Asynchronous MPI for the Masses

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Abstract. We present a simple library which equips MPI implementations with truly asynchronous non-blocking point-to-point operations, and which is independent of the underlying communication infrastructure. It utilizes the MPI profiling interface (PMPI) and the \texttt{MPI\_THREAD\_MULTIPLE} thread compatibility level, and works with current versions of Intel MPI, Open MPI, MPICH2, MVAPICH2, Cray MPI, and IBM MPI. We show performance comparisons on a commodity InfiniBand cluster and two tier-1 systems in Germany, using low-level and application benchmarks. Issues of thread/process placement and the peculiarities of different MPI implementations are discussed in detail. We also identify the MPI libraries that already support asynchronous operations. Finally we show how our ideas can be extended to MPI-IO.

Keywords: asynchronous MPI, overlap, progress threads

1 Introduction

A widespread misconception about MPI’s non-blocking point-to-point and I/O routines is that communication and I/O necessarily overlaps with computation. According to the MPI standard \cite{MPIStandard} non-blocking semantics does not require asynchronous progress. Some MPI implementations do support asynchronous progress. However, this feature often needs to be explicitly enabled at compile time (e.g., with “progress threads”), requires the cooperation of several components of the used software stack, or needs special start-up parameters.

Surprisingly, many applications show performance improvements when non-blocking point-to-point communication is employed, even when the MPI library does not feature asynchronous progress. This is because of the other beneficial consequences of using non-blocking MPI, such as full-duplex transfers and avoidance of frequent explicit mutual synchronization.

In this work we describe a library which achieves asynchronous data transfer by utilizing the profiling interface of MPI (PMPI) and a separate progress thread. Therefore the MPI implementation must support the MPI-2 standard \cite{MPI2Standard} and must provide the \texttt{MPI\_THREAD\_MULTIPLE} compatibility level to allow several threads of a process to perform concurrent calls to MPI routines.

The library supports the C and Fortran MPI interfaces and requires no code changes to the target application. If the target application is statically linked against the MPI
library, relinking may be required. The method should work independently of the underlying interconnect.

This paper is organized as follows: In Sect. 2 we review related work on asynchronous data transfer with non-blocking point-to-point MPI or MPI I/O. The implementation details of the library are discussed in Sect. 3, and the test bed (hardware and software used for benchmarking) is introduced in Sect. 4. In Sect. 5 we evaluate the point-to-point messaging capabilities of our library using low-level benchmarks and hybrid-parallel sparse matrix vector multiplication. Asynchronous I/O is discussed in Sect. 6. Sect. 7 gives a conclusion and an outlook.

2 Related Work

Overlapping data transfer can be achieved on three different levels [5]: either by manual progression, progress threads, or communication offload.

Offloading  At the lowest level the transfer can be offloaded to the corresponding network interface, if supported. In principle this can be done for example with Myrinet or InfiniBand if the host channel adapter (HCA) is capable of it. In [8] KOOP et al. describe a protocol which enables full asynchronous progress by completely offloading the message transfer and matching to the InfiniBand HCA.

Progress Threads  Another option to handle communication and/or I/O while the user application can proceed is to use dedicated threads. One option is to have these threads be controlled by the MPI library. This technique was used for Open MPI until version 1.5.3 [18]; however, Open MPI could still support threads in some layers of its architecture. Other implementations, such as MPICH2, MVAPICH2, and Cray MPI [2] also feature special settings for enabling internal progress threads. Also several not so familiar MPI implementations have been built with this idea in mind, e.g. FiT MPI in MAO et al. [10] or USFMPI in CAGLAR et al. [1]. In [5] HOEFLER et al. analyze the impact of progress threads for non-blocking collectives inside their own reduced MPI implementation. Their findings are that polling for progress is beneficial if spare cores are available. Interrupt-driven progress threads are advantageous if all cores are fully utilized. DICKENS et al. [3] use progress threads for collective MPI-I/O. They have found that naïve usage of threads decreases performance. This might no more be true on current systems as the amount of available cores has increased. A similar approach has been followed by PATRICK et al. [13] by spawning a thread when the non-blocking I/O functions are called. The thread then calls the blocking counterpart. SHAHZAD et al. [16] use explicit progress threads inside an application for performing checkpoints of the application. Here the performance of the application was only marginally reduced compared to the case without any checkpointing. Using application-level progress threads SCHUBERT et al. [15] could significantly improve the performance of hybrid-parallel sparse matrix-vector multiplication.

