Autotuning MPI Collectives using Performance Guidelines

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ABSTRACT

MPI collective operations provide a standardized interface for performing data movements within a group of processes. The efficiency of collective communication operations depends on the actual algorithm, its implementation, and the specific communication problem (type of communication, message size, and number of processes). Many MPI libraries provide numerous algorithms for specific collective operations. The strategy for selecting an efficient algorithm is often times predefined (hard-coded) in MPI libraries, but some of them, such as Open MPI, allow users to change the algorithm manually. Finding the best algorithm for each case is a hard problem, and several approaches to tune these algorithmic parameters have been proposed. We use an orthogonal approach to the parameter-tuning of MPI collectives, that is, instead of testing individual algorithmic choices provided by an MPI library, we compare the latency of a specific MPI collective operation to the latency of semantically equivalent functions, which we call the mock-up implementations. The structure of the mock-up implementations is defined by self-consistent performance guidelines. The advantage of this approach is that tuning using mock-up implementations is always possible, whether or not an MPI library allows users to select a specific algorithm at run-time. We implement this concept in a library called PGMPITuneLib, which is layered between the user code and the actual MPI implementation. This library selects the best-performing algorithmic pattern of an MPI collective by intercepting MPI calls and redirecting them to our mock-up implementations. Experimental results show that PGMPITuneLib can significantly reduce the latency of MPI collectives, and also equally important, that it can help identifying the tuning potential of MPI libraries.

CCS CONCEPTS

• **Computing methodologies → Parallel computing methodologies**;

KEYWORDS

MPI, collective operations, autotuning, performance guidelines

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1 INTRODUCTION

The Message Passing Interface (MPI) is still the most prominent and probably the most frequently used programming model for supercomputers, for example, MPI is driving most of the machines on the TOP500 list. The scalability of parallel applications running on these large platforms is therefore directly dependent on the performance of the underlying MPI implementations. The performance of MPI libraries is therefore of utmost importance for the overall efficiency of the software stack.

In the present article, we address the problem of optimizing the performance of MPI libraries, that is, we want to minimize the latency of a given MPI function for a given payload and a specific number of processes. The performance of MPI libraries can be improved in different ways. One possibility is to devise better algorithms for various communication patterns. Another possibility is to better exploit current hardware, e.g., by aligning memory segments to cache lines or by respecting ccNUMA domains when allocating memory chunks. Altogether, typical open-source MPI implementations, such as MPICH, MVAPICH, or Open MPI, provide several algorithms for each MPI function, and each of these individual implementations may be able to leverage some hardware-specific optimizations.

Now, the problem is that potentially all algorithmic and hardware parameters that an MPI library provides must be considered when tuning on a given parallel machine. The goal of such a tuning process is to select the best possible algorithm for a given message size and number of processes (and possibly other factors like the process-to-core mapping, etc.). Since MPI libraries allow developers to vary hundreds of parameters (e.g., Open MPI), the search space can be extremely large and tuning will be costly. Moreover, parameter tuning may suffer from the fact that tuning is done for individual MPI functions, often in isolation and without a baseline implementation. Thus, having found the best set of parameters for a specific function (e.g., `MPI_Bcast`) will not guarantee its efficiency.

Self-consistent performance guidelines can help to provide such a performance baseline. An MPI performance guideline states that the currently inspected, specialized MPI functionality, say functionality A, should not be slower than a less specialized, but semantically equivalent functionality, say B ($A \preceq B$). For example, the specialized `MPI_Gather` function, which only works with equal-sized messages, should not take longer than the more generic `MPI_Gatherv` function on the same equal-sized problem.

In previous work [7], we have shown that many MPI libraries—available on production systems—violate performance guidelines for several blocking MPI collective operations. We have also demonstrated that guideline violations can be avoided by changing the algorithm used in a specific case. However, not all guideline violations could be fixed by changing the algorithm. First, only a few MPI libraries provide multiple algorithmic strategies for some MPI functions. Second, many proprietary libraries do not expose algorithmic variants in the form of adjustable parameters to the programmer. In both cases, performance violations of MPI libraries cannot be repaired at library level, and in these cases, a programmer would have to adapt the application code (e.g., switching from `MPI_Allgather` to `MPI_Allgatherv`).

To overcome these limitations, we employ self-consistent performance guidelines for tuning MPI libraries, and we make the following contributions:

(1) We propose the *library PGMPITuneLib*, which can be used to *automatically tune* the performance of *any* MPI library. PGMPITuneLib can *replace the default implementation of an MPI function* with one of the semantically equivalent mock-up versions, if the corresponding performance guideline is violated.
(2) To the best of our knowledge, we are the *first* to use *self-consistent performance guidelines for automatically tuning MPI libraries*, in contrast to the traditional way of tuning library-provided algorithmic parameters. As the DRAM memory per core is a scarce resource on larger parallel machines, our implementation of the tuning library takes special care about additional memory requirements.
(3) The experiments provide evidence that our tuning strategy can *automatically repair all guideline violations* on three different test machines, including an IBM BlueGene/Q.
(4) We also propose an *algorithm for solving the NREP problem*, i.e., obtaining reproducible experimental results while keeping the number of measurements small.
(5) Our proposed tuning process is also able to reveal algorithmic variants that have not yet been implemented in MPI libraries. In the present paper, we *show how a new and faster algorithm for* `MPI_Allreduce` *in Open MPI can be derived.*

2 BACKGROUND AND RELATED WORK

Due to the diversity of parallel hardware, it is not surprising that MPI libraries only provide implementations of the MPI standard in a best-effort manner, i.e., the decision which underlying algorithm to use for a given case is predefined in a library. Nonetheless, as systems are, among themselves, usually very heterogeneous, it is necessary to adapt/tune MPI libraries to hardware. This tuning process is very difficult for two main reasons: first, the number of parameters that MPI libraries (e.g., Open MPI) expose for tuning can be very large. In addition, theoretically one would need to examine all possible process-to-core mappings and all possible message sizes, which is simply infeasible. Second, the optimization functions (for minimizing the run-time) are often neither linear nor convex, which makes it harder to find the optimal value as the problems may become intractable. Previous work on library tuning faced these problems, and we will summarize three approaches.

Chaarawi et al. [2] developed the Open Tool for Parameter Optimization (OTPO), whose task is to find a good set of parameter values for a given number of processes and an MPI function. It basically performs a brute-force search over all specified parameters and their ranges in Open MPI. A related method was proposed by Pjesivac-Grbovic et al. [8], in which a quadtree scheme is used to encode the best collective algorithm for a given pair of (number of processes, message size). The quadtree is the internal data structure for allowing a fast lookup of the best-suited algorithm. Since the quadtree can be limited in its depth and granularity, this tuning approach avoids a full enumeration of the search space. A different method was proposed by Sikora et al. [11], where a user can specify parameters and their ranges that should be tuned. Then, a plugin of the Periscope Tuning Framework tries to find the best configuration of these parameters by applying a meta-heuristic, in this case a genetic algorithm. In contrast to previous approaches, the tool of Sikora et al. [11] benchmarks and optimizes the run-time of entire MPI applications instead of optimizing individual MPI functions.

The mentioned approaches try to optimize the run-time of MPI functions for different message sizes but only for a fixed number of processes. It is also possible to search for optimization potential by looking at the scalability behavior of MPI functions. In general, MPI functions have an expected and an actual performance, and the expected performance depends on the theoretical lower bound of an algorithm, which can be obtained analytically for different network topologies [3]. Shudler et al. [10] compared the expected scalability curve of an MPI function to the actual, measured scalability curve. A mismatch between the curves indicates that an MPI function has tuning potential.

