Towards Achieving Transparent Malleability Thanks to MPI Process Virtualization

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Abstract. The field of High-Performance Computing is rapidly evolving, driven by the race for computing power and the emergence of new architectures. Despite these changes, the process of launching programs has remained largely unchanged, even with the rise of hybridization and accelerators. However, there is a need to express more complex deployments for parallel applications to enable more efficient use of these machines. In this paper, we propose a transparent way to express malleability within MPI applications. This process relies on MPI process virtualization, facilitated by a dedicated privatizing compiler and a user-level scheduler. With this framework, using the MPC thread-based MPI context, we demonstrate how code can mold its resources without any software changes, opening the door to transparent MPI malleability. After detailing the implementation and associated interface, we present performance results on representative applications.

Keywords: MPI · Malleability · Compiler

1 Introduction

The field of High-Performance Computing (HPC) is witnessing an increasing complexity in hardware, with hybridized architectures combining distributed and shared-memory parallelism along with accelerators. This requires programs to incorporate multiple programming models, potentially with diverse computing abstractions, to fully utilize the capabilities of the underlying computing substrate. This complexity has consequences both on the programs themselves and on their efficient utilization of the hardware. Programs in HPC are typically large simulation codes, often consisting of millions of lines of code. Therefore, adapting to new architectures is a planned and complex process. The chosen technology should be able to remain relevant for a sufficient duration to avoid tying the codebase to a particular technology or vendor, necessitating parallelism abstractions [4]. The process is often piece-wise, leading to incomplete parallelism and parallel limitations due to fork-join patterns. Parallel runtimes play a

crucial role in abstracting hardware changes. However, due to increasing hardware constraints, low-level behaviours start to impact applications. OpenMP is successful in porting *existing* code to new architectures in a piece-wise manner by adding `#pragma parallel for`. However, the slower adoption of recent OpenMP advances suggests that this is less effective for tasks and OpenMP targets, despite the preservation of optional pragmas. On the MPI side, the programming model is deeply embedded in most of the HPC payloads due to its robustness and ability to constantly evolve to handle new hardware while providing bare-metal performance. However, this strength is also a weakness as it encloses parallelism expression in a relatively low-level and fine-grained form. The end-users are directly using what could have become the "assembly" of a higher-level abstraction.

Our paper highlights the imminent complexity barrier that HPC is facing due to architectural evolutions and technical debt accumulated by HPC applications. Although runtimes have evolved and new abstractions have been provided, they often do not translate to applications [5, 19]. The empirical nature of the usage of supercomputers, driven by domain-specific scientists who are mainly interested in their results and given virtually unlimited computing power with little or no quota, has resulted in heuristics of doing good science that prioritize final results over efficient use of parallel machines. However, with the rise of GPUs and multi-level parallelism, the need for efficient use of parallel machines is more pressing than ever. Ideally, the solution would be to rewrite applications using new abstractions to address new hardware. However, this requires teaching domain-specific scientists how to code in parallel abstractions or providing them with tools that hide the complexity of parallelism. Several languages, including domain-specific ones, have tried to define more expressive ways of parallelizing programs [4, 17, 28]. Acknowledging the existence of inefficient (by design) and potentially transitively inefficient parts of parallel programs, the question of malleability then becomes preponderant.

2   Fast is not Efficient

Time to result is not a correct heuristic to define how efficient a computation is. Indeed, from the well-known parallel efficiency formula, one may add computing resources to a computation while contributing only at the margin to the final result. As a consequence, sometimes a slower run is making much better use of the underlying hardware while leaving space for other runs on the freed resources [10, 3]. Malleability is the systematic and automated application of such reasoned running configuration for a given heuristic. And for more optimized applications, co-scheduling also provides opportunities for resource sharing for example during alternating phases of computing or to cope with load imbalance. In this work, we propose to implement transparent application co-location using the MPC thread-based MPI and a specialized compiler enabling the conversion of MPI+OpenMP applications to threads.