Manual Progression  The idea of manual progression is to repeatedly call MPI_Test to check for completion. Hereby the assumption is made that every call into the library drives the progress. An evaluation of how frequent these calls should be performed has been done by HOEFLER et al. in [6].

Benchmarks  WHITE and BOVA [19] have performed an early investigation of asyn-
Fig. 1. (a) The APSM intercepts the initialization stage of the MPI library and enforces the MPI_THREAD_MULTIPLE level. Finally the progress thread is started. (b) The non-blocking MPI calls (e.g., MPI_Isend) are intercepted and executed by the application thread. The returned request handle is put into an internal queue, which is consumed by the progress thread. A generalized request handle is returned to the application. This handle will receive the status of the original request once it has been completed.

chronous progress in MPI libraries. In [9] LAWRY et al. describe a benchmark for detecting possible overlap. The Sandia MPI Micro-Benchmark Suite [14] contains a component that measures the host processor overhead during non-blocking MPI send and receive operations. The overhead introduced with using the MPI_THREAD_MULTIPLE level was analyzed by THAKUR et al. in [17]. Depending on the implementation quality of the library the overhead ranges from negligible to large.

3 Solution

The APSM library (Asynchronous Progress Support for MPI) is designed to work with every MPI library and any interconnect, as long as following conditions are met:

- Every call into the MPI library drives the internal progress engine.
- The MPI library supports MPI_THREAD_MULTIPLE.
- The MPI library supports the MPI profiling interface (PMPI), i.e., for every relevant MPI symbol (MPI_Xxx...) there is a corresponding symbol PMPI_Xxx... A library can then implement the MPI functions it wants to intercept and can then call the corresponding PMPI routine.

The PMPI interface is used to intercept all MPI calls that are relevant for non-blocking point-to-point messages or non-blocking MPI-IO.

3.1 Initialization and Finalization

The initialization process is depicted in Fig. 1a. To setup the library the MPI_Init* functions are intercepted. In MPI_Init_thread the MPI_THREAD_MULTIPLE level is requested; if the library does not support this level, the application is aborted. (For convenience calls to MPI_Init are rerouted to MPI_Init_thread so that applications
which do not call the threaded initialization require no code changes.) Next, the progress
thread is created using pthread_create. In our experience the Pthreads primitives
used by APSM do not interfere with any other threading model employed in the user
program, such as OpenMP.

The progress thread is terminated by intercepting MPI_Finalize, which first stops
the progress thread before calling PMPI_Finalize.

3.2 MPI Point-to-Point Functions

All intercepted non-blocking point-to-point functions are handled in the same way (see
Fig. 1b). If such a function is called by the application the actual requested operation,
e.g., MPI_Isend, is carried out by calling the corresponding PMPI function.

The returned request handle is enqueued to an internal queue, and a newly created
generalized request handle is returned to the application. This handle will act as a
“proxy” of the original request. This process is transparent to the application, and no
code changes are necessary.

The queued original requests which are bound to the message transfers are pro-
cessed from the internal queue by the progress thread. If, at any time, a bunch of
requests is waiting in the queue, they are served simultaneously by calling either
MPI_Test(some|any) or MPI_Wait(some|any) for driving the progress of data
transfer and waiting for the completions. Which of the four alternatives is chosen in
practice depends on the MPI library (see below). If a request completes, its status is
 propagated to the associated generalized request, notifying the application.

Since all non-blocking MPI functions return an MPI request handle, this method
will work for them. Note that the call to the PMPI functions happens still in the context
of the application’s thread. This is necessary to provide a correct MPI program, since
a pair of matching non-blocking send and receive calls in the same MPI process are
guaranteed to complete. This would not be ensured if the PMPI calls were done inside
the progress thread and MPI_Wait(some|any) were used to wait for completion: After
the application posts the send, the progress thread would detect it in the internal queue,
execute it, and wait for it. Then, a matching receive could be posted next by the appli-
cation, but it would never be handled by the progress thread, which would wait forever
for the completion of the send request.

3.3 MPI-IO Functions

Calls to non-blocking MPI-IO functions are handled slightly differently. The call to the
PMPI function (e.g. PMPI_File_iwrite) is performed in the context of the progress
thread. Since the MPI standard allows MPI-IO progress to occur within the initial non-
blocking call, this is the more general (and, in this case, safe) way to ensure asyn-
chronous I/O.

