times$ for contiguous types to $140,000\times$ objects with small x dimensions.

Fig. 7. TEMPI speedup for objects vs mvapich (mv), openmpi (op), and Summit (sp). Each object is equivalently represented through a vector, hvector, and subarray. MPI_Pack small 2D, large 2D, and 3D objects. Speedup varies from 0.89 to 720, 400. mvapich contiguous results (1|256|256, 2|256|256, 1|1024|1024|1 and 2|1024|1024|1) are omitted due to a bug that impacts its correctness. MVPAICH2 tends to perform best, and Spectrum MPI the worst, due to MVAPICH2's minimal synchronization, and SpectrumMPI's multiple transfers for large contiguous regions. As most types are handled with the copy-per-block method, performance is best when blocks are larger and fewer. In nearly all cases, TEMPI dramatically exceeds existing performance.

better when the contiguous regions are smaller or the total data is larger. In the first case, more memory copies are consolidated into a single kernel, and in the second case, the GPU resources in the kernel are more fully utilized.

MVPIACH2 2.3.4 has a semantic bug for support for continuous datatypes. It uses cudaMemcpy for device-to-device copies, but cudaMemcpy is not synchronous with the host in that specific scenario. Therefore, MPI_Pack may return before the input buffer is transferred to the output buffer, allowing the input buffer to be modified while the MPI_Pack is

still executing. For this reason, we omit MVAPICH2's contiguous data transfer performance in this comparison. Mvapich also shows the fragility of specializing to particular types. It handles a vector of subarrays hundreds or thousands of times faster than a single subarray describing the same region.

5.4 MPI_Send

MPI allows datatypes to be directly used with MPI_Send and other communication routines. We consider three ways to jointly handle datatypes with communication. All experiments are limited to the Summit platform, the only evaluation platform with multiple GPUs and multiple nodes.

In the "device" packing method (T_{device}), the strided object is packed from the original GPU buffer into an intermediate GPU buffer ($T_{gpu-pack}$), then transferred to an intermediate buffer on the destination GPU with CUDA-aware MPI_Send ($T_{gpu-gpu}$, then unpacked into the strided destination object ($T_{gpu-unpack}$).

$$T_{device} = T_{gpu-pack} + T_{gpu-gpu} + T_{gpu-unpack} \tag{1}$$

In the "oneshot" packing method (T_{device}), the strided object from the original GPU buffer into intermediate mapped CPU buffer ($T_{host-pack}$), transferred to an intermediate mapped buffer at the destination ($T_{cpu-cpu}$, then unpacked directly into GPU memory ($T_{host-unpack}$).

$$T_{oneshot} = T_{host-pack} + T_{cpu-cpu} + T_{host-unpack} \tag{2}$$

Finally, in the "staged" method (T_{device}) matches the device method, except the intermediate GPU buffer is transferred to a pinned buffer on the host (T_{h2d}), where it is transferred to the destination rank's CPU before being copied to the destination GPU (T_{h2d}). This method would only be faster than the device method if $T_{cpu-cpu} + T_{h2d} + T_{d2h} < T_{gpu-gpu}$.

$$T_{staged} = T_{device-pack} + T_{d2h} + T_{cpu-cpu} + T_{h2d} + T_{gpu-unpack} \tag{3}$$

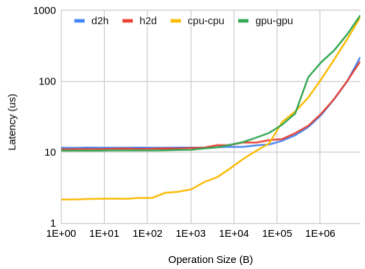
To understand which method is fastest, we measure the performance of several primitives.

- $T_{cpu-cpu}$: MPI_Send/MPI_Recv on CPU buffer
- $T_{gpu-gpu}$: MPI_Send/MPI_Recv on GPU buffer
- T_{d2h}: cudaMemcpyAsync from device (GPU) to host (CPU) and cudaStreamSynchronize
- T_{h2d}: cudaMemcpyAsync from host to device and cudaStreamSynchronize

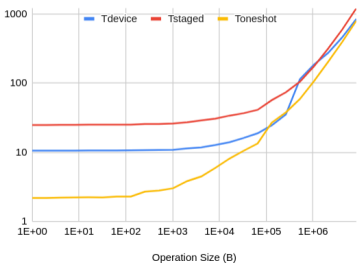
The MPI operations are measured through a ping-pong between two ranks, and the reported time is half of the total ping-pong time. The two ranks are on separate nodes. The CUDA operations are recorded using wall-time around the first and last calls, reflecting when control leaves and returns to the application.