3   The Multi-Processor Computing Runtime

MPC is a thread-based implementation of MPI, where MPI processes run in threads instead of traditional UNIX processes. This approach has various benefits, including reduced memory usage, faster launch times, and improved intra-node messaging (see section 6). Moreover, MPC has its own implementation of OpenMP and a user-level scheduler that is necessary for transparently running programs in co-routines, as discussed in Section 3.2. Additionally, MPC provides a specialized compiler that facilitates the porting of regular MPI+OpenMP codes to a thread-based context.

3.1   MPC Compiler Additions: privatization

The process of converting global variables to Thread-Local Storage (TLS) variables using MPC's privatizing compiler [6] is crucial to enable the thread-based execution of regular MPI programs inside threads. This is necessary because global variables can cause conflicts when loaded in the same address space. The MPC privatizing compiler converts these global variables to MPC's TLS variables, which enables loading the same program multiple times in a single address space without any conflicts. The privatizing compiler is based on a modified version of GCC and includes a pass that converts global variables and other TLS levels (such as OpenMP thread-locals) to MPC's TLS. This pass has been implemented in a component called libextls (extended TLS) [6].

After a program has been privatized, it can be executed in the context of a thread, initially to meet the needs of a thread-based MPI. However, as we will discuss later in this paper, we aim to expand this concept to hybrid computing, where various executables are loaded in the same address space. In such a setup, the MPC runtime (MPI and OpenMP) can better address performance differences between the different applications.

3.2   User-Level Threads

Once MPI processes are threads, it becomes interesting to consider their execution inside user-level threads. This is a convenient way to hide waiting time, replacing it with context switches [30]. When a *task* is delayed, the resources can be used productively by moving to another task, instead of remaining in a busy loop. MPC is built around the concept of co-routines, and to make this approach viable, it is crucial to not only privatize threads but also to wrap the complete Pthread interface to capture potentially blocking calls, redirecting them to the scheduling loop inside MPC. Otherwise, a lock could be held by a pending task. Using MPC's $m{:}n$ scheduler, it is already possible to run two programs on the same resources in an oversubscribed fashion, meaning that the two programs will alternate on the underlying Pthread (co-routines).

By extending this idea to malleable programs, two programs can run on the same resources [25]. In addition, since MPI programs are now running inside threads, it is possible to move them on the node, changing their affinities. This

is analogous to changing the target pending list in the scheduler without having to handle data dependencies, which can be complex in the case of regular MPI processes, but trivial in shared-memory. This extended support for threads and the user-level scheduler provides opportunities for fine-grained control over cross-scheduling of runtimes [13, 31, 18].

3.3   OpenMP Runtime

The MPC framework includes an OpenMP runtime that utilizes the same user-level thread and privatization infrastructures as the MPI runtime. This runtime is designed to be compatible with both GOMP and Intel/LLVM ABIs, enabling it to run OpenMP programs generated by different compilers. One significant advantage of co-locating both OpenMP and MPI threads in the same scheduler is the potential for runtime-stacking [11, 27]. This refers to the idea of combining multiple runtimes for improved scheduling. Recent research has shown that it is possible to convert MPI waiting time into OpenMP task progress [31]. We aim to utilize this feature, in conjunction with privatization, in our co-scheduling approach, which relies on MPI process virtualization.

4   MPI Process Virtualization

MPI process virtualization is the process of converting MPI processes into threads within compute nodes [6, 30]. This approach allows for new scheduling opportunities for parallel applications by implementing cross-job malleability at the node level, instead of relying on a single scheduler. In this section, we will provide an overview of this concept. We will discuss how it involves using a node-level scheduler, specifically MPC, to enable job malleability, resource sharing, and mitigation. Additionally, we will explore the compilation aspect of gathering multiple programs in the same binary and the executive part of leveraging OpenMP tasking, building on previous work [31], to optimize performance.