3.4 Fortran Interface

The Fortran interface poses a slight problem, since different MPI implementations use
different strategies to implement the MPI interface. Internal MPI routines may be called
3.5 Affinity of the Progress Thread

Since the application and the MPI library are not aware of the progress thread, they cannot control its affinity (i.e., which logical core it is bound to) in a meaningful manner. If there is no general way to handle excess threads (e.g., with the -d option in Cray’s `mpirun`), this can be set by the environment variable `MPI_ASYNC_CPU_LIST`. The specified core list relates to the MPI processes on a node. For example, the list `0_2_4` would pin the progress thread of the first MPI process on every node to core 0, the progress thread of the second MPI process to core 2, and the progress thread of the third MPI process to core 4. 

4 Test Bed

We have used three cluster systems for our tests: “Lima” at the Erlangen Regional Computing Center (RRZE) in Erlangen, Germany, “SuperMUC” at the Leibniz Supercomputing Center (LRZ) in Garching, Germany, and “Hermit” at the High Performance Computing Center (HLRS) in Stuttgart, Germany. Their system parameters can be found in Table 1.

There is the residual problem of how to determine the number of processes per node. This can be solved in a general way, but an in-depth description would be out of scope for this work.
5 Overlap of Point-to-Point Messages

In this section we demonstrate the capabilities of the APSM library using simple low-level benchmarks and a hybrid-parallel sparse matrix-vector multiplication kernel. Since it is impossible to show all benchmark results due to the vast number of parameters, we will concentrate the discussion on the most prominent aspects. The complete set of benchmark results can be reviewed online [20].

5.1 Simple Overlap Benchmark

A simple benchmark is used to test the ability of MPI libraries to overlap computation with communication using non-blocking point-to-point calls [4]. Two MPI processes are run, each on its own compute node. The first process initiates a non-blocking send (MPI_Isend), performs (CPU-bound) work for a time \( t_w \), and finally calls MPI_Wait. The total time \( t_t \) taken for all three steps is measured. The second process immediately posts a blocking receive (MPI_Recv). This can also be varied with MPI_Irecv/MPI_Send or MPI_Isend/MPI_Irecv instead of MPI_Isend/MPI_Recv.

When \( t_t \) is plotted against \( t_w \) and no asynchronous progress has occurred a straight line can be seen with an offset on the \( y \) axis:

\[
t_t = t_c + t_w,
\]

where the communication time \( t_c = V / B_N + t_l \). Here \( V \) is the message volume, \( B_N \) is the network bandwidth, and \( t_l \) is the network latency. If there is fully asynchronous progress, we have

\[
t_t = \max(t_c, t_w).
\]

The results for Intel MPI 4.0.3 are shown in Fig. 2a. Intel MPI currently does not provide asynchronous progress over InfiniBand. Using it together with APSM provides full overlap for non-blocking point-to-point communication and “large” messages (see below for details on how smaller messages must be handled). The only test/wait function of MPI which was usable in the progress thread without deadlocking was MPI_Waitany. We attribute this to problems with thread safety in Intel MPI.

Open MPI (version 1.6.3) provides overlap for non-blocking point-to-point communication, at least for MPI_Isend. However, Open MPI cannot use InfiniBand with the MPI_THREAD_MULTIPLE threading level as the corresponding OpenIB module is not thread safe. In this case the implementation falls back to TCP, which in our case takes place using IP-over-IB or Gigabit Ethernet. This can be seen from the simple ping-pong benchmark in Fig. 2b. Here only around 200 MB/s compared to the 3.0 GB/s with IB can be achieved when the highest threading level is requested.

MPICH2 only supports Gigabit Ethernet (GE) and no InfiniBand. With the internal progress thread enabled (by setting MPICH_ASYNC_PROGRESS=1) overlap can be achieved. APSM can be used as an alternative.

MVAPICH2 (version 1.9a2) can overlap non-blocking point-to-point messages with communication if the internal progress threads are enabled via MPICH_ASYNC_PROGRESS=1. This MPI library also works with APSM.
IBM MPI (version 1.2) can by default only overlap MPI_Isend with computation. However specifying MP_CSS_INTERRUPT=yes [7], which causes arriving packets to generate interrupts, leads to overlapping behavior in all other situations. Utilizing APSM delivers in principle the same result, but introduces a lot of variability in execution times; sporadically, MPI calls take an exceedingly long time. The reason for this behavior has not been investigated yet.

