PGMPI: Automatically Verifying Self-Consistent MPI Performance Guidelines

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Abstract. The Message Passing Interface (MPI) is the most commonly used application programming interface for process communication on current large-scale parallel systems. Due to the scale and complexity of modern parallel architectures, it is becoming increasingly difficult to optimize MPI libraries, as many factors can influence the communication performance. To assist MPI developers and users, we propose an automatic way to check whether MPI libraries respect self-consistent performance guidelines. We introduce the PGMPI framework that can benchmark and detect violations of performance guidelines. Our experimental results show that PGMPI can indeed help to pinpoint undesired and often unexpected performance degradations of collective MPI operations. We demonstrate how to overcome these performance issues of several libraries by adapting the algorithmic implementations of their respective collective MPI calls.

Keywords: MPI, performance guidelines, benchmarking

1 Introduction

Communication libraries implementing the Message Passing Interface (MPI) are major building blocks for developing parallel, distributed, and large-scale applications for current supercomputers. The performance of these parallel codes is therefore highly dependent on the efficiency of the MPI implementations. A lot of research effort is currently conducted to improve existing MPI libraries, as one of the key problems on the way to Exascale computing.

Assessing the performance of MPI libraries is vital for developers, vendors, and users of those libraries. However, the performance of MPI libraries can be assessed in different ways. A common approach is to run a set of MPI micro-benchmarks, such as SKaMPI [11] or ReproMPI [7]. Micro-benchmarks usually report the measured (mean or median) run-time of a given MPI function for different message sizes, e.g., the run-time of MPI_Bcast for broadcasting a 1 Byte message. Developers can gain insights on how the run-time of an MPI function

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depends on the message size for a fixed number of processes. It is also possible to assess the scalability of MPI functions when the number of processes is increased, when keeping the message size fixed.

Verifying self-consistent MPI performance guidelines is an alternative, orthogonal method for analyzing the performance of MPI libraries [14]. This approach does not require explicit performance models. Instead, performance guidelines form a set of rules that an MPI library can be expected to fulfill. A performance guideline usually defines an upper bound on the run-time behavior of a specialized MPI function. For example, one performance guideline states that a call to \texttt{MPI\textunderscore Scatter} of \( n \) data elements should “not be slower” than a call to \texttt{MPI\textunderscore Bcast} with \( n \) data elements, as the semantics of an \texttt{MPI\textunderscore Scatter} operation could be emulated using \texttt{MPI\textunderscore Bcast} [14]. Only minor efforts have been made to systematically test self-consistent performance guidelines for MPI implementations in practice, one example being the mpicroscope benchmark [13]. To close this gap, we introduce the benchmarking framework PGMPI that can automatically verify performance guidelines of MPI libraries.

We make the following contributions: (1) We propose the benchmarking framework PGMPI to detect performance-guideline violations. (2) We present a systematic, experimental verification of performance guidelines for several MPI libraries. (3) We examine different use cases, for which the detection of the guideline violation helped to tune and improve the libraries’ performance.

In Sect. 2, we state the scientific problem and introduce our notation. We continue with summarizing related work and comparing it to our approach in Sect. 3. We introduce the PGMPI framework in Sect. 4 and present an experimental evaluation of different MPI libraries using our performance-guideline framework in Sect. 5. We summarize our findings and conclude in Sect. 6.

2 Problem Statement and Notation

Träff et al. [14] introduced self-consistent performance guidelines for MPI libraries as follows: The run-time of two MPI functionalities \( A \) and \( B \) can be ordered using the relation \( \preceq \) as \( \texttt{MPI\textunderscore A}(n) \preceq \texttt{MPI\textunderscore B}(n) \), which means that functionality \( \texttt{MPI\textunderscore A}(n) \) is possibly faster than functionality \( \texttt{MPI\textunderscore B}(n) \) for (almost) all communication amounts \( n \). Performance guidelines are defined for a fixed number of processes \( p \), and thus, they do not mention \( p \) explicitly. However, the communication volume per process may vary depending on the semantics of a given MPI function and the number of processes. For example, in the case of \texttt{MPI\textunderscore Bcast}, the total size \( n \) is equal to the message size being transferred to each process. In contrast, the individual message size for an \texttt{MPI\textunderscore Scatter} is a fraction of the total communication volume \( n \), i.e., each process receives \( n/p \) elements.