4.1   The Need for Node-Level Schedulers

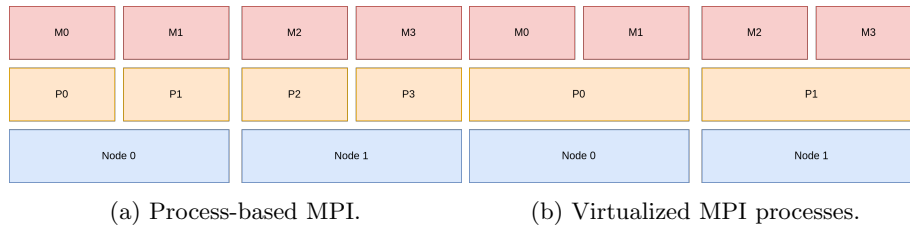(a) Process-based MPI.   (b) Virtualized MPI processes.

Fig. 1: Comparison between regular scheduling approach and virtualized MPI processes.

As shown in Figure 1a, a traditional HPC scheduler allocates resources based on UNIX processes. Typically, there is a one-to-one correspondence between UNIX processes and MPI processes. In contrast, our approach using MPC involves colocating and co-scheduling multiple programs within a single address space on each node, as illustrated in Figure 1b. One advantage of this approach is that it requires fewer processes to run a given program. This is because there is no longer a direct mapping between UNIX and MPI processes; MPI processes are now threads. Furthermore, the work we present in this paper has indirect implications for malleability pivoting with a centralized scheduler (e.g., using the Process Management Interface or PMIx), as it can now be partially a local scheduling decision that is fully dynamic and arbitrary. Our two-level scheduling approach can leand to multiple profitable scenarios that have been explored in the literature:

- **Ressource sharing** [16, 22, 24, 12, 29, 1]: two applications residing in the same address space can dynamically exchange their resources without the need for copying or remapping of data. This allows the underlying scheduler to balance the compute resources from all collocated applications without complex code adaptation. For instance, two applications that require linear algebra computations on the node could have their respective tasks scheduled on the GPUs with a global view of the system, potentially achieving higher utilization than when allocating GPUs to each program separately.
- **Overprovisionning** [8, 21, 35, 25]: in this configuration we run multiple applications per core, forcing them to alternate on the resources. In this case, the waiting time is directly recovered by the yield mechanism of the user-level scheduler, hiding latency. This case is of course bound to the availability of enough memory on the node.
- **Specialization** [14, 34, 15]: this opens the way to define in-process services providing facilities such as I/O to all programs running on the node in a very efficient manner (true zero-copy). Doing so may open the way to machines with smaller service islands, I/O being part of the job themselves with dedicated resources. This provides strong advantages to in-situ scenarios.

Overall, the main advantage of this two-level scheduler model is that scheduling decisions at the node level is now local, and there is no need to rely on an external component, except when more resources are needed. In the context of this work, we consider that we have colocated multiple applications in the same address space, and they now share their CPUs. Moving an application is now equivalent to moving a simple thread.

Therefore, as shown in Figure 2, malleability inside the node becomes practical for any MPI+OpenMP application without requiring specific porting or modification. This is due to MPC's privatizing compiler that ensures applications can run inside threads, and we can simply adjust the resources allocated to each of these applications while sharing all the runtime components between the two programs. In the next section, we will describe how an application can be converted to a virtualized program inside MPC.
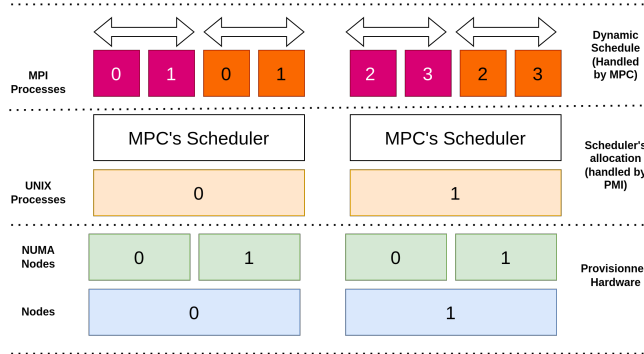
Fig. 2: Illustation of node-level malleability in the context of virtualized MPI processes.