Fig. 8a shows the results of the four operations for various data sizes. CUDA-aware MPI transfers show a latency floor of about ≈11 µs. This almost exactly equal to the floor for CUDA device-to-host and host-to-device transfers, suggesting that the same overhead dominates both operations. For the CUDA operations, the latency is from overhead of both cudaMemcpyAsync() and cudaStreamSynchronize(). The equivalent CPU-CPU MPI transfer has a minimum latency of 2.2 µs.

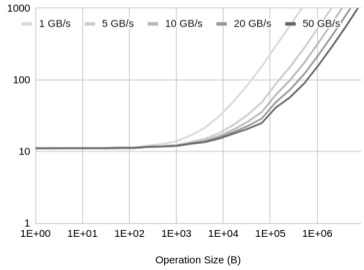
Fig. 8b partially the measurements to Eqs. 1, 2, 3 while holding $T_{gpu-gpu}$ and $T_{cpu-cpu}$ to zero. Therefore, $T_{oneshot} = T_{cpu-cpu}$, and $T_{device} = T_{gpu-gpu}$. These results show that while there is a small region where $T_{cpu-cpu} < T_{gpu-gpu}$, that difference is not enough to make the "staged" method competitive, and it will be disregarded in further discussion. The largest gap is 80 µs at 1 MiB, which is consumed by the D2H and H2D transfer time at that size.



(a) Measurements of T_{d2h}, T_{h2d}, $T_{cpu-cpu}$, and $T_{gpu-gpu}$ on Summit.

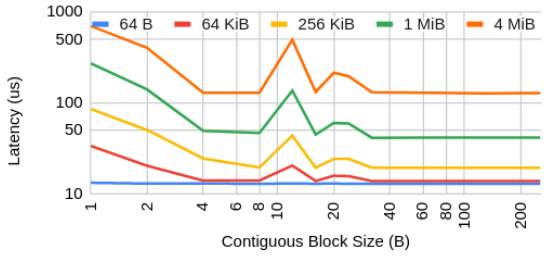


(b) Models of T_{device}, $T_{oneshot}$, and T_{staged}, **excluding** pack time, using the values in (a).

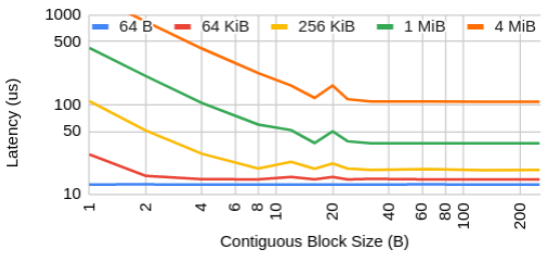


(c) Model of $T_{oneshot}$ using the values in (a) for various pack/unpack bandwidths.

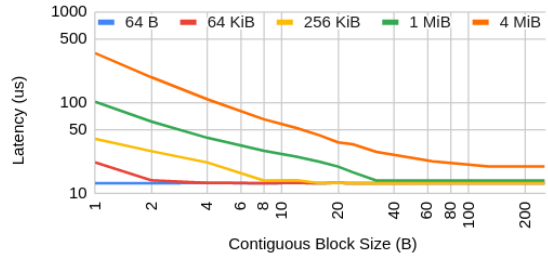
Fig. 8. Raw measurements and resulting performance models for various data transfer methods on OLCF Summit. At 8 MiB, d2h reaches 38.2 GB/s, h2d reaches 43.8 GB/s, cpu-cpu reaches 10.42 GB/s, and CUDA-aware MPI reaches 9.79 GB/s.



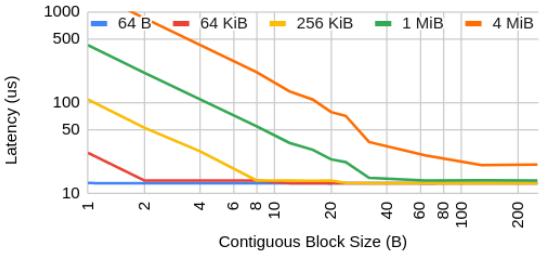
(a) Oneshot pack performance.