We examine three types of performance guidelines: (1) \textit{monotony}, (2) \textit{split-robustness}, and (3) \textit{pattern}. The monotony guideline

\[
\texttt{MPI\textunderscore A}(n) \preceq \texttt{MPI\textunderscore A}(n + k)
\]

ensures that communicating a larger volume should not decrease the communication time. The split-robustness guideline

\[
\texttt{MPI\textunderscore A}(n) \preceq k \texttt{MPI\textunderscore A}(n/k)
\]

...
states that communicating a total volume of \( n \) data elements should not be slower than sending \( \frac{n}{k} \) elements in \( k \) steps. Pattern guidelines define upper bounds on the performance of MPI communication operations. The idea is that a specialized MPI function should not have larger running time than a combination of other MPI operations, which emulate the functionality of the specialized function. Let us consider the following pattern performance guidelines:

\[
\begin{align*}
\text{MPI	extunderscore Scatter}(n) & \leq \text{MPI	extunderscore Bcast}(n), \text{ and } \\
\text{MPI	extunderscore Bcast}(n) & \leq \text{MPI	extunderscore Scatter}(n) + \text{MPI	extunderscore Allgather}(n).
\end{align*}
\]

The first states that a call to \texttt{MPI	extunderscore Scatter} should not be slower than a call to \texttt{MPI	extunderscore Bcast}, of course, given the same overall communication volume and the same number of processes. The reason is that \texttt{MPI	extunderscore Scatter} could be implemented using \texttt{MPI	extunderscore Bcast}, by broadcasting the entire vector, and then processes can take their share by using their ranks. The second guideline states that a call to \texttt{MPI	extunderscore Bcast} should be at least as fast as a combination of calls to \texttt{MPI	extunderscore Scatter} and \texttt{MPI	extunderscore Allgather}, which we call the mock-up version of \texttt{MPI	extunderscore Bcast}, as it emulates its semantics [2].

3 Related Work

Collective communication operations are a central part of the MPI standard, as collectives are important for large-scale applications. Chan et al. [2] provide an overview of typical, blocking collectives and their implementations, as well as lower bounds for the communication cost of each function. For different network topologies, the authors devise algorithms that achieve the lower bounds for either the latency or the bandwidth component. As the model of parallel computation in this paper is rather simplistic, we need to complement this study by carefully benchmarking MPI collectives on actual hardware.

Träff [13] proposed the MPI benchmark mpicroscope, which can verify two self-consistent performance guidelines: “split-robust” and “monotone”. In the present work, we extend this functionality by testing various pattern violations, using the experimental framework that was proposed by Hunold et al. [7] for better reproducibility of the experimental results. While we focus on performance guidelines for collectives, previous works have also formulated performance guidelines for derived datatypes [4] and MPI-IO operations [5].

As hardware and software factors can influence the performance of MPI collectives, the tuning of MPI parameters is an essential part when installing an MPI library. Yet, optimizing and tuning MPI operations are orthogonal steps compared to the verification of self-consistent performance guidelines, i.e., the latter can help us to verify whether run-times of collectives are logically consistent. For example, the guidelines can be used to ensure that \texttt{Gather} is faster than \texttt{Allgather} for the same problem size. Thus, if a violation occurs, it usually means that one collective can be tuned. To optimize the latency of collectives at run-time, one can employ the STAR-MPI routines [3]. When a call to a specific
MPI function is issued, STAR-MPI selects one of the available algorithms and measures its run-time. After some time, STAR-MPI has enough knowledge to pick a good algorithm for a specific case.

Selecting the right algorithm to implement a given MPI function is only one step towards tuning MPI libraries. Another problem is finding the right parameter settings that run-time systems of MPI libraries like Open MPI or MVAPICH offer. Chaarawi et al. [1] introduced the OTPO tool that can be used to tune Open MPI run-time parameters. OTPO takes as input the run-time parameters to be tuned as well as their respective ranges, and then starts measuring for all combinations the parameter values. Another approach to tune Open MPI parameters has been proposed by Pellegrini et al. [9], where the parameter values are predicted using machine learning techniques.

The performance guidelines are formulated as a function of the communication volume. It is also possible to examine the scalability of MPI collectives when increasing the number of processes. Shudler et al. [12] proposed a framework that compares performance characteristics of HPC applications with a theoretical performance model. The framework fits the recorded benchmarking data to analytic speedup functions and compares the experimentally determined scalability behavior to an expected, provided performance model. If the models do not match, it indicates a scalability problem of the parallel code section.