4.2   Virtualizing Programs

The process of virtualizing an existing program is very similar to the one done inside MPC for privatization purposes, which involves running the same program image multiple times in a single process [6]. It consists of compiling the program with a modified compiler that converts global variables and thread-local variables to the extended TLS hierarchy of MPC, which features an additional "process" level that matches each MPI process in the final runtime memory image. This process preserves TLS optimizations [6]. As shown in Figure 1b, once this is done, and because the `main` function of the application has been renamed using a preprocessor directive, MPC simply launches N threads with their respective pinning, TLS context, and ranks to mimic the execution of the process in MPI, except that it is now in threads. This process has been reliably used by MPC to run C, Fortran, and C++ applications, with C++ being the most complex due to potential dynamic initializers, global objects, and templates. The idea of virtualizing MPI processes is not new and has a long research history [30, 25, 20]. AMPI [30], FG-MPI [?] and the Charm++ [24] runtimes have demonstrated many benefits of virtualized MPI processes, such as load-balancing [30] and dynamicity [23]. The closest related work to the idea we present in this paper is Adaptive Jobs [23]. This work moves the scheduler inside virtualized MPI processes and proposes to allocate programs in these address spaces. Conversely, in our approach, we stay much closer to the existing parallelism interfaces and runtimes, with the goal of transparently running *existing* programs in a virtualized configuration. This is only possible because MPC features its own OpenMP implementation and a Pthread interface to redirect locking calls to the user-level scheduler. When multiple programs are living in the same address space, there are opportunities for *runtime stacking*, and it is this aspect that we aim to highlight in this paper.

Returning to our initial goal of generalizing the approach to multiple programs, we needed to load multiple privatized programs in the same address space.

To achieve this, we compiled the codes with the `-fpic -rdynamic -shared` flags, making the code position independent (as shared libraries) and exposing symbols in the final binary (and therefore the main). With this done, we were able to dynamically open binaries and their shared library dependencies with the help of the loader. The programs now run inside the same process, and we eventually replace their `MPI_COMM_WORLD` with a subset of the actual world, matching the actual program splitting. As MPC is also an MPI runtime, doing so is straightforward, as it simply involves replacing the communicator in the MPI process context. Note that this last step can become even more transparent using the session model, in which the application builds its `COMM_WORLD`, enabling explicit redirection. There are of course security issues when colocating programs in a single address space, and therefore such a scenario can only be envisioned for binaries belonging to the same user, and not as a way to run general programs in such a configuration. Memory segmentation from the Operating System and the zero-page mechanism are essential security measures to ensure perfect impermeability in between address spaces. Besides, signals are also handled by the controlling process and therefore, events such as `SIGINT` cannot be handled individually in such a configuration.

4.3   Co-Scheduling Multiple Programs in a Single Process

Thanks to the nature of the MPC thread-based MPI+OpenMP runtime, multiple programs can run within a single UNIX process. Now comes the question of *co-scheduling* [2] each program to guarantee efficient progression of each application. The first possibility is through cores oversubscription with kernel threads (e.g., *pthreads*), letting the operating system preemptively schedule threads of each program. With n cores and $m > n$ threads, this is the $m{:}n$ co-scheduling approach. Oversubscription has been widely adopted in runtimes for overlapping synchronization idleness on cores, on AMPI [30] or LLVM OpenMP [33] for instance. Yet, it can degrade performances when a high number of asynchronous operations concurrently progresses [21, 35], one source of overheads being the operating system [7, 32]. The second possibility is an $n{:}n$ approach: each core is assigned a single kernel thread, and the scheduling decision is taken by the MPC user space scheduler. In particular, recent work on the MPC OpenMP *task* scheduler has shown improvement over the LLVM $m{:}n$ approach for target tasks offloading [18].

   The final goal of our work, which we are yet to reach, is to deploy a co-scheduling approach as depicted on Listing 1.1. Line 1 to 6 corresponds to program dynamic loading, line 10 the $n{:}n$ threads binding is created. From lines 11 to 19, each program starts execution within an OpenMP task with its own *fiber*, which is an MPC extension hinting at the OpenMP runtime to execute tasks on their stack, enabling more scheduling flexibility. Descendant MPI processes, OpenMP parallel regions, and tasks created by each program will then run as part of a single MPC OpenMP task scheduler responsible for co-scheduling. Note that our execution model assumes tasks can migrate between *teams* which is not

compliant with current OpenMP specifications and therefore still requires dedicated work. Recent work on Free Agent Threads [26] provided a solution to this limitation, improving the malleability of OpenMP tasking. Our execution model also relies on runtimes interoperability [31] so that a task blocking within an MPI call is automatically preempted instead of retaining its core.