Cray MPI in the standard configuration provides no asynchronous message transfer, but it supports an option to activate an extra progress thread by setting the environment variable MPICH_NEMESIS_ASYNC_PROGRESS=1 [2] and reserving one core with the aprun option -r 1 for the additional thread. With the simple overlap benchmark this yields better results than with APSM.

Table 2 summarizes these results in columns 3 and 5.

5.2 Prototype Ghost Cell Exchange Benchmark

This benchmark simulates strong scaling of an application which performs exchange of ghost cells in one dimension. A number of MPI processes are running, each of which exchanges a “halo” of fixed size with its two neighbors. After the exchange, each process executes a workload which is subject to strong scaling with the number of processes. Computations which would be required in a real application for the boundary cells in preparation of the halo exchange are neglected.

In order to better mimic the execution behavior of real applications but still achieve good reproducibility of time measurements, a simple triad loop benchmark ($a(:) = b(:) \ast c(:) + d(:)$) was chosen as the workload. The size of the working set was adjusted to fit into each core’s own L2 cache.
Table 2. Overview of all MPI implementations and the system they were evaluated on.

| Name         | Version | Overlap | Works w/ APSM | Improvement | System         |
|--------------|---------|---------|---------------|-------------|----------------|
| Intel MPI    | 4.0.3   | No      | No            | Yes         | No            |
| Open MPI     | 1.6.3   | Yes     | No            | Partial     | No            |
| MPICH2       | 1.5     | Partial | Partial       | Yes         | No            |
| MVAPICH2     | 1.9a3   | Yes     | No            | Yes         | Yes           |
| IBM MPI      | 1.2     | Yes     | No            | Yes         | No            |
| Cray MPI     | 5.6.1   | Yes     | No            | Yes         | Yes           |

We used the Lima cluster with Intel MPI and up to twelve nodes, with twelve MPI processes per node (PPN). Each process was bound to its own physical core. In the case where the APSM library was used, the progress thread was pinned to the other SMT thread.

The performance results for a communication buffer size of 10 MiB can be found in Fig. 3a. Use of the APSM library achieves superior performance and scalability up to the point where communication takes longer than computation (at about three nodes). This can be seen from Fig. 3b, which shows a breakdown of time contributions in the duration of work, i.e., the computation (filled symbols), and the “visible” communication time, which is in case of overlap the difference between overall time and working time (open squares). Without overlap, the communication time is independent of the number of processes (open circles), since the message length is always the same.

Beyond three nodes, performance saturates in the overlapped case, whereas it continues to rise without overlap. At large node counts, both numbers coincide, since communication absolutely dominates in this case and computation time is negligible. However, this is not the limit in which one would want to run any real application code in practice, since parallel efficiency has dropped to unacceptable levels. The “sweet spot” in terms of efficient execution is at the point where the overlapped performance saturates. This is also where the advantage compared to the non-overlapped case is at a maximum.

As the difference in \( t_w \) between overlapped and non-overlapped cases shows, the progress thread requires additional resources, reducing the worker thread’s performance accordingly. In cases where spare physical cores are available, e.g., if the application is strongly memory-bound with saturation across the cores of a socket, the progress threads can be bound to those. This would strongly reduce the interference of MPI progress with application execution.

5.3 Sparse Matrix Vector Multiplication (spMVM)

We use a hybrid (OpenMP + MPI) sparse matrix vector multiplication \( (y = y + M \times v) \) as a relevant real-world test case to demonstrate the applicability of our approach. MPI
parallelization is done by distributing the matrix rows across processes so that each process has (approximately) the same number of nonzero entries. The right-hand side (RHS) vector $v$ is distributed in the same way. Consequently, overlapping computation with the required communication of the RHS vector parts requires splitting the spMVM operation in two phases: A “local” phase, in which a process multiplies its local part of the RHS vector to the corresponding diagonal block of the matrix, and a “non-local” phase, in which the parts of the RHS vector that have been received by other processes are multiplied to the remaining matrix entries.

There are two ways in which communication overlap may be achieved, “vector model with naive overlap” and “task mode with explicit overlap” [15]. The former uses all OpenMP threads to perform the local spMVM part and relies on non-blocking MPI calls and a subsequent MPI_Waitall for asynchronous MPI progress, while the latter uses a dedicated communication thread. After the local spMVM and the communication are both over, both approaches perform the non-local spMVM with all threads (see [15] for a full description).