4 PGMPI: Verifying MPI Performance Guidelines

We now introduce the PGMPI framework, which can verify self-consistent performance guidelines of MPI libraries. In the first step, PGMPI experimentally determines the number of repetitions needed to obtain stable, reproducible run-time measurements (Step NREP). In the second step, the framework performs run-time measurements of all functions that are part of performance guidelines (Step MEASURE). The data analysis and the statistical verification of the specified guidelines is carried out in the last step (Step ANALYZE).

4.1 Obtaining Reproducible Results

We start by looking at the main (second) step of PGMPI (Step MEASURE), in which the run-times of MPI functions and their emulating counterparts are measured. The guideline-checking program takes as input a set of pattern guidelines, each defined by a pair consisting of an MPI function and its emulating function. Our PGMPI framework will measure the run-time of one of the specified MPI functions $f_j$ for all given message sizes $m_i$ and the number of processes $p$ that are given in the input file. Within one call to mpirun, each individual measurement for $(f_j, m_i)$ is repeated $r_i$ times, where $r_i$ is defined for each $m_i$. As we expect to obtain varying means (or medians) between different calls to mpirun [7], PGMPI measures the run-time of one function $f_j$ over $R$ mpiruns.
4.2 Determining the Number of Repetitions

A major problem in MPI benchmarking is the question of how long (how many times) to measure. We need to find the right trade-off between time and accuracy. One way of dealing with this problem is by executing the experiment sufficiently often, e.g., 1000 times. This would alleviate the problem of low accuracy, but, most often, we cannot afford long-running benchmarking experiments. Therefore, we formulate the following problem:

**Definition 1.** The NREP problem is the problem of finding a suitable number of repetitions \( r_i \) for the tuple \( \langle f_j, m_i, p \rangle \), such that the obtained mean (or median) run-time after \( r_i \) repetitions of function \( f_j \) with \( m_i \) Bytes on \( p \) processes is reproducible between different calls to `mpirun`. Reproducible means that the distribution of means (or medians) obtained from \( R \) `mpirun`s is not significantly different if repeated.

We have experimented with various ways to estimate the number of repetitions needed to obtain reproducible results. One possibility is to monitor the relative standard error of the mean (RSE). SKaMPI, for example, stops the measurements when the RSE falls below a threshold of 0.1 [11]. Although we have tested many different ways to solve the NREP problem, we could not find a generally superior approach. We therefore designed the NREP predictor for Step NREP of the PGMPI framework in a flexible manner. The framework currently provides three different methods (metrics) for solving the NREP problem, but new metrics can be added. The NREP prediction stops

1. when the relative standard error (RSE) is smaller than some predefined threshold \( t_{RSE} \); or
2. when the coefficient of variation of the mean run-time (COV<sub>mean</sub>) is smaller than some predefined threshold \( t_{COV_{mean}} \). The value of the COV<sub>mean</sub> is computed over the last \( w_{COV_{mean}} \) means (window size); or
3. when the coefficient of variation of the median run-time (COV<sub>median</sub>) is smaller than some predefined threshold \( t_{COV_{median}} \) using a window size of \( w_{COV_{median}} \).

Users can select their favorite method on the command line like this

```
mpirun -np 4 ./mpibenchmarkPredNreps --calls-list=MPI_Reduce --msizes-list=8 --rep-prediction min=20,max=1000,step=10 --pred-method=rse --var-thres=0.025
```

It is also possible to combine different metrics, i.e., the NREP prediction stops when all selected metrics have been positively evaluated. An example is shown in Fig. 1, in which both the RSE and the COV<sub>mean</sub> need to be below a specific threshold. The prediction function for the RSE metric stops after 85 iterations, at which the COV<sub>mean</sub> value is also below its threshold. As a result, 85 is the number of iterations that will be used when collecting benchmark data in Step MEASURE of our framework. To cope with the run-time variation between different `mpirun`s, we perform three NREP predictions for each message size and select the maximum number of repetitions obtained.
Fig. 1. Example of estimating the required number of repetitions for MPI_Allgather (16 B, 16 × 1 processes, Jupiter, $t_{RSE} = 0.025, t_{COV_{mean}} = 0.01, w_{COV_{mean}} = 20$)

4.3 Statistically Verifying Performance Guidelines

After gathering the measurement results, PGMPI can proceed to Step ANALYZE, the data processing and the verification of performance guidelines. We now explain which statistical methods are applied for guideline verification. For each MPI function, for which guidelines were formulated, the experimental results comprise $R$ (number of mpiruns) data sets for a specific number of processes $p$. Each data set contains $r_i$ run-time measurements for a specific message size $m_i$. We first reduce the number of measurements per tuple (mpirun, $m_i$, $p$) to a single value, by computing the median run-time over the $r_i$ measurements. In this way, we obtain a distribution of $R$ medians (median run-times) for each message size $m_i$. The various performance guidelines will then be verified using these distributions of medians.