Listing 1.1: Pseudo-code of the launcher wrapper

```
1   extern struct program_t {
2       int argc;
3       char ** argv;
4       int (*main)(int, char **);
5   } * programs;
6   extern int n_programs;
7
8   int main(void)
9   {
10      # pragma omp parallel
11      # pragma omp single
12      {
13          for (int i = 0 ; i < n_programs ; ++i)
14          {
15              program_t * p = programs + i;
16              #pragma omp task fiber
17                  p->main(p->argc, p->argv);
18          }
19      }
20      return 0;
21  }
```

5   Co-Scheduling Experiment

In this section, we present the results of our initial experiments, which involved running applications on the same node in order to identify optimal execution times. The purpose of this setup was to identify potential "sweet spots" for execution time, which could eventually become more dynamic as shared-memory models used within applications become more flexible, particularly in terms of their ability to be invasive. However, it is important to note that the results presented here are limited by the static nature of the allocation used in our experiments.

In Figure 3a, we show the scalability of the various kernels, which have different problem sizes and exhibit different strong scaling behavior. The smaller kernels exhaust their parallelism more quickly than the larger ones. This behavior is also present in the individual nodes of larger simulations, particularly when considering dynamic behavior over time.

To further investigate co-location, we selected four of these benchmarks (bt.A, lu.C, ft.C, and mg.C) and ran them on a single node. As expected from

(a) Scalability of the individual kernels on the machine.

(b) Combination of four programs bt.A, lu.C, ft.C and mg.C over the machine (walltimes)
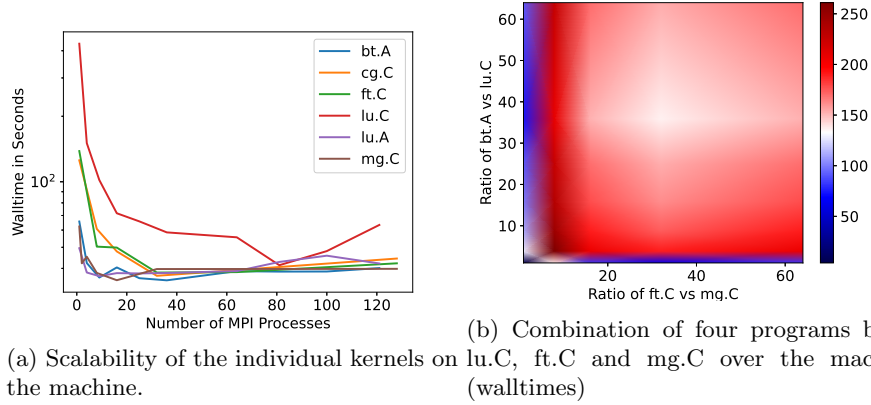
Fig. 3: Walltime for various resource breakdowns for co-located NAS MPI benchmarks.

the scaling behavior, there are sweet spots of scheduling for these four programs, which are indicated by the lower values in Figure 3b. This suggests that dynamically reshaping jobs over time to follow these sweet spots could lead to improved performance. However, this can be difficult to accomplish through models alone, which is why our future work will focus on developing a node-level shared runtime to support malleability.

Co-locating programs is not a new idea, and several MPI runtimes and experiments dedicated to malleability have demonstrated similar gains to the ones we present here [29, 9, 24, 2]. However, one of the main motivations for our work is that MPC can convert existing programs to shared-address space transparently, while still supporting regular MPI and OpenMP. This simplifies the process of making programs malleable and expands the range of applications that can benefit from this approach.

6   Networking Performance

As a thread-based MPI, MPC is capable of exchanging MPI messages between MPI Processes (now threads) running in the same process. In addition, it also supports all intermediate configurations, including a regular process-based execution. Besides, MPC has support for standard HPC networks, including SHM, Infiniband, Portals 4 BXI [?] interconnect and libFabric. It means co-scheduled programs can run distributed as regular MPI applications, malleability would only occur at the level of nodes, in between colocated programs thanks to the shared runtimes (mostly OpenMP for compute).