Self-consistent performance guidelines (previously called "performance requirements") can be used to verify the consistency of an MPI library. In MPI, several communication patterns can be expressed in semantically equivalent ways. For example, the specialized MPI function `MPI_Allreduce` can also be implemented by chaining calls to `MPI_Reduce` and `MPI_Bcast` together. The user's expectation is that the composition of the latter two functions should not be faster than executing the specialized one. In a more formal definition [12], a performance guideline is defined between two functionalities A and B, which semantically implement the same operation. If functionality A is the more specialized of the two, we can state that $\texttt{MPI\_}A(n) \preceq \texttt{MPI\_}B(n)$, which means that A should complete faster than B for a comparable communication volume n. The communication volume n should be understood as the amount of "actual" data items. It is possible that functionality B needs to transfer messages of larger size, e.g., pn, to mimic functionality A with n data items and p processes. However, as B mimics A, only a communication volume of size n is relevant. The majority of MPI performance guidelines are defined for a fixed number of processes and for the same communicator. Guidelines for different communicators can also be devised, but they are not considered in this work.

In previous work [7], we implemented and tested several performance guidelines for blocking, collective MPI operations, such as `MPI_Bcast`. Our goal was to get an overview of how many libraries violate such guidelines in practice. For that task, we implemented

the toolkit PGMPI,[1] which distinguishes three classes of performance guidelines: monotony, split-robustness, and pattern. The monotony guideline ensures that increasing the message size(s) also increases the run-time. The goal of the split-robustness guideline is to ensure that splitting one large communication operation into several smaller chunks does not improve the overall performance. Last, pattern guidelines are defined between semantically equivalent operations, e.g., `MPI_Allreduce` $\preceq$ `MPI_Reduce` + `MPI_Bcast`. We showed that all tested MPI libraries (MVAPICH, Open MPI, Intel MPI, IBM MPI) violate performance guidelines in various cases. In addition, we demonstrated how violations of performance guidelines can be fixed, e.g., by selecting a better underlying algorithm for a specific communication operation.

In the present paper, we combine the detection of performance-guideline violations with the tuning of MPI libraries. Our previous work [7] pointed out two problems: first, several, often vendor-provided MPI implementations lack user-controlled parameters for algorithmic tuning. Second, some MPI libraries only provide a small set of algorithmic choices for several MPI functions. In such cases, even though a performance violation has been detected, it cannot be repaired due to the limited number of algorithms provided.

Therefore, we propose to use performance-guideline variants as possible replacement implementations. The idea is the following: a guideline may state `MPI_Gather` $\preceq$ `MPI_Gatherv`, which is a natural and almost trivial requirement. If an MPI library violates this guideline and if no other (or faster) variant (algorithm) implementing `MPI_Gather` is available, scientific programmers either accept inferior performance, or they refactor the code and replace calls to `MPI_Gather` with calls to `MPI_Gatherv`. Yet, as this optimization might only be useful on machine Z with K processes, substituting MPI calls manually does not seem to be a good strategy, in general. We solve this problem by introducing PGMPITuneLib,[2] which sits between the MPI user code and the MPI library. By using the `PMPI`-interface, it intercepts calls to a specific MPI function, say `MPI_Gather`, and redirects them to an internally implemented `MPI_Gather` function, which uses `MPI_Gatherv` as its base implementation. Our approach is in the spirit of the approaches of Pjesivac-Grbovic et al. [8] and Faraj et al. [4]. The latter authors proposed the STAR-MPI library, which selects an algorithm for a collective operation (online) after benchmarking (timing) several algorithmic variants during the run-time of an application. Our PGMPITuneLib library instead provides several implementations of a specific collective `MPI_`C, and each variant corresponds to one performance guideline. We then profile MPI functions in isolation (*offline*) and check for performance-guideline violations. If violations occur, we record these cases and later redirect MPI calls (*online*) to faster implementations during application runs. Instead of quadtrees, PGMPITuneLib uses a combination of hash functions and binary searches, ensuring an efficient lookup of algorithmic variants for a given number of processes and message size, which in our case can be done in time $O(\log m)$, where m denotes the largest message size that may occur.

[1] https://github.com/hunsa/pgmpi
[2] https://github.com/hunsa/pgmpitunelib

3 AUTOTUNING MPI LIBRARIES WITH PGMPITUNELIB

Now, we describe our approach for autotuning blocking MPI collective operations using PGMPITuneLib. First, we show all performance guidelines that our library comprises and give a short explanation for each of them. Second, we discuss implementation details of the library and describe the tuning process.

3.1 Performance Guidelines and Semantics

Currently, PGMPITuneLib contains implementations of the performance guidelines listed in Equations (GL1)–(GL22), some of which were introduced before [7, 12]:

$$\texttt{MPI\_Allgather}(n) \preceq \texttt{MPI\_Gather}(n) + \texttt{MPI\_Bcast}(n)\,, \tag{GL1}$$
$$\texttt{MPI\_Allgather}(n) \preceq \texttt{MPI\_Alltoall}(n)\,, \tag{GL2}$$
$$\texttt{MPI\_Allgather}(n) \preceq \texttt{MPI\_Allreduce}(n)\,, \tag{GL3}$$
$$\texttt{MPI\_Allgather}(n) \preceq \texttt{MPI\_Allgatherv}(n)\,, \tag{GL4}$$
$$\texttt{MPI\_Allreduce}(n) \preceq \texttt{MPI\_Reduce}(n) + \texttt{MPI\_Bcast}(n)\,, \tag{GL5}$$
$$\texttt{MPI\_Allreduce}(n) \preceq \texttt{MPI\_Reduce\_scatter\_block}(n) + \texttt{MPI\_Allgather}(n)\,, \tag{GL6}$$
$$\texttt{MPI\_Allreduce}(n) \preceq \texttt{MPI\_Reduce\_scatter}(n) + \texttt{MPI\_Allgatherv}(n)\,, \tag{GL7}$$
$$\texttt{MPI\_Alltoall}(n) \preceq \texttt{MPI\_Alltoallv}(n)\,, \tag{GL8}$$
$$\texttt{MPI\_Bcast}(n) \preceq \texttt{MPI\_Allgatherv}(n)\,, \tag{GL9}$$
$$\texttt{MPI\_Bcast}(n) \preceq \texttt{MPI\_Scatter}(n) + \texttt{MPI\_Allgather}(n)\,, \tag{GL10}$$
$$\texttt{MPI\_Gather}(n) \preceq \texttt{MPI\_Allgather}(n)\,, \tag{GL11}$$
$$\texttt{MPI\_Gather}(n) \preceq \texttt{MPI\_Gatherv}(n)\,, \tag{GL12}$$
$$\texttt{MPI\_Gather}(n) \preceq \texttt{MPI\_Reduce}(n)\,, \tag{GL13}$$
$$\texttt{MPI\_Reduce}(n) \preceq \texttt{MPI\_Allreduce}(n)\,, \tag{GL14}$$
$$\texttt{MPI\_Reduce}(n) \preceq \texttt{MPI\_Reduce\_scatter\_block}(n) + \texttt{MPI\_Gather}(n)\,, \tag{GL15}$$
$$\texttt{MPI\_Reduce}(n) \preceq \texttt{MPI\_Reduce\_scatter}(n) + \texttt{MPI\_Gatherv}(n)\,, \tag{GL16}$$
$$\texttt{MPI\_Reduce\_scatter\_block}(n) \preceq \texttt{MPI\_Reduce}(n) + \texttt{MPI\_Scatter}(n)\,, \tag{GL17}$$
$$\texttt{MPI\_Reduce\_scatter\_block}(n) \preceq \texttt{MPI\_Reduce\_scatter}(n)\,, \tag{GL18}$$
$$\texttt{MPI\_Reduce\_scatter\_block}(n) \preceq \texttt{MPI\_Allreduce}(n)\,, \tag{GL19}$$
$$\texttt{MPI\_Scan}(n) \preceq \texttt{MPI\_Exscan}(n) + \texttt{MPI\_Reduce\_local}(n)\,, \tag{GL20}$$
$$\texttt{MPI\_Scatter}(n) \preceq \texttt{MPI\_Bcast}(n)\,, \tag{GL21}$$
$$\texttt{MPI\_Scatter}(n) \preceq \texttt{MPI\_Scatterv}(n)\,. \tag{GL22}$$

All inequalities have a regular, blocking MPI collective on the left-hand side. Regular means that all processes use the same send buffer size (e.g., in `MPI_Allreduce`, `MPI_Gather`), and in the case of `MPI_Bcast`, equal-sized receive buffers. We only included regular collectives as their use cases seem to be better defined. However, in the irregular case (∗v functions), we have another degree of freedom (how much data each process contributes), which makes global tuning harder. Thus, it seems unrealistic that offline-tuned irregular collectives will actually be (re-)used. For such irregular collectives, an online tuning approach (such as done by STAR-MPI) seems to be more promising.