Monotony Guideline PGMPI checks for each pair of adjacent message sizes $m_i$ and $m_j$, $m_i < m_j$ that the run-time of an MPI function with a message size of $m_i$ is not larger than the run-time with a size of $m_j$. We use the Wilcoxon rank-sum test [6] to test whether the distribution of medians at $m_i$ is smaller or equal than the one at $m_j$. If the test rejects our hypothesis, we have statistical confidence (at the provided confidence level) that the monotony between message sizes $m_i$ and $m_j$ is violated.

Split-Robustness Guideline We want to check whether communicating a large message in $k$ smaller blocks of size $m_i$ is faster than communicating one large block of size $m_j$. We are only given the run-time distribution of one MPI function at $m_i$. Unfortunately, we have no knowledge about the shape of the run-time distribution when messages of size $m_i$ are communicated in $k$ rounds. We cannot simply shift the distribution at $m_i$ by some constant factor. Since it is not easy to apply the right statistical test in this case, we decided to rely on (and to compare) the median values of the distributions.
Table 1. Overview of parallel machines used in the experiments

| name   | hardware                          | MPI libraries / Compiler          |
|--------|-----------------------------------|-----------------------------------|
| Jupiter| 36 × Dual Opteron 6134 @ 2.3 GHz  | NEC MPI 1.3.1, MVAPICH2-2.1       |
|        | IB QDR MT4036                     | Open MPI 1.10.1/ gcc 4.4.7       |
| VSC-3  | 2000 × Dual Xeon E5-2650V2 @ 2.6 GHz | Intel MPI Library 5.9 (Update 3) |
|        | IB QDR-80                         | gcc 4.4.7                         |

We compute the factor \( k = \min_{l \in \mathbb{N}} (lm_i \geq m_j) \), which denotes the smallest multiple of \( m_i \) such that the resulting product is at least \( m_j \). Notice that we explicitly allow \( lm_i \) to be larger than \( m_j \), which enables us to check whether sending two messages of size 1024 B is faster than sending one message of size 2000 B. The PGMPI framework verifies that the time to communicate messages of size \( m_i \) in \( k \) rounds is indeed smaller than the time to communicate \( m_j \). If we find a violation for a message size \( m_j \), we only report the largest message size \( m_i \) (the smallest factor \( k \)) for which the violation occurred; otherwise too many violations would be reported in some cases. It happens often that the predicted run-time for \( lm_i \) is very similar to the run-time for \( m_j \). To avoid reporting split-robustness violations, for which only marginal relative run-time differences have been measured, we use a 5% tolerance level when verifying this guideline. Currently, PGMPI does not empirically test whether communicating \( k \) messages of size \( m_i \) is indeed faster than communication a message of size \( m_j \) in practice. This additional check would require an additional benchmarking round, and will be added to PGMPI in future versions.

**Pattern Guidelines** The verification of pattern guidelines is done similarly to checking the monotony guideline, except that we now compare two run-time distributions of two distinct functions, which are the MPI function and its mock-up version. We apply the *Wilcoxon rank-sum test* on the two distributions, which tests if the run-time distribution of the MPI function is not significantly shifted to the right of the distribution obtained with the mock-up version. The *Kolmogorov-Smirnov test* [6] can be an alternative, as it is less sensitive to ties. Overall, both tests led to similar results in the majority of the considered cases.

5 Experimental Evaluation and Results

We evaluate our proposed PGMPI framework\(^1\) experimentally using the hardware and software setup listed in Table 1. First, we present a summary of detected performance-guideline violations for several MPI libraries. Second, we demonstrate in two case studies that the knowledge about specific guideline violations can help us tuning and adapting MPI implementations to parallel systems.