(b) Oneshot unpack performance.



(c) Device pack performance.

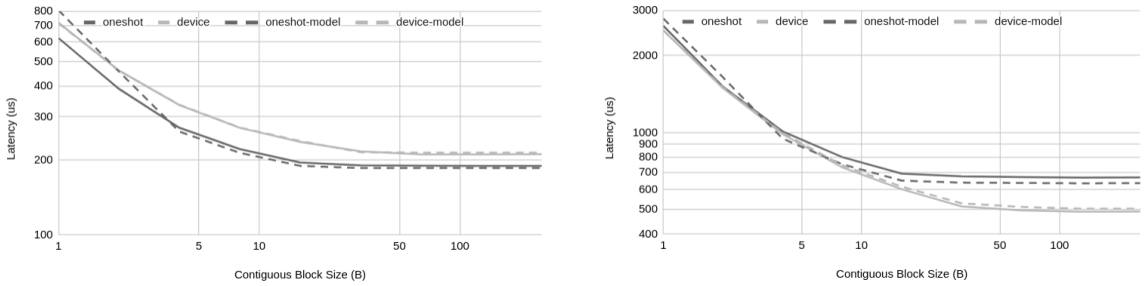


(d) Device unpack performance.

Fig. 9. Pack/unpack performance using the "oneshot" and "device" strategies for objects from 64 B to 4 MiB. For smaller contiguous regions, performance is reduced due to low memory or interconnect efficiency for non-coalesced accesses. For larger objects, performance increases as GPU resources are more fully utilized. The maximum achieved oneshot pack throughput is 32.5 GB/s (39 GB/s for unpack). For device, it is 212 GB/s (202 GB/s for unpack).

Fig. 8c shows $T_{oneshot}$, with various hypothetical pack/unpack bandwidths. It also includes a measured kernel launch time of 4.5 µs. It is clear that the latency of the oneshot method depends heavily on the pack/unpack performance. The same is true for the device method.

In contrast with the hypothetical values from Fig. 8c, Fig. 9 shows the actual performance of pack and unpack operations for "oneshot" ($T_{cpu-pack}/T_{cpu-unpack}$) and "device" ($T_{gpu-pack}/T_{gpu-unpack}$). The recorded time includes all



(a) 1 MiB object (b) 4 MiB object

Fig. 10. Measured and modeled MPI_Send performance for the "oneshot" and "device" packing strategies.

of the operations described in Section 4.3; dispatching a specialized kernel based on that word size, selecting appropriate grid dimensions, executing the kernel, and synchronizing after execution.

Fig. 9a (9b) shows the time for GPU (un)packing from (to) device memory to (from) mapped host memory. Fig. 9c (9d) shows the time for GPU (un)packing from (to) device memory to (from) mapped host memory. The performance depends both on the object size and the size of the contiguous blocks in the object. Generally, larger objects are faster as GPU resources are more fully utilized. Larger blocks also tend to be faster as more memory accesses are contiguous. For the in-device pack this effect disappears once the block is 32 B as all measured transfers larger than that fully utilize a memory transaction. For oneshot, the effect disappears at 128 B, suggesting that is the transaction size over NvLink. The unpack operation tends to be slower than the pack operation, as unpack involves uncoalesced writes and coalesced reads instead of coalesced writes and uncoalesced reads. Also noteworthy is the irregular performance for 12 B, 20 B, and 24 B measurements in the one-shot execution.

Depending on the object size and contiguous block size, $T_{oneshot}$ or T_{device} is faster. Intuitively, oneshot is faster when objects are smaller (affording less time to hide the overhead of the CUDA-aware MPI) and more contiguous (where packing over the interconnect performs best), and device is faster when objects are larger and less contiguous (where wasting the higher on-device bandwidth during packing is less costly). Fig. 10 compares the modeled and measured performance for 1 MiB and 4 MiB objects across a variety of contiguous data sizes. The "oneshot" model departs the measured performance for very small block sizes, but otherwise, the models provide a faithful prediction of the measured performance.

Finally, Fig. 11 shows the application-visible performance of the two methods MPI_Send/MPI_Recv compared to the baseline. A ping-pong of MPI_Send/MPI_Recv between a pair of ranks on different nodes is measured 1000 times. The results presented are half of the trimean of those samples, to measure a single send/recv pair.

