Abstract—Over the past two decades, C++ has been adopted as a major HPC language (displacing C to a large extent, and Fortran to some degree as well). Idiomatic C++ is clearly how C++ is being used nowadays. But, MPI’s syntax and semantics defined and extended with C and Fortran interfaces that align with the capabilities and limitations of C89 and Fortran-77. Unfortunately, the language-independent specification also clearly reflects the intersection of what these languages could syntactically and semantically manage at the outset in 1993, rather than being truly language neutral.

In this paper, we propose a modern C++ language interface to replace the C language binding for C++ programmers with an upward-compatible architecture that leverages all the benefits of C++11–20 for performance, productivity, and interoperability with other popular C++ libraries and interfaces for HPC. Demand is demonstrably strong for this second attempt at language support for C++ in MPI after the original interface, which was added in MPI-2, then was found to lack specific benefits over the C binding, and so was subsequently removed in MPI-3.

Since C++ and its idiomatic usage have evolved since the original C++ language binding was removed from the standard, this new effort is both timely and important for MPI applications. Also, many C++ application programmers create their own, ad hoc shim libraries over MPI to provide some degree of abstraction unique to their particular project, which means many such abstraction libraries are being devised without any specific commonality other than the demand for such.

I. INTRODUCTION

The Message Passing Interface (MPI) has been the ubiquitous programming model for scalable computing since 1994. But, as MPI ages, it is clear it is held back in terms of function and performance by the close ties between the concepts that constitute MPI and the languages in which it was originally expressed. This drawback was most recently evidenced by the introduction of the large-count procedures, which doubled and wrapped the key MPI concepts as classes and for operations naturally. We use C++ as the target language in the bulk of this paper, and show how even minimal C++ features of which MPI could take advantage. Section V considers the consequences of introducing new language interfaces to MPI. Section VI explores approaches that have been taken in the community to introduce higher level language interfaces to MPI. The gap addressed by these community-led projects is that, as it is currently standardized, does not allow for modern applications or languages to make use of it idiomatically. The language-independent specification effectively gates MPI concepts behind the C89 and Fortran-77 languages.

Here, we propose the official introduction of higher level languages to the MPI Standard in addition to the standardized C and Fortran interfaces. By introducing a common layer for a given language, we fulfill the same goal as the originally standardized languages: to enable development of an MPI application with performance-portability between implementations. For each such standardized language, we could choose to accommodate language features that are either difficult or impossible to support effectively through a community-led project based on the current MPI Standard. This approach enables expression of MPI idiomatically for each language while keeping the core concepts uniform across all expressed languages. First-class MPI concepts are thereby standardized for all languages while each language expresses those semantics and operations naturally. We use C++ as the target language in the bulk of this paper, and show how even minimal use of C++ can make huge improvements over the C interface.

The remainder of this paper is organized with Section II discussing the MPI C++ interface that was introduced in MPI 2.0, and mention its shortcomings; then, Section III examines how the C MPI interface holds MPI back as a whole. Section IV explores approaches that have been taken in the community to introduce higher level language interfaces to MPI. Section V considers the consequences of introducing new language interfaces to MPI. Section VI looks at potential C++ features of which MPI could take advantage. Section VII introduces a minimally extended C++ language interface to MPI that attempts to remain as close to the present C interface as possible while still introducing C++ concepts. Section VIII discusses mixing C++ and C MPI code and libraries. Finally, we conclude and offer final recommendations in Section IX.

II. THE FAILURE OF C++ BINDINGS IN MPI 2.0

The MPI C++ bindings extended the MPI C object-based design and wrapped the key MPI concepts as classes and for the most part retained a one-to-one correspondence between
the C and C++ APIs. This was a deliberate decision of the MPI Forum [5]: many of the object-oriented features provided by C++ were therefore not fully utilized. In addition, as the C++ language evolved, there was no effort to update the MPI C++ bindings. As a result, the MPI C++ bindings were not widely used by newly designed C++ applications. MPI implementers were faced with a daunting task of supporting these bindings that were not widely used. Eventually, the MPI Forum decided to deprecate the MPI C++ bindings in the MPI-2.2 [6] standard and removed this feature in the MPI-3.0 [7] standard.