\(^1\) https://github.com/hunsa/pgmpi
Table 2. Performance-guideline violations of different MPI libraries \((R = 10)\); violation types: \textit{monotony, split-robustness, pattern}; message sizes between 1 B and 100 KiB

(a) \textit{Jupiter}

| # processes | type | MV APICH2-2.1 | NEC MPI 1.3.1 | Open MPI 1.10.1 |
|-------------|------|--------------|--------------|----------------|
| 16x1        | m    | 7/9          | 6/9          | 7/9            |
| 16x1        | s    | 1/9          | 0/9          | 3/9            |
| 16x1        | p    | 12/15        | 7/15         | 9/15           |
| 32x16       | m    | 5/9          | 4/9          | 4/9            |
| 32x16       | s    | 3/9          | 0/9          | 3/9            |
| 32x16       | p    | 8/15         | 7/15         | 7/15           |

(b) \textit{VSC-3}

| # processes | type | MV APICH2-2.1 | NEC MPI 1.3.1 | Open MPI 1.10.1 |
|-------------|------|--------------|--------------|----------------|
| 16x16       | m    | 7/9          | 6/9          | 7/9            |
| 16x16       | s    | 6/9          | 4/9          | 4/9            |
| 16x16       | p    | 9/15         | 7/15         | 7/15           |
| 64x16       | m    | 6/9          | 7/9          | 6/9            |
| 64x16       | s    | 7/9          | 6/9          | 7/9            |

Table 3. Pattern guideline violations of different MPI libraries with \(32 \times 16\) processes on \textit{Jupiter}, \(R = 10\); message sizes between 1 B and 100 KiB

| guideline                        | MV APICH2-2.1 | NEC MPI 1.3.1 | Open MPI 1.10.1 |
|----------------------------------|--------------|--------------|----------------|
| MPI_Allgather \(\preceq\) Allreduce | *            | *            | *              |
| MPI_Allgather \(\preceq\) Alltoall  |              | *            | *              |
| MPI_Allgather \(\preceq\) Gather+Bcast | *            |              | *              |
| MPI_Allreduce \(\preceq\) Reduce+Bcast | *            | *            | *              |
| MPI_Allreduce \(\preceq\) Reduce_scatter_block+Allgather | *            |              | *              |
| MPI_Bcast \(\preceq\) Scatter+Allgather |              |              | *              |
| MPI_Gather \(\preceq\) Allgather | *            |              | *              |
| MPI_Gather \(\preceq\) Reduce | *            |              | *              |
| MPI_Reduce_scatter_block \(\preceq\) Reduce+Scatter | *            | *            | *              |
| MPI_Reduce_scatter \(\preceq\) Allreduce | *            | *            | *              |
| MPI_Reduce_scatter \(\preceq\) Reduce+Scatterv | *            |              | *              |
| MPI_Reduce \(\preceq\) Allreduce | *            |              | *              |
| MPI_Reduce \(\preceq\) Reduce_scatter_block+scatter | *            | *            | *              |
| MPI_Scan \(\preceq\) Exscan+Reduce_local | *            |              | *              |
| MPI_Scatter \(\preceq\) Bcast | *            |              | *              |

5.1 Assessing the Guideline Compliance of MPI Libraries

We used the PGMPI framework to verify performance guidelines for different MPI libraries that are listed in Appendix A. On \textit{Jupiter}, we evaluated NEC MPI 1.3.1, MVAPICH2-2.1, and Open MPI 1.10.1. The NEC MPI 1.3.1 library was delivered by NEC pre-compiled for our system and we therefore do not know the internals. The other two libraries, MVAPICH2-2.1 and Open MPI 1.10.1, were compiled using the default settings. On \textit{VSC-3}, we recorded guideline violations for the Intel MPI Library 5.0 (Update 3), for which we also do not have the source code.

Table 2 presents an overview of the detected guideline violations for several MPI libraries on \textit{Jupiter} and \textit{VSC-3}. In total, performance guidelines for nine different MPI collectives were verified. If a guideline violation is revealed for any message size of a particular MPI function, we say that this particular guideline is unsatisfied, i.e., a violation is only counted once across all message sizes. We can observe in Table 2 that the monotony and the split-robustness guidelines are violated by approximately 50% of the collectives. The table also reveals that more than 40% of the examined pattern guidelines were violated. The guideline violations occurred across different numbers of processes, message sizes, libraries, and machines. We therefore contend that there is a large potential for optimization of the individual MPI libraries on our machines.
Table 4. Performance-guideline violations of MVAPICH2-2.1 using $32 \times 16$ processes on *Jupiter* ($R = 10$); violation types: monotony, split-robustness, pattern