We want to stress that PGMPITuneLib contains an actual implementation of the right-hand side of each performance guideline shown above. That means, in some cases (detailed below) it is necessary to allocate additional buffer space and to perform data

Table 1: Performance guidelines implemented in PGMPITuneLib. Variable n denotes the number of elements of basetype in the send count of an operation, p denotes the number of processes in the communicator, and I denotes the size of `MPI_INT`.

MPI collective	max memory requ. per proc.	guidel.	mock-up	additional memory requirement
`MPI_Allgather`	$n + pn$	GL1	`MPI_Gather` + `MPI_Bcast`	none
		GL2	`MPI_Alltoall`	pn (p times larger send buffer)
		GL3	`MPI_Allreduce`	pn (p times larger send buffer)
		GL4	`MPI_Allgatherv`	$2pI$ (displs, recvcounts)
`MPI_Allreduce`	$2n$	GL5	`MPI_Reduce` + `MPI_Bcast`	none
		GL6	`MPI_Reduce_scatter_block` + `MPI_Allgather`	$(n + c)/p + (n + c)$ (small c for padding)
		GL7	`MPI_Reduce_scatter` + `MPI_Allgatherv`	$2pI$ (displs, recvcounts)
`MPI_Alltoall`	$2pn$	GL8	`MPI_Alltoallv`	$2pI$ (displs, recvcounts)
`MPI_Bcast`	n	GL9	`MPI_Allgatherv`	$2pI$ (displs, recvcounts)
		GL10	`MPI_Scatter` + `MPI_Allgather`	$(n + c)/p + (n + c)$ (small c for padding)
`MPI_Gather`	$n + pn$	GL11	`MPI_Allgather`	none on root, pn on other processes
		GL12	`MPI_Gatherv`	$2pI$ (displs, recvcounts)
		GL13	`MPI_Reduce`	pn (for new send buf)
`MPI_Reduce`	$n + n$ (on root)	GL14	`MPI_Allreduce`	extra n (on processes other than root)
		GL15	`MPI_Reduce_scatter_block` + `MPI_Gather`	$(n + c)/p + (n + c)$ (small c for padding)
		GL16	`MPI_Reduce_scatter` + `MPI_Gatherv`	$(\lfloor n/(Cp) \rfloor + 1)C + 2pI$ (displs, recvcounts), chunk size C
`MPI_Reduce_scatter_block`	$n + n/p$	GL17	`MPI_Reduce` + `MPI_Scatter`	n (for first reduce)
		GL18	`MPI_Reduce_scatter`	pI (recvcounts)
		GL19	`MPI_Allreduce`	n (for new recv buffer)
`MPI_Scan`	$2n$	GL20	`MPI_Exscan` + `MPI_Reduce_local`	none
`MPI_Scatter`	$n + n/p$	GL21	`MPI_Bcast`	extra n (on processes other than root)
		GL22	`MPI_Scatterv`	$2pI$ (displs, recvcounts)

movements between buffers for obtaining a semantically equivalent implementation of the left-hand side. A brief description of the semantics and some implementation details of the considered performance guidelines is given in Appendix A. Table 1 summarizes the additional memory requirements for each guideline implementation. When referring to guidelines of the form $\texttt{MPI\_}A \preceq \texttt{MPI\_}A'$, we say that an implementation of A' is a mock-up version of functionality A. Our notation of n and p in Table 1 is as follows. The number p denotes the number of processes involved in the MPI collective. As in most cases the memory requirements are different among the processes, the table lists the maximum memory requirement of any process, which is often the root process for rooted operations like Gather and Scatter. The number n denotes the number of elements that are placed in the send buffer by a process. For example, in `MPI_Alltoall`, n elements are sent from each process to every other process, and thus overall, each process sends pn elements. Since a process also receives pn elements, the total memory requirement for `MPI_Alltoall` is $2pn$.

`MPI_Reduce_scatter_block` is a special case, as it has no explicit send count. Therefore, the initial send buffer holds n elements, on which the reduction will be performed. After the scatter step, each process receives n/p elements, and overall, the memory requirement for this routine is $n + n/p$.

When referring to n as the memory space needed for one process, we would have to say precisely nE, where E is the extent of the base datatype used. However, for the sake of a better readability we omit E and simply say n for the memory requirement. Table 1 also uses variable I, which denotes the extent of `MPI_INT`, which is commonly needed when specifying the displacement and the receive (send) count vectors.

3.2 Library Design and Implementation

3.2.1 General Design. Since PGMPITuneLib uses the PMPI interface of MPI, it is layered between the MPI user code and the MPI library. If the user code makes a call to an MPI function, in our case a blocking MPI collective function, PGMPITuneLib intercepts the call and may select one of the mock-up implementations. Figure 1 shows an example: the MPI user code calls `MPI_Allreduce`, which is intercepted by PGMPITuneLib. Internally, PGMPITuneLib uses performance *profiles* containing identifiers of possible replacement algorithms for various message sizes. Then, PGMPITuneLib searches for a replacement algorithm for `MPI_Allreduce`. If such a replacement algorithm can be found, PGMPITuneLib emulates the original call by using its replacement, which is in our example the combination of Reduce and Bcast. If no replacement algorithm is found, PGMPITuneLib uses the default implementation, i.e., it calls `PMPI_Allreduce`.

3.2.2 Tuning Workflow and Modes of Operation. PGMPITuneLib provides two modes of operation, which are encapsulated in different libraries and which can be linked with any MPI application (or benchmark). Figure 2 shows the general architecture, where PGMPITune provides the basic API. On top of that core API, two different libraries exist. One is the PGMPITuneCLI library (CLI stands for command line interface), which is used for measuring the performance of mock-up implementations. To that end, MPI developers link their applications against the CLI version of PGMPITuneLib. It is now possible to select a mock-up version for a specific MPI function as follows:

```
mpicc *.c -o mympicode -lpgmpitunecli -lmpi
mpirun -np 2 ./mympicode
   --module=allgather:alg=allgather_as_gather_bcast
```

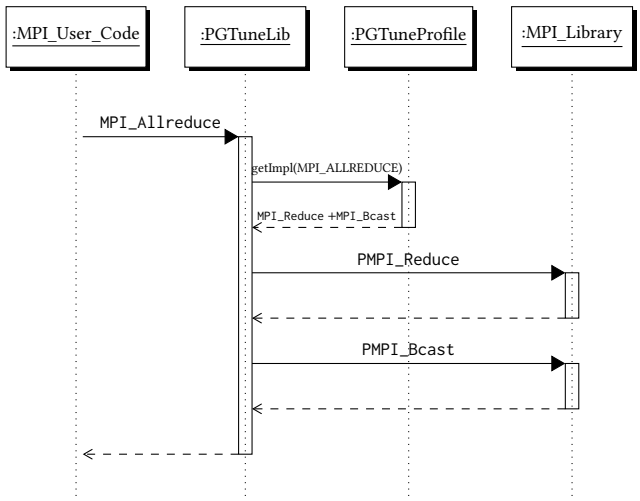


Figure 1: Example of intercepting `MPI_Allreduce` and replacing it with calls to `MPI_Reduce` and `MPI_Bcast`.