III. THE C INTERFACE HOLDS C++ PROGRAMMERS BACK

Using MPI in a C application is not an issue. But, many issues arise for C++ using MPI using the C interface:

- All C++ data structures need either to be converted to or be native to C.
- One cannot use a huge part of the C++ language: templates, classes, type specialization, lambdas, polymorphism, exceptions, iterators, ranges, etc.
- Info arguments and assertions that could be compile-time-optimized must be runtime analyzed with C.
- Efficient C++ constructs, such as smart pointers and reference-counted arrays, are useless with the C interface. All memory and scope management of objects and aliases are manual and must be handled with extreme care whereas these are easy to manage in modern languages.
- There is no encapsulation. MPI specifies a global set of functions, without name-spacing; many procedures take weakly typed request objects, which are polymorphic.
- C is not flexible/expressive enough to address 64-bit support vs. 32-bit legacy issues. Big count needed to double up 157 C interfaces. C++ and modern Fortran have overloading and largely skirt this issue.

It also should be noted the purely layered C++ interfaces aren’t enough, because a native C++ library should be optimized to be as fast as faster than a C interface when coupled with a suitable MPI implementation. Therefore, a standard language interface is needed to justify optimizing the critical path for C++ programmers.

IV. BACKGROUND AND RELATED WORK

C++ bindings for MPI began while MPI-1 was still being ratified [9]. [10]. [11]. [12] and continued until the official introduction of the C++ bindings in MPI-2. After MPI-3 discarded the interface, work evidently resumed. Prior and ongoing efforts are noted that sought to provide third-party MPI language interfaces including Java [13], C++ (e.g., [9], [11]), Spark [14], and Python [15].

A. MPJ: MPI-like Message Passing for Java

In Carpenter et al. [13], the MPJ notation for Java was introduced, providing a means to program Java with MPI-like type operations. This project has been inactive since 2000.

B. Boost MPI

Boost MPI is a historical, header-only library on top of MPI-2 that leverages the Boost library [16]. The goal was evidently to provide a higher-level abstraction like C++ STL. Boost MPI has not been widely used by major MPI applications due to its complex dependencies and use of serialization to handle user defined datatypes. Recent minor updates in 2019 follow minor updates in 2013, and end of active development in 2008.

C. MPP

MPP [17] is a header only, C++ MPI interface that uses some of the object oriented programming features of C++ such as generic programming, type traits, futures, and also supports the use of user defined datatypes. Initial performance evaluation indicated better performance when compared with Boost MPI. This interface has not been updated since 2013.

D. MPL

MPL [18] is an open-source, header-only, C++11-based implementation of a layered library on top of significant portions of MPI-3.1 [13]. The key features are as follows:

- use of `comm` and `group` objects with MPI APIs refactored into member functions (like MPI-2 C++ interface)
- reduced argument sets compared to the C interface, including polymorphic variations with functions like `gatherv` (e.g., non-root processes specify less arguments)
- return of values and request objects in non-blocking operations, not error codes like C.

MPL does not support one-sided, dynamic process management, or MPI I/O. Exceptions are thrown for various detected errors in MPL but there is no formal connection of the five exceptions it can throw to all the MPI error codes and classes.

Lastly, MPL provides useful abstractions built on top of MPI, (e.g., logical process grids and a MPI derived datatype encapsulation).

E. Ad Hoc C++ APIs

A large-scale study of MPI usage in open-source HPC applications [19] found that C++ was the most widely used language among open-source HPC applications. It appears that layering on top of the C interface is done commonly in C++-based MPI applications, particularly after MPI-3 deprecated the old C++ interface. For example, Comb [4] and HemelB [20] are two particular examples of this trend.

F. MPI4Py

MPI4Py [15] provides a Python-friendly layer on top of MPI-3.1, and works closely with NumPy [21]. While MPI4Py enables access to MPI for Python developers, it is heavily influenced by the C interface. However, the implementation of the futures package in MPI4Py shows an attempt at creating a more pythonic interface.