| type function | m MPI_Allgather | m MPI_Allreduce | m MPI_Gather | m MPI_Reduce | m MPI_Scatter | s MPI_Gather | s MPI_Reduce | s MPI_Reduce_scatter_block | p MPI_Allreduce ⪯ Allreduce | p MPI_Allreduce ⪯ Reduce+Bcast | p MPI_Gather ⪯ Reduce | p MPI_Reduce ⪯ Reduce | p MPI_Reduce_scatter ⪯ Allreduce | p MPI_Reduce_scatter ⪯ Allreduce | p MPI_Reduce_scatter ⪯ Allreduce | p MPI_Reduce ⪯ Allreduce | p MPI_Reduce ⪯ Reduce_scatter_block+Gather | p MPI_Scatter ⪯ Bcast |
|---------------|----------------|----------------|-------------|-------------|-------------|-------------|-------------|----------------------------|-------------------------|--------------------------|----------------|-------------|-----------------------------|------------------------|------------------------|-------------------------|---------------------------|------------------------|
|               |                |                |             |             |             |             |             |                           |                         |                          |                |             |                            |                        |                        |                          |                           |                        |
5.2 Case Study 1: MPI_Gather ⪯ MPI_Allgather, MVAPICH2-2.1

We consider the violation of this performance guideline that was detected using 32 × 1 processes and MVAPICH2-2.1 on Jupiter and is shown in Fig. 2a. When the Wilcoxon rank-sum test reports a violation for a particular message size, we mark this case in the figure with a red background and add asterisks to show the statistical significance. Here, executing MPI_Gather using 32 × 1 processes (one process per compute node) is slower than performing a Gather using MPI_Allgather. When calling MPI_Gather in the default installation of MVAPICH2-2.1, it will use the internal function MPIR_Gather_intra for the first 14 invocations and then switches to MPIR_Gather_MV2_Direct for subsequent calls. The direct implementation of Gather performs \((p - 1)\) MPI_Irecv operations.
on the root process and an MPI_Send on the other processes. We can set the environment variable MV2_USE_DIRECT_GATHER=0 to force MVAPICH to use MPIR_Gather_intra only. The intra-version on our machine uses a binomial tree algorithm to implement Gather, and forcing this algorithm fixes the violation (cf. Fig. 2b). Let us check that the algorithmic change for small message sizes is indeed favorable. We use the Hockney model for MPI_Reduce given by Pjesivac et al. [10], but omit the computational term. As the direct algorithm issues \((p-1)\) receive operations, we obtain a run-time for small message sizes (we neglect the bandwidth term) of about 52.7 \(\mu s\), for a network latency of roughly 1.7 \(\mu s\). If we use a binomial tree algorithm instead, the latency cost grows only logarithmically in the number of processes, i.e., \(\log 32 \times 1.7 \mu s = 8.5 \mu s\). Even though our estimation does not perfectly match the experimental data, it explains why the binomial tree algorithm performs better.

5.3 Case Study 2: MPI_Reduce \(\preceq\) MPI_Allreduce, Open MPI

In the second case study, we consider the guideline violations that occurred for MPI_Reduce using Open MPI 1.10.1 on the Jupiter system. Here, in contrast to the first case study, violations have only been measured for larger message sizes \(> 2^{16}\)B), but for various numbers of processes: \(16 \times 1\), \(32 \times 1\), \(16 \times 16\), and \(32 \times 16\). Figure 3 limits the view to message sizes for which violations were detected. Since Open MPI is highly configurable via the MCA parameters, we have tried to find parameter settings for MPI_Reduce, such that executing the latter would be faster than executing MPI_Allreduce. We have tried various segment sizes and fan-outs (where the parameters were applicable). Unfortunately, we failed to tune the parameters in such a way that the violations would disappear on our machine. For that reason, we implemented our own Reduce algorithm, which is based on the MPI_Allreduce algorithm found in Open MPI 1.10.1. Here, MPI_Allreduce is implemented using a Reduce-scatter followed by an Allgatherv on a ring of processes [8]. We modified this algorithm to become an MPI_Reduce by replacing the final Allgatherv by a Gatherv to the root. The Gatherv was realized using a direct Irecv/Send scheme. In the MPI semantics of Reduce, only the root process has a receive buffer. We therefore need to allocate additional buffer space to send and receive data segments in the Reduce-scatter phase. We found that executing malloc in each Reduce call has a severe impact on the performance of Reduce. To overcome this problem, we allocate a temporary buffer outside of Reduce but accessible to the Reduce implementation. This modification helped us to significantly speed up the run-time, and made this Reduce implementation a suitable candidate to be included in the Open MPI library. In sum, our Reduce implementation avoids violations for larger messages sizes, as shown in Figure 3b.