Figure 4 presents the performance results of running the Intel IMB-MPI1 Ping-Pong benchmark between two processes co-located on the same node. This
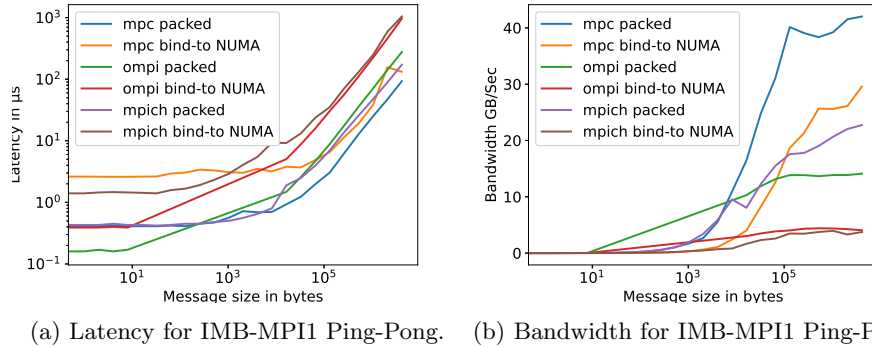
(a) Latency for IMB-MPI1 Ping-Pong.   (b) Bandwidth for IMB-MPI1 Ping-Pong.

Fig. 4: Comparison of MPC, OpenMPI and MPICH over various biding config-
uration using the IMB-MPI1 Ping-Pong benchmark.

simple benchmark allows us to assess the relative bandwidth and latency per-
formance between co-located programs. The tests were conducted on a bi-socket
AMD EPYC 7413 machine with a total of 48 cores. The "packed" configuration
means processes are running on nearby cores, while the "scattered" configura-
tion means processes are spread across the two NUMA nodes. We measured the
performance using MPC 4.1.0, OpenMPI 4.1.5, and MPICH 4.1, all of which
were installed through spack using the default configuration flags.

In Figure 4a, we observe that MPC has lower latencies for larger messages.
However, for smaller messages, other runtimes, particularly OpenMPI, can per-
form better. The main reason for this is that in MPC, the `THREAD_MULTIPLE`
support is always on, due to its thread-based nature, which leads to locking re-
quirements and impacts the micro-optimizations needed to reach performance
levels comparable to OpenMPI. However, thanks mostly to the improved band-
width as messages are moved through direct `memcpy` (as shown in Figure 4b),
MPC yields lower latencies for larger messages. Other runtimes may use SHM
fragments or more optimal Cross-Memory Attach (CMA) to transfer such large
buffers, which are less direct than a regular *memcpy*.

Overall, we have demonstrated that running programs in shared memory
with MPC can result in improved messaging bandwidth in some cases. This
improvement is more pronounced for larger messages, but smaller messages still
suffer from locking overhead. To address this limitation, we are currently in the
process of fully rewriting the networking stack in the MPC runtime. Our goal
is to improve performance and reduce overhead for all message sizes, further
enhancing the benefits of running programs in shared memory with MPC.

7   Conclusion

High-performance computing architectures are evolving towards increased flex-
ibility in utilizing node-level resources. However, shared-memory resources are

often underutilized due to a lack of collaboration between programming models. For instance, MPI may get stuck in a busy-wait loop while OpenMP may have pending tasks. To address this issue, we utilized the virtualization capabilities of the MPC thread-based MPI + OpenMP runtime to transparently port MPI applications to a space where they can be adapted to shared memory with less effort. This process is analogous to what MPC does for MPI programs, utilizing its Extended TLS model. In this work, we presented two types of co-scheduling: oversubscription to eliminate busy waiting by using context yields and a unified scheduler that balances computing on a whole node, including between different virtualized programs. We also showcased the OpenMP code that we plan to use to achieve this.

We then conducted co-scheduling experiments that showed the potential for dynamic scheduling at the node level to compensate for imbalance and inefficiencies by opening