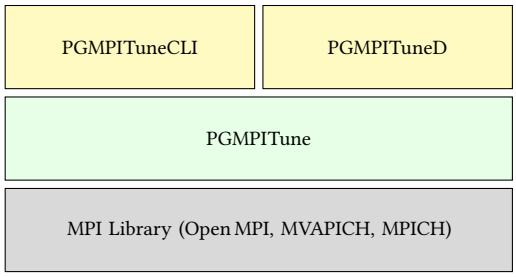


Figure 2: PGMPITuneLib architecture.

In this example, all calls to `MPI_Allgather` will be replaced with the mock-up implementation of guideline (GL1). By using this CLI version of PGMPITuneLib, we can analyze the latency of all implemented collective algorithms for different message sizes. Any MPI benchmark suite can be used to measure the latency of MPI collective operations. Benchmarking allows us to detect message sizes for which performance guidelines are violated. When violations occur, PGMPITuneLib stores the message sizes for which a possible replacement mock-up was found. After scanning over all collectives and selected message sizes, PGMPITuneLib writes a performance *profile* for each MPI collective. Performance *profiles* contain the replacement algorithms for specific message ranges. Listing 1 shows a sample *profile* for `MPI_Scatter` that was recorded with 64×16 processes on *JUQUEEN*. Each *profile* only contains message ranges for which violations have occurred and for which a replacement algorithm should be used. As we have measured (in the example shown in Listing 1) for discrete message sizes, the sample profile uses the same message size for the start and the end of a message range. For example, algorithm 2 (`scatter_as_bcast`) should be applied for the message ranges 1 Byte to 1 Byte, 8 Bytes to 8 Bytes, and so on.

Listing 1: Profile of `MPI_Scatter` on *JUQUEEN*.

```
1  # pgtune profile
2  MPI_Scatter
3  1024  # nb. of. processes
4  2     # nb. of mock-up impl.
5  2 scatter_as_bcast
6  3 scatter_as_scatterv
7  8     # nb. of ranges
8  1 1 2 # byte_range_start byte_range_end alg_id
9  8 8 2
10 32 32 2
11 64 64 2
12 100 100 2
13 512 512 2
14 1024 1024 2
15 10000 10000 3
```

Once performance *profiles* are created, any MPI application can use them. Developers can simply link their applications against the PGMPITuneD library. Similar to PGMPITuneCLI, the PGMPITuneD library intercepts MPI calls and redirects them to the mock-up versions implemented in the core library. PGMPITuneD reads in all performance *profiles* from disk, which happens transparently when intercepting `MPI_Init`. Then, PGMPITuneD has all the information required to select a (possibly) better mock-up version for a collective MPI operation at run-time.

3.2.3 Implementation Details. It seems obvious that a tuned MPI library should be implemented as efficiently as possible. We have therefore tried to keep the overhead incurred by PGMPITuneLib very low. As mentioned before, some mock-up implementations require the allocation of additional memory, e.g., for padded data or for displacement or send/receive count vectors. PGMPITuneLib avoids additional system calls (e.g., `malloc`) by allocating two extra memory chunks at the start of the MPI program, one for additional message buffers and one for displacement or send/receive count vectors. The size of both buffers can be controlled by the user with the variables `size_msg_buffer_bytes` and `size_int_buffer_bytes`, which can be set in the configuration file of PGMPITuneLib. Another advantage of this additional memory management is that users can accurately control how much extra memory they want to dedicate for possibly faster MPI functions. It could be that a replacement algorithm was found to be faster than the default implementation provided by the MPI library, but if this mock-up needs too much extra memory, then it will not be selected.

For providing an efficiently tuned library, it is also important to perform fast look-ups to check whether a replacement algorithm is available. Currently, performance profiles are read for a specific number of processes only. Thus, PGMPITuneLib can look up the right performance *profile* for a certain collective and can check whether the profile is compatible with the current number of processes in time $O(1)$. Then, PGMPITuneLib only needs to verify whether the profile contains a replacement algorithm for the current message size. As we sort the M different message ranges at program start, such a lookup of the replacement algorithm is performed in time $O(\log M)$ using binary search.

Table 2: Parallel machines used in our experiments.

Name	Hardware	MPI Libraries	Compiler
Jupiter	36 × Dual Opteron 6134 @ 2.3 GHz IB QDR MT26428	MVAPICH2-2.2 Open MPI 2.1.0	gcc 4.4.7
VSC-3	2000 × Dual Xeon E5-2650V2 @ 2.6 GHz IB QDR-80	Intel MPI 2017 (Update 2)	icc 16.0.4
JUQUEEN	28 672 × IBM PowerA2 @ 1.6 GHz IBM-BlueGene/Q, 5D Torus interconnect	IBM BG MPI	IBM XL

4 EXPERIMENTAL EVALUATION

4.1 Hardware Setup

We evaluated PGMPITuneLib on three different machines, whose characteristics are summarized in Table 2. The systems *Jupiter* and *VSC-3* are rather similar when comparing their hardware setup. The advantage of having similar architectures is that the reproduction of phenomena on other systems increases the confidence in the significance of our findings. The BlueGene/Q called *JUQUEEN* allows us to study a vendor-provided, tailor-made MPI library on an actual supercomputer.

4.2 Tuning Workflow

The tuning process of PGMPITuneLib first checks whether the performance guidelines defined for blocking collective MPI operations are fulfilled. If violations occur, these cases are recorded and a *profile* is written. In a subsequent execution, PGMPITuneLib can then change to a different mock-up implementation at run-time.

In order to automatically tune an MPI library, we need to benchmark the latency of the default implementations of blocking collectives and their mock-up versions that are part of PGMPITuneLib. For measuring the latency, one could employ any type of MPI benchmark suite, e.g., OSU Micro-Benchmarks [1] or SKaMPI [9]. It is only required that the benchmark suite is linked against PGMPITuneLib.

For the analysis shown in the present paper, we have used our own benchmark suite called ReproMPI,[3] which allows to record raw data (the latency of every single measurement) from each experiment [5]. In contrast to other benchmark suites, it refrains from performing any kind of data aggregation (e.g., computation of means) or data removal (e.g., discarding the first X measurements for "warming up" the system). By using ReproMPI, we can record every single measurement and perform the data analysis in R, Python, or Julia later.

The autotuning process with PGMPITuneLib is divided into *three* steps. The *first* and a critical step is to estimate the number of repetitions (*nrep*) of measurements that have to be conducted for a specific MPI function with a given message and communicator size (number of processes). *Second*, we benchmark the MPI collectives and their mock-up counterparts using the CLI version of PGMPITuneLib (cf. Figure 2). From the performance data gathered, we can then detect violations of the performance guidelines (GL1)–(GL22). Among all mock-up functions for which guideline violations have occurred, the mock-up version that performs best for a given message range is selected and written into a performance *profile* (cf. Listing 1). *In a last step*, we re-link the ReproMPI benchmark suite against the *tuned* version of PGMPITuneLib. Now, PGMPITuneLib can replace individual MPI collectives with their faster mock-up counterparts.

[3] https://github.com/hunsa/reprompi

Algorithm 1 MPI timing procedure ([5]).

```
1: procedure TIME_MPI_FUNCTION(func, msize, nrep)
                // func - MPI function; msize - message size; nrep - nb. of observations
2:     initialize time array l with nrep elements
3:     for obs in 1 to nrep do
4:         BARRIER()          // use external dissemination barrier implementation
5:         t = GET_TIME()
6:         execute func (msize)
7:         l[obs] = GET_TIME() - t
```

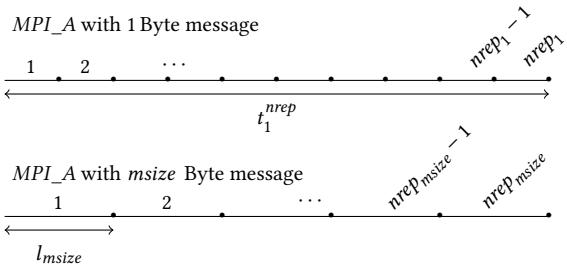


Figure 3: Estimating the number of repetitions (NREP) based on the time obtained for 1 Byte **messages.**

ReproMPI supports different synchronization strategies and different ways (clocks) to measure the run-time (latency) of collective calls. For the presented experiments, we have used the timing procedure shown in Algorithm 1: Before every individual measurement, processes are synchronized with a barrier. Here, we use a dissemination barrier, which—due to its structure—ensures that processes leave this barrier relatively synchronized (which would not be the case for tree-based barriers for example).

The "NREP problem" consists of finding a suitable (and possibly minimal) number of repetitions, such that the derived statistical measures (mean, median) are reproducible [7].

We use the following method to address the **NREP problem**: for each MPI function `MPI_A`, the *general idea* is to determine the time (t_1^{nrep}) until the latency measurements with a 1 Byte message have stabilized (e.g., a small variance). This time is further used as the reference time for other message sizes (cf. Figure 3). Our assumption is that the relative system noise decreases when the message size increases, as the run-time of each collective function grows with the message size. Thus, we measure the latency of `MPI_A` with a different message size *msize* (*msize* > 1 Byte) for at least time t_1^{nrep}.

More precisely, in step (1), we repeat the measurement of the latency of function `MPI_A` with 1 Byte messages until the current relative standard error (*RSE*) over the measured latencies is below some user-defined threshold. We repeat this process over several calls to `mpirun` and take the longest time that was required to make the *RSE* drop below the threshold, and we denote this time as t_1^{nrep}. As this process can take hundreds of repetitions, we only want to do that for a message size of 1 Byte. For all the other messages sizes, we measure for at least time t_1^{nrep}. As many benchmarking tools require the number of repetitions as an input, we convert the time t_1^{nrep} into a number of repetitions $nrep_{msize}$ of `MPI_A` for any other

message size *msize*. To that end, in step (2), we run two batches of measurements called batches b_1 and b_2, and the user-defined number of repetitions for both batches should be relatively small (< 10) or even zero in case of b_2. We compute the *RSE* value of these b_1 measurements. If that value is smaller than some predefined threshold (note that this is a different threshold than the one used for 1 Byte messages), the measuring process is stopped. Otherwise, another batch with b_2 measurements is started. For larger message sizes, taking only one batch with b_1 elements leads to a very small variance, and thus, we can return quickly. However, for smaller message sizes, we need a few more measurements to get a reasonable value of the latency. In step (3), we compute the minimum of these measured latencies l_i, $1 \leq i \leq b_1 + b_2$, as

$$l_{msize} = \min_{1 \leq i \leq b_1 + b_2} l_i \quad ,$$

and use this value as the "expected" latency. Then, we compute the estimated number of repetitions needed for `MPI_A` and message size *msize* as

$$nrep_{msize} = \max \left\{ \left\lceil \frac{t_1^{nrep}}{l_{msize}} \right\rceil, K \right\} \quad .$$

The value $K \geq 1$ ensures that at least K latency measurements for every collective and message size are performed, especially when l_{msize} becomes very large (even larger than t_1^{nrep}).

In our experiments, we use the following values to estimate the *nrep* value for each collective or mock-up: we repeat measuring the latency with *msize* = 1 Byte until the *RSE* value is smaller than 0.01 (1%). We perform $b_1 = 5$ and possibly $b_2 = 5$ more measurements for each collective (and mock-up) with larger message sizes and then compute $nrep_{msize}$. We measure the latency of each collective and its mock-ups for $nrep_{msize}$ iterations and repeat this process for *nmpiruns* = 5 different calls to `mpirun`. The selection of the mock-up function is done *statically* on the command line (PGMPITuneCLI). We check for guideline violations of each collective and write a performance *profile* to disk, if violations have occurred. In our particular case, we only replace a collective if the best performing mock-up is at least 10% faster than the default implementation. Then, we run another set of experiments with the tuned version of the MPI library, where the selection of the best implementation (default or mock-up) is done *dynamically* at run-time by PGMPITuneD.

Listing 2 shows the output of ReproMPI when being run and linked against PGMPITuneLib. The output is directly readable as CSV data into data processing frameworks like R. The header contains information about the specific benchmarking run, e.g., how many processes, which clock, or which barrier implementation have been used. However, the footer is written by PGMPITuneLib and shows whether certain calls to MPI collectives have been replaced. In the example, for a message size of 100 Bytes, the default implementation of `MPI_Allgather` was replaced by the mock-up implementation `MPI_Gather` + `MPI_Bcast`. In some other cases, for example with 8 Bytes, the *Default* implementation was used. The footer also contains information about how much memory was reserved for the temporary buffers in PGMPITuneLib. Here, PGMPITuneLib could use additional 100 MBytes for allocating message buffers and 10 kBytes for displacement and count vectors.

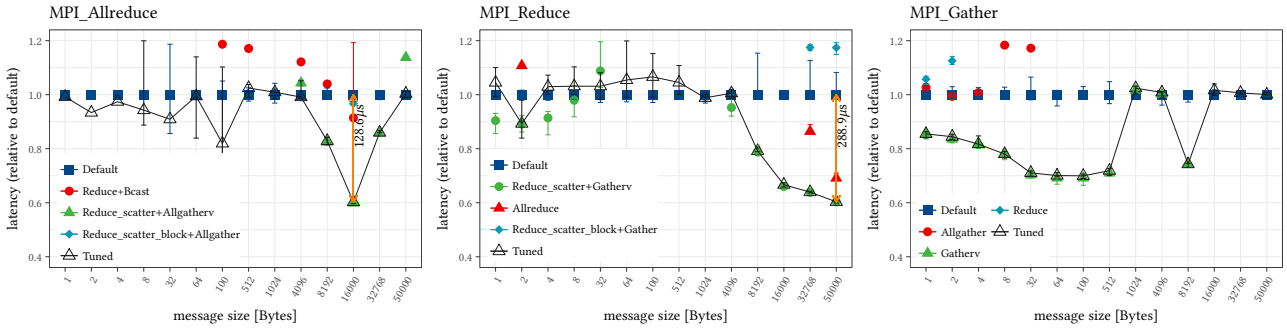
Listing 2: ReproMPI output when benchmarking a tuned MPI library; some lines were omitted for better readability.

```
#@operation=MPI_BOR
#@datatype=MPI_CHAR
#@root_proc=0
#@reproMPIcommitSHA1=unknown
#@nprocs=1024
#@clocktype=local
#@clock=MPI_Wtime
#@sync=BBarrier
#@nrep=0
test nrep msize runtime_sec
MPI_Allgather 0 1 0.0002306175
MPI_Allgather 1 1 0.0001389663
MPI_Allgather 2 1 0.0001024431
MPI_Allgather 3 1 0.0001023700
MPI_Allgather 4 1 0.0001029038
#@pgmpi alg MPI_Allgather 16000 default
#@pgmpi alg MPI_Allgather 8 default
#@pgmpi alg MPI_Allgather 100 allgather_as_gather_bcast
#@pgmpi alg MPI_Allgather 32 default
#@pgmpi alg MPI_Allgather 32768 default
#@pgmpi alg MPI_Allgather 4 default
#@pgmpi alg MPI_Allgather 50000 default
#@pgmpi alg MPI_Allgather 8192 default
#@pgmpi alg MPI_Allgather 100000 default
#@pgmpi alg MPI_Allgather 2 allgather_as_gather_bcast
#@pgmpi alg MPI_Allgather 1024 allgather_as_gather_bcast
#@pgmpi alg MPI_Allgather 64 allgather_as_gather_bcast
#@pgmpi alg MPI_Allgather 4096 allgather_as_gather_bcast
#@pgmpi alg MPI_Allgather 512 allgather_as_gather_bcast
#@pgmpi alg MPI_Allgather 1 allgather_as_gather_bcast
#@pgmpi config size_msg_buffer_bytes 100000000
#@pgmpi config size_int_buffer_bytes 10000
```

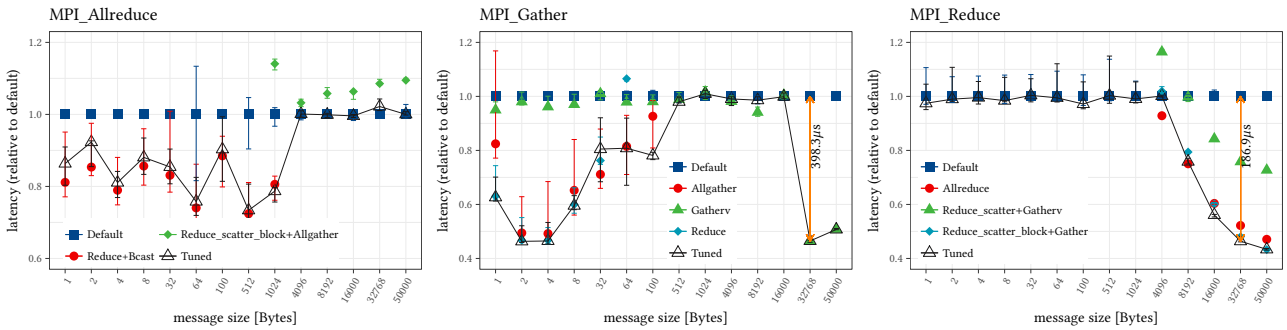
4.3 Experimental Results

Figure 4a summarizes the tuning results that were obtained for 32×1 processes and Open MPI 2.1.0 on *Jupiter*. Each plot contains the performance of the *Default* algorithm, the *Tuned* version, and the individual mock-up implementations. As latencies for small and large messages differ by orders of magnitude, we plot the relative performance of each implementation, where the latency of the *Default* implementation is used as the reference. As we measure over multiple calls to `mpirun` (*nmpiruns*), we use the median over the *nmpiruns* = 5 median latencies measured. The error bars denote the minimum and the maximum of these *nmpiruns* medians to reflect the variance of the data. For a better comprehension, let us look at the plot on the right-hand side of Figure 4a, which compares the *Tuned* and the *Default* version of `MPI_Gather`. The figure also includes the performance data of three different mock-up implementations of `MPI_Gather` (Allgather, Gatherv, Reduce). We can observe that the *Tuned* version uses Gatherv as replacement up to a message size of 1024 Bytes, for which PGMPITuneLib switches back to the *Default* version. Except for 8192 Bytes, the *Default* version was found to perform best for message sizes larger than 1024 Bytes. As the scale of the y-axis is limited, not all individual points can be shown, e.g., the red points for the Allgather mock-up are absent for more than 32 Bytes. As shown Figure 4a, `MPI_Allreduce` and `MPI_Reduce` can also be significantly improved by PGMPITuneLib. The data shown for `MPI_Reduce` (center) suggest that a large tuning potential for larger messages exists in Open MPI, and we will consider this case in Section 4.4.

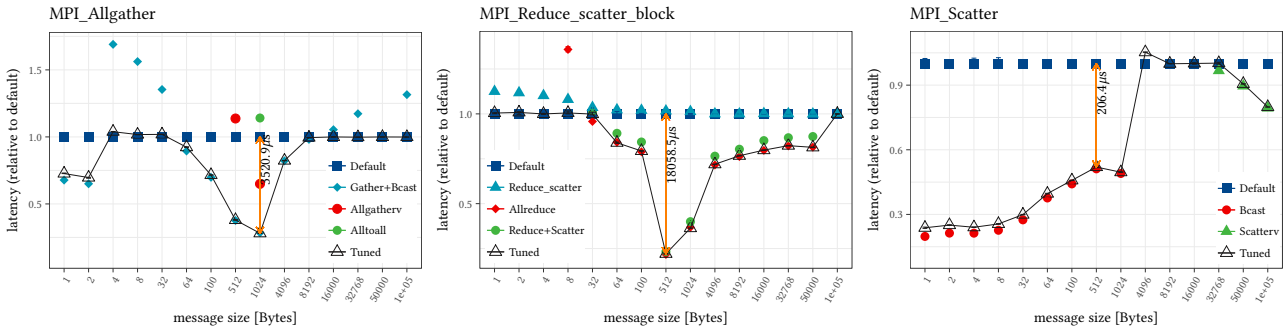
With MVAPICH2-2.2, different cases were detected for which PGMPITuneLib can improve the performance (see Figure 4b). As the relative latency can sometimes be misleading, we also indicate the absolute performance difference for a few cases. For example, the latency of `MPI_Reduce` or `MPI_Gather` with 32 KiBytes of data



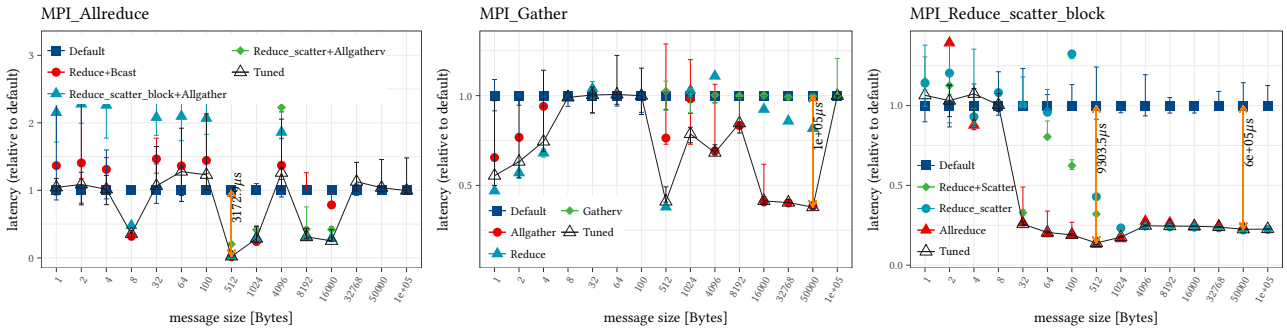
(a) Open MPI 2.1.0, 32×1 processes, *Jupiter*



(b) MVAPICH2-2.2, 32×1 processes, *Jupiter*



(c) IBM BG MPI, 64×16 processes, *JUQUEEN*



(d) Intel MPI 2017 (Update 2), 64×16 processes, *VSC-3*

Figure 4: Performance comparison between *Default* and *Tuned* versions of MPI functions.

can be reduced up to 180 µs or 400 µs, respectively (an improvement of roughly 50%).

Figure 4c shows the performance improvement observed on *JUQUEEN* and 64 × 16 processes. It is interesting to note, but perhaps not surprising, that many performance violations occur when MPI functions were tested against mock-up versions that rely on `MPI_Bcast`, e.g., the mock-up in guideline (GL1) is composed of Gather and Bcast. It seems often beneficial to employ `MPI_Bcast` whenever possible, as the BlueGene/Q has hardware support for Bcast. As a consequence, the performance of `MPI_Allgather` and `MPI_Scatter` could significantly be improved.

With a last set of plots, given in Figure 4d, we highlight the tuning potential of Intel MPI 2017 (Update 2) on *VSC-3* using 64 × 16 processes. We can observe that the *Default* versions of `MPI_Gather` and `MPI_Reduce_scatter_block` can substantially be improved by PGMPITuneLib. In the case of `MPI_Reduce_scatter_block`, we obtain a 4x speedup by using Allreduce within the *Tuned* version. However, the largest relative improvements were recorded for `MPI_Allreduce` with 512 and 1024 Bytes of payload. For messages of 1024 Bytes, we observed a 45x speedup when using the mock-up functions (that either combine Reduce_scatter_block and Allgather or Reduce and Bcast). Since we deal with a proprietary MPI library, it was not possible to find the root cause of that performance issue. Nevertheless, it is possible to work around that problem by using PGMPITuneLib.

Notice that we only present a selection of the performance plots, showing the most significant results. More performance graphs can be found in our technical report [6].

4.4 Parameter vs. Guideline-based Tuning

Now, we inspect two performance guideline violations, one of which we had already examined in our previous work [7].

4.4.1 Case `MPI_Reduce` ⪯ `MPI_Allreduce`. We had shown that `MPI_Reduce` in Open MPI 1.10.1 violates the Allreduce guideline (GL14) for message sizes ranging from 128 kBytes to 725 kBytes and for 32 × 16 processes on *Jupiter*. We were able to overcome this violation by implementing our own `MPI_Reduce` function. Now, we go one step further and compare two versions of `MPI_Reduce` that were obtained through different tuning strategies: (1) the best mock-up algorithm found by PGMPITuneLib and (2) the best algorithm found after an exhaustive search using the MCA parameters of Open MPI. To that end, we varied the relevant MCA parameters (e.g., segment size, fan-out) for all Reduce algorithms provided by Open MPI. The result of this brute-force tuning and the results from PGMPITuneLib are compared in Figure 5. We can observe that the `MPI_Allreduce` mock-up is faster than the *Default* `MPI_Reduce` implementation over the entire range of message sizes. However, the latency can further be improved (although only moderately) by using the `in-order_binary`-algorithm of Open MPI. This case exemplifies that scanning for guideline violations and performing a serious parameter tuning (e.g., MCA parameters in Open MPI) should complement each other. In this case, a fully parameter-tuned version of Open MPI would not have violated the `MPI_Reduce` performance guidelines in the first place. The downside is that such an exhaustive search is very time-consuming.

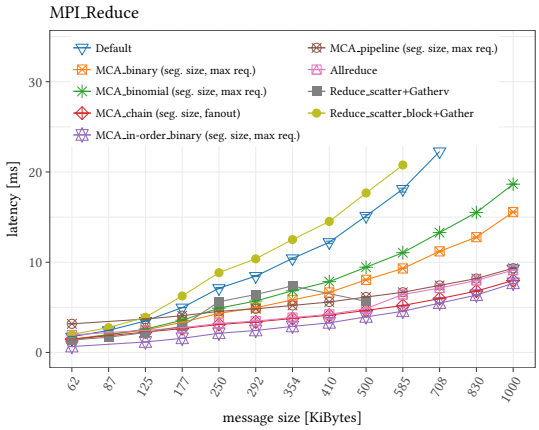


Figure 5: Violation of `MPI_Reduce` ⪯ `MPI_Allreduce`. Comparing latencies of mock-ups with algorithmic variants (Open MPI 2.1.0, 32 × 16 processes, *Jupiter*).

4.4.2 Tuning Potential of `MPI_Allreduce` *in Open MPI.* Our extensive experimental analysis also revealed other interesting cases. One of them is shown in Figure 6. The plot shows latencies measured for `MPI_Allreduce`, its mock-up variants implemented in PGMPITuneLib, and several algorithmic versions found in Open MPI 2.1.0 (the latencies of the algorithm "`basic linear`" were omitted, since they were too large). Here, the algorithmic version called `MCA_nonoverlapping` performs almost identical to our Reduce+Bcast mock-up variant. Indeed, when inspecting the internals of Open MPI, this algorithmic variant uses exactly these two collectives. Additionally, we discovered that the mock-up version combining Reduce_scatter and Allgatherv outperforms all other algorithms, even all versions provided by Open MPI after the exhaustive search was done. Thus, PGMPITuneLib helps developers to detect cases for which a better algorithmic variant exists. We implemented the Allreduce variant based on Reduce_scatter and Allgatherv within Open MPI 2.1.0 [6]. The plot shows that this new algorithm, denoted as `MCA_NEW_Reduce_scatter+Allgatherv`, exactly matches the expected latency achieved by combining Reduce_scatter and Allgatherv, and it outperforms all other variants.

5 CONCLUSIONS

Tuning MPI libraries can help to improve the overall parallel efficiency of applications on supercomputers, as MPI is the de-facto standard for data communication on these machines. Parameter tuning is a valuable method for achieving the goal of improving the MPI software layer. The downsides of parameter tuning are twofold: (1) the method is relatively expensive, as MPI libraries such as Open MPI provide hundreds of possibly interacting parameters, and (2) a performance baseline is often missing, i.e., how fast is fast enough since global minima are usually unknown.

Tuning MPI libraries by using performance guidelines can complement the traditional parameter-based approach. Self-consistent performance guidelines define relations between the performance of a specialized functionality and a less specialized functionality, both of which realize the same, semantically equivalent operation.

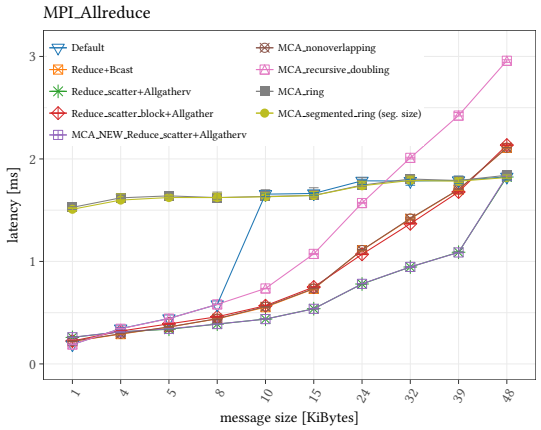


Figure 6: Performance comparison of `MPI_Allreduce`, its mock-ups, and MCA-tuned variants of `MPI_Allreduce` (Open MPI 2.1.0, 32×16 processes, *Jupiter*).

For example, the latency of `MPI_Allgather` should be smaller than combining `MPI_Gather` with a subsequent call to `MPI_Bcast`.

In the present paper, we extended the set of performance guidelines for blocking, collective MPI operations and implemented each guideline as a mock-up function in a library. With this library called PGMPITuneLib, it is possible to find performance deficits of MPI implementations by scanning for guideline violations. If violations are detected, we create so-called performance profiles, which can be used by PGMPITuneLib to replace specific MPI functions by their mock-up version at run-time. As a result, the obtained, tuned collective MPI operations are self-consistent with respect to the performance guidelines and their latencies are significantly shorter.

Our experimental results show that PGMPITuneLib overcomes performance deficits of MPI libraries for all systems that we tested on. In addition, PGMPITuneLib also revealed cases in MPI libraries (e.g., Open MPI) for which even better algorithms exist. The biggest advantage of PGMPITuneLib, however, is the fact that it can be used with any MPI library, whether or not it exposes parameters for tuning purposes.

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A APPENDIX

`MPI_Allgather` and its Mock-ups

(GL1) `MPI_Gather` + `MPI_Bcast`: trivially composes `MPI_Gather` with `MPI_Bcast` to obtain a functionally equivalent version of `MPI_Allgather`.

(GL2) `MPI_Alltoall`: uses a p times larger send buffer, in which each process puts p copies of its own buffer contents. Afterwards, `MPI_Alltoall` is called to mimic `MPI_Allgather`.

(GL3) `MPI_Allreduce`: uses, similar to the `MPI_Alltoall` mock-up, a p times larger send buffer. This larger buffer is initialized with zeros, and the actual message of each process i is copied into the large buffer starting at index $i \cdot n$. Then, an `MPI_Allreduce` is applied to all buffers and a bitwise or-operation ensures that the result is semantically equivalent to the result of `MPI_Allgather`.

(GL4) `MPI_Allgatherv`: calls `MPI_Allgatherv` instead, and therefore needs to allocate two additional buffers of size p (p elements of type `MPI_INT`) for the receive counts and the displacements. **Note** that we will *not further comment* on any other mock-up implementation using an *irregular operation* (e.g., `MPI_Gatherv`, `MPI_Alltoallv`, etc.), as they are all straightforward to implement.

`MPI_Allreduce` and its Mock-ups

(GL5) `MPI_Reduce` + `MPI_Bcast`: is implemented as the straightforward composition of `MPI_Reduce` and `MPI_Bcast`.

(GL6) `MPI_Reduce_scatter_block` + `MPI_Allgather`: first calls `MPI_Reduce_scatter_block`, which needs equal-sized blocks in the Scatter phase. As the send buffer of the original `MPI_Allreduce` function does not have to be a multiple of the number of processes, our mock-up version will add c dummy elements (with a maximum of $p - 1$ elements) of the send type as additional padding, such that `MPI_Reduce_scatter_block` can be called. By construction, it is also possible to perform an `MPI_Allgather` on the receive buffer of the previous stage. After this `MPI_Allgather` is completed, the mock-up version only copies the first n elements (ignoring the

padded elements) back to the original receive buffer.

(GL7) `MPI_Reduce_scatter` + `MPI_Allgatherv`: applies the same strategy as the previous mock-up. Since `MPI_Reduce_scatter` and `MPI_Allgatherv` work with send buffers of arbitrary size, the mock-up function needs to allocate buffers for the receive counts and for the displacements. However, `MPI_Reduce_scatter` gives us the freedom to choose how many elements end up on each process after the Scatter phase. We balance the number of elements using the chunk size C, $1 \leq C \leq n$. Each process receives approximately $n/(C \cdot p)$ elements after `MPI_Reduce_scatter`. The remaining elements are distributed in a round-robin fashion onto the processes. By using the chunk size C, we can avoid cases where each process would receive only 1 Byte of data after the execution of `MPI_Reduce_scatter`. In our implementation, we use the receive buffer of the emulated `MPI_Allreduce` function as the receive buffer for `MPI_Reduce_scatter`. Then, we can call `MPI_Allgatherv` using the previous receive buffer as the final receive buffer and `MPI_IN_PLACE` as the send buffer, which allows us to avoid allocating extra message buffers and performing extra memory copies in the implementation of this mock-up.

`MPI_Bcast` and its Mock-ups

(GL9) `MPI_Allgatherv`: The idea is that `MPI_Allgatherv` copies the buffer contents of the root rank of the original Bcast to all other processes in a broadcast-to-all fashion. Therefore, only the process that emulates the Bcast root sends n elements, and all other processes send 0 elements. Our implementation uses `MPI_IN_PLACE` as the value of the send buffer, which avoids the allocation of one additional chunk of memory.

(GL10) `MPI_Scatter` + `MPI_Allgather`: uses the van de Geijn version to implement the Broadcast, which calls Scatter followed by Allgather [3]. As Scatter requires the same send count on each process, we need to allocate one padded buffer holding all elements to be sent and one buffer that stores the elements after the Scatter phase.

`MPI_Gather` and its Mock-ups

(GL11) `MPI_Allgather`: simply uses `MPI_Allgather` behind the `MPI_Gather` interface. As now every process needs to receive n elements of the base datatype from every other process, we need to allocate a buffer with space for $p \cdot n$ elements of basetype on each process.

(GL13) `MPI_Reduce`: Similarly to (GL3), we allocate a p times larger send buffer on all processes and intialize it with zeros. Each process copies the contents of its send buffer into the larger temporary buffer. Then a call to `MPI_Reduce` with an `MPI_BOR` operation results in the correct emulation of `MPI_Gather`.

`MPI_Reduce` and its Mock-ups

(GL14) `MPI_Allreduce`: uses the same strategy as guideline (GL11). Every process, except the root process of the operation, needs to allocate a receive buffer that can accommodate n basetype elements. Calling `MPI_Allreduce` will not only give root the result but also the other processes, which then simply ignore it.

(GL15) `MPI_Reduce_scatter_block` + `MPI_Gather`: This mock-up is a rather heavyweight replacement of `MPI_Reduce`. It first performs an `MPI_Reduce_scatter_block` on the send buffer. For the scatter part, the vector size must be a multiple of the number of processes, as `MPI_Reduce_scatter_block` requires receive buffers of the same size on all processes. To achieve that, an extra padding is added to the end of the send buffer. Two new buffers are allocated, one holding the new, padded send buffer and another one for the result of the `MPI_Reduce_scatter_block` operation, which is exactly p times smaller than the new send buffer. Upon completion of this operation, we can call `MPI_Gather` on the result buffers of `MPI_Reduce_scatter_block`, which finally gives us an emulated version of `MPI_Reduce`.

(GL16) `MPI_Reduce_scatter` + `MPI_Gatherv`: The idea of this mock-up is similar to the one above. The only difference is that we do not need the additional padding, as `MPI_Reduce_scatter` works on vectors of arbitrary size. However, to accomplish an emulation, we need to allocate two buffers for the displacement and the count information that will be used for `MPI_Reduce_scatter` and the following `MPI_Gatherv`. We also need to allocate an additional message buffer that holds on each process the result of `MPI_Reduce_scatter`. We again distribute the elements in a round-robin fashion in chunks of C elements, as done in the implementation of guideline (GL7).

`MPI_Reduce_scatter_block` and its Mock-ups

(GL17) `MPI_Reduce` + `MPI_Scatter`: This mock-up function uses a straightforward composition of `MPI_Reduce` and `MPI_Scatter`. As the result of the first step (`MPI_Reduce`) requires a receive buffer of size n (elements), we need to allocate this additional buffer between the two calls.

(GL18) `MPI_Reduce_scatter`: is a trivial emulation using the irregular counterpart, for which an additional buffer holding the receive counts is required.

(GL19) `MPI_Allreduce`: The `MPI_Reduce_scatter_block` functionality can also be emulated with `MPI_Allreduce`. We need to allocate an additional receive buffer on each process but the root with space for n elements. Allreduce will then distribute the reduction result to all processes. Now, each process picks its part of the reduction result, which it would have received from the scatter phase of the original operation. This completes the emulation of `MPI_Reduce_scatter_block`.

`MPI_Scan` and its Mock-ups

(GL20) `MPI_Exscan` + `MPI_Reduce_local`: This mock-up version performs first an exclusive scan on the same data as the inclusive scan would have performed. In order to obtain the same result as the inclusive scan, we need to perform a local reduction operation on all processes but the root. Overall, no additional buffers are needed.

`MPI_Scatter` and its Mock-ups

(GL21) `MPI_Bcast`: This version allocates on all processes but the root an additional receive buffer for the n elements of the root process. The root process then broadcasts all its data to the others. Now, every process (also the root) copies its part of the data (n/p elements) to the receive buffer of the scatter operation.