If the MPI implementation does not support asynchronous progress, communication only takes place during the MPI_Waitall call. This results in overlap only with task mode, at the price of sacrificing one worker thread for the local spMVM.

For evaluation we selected two sparse matrices “HV15R” and “DLR1,” where the former has about $2 \cdot 10^6$ rows and $2.8 \cdot 10^8$ nonzeros, and the latter has $2.8 \cdot 10^9$ rows and $4 \cdot 10^7$ nonzeros. DLR1 uses only around 480 MB of memory and thus fits completely in the L3 caches of 24 Lima compute nodes.

Task mode shows best performance with Intel MPI in all cases (see Fig. 4). For the HV15R matrix (Fig. 4a) vector mode with APSM is better than without and nearly achieves the performance of task mode. The DLR1 matrix reveals a specific problem due to the very small message sizes that occur as the number of MPI processes is increased. These are usually handled by MPI implementations using a so-called eager protocol: If a message is small enough it can directly be sent to a predefined buffer at the destination. Otherwise the sender and the receiver must synchronize to initiate the actual transfer (rendezvous protocol).
Fig. 4. Performance comparison of spMVM with Intel MPI on Lima, running one MPI process with twelve OpenMP threads per node

If every message were handled in the same way by the APSM library independent of size, the latency for potential eager messages would increase since the whole mechanism of processing queued requests by the progress thread would add nothing but overhead. When the library is made aware of the threshold, request handles for eager messages are directly obtained from MPI and passed back to the application, with no interference from the progress thread. The difference between both behaviors can be seen in Fig. 4b, where the performance of APSM without eager awareness becomes unacceptable beyond 16 nodes (diamonds). With eager awareness, however (at a message size of \( \leq 256 \text{ KiB} \) in this case), the performance reaches the level of vector mode without APSM (triangles). The reason why task mode is still measurably better at large node counts is that all overheads connected with MPI communication can be hidden by an explicit communication thread, whereas the eager protocol alone (which is also in effect when APSM is used with eager awareness) still suffers from unavoidable communication latencies.

6 Overlap of MPI-IO

The APSM library can also be used to overlap computation and MPI-IO. To evaluate the state of the MPI implementations and the usefulness of APSM a modified version of the overlap benchmark (see Sect. 5.1) was used, where point-to-point communication was substituted by I/O via `MPI_File_iwrite`. Only one process per node was used, writing 6 GiB of data to a parallel file system. All processes wrote to the same file. Care was taken to rule out caching effects, i.e., the measured I/O times included real disk I/O only. In general, getting reliable timing for I/O is not easy since the parallel filesystems are usually under load by other users, which leads to fluctuating bandwidths.

The results can be summarized as follows. The Intel MPI library does not overlap computation and I/O. Using it together with APSM is not possible due to frequent deadlocks. Open MPI does not provide asynchronous I/O on the Lustre filesystem of Lima, but overlap can be seen with APSM (see Fig. 5a). The main disadvantage with this solution is that Open MPI can not use native InfiniBand for point-to-point communication.
Fig. 5. Results for the MPI-IO overlap benchmark on Lima using (a) Open MPI and (b) MVAPICH2, on eight Lima nodes, one process per node, and 6 GiB of I/O volume per process.

with APSM (see Sect. 5.1 above). MVAPICH2 does not support asynchronous I/O even with its internal progress thread enabled. However, overlap is available with APSM (see Fig. 5b). Cray MPI does not feature asynchronous I/O (with and without the internal progress thread) but can benefit from the APSM library.

Table 2 gives an overview of the results in columns 4 and 7.

7 Summary

We have demonstrated how asynchronous point-to-point communication and MPI-IO can be achieved for MPI implementations that have no native support for asynchronous progress. By overloading some MPI functions using the PMPI interface, an internal progress thread is used to handle non-blocking requests in the background with minimal impact on the performance of code execution in the application program. In cases where no dedicated physical cores are available for the progress thread, virtual cores can be used. Most current MPI implementations are compatible with our method. However, strict MPI_THREAD_MULTIPLE compatibility and thread safety is required.

Possible future work includes support for persistent communication and split-collective MPI-IO functions. The library is freely available under an LGPL license [20].

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