Speedup varies from 1.07× for large contiguous regions to 59000× for large objects with small blocks. Most of the performance improvement comes from the pack/unpack kernels, with the rest from the choice of "device" or "oneshot" packing. This is substantially less than the raw MPI_Pack and MPI_Unpack times (Section 5.3), as the contiguous transfer time (Fig. 8a) also contributes significantly to the overall time and is not accelerated by TEMPI.

5.5 Case Study: 3D Stencil

The enormous datatype handling performance has a commensurate impact on application performance. Here we consider a 3D stencil code, where the total stencil region is $512^3 \times P$ gridpoints and P is the number of ranks. Each

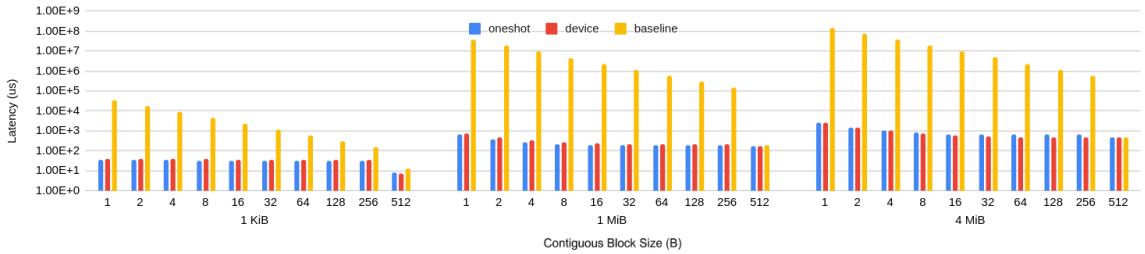


Fig. 11. Time for an MPI_Send/MPI_Recv pair for 1KiB, 1MiB, and 4MiB 2D objects with contiguous blocks of various sizes.

gridpoint is a single four-byte value, and the stencil radius is 2. Each halo region is defined in a separate MPI dervied datatype and packed into the single buffer using MPI_Pack. Halo exchange is implemented as an MPI_Alltoallv on that single buffer. Then, the recieve buffer is unpacked. The stencil kernel is a standard 26 point, yeilding 26 neighbors for each rank with periodic domain boundaries. This means each rank engages in 26 MPI_Pack and 26 MPI_Unpack operations on a variety of different 3D strided datatypes.

Fig. 12 shows TEMPI's speedup vs the baseline SpectrumMPI implementation, broken into total speedup, pack speedup, and unpack speedup. The difference between pack and unpack speedup is solely related to the elided synchronization described in Section 5.3. The speedup is smallest for larger number of ranks, as the communication takes up a relatively larger amount of the total iteration time compared to the pack and unpack operations.

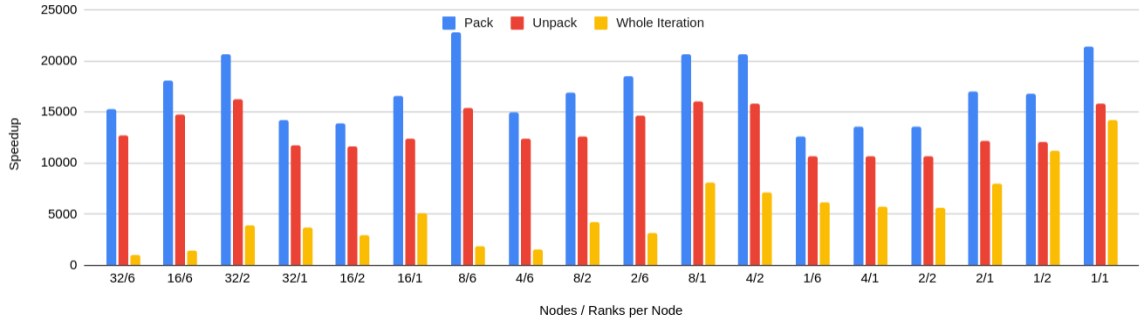


Fig. 12. Speedup of 3D stencil halo exchange operation using TEMPI vs SpectrumMPI 10.3.1.2. The variation in pack/unpack speedup is driven by the aspect ratio of the subdomain on each GPU. The larger the x-dimension, the lower the TEMPI speedup is. The iteration speedup is smaller for more ranks because the inter-GPU communication takes relatively longer part of the interation time.

6 FUTURE WORK

This work could be extended to cover indexed and struct types with some additional kernels. Prior work also suggests that pipelining packing operations with MPI send operations is optimal. The performance model in this work could be extended to model that case. CUDA provides native APIs to handle 2D and 3D objects using the DMA engine: cudaMemcpy2D* and cudaMemcpy3D*. For scenarios where those functions apply, they could be used for packing and unpacking data. Finally, the type analysis is restricted to a tree, where MPI datatypes are more properly modeled as DAGs. A more complicated type analysis could be executed for non-tree derived types.

7 RELATED WORK

Prior work has tended to focus on an implementation of GPU datatype handling that is integrated with MPI communication. While this allows low-level optimization to improve latency, it hinders adoption of the improvements since they must be integrated with an MPI implementation. TEMPI wraps the relevant portion of an existing MPI interface to allow applications to gain some improvement without waiting for MPI upgrades or managing datatypes explicitly in application code.

Further, substantial prior work uses GPU kernels to accelerate datatype operations. TEMPI is the first work that shows transformations on structured datatypes for canonicalization (as opposed to reducing everything to a list of offsets and lengths). This has the advantage of a wide coverage using a few simple, fast kernels, at the expense of complete support for all possible MPI types.

The MPITypes library [10] appears to represent one of the first attempts to generalize datatype handling outside of MPI. It provides several functions for flattening and copying datatypes, and a framework for extending those operations. As TEMPI tries to maintain the strucured information of types to facilitate GPU acceleration.

[13] describes an early approach in MVAPICH2. cudaMemcpy2D was used to move GPU data either directly to the destination GPU, or into a contiguous buffer before being sent over the network. Since MVAPICH 1.92a, MVAPICH has used kernels to handle vector and hindexed datatypes [8], which is still the case as of 2.3.4. Different kernels for different named datatypes exist, but no optimizations are present for nested datatypes, or operations on more than one datatype.

[7] attempts to provide fast handling of arbitrary MPI datatypes on the GPU. It is similar to TEMPI structurally, with a transformation phase and a kernel selection heuristic. Unlike TEMPI, nested types are represented by a tree structure that must be traversed by each GPU thread using division, modulo, and binary search operations. Furthermore, data is written directly to mapped host memory instead of staging in the GPU. This may accelerate data transfer when CPU-CPU sends are faster than GPU-GPU sends.

[11] also explicitly breaks the problem into transformation and kernel selection phase. Hand defines specific kernels for handling VectorHvector, Subarray, and indexed Block types. For other datatypes, it transforms a variety of datatypes into a blocklist, for which it has a specific kernel implementation. TEMPI recognizes that many nested regular types reduce to (essentially) a subarray, and explicitly designs a transformation and optimal packing kernel to cover all of those scenarios.

[14] describe a fork of OpenMPI that integrates derived datatype handling both on the GPU itself as well as communication between nodes. The datatype is ultimately represented as a list of blocks, and blocks are partitioned among separate kernels with pipelined communication. It also identifies that full GPU resources for handling non-contiguous data are not needed to saturate the communication links. This fork has remained unmerged and not publicly available - TEMPI can currently be used with OpenMPI.

[1] recognizes that one of the challenges of all prior work is the latency of kernel launches. Like prior work, it also represents the datatypes as a list of displacements and lengths. Similar to this work, it defines extraction, conversion, and caching steps. It defines a “one-shot” packing and unpacking, where the non-contiguous GPU data is directly packed into (or unpacked from), a CPU buffer. TEMPI is also able to pack with a single kernel launch. It does not identify that there are certain scenarios where the one-shot method may not be fastest due to inefficiency of packing and unpacking over the interconnect.

[2] identifies that a major cost of transfer is the launch of the packing kernels. They develop an engine that is able to merge various packing requests into a single kernel launch. TEMPI addresses the packing kernel launch cost only by issuing a single kernel for multiple copies of the same MPI datatype.

[5] describes a wholistic zero-copy-based data movement system for MPI datatypes. They include kernels where a warp is responsible for a contiguous block in a block list. They also describe a variety of integrations with the underlying communication library, which TEMPI does not address.

8 CONCLUSION

ACKNOWLEDGMENTS

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A ONLINE RESOURCES

TEMPI is hosted at https://github.com/cwpearson/tempi