6 Conclusions

The experimental verification of performance guidelines is an orthogonal approach to traditional MPI library tuning. It allows to find performance degra-
dations of MPI functions, which would be hidden otherwise. For example, it is possible to optimize several existing implementations of MPI_Gather, but even the fastest of these Gather algorithms might be slower than the call to MPI_Allgather.

We have introduced the PGMPI framework to verify self-consistent performance guidelines of MPI functions. Currently, the framework supports blocking MPI collective communication operations, but it can and will be extended to support MPI derived datatypes. We have evaluated 17 different guidelines for collective communication operations for several MPI libraries such as MVAPICH and Open MPI. The experimental results reveal that none of the libraries is perfectly adapted to a parallel machine, which might not be surprising. However, PGMPI was able to pinpoint exactly which MPI functions should be tuned and which message sizes should be considered. Thus, PGMPI is a useful tool that allows MPI developers and system administrators to easily spot tuning potentials.

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A Self-Consistent Performance Guidelines in PGMPI

Monotony Guideline

$$\text{MPI}_A(n) \preceq \text{MPI}_A(n + k)$$  (GL1)

Split-Robustness Guideline

$$\text{MPI}_A(n) \preceq k \cdot \text{MPI}_A(n/k)$$  (GL2)

Pattern Guidelines

$$\text{MPI}_\text{Gather}(n) \preceq \text{MPI}_\text{Allgather}(n)$$  (GL3)
$$\text{MPI}_\text{Gather}(n) \preceq \text{MPI}_\text{Reduce}(n)$$  (GL4)
$$\text{MPI}_\text{Allgather}(n) \preceq \text{MPI}_\text{Alltoall}(n)$$  (GL5)
$$\text{MPI}_\text{Allgather}(n) \preceq \text{MPI}_\text{Allreduce}(n)$$  (GL6)
$$\text{MPI}_\text{Scatter}(n) \preceq \text{MPI}_\text{Bcast}(n)$$  (GL7)
$$\text{MPI}_\text{Reduce}(n) \preceq \text{MPI}_\text{Allreduce}(n)$$  (GL8)
$$\text{MPI}_\text{Reduce\_scatter}(n) \preceq \text{MPI}_\text{Allreduce}(n)$$  (GL9)
$$\text{MPI}_\text{Bcast}(n) \preceq \text{MPI}_\text{Scatter}(n) + \text{MPI}_\text{Allgather}(n)$$  (GL10)
$$\text{MPI}_\text{Allgather}(n) \preceq \text{MPI}_\text{Gather}(n) + \text{MPI}_\text{Bcast}(n)$$  (GL11)
$$\text{MPI}_\text{Allreduce}(n) \preceq \text{MPI}_\text{Reduce}(n) + \text{MPI}_\text{Bcast}(n)$$  (GL12)
$$\text{MPI}_\text{Allreduce}(n) \preceq \text{MPI}_\text{Reduce\_scatter\_block}(n)$$  (GL13)
$$\quad + \text{MPI}_\text{Allgather}(n)$$
$$\text{MPI}_\text{Reduce}(n) \preceq \text{MPI}_\text{Reduce\_scatter\_block}(n)$$  (GL14)
$$\quad + \text{MPI}_\text{Gather}(n)$$
$$\text{MPI}_\text{Reduce\_scatter\_block}(n) \preceq \text{MPI}_\text{Reduce}(n) + \text{MPI}_\text{Scatter}(n)$$  (GL15)
$$\text{MPI}_\text{Scan}(n) \preceq \text{MPI}_\text{Exscan}(n) + \text{MPI}_\text{Reduce\_local}(n)$$  (GL16)
$$\text{MPI}_\text{Reduce\_scatter}(n) \preceq \text{MPI}_\text{Reduce}(n) + \text{MPI}_\text{Scatter\_v}(n)$$  (GL17)