1Recent check-ins only as of May, 2021 have required C++17, but for superficial reasons such as adding `[[nodiscard]]` specifiers for returned values in certain functions.
V. A CAUTIONARY TALE ABOUT LANGUAGES

The introduction of new MPI language interfaces is an enticing opportunity for change. The benefits brought by this change can be of great benefit to those currently tied to using a C interface from a language that is dissimilar to C, which forces design decisions and unidiomatic language usage.

This section aims to serve as a note of caution. While introducing new features is required to advance any product, introducing too many leads to feature bloat, which is something MPI standardizers and users are intimately familiar. Therefore, the introduction of more languages and especially expressions of underlying concepts in these new languages that are unlike prior expressions must be thoroughly considered. The previously introduced C++ interface, which was deprecated and removed one major version later, shows the danger.

The central problem to introducing more languages is that the current Standard has only considered MPI through the lens of the intersection of both C and Fortran. This has resulted in a document that fundamentally ties and limits the concepts seriously considered to what is expressible in C and Fortran.

In fact, Fortran is held back in many ways given the languages advancement compared to C. If one were to decouple those two languages, accepting the cost of such an action (more complex language interaction), then each language could serve as its own interpretation of the concepts of MPI.

To introduce any additional language or extend and change the current languages in an idiomatic way, we first need to conceptually separate the core MPI from the expressions in C and Fortran. This is a formidable challenge in itself.

With the large variance in programming languages for which community language bindings have been developed, it is also important to consider that not all languages will support the same functionality. An example of this would be the profiling interface (PMPI); it provides an intercept functionality that is baked into C from the underlying method by which computers operate. However, in higher level languages such as Python, which is executed in the Python Virtual Machine, the functionality of PMPI can only be emulated and not replicated with decorators.

The MPI Forum must be cautious with introducing new language interfaces. The standard should not convert from its language-independent binding and C, Fortran bindings, to a C++-centric or Python-centric standard, per se. The key semantics and services of MPI should be contained in the core standard. The language interfaces should deliver these services in idiomatic ways without creating huge impacts on the main standard. In fact, with a division of the language-neutral specification from the language interfaces, the main document should shrink considerably in length and complexity.

VI. WHAT DOES AN IDIOMATIC C++ LANGUAGE GIVE US?

The C++ language has many powerful constructs and concepts that MPI could take advantage of, and such ideas are potential avenues for more performant or productive code. These ideas, some of which stray far from the current C bindings, are likely not to work with existing C++ applications using the C interface without code adaptations from MPI libraries and applications; see Section VII for further discussion. Despite that caveat, some of these benefits include:

- Pervasive Polymorphism—This enables extension libraries to provide the same MPI object with new features
- Compile-time Optimizations—In a C++ interface, certain MPI_Info objects could be treated as templates, and affect code paths at compile time instead of runtime. Additionally, MPI_Datatypes could also have compile-time components. An example of this is constexpr plus C++20 ranges to create compile-time derived datatype specifications for faster runtime gather or scatter of non-contiguous data.
- Factory-based MPI functions—Certain MPI functions could be altered to become factories for certain objects (such as for MPI_Requests). For instance, all Sends and Receives could be generated by a general factory for that kind of operation; even blocking ones could fit this model with some special thinking for that case.
- Delegates—We could endow each object a set of allowable actions that return other objects with other/different allowable actions. This would help both MPI application developers and compilers know at compile time what actions can and cannot be performed compliant with the standard. Concepts, introduced in C++20, may also be useful in this regard.

VII. ZEROTH INTERFACE IN C++

The first incremental change from a C interface to a C++ interface introduces overloaded MPI procedures with a “Big Count” variant. An example is shown below in Listing 1. Here, the procedure names remain the same while the definitions change. The specific procedure will be automatically picked by the compiler based on the variables passed by the user. With that change, most C++ applications could easily stop using the _c procedures and maintain support for large counts, or gain support for them if they weren’t using them.

```c++
/* MPI 4.0 C Bindings */
int MPI_Type_size(MPI_Datatype datatype, int *size)
int MPI_Type_size_c(MPI_Datatype datatype, MPI_Count *size)

/* Potential C++ Bindings */
int MPI_Type_size(MPI_Datatype datatype, int *size)
int MPI_Type_size(MPI_Datatype datatype, MPI_Count *size)
```

Listing 1. Example of overloaded C++ MPI bindings

The remaining examples below are more design-specific decisions on how to implement MPI operations in a manner that is consistent with modern C++ style. As such, these examples are listed just to show possibilities, rather than purporting to be mature proposals for future C++ MPI bindings.

The first such possible change the C++ interface would bring relates to how MPI returns errors. In Listing 1 the function signatures still return an error code akin to the normal
C bindings. In C++, such errors could potentially be returned through exceptions (with the specific error code accessible in the caught exception). Exceptions would allow applications that don’t care about errors to continue writing MPI applications without change. For applications that are interested, they would use C++’s try ... catch mechanism instead of checking the return code manually. An example of this is shown in Listing 2. Further, applications could also do multiple MPI function calls inside a single try-block if they are willing to ignore which of the enclosed MPI procedures failed. Compatibility of this change with a C-based library is also possible. In the C interface, the implementation should capture the exceptions in the bindings, and return the error codes for the user; in short, the C binding should contain the try ... catch shown below.

```c
int rc = MPI_Func();
if (rc != MPI_SUCCESS)
    MPI_Abort(MPI_COMM_WORLD, rc);
```

Listing 2. Example of MPI error codes in C++

Next, if a C++ interface removes the obligation to return error codes, then that frees up some MPI procedures to return values instead of requiring them to be OUT parameters. For example, MPI_COMM_RANK would return an integer representing a process’ rank inside a communicator, and MPI_COMM_DUP would return the new, duplicated communicator. These examples can be seen in Listing 3.

```c
int rank = MPI_Comm_rank(dp);
```

Listing 3. Example MPI functions returning objects and values in C++

### VIII. MIXING C AND C++ MPI

There are, loosely speaking, two categories of MPI C++ application developers. The first consists of programmers who choose to develop their entire application using modern C++ features and libraries. The second consists of those who aim to modernize or convert their application to C++, but must rely on a C-based library or libraries over which they have no control. This second category is the focus of this section.

Currently, the MPI C bindings can be called from C++ applications without any complications. In the previous section, we introduced a set of changes that progressively utilize more C++ features. Besides a few changes to specific functions, additional benefits of a C++ interface become limited by the second category of developers noted above if the C++ MPI implementation must keep some of the C interface rules. However, a C++ interface could provide both the original C interface and the new C++ interface by providing additional namespaces or headers that a library or application could use.

An additional namespace requires that legacy C-based MPI libraries or applications add a small wrapper that includes the code (e.g., using namespace MPI_C); while a different header requires a simple #include change.

The separate-header solution may indeed work for some applications. Some applications may wish to use the C++ bindings, but are stuck with a library that uses the C bindings and requires base MPI objects to be passed to them (such as an MPI_Comm). Such an application could also benefit from this dual-binding approach, but will require C++-to-C conversion functions for MPI objects to be provided by the implementation. To support such applications, the C++ MPI API would require functions to convert objects from their C++ representation to their C (or Fortran) representation (or vice versa). A separate namespace for the bindings would also help limit any potential mixing of MPI objects from different bindings without conversion. For example, the underlying type implementing an MPI_Comm in the C bindings namespace would be incompatible in a function argument that takes a MPI_Comm as defined in the C++ bindings.

Lastly, we recommend that, as MPI supports more languages, such conversion functions be kept to a minimum to avoid namespace pollution in MPI. Since C++ is still close to C, such conversion functions could prove useful to developers, but conversion functions for other languages may not be as straightforward or needed as often as between C and C++.

### IX. CONCLUSIONS

This paper motivated the need for a first-class C++20-based language interface for MPI, and strong consideration of such interfaces for other modern languages. Historical and ad hoc systems were discussed and possible design options for C++ in particular were mentioned. The next major standard release for MPI should seriously consider modern language interfaces for multiple languages, and permit these to decouple from the extent language-independent specification that is firmly rooted in C89 and Fortran-77, and those languages’ idiosyncrasies.

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1It is possible to have the exception handler return the request of a failed operation. In that case, blocking requests would only be made programmer accessible when exceptions occur.

2A C++ implementation could also provide several versions of the C++ bindings.

3Fortran to C++ conversions may not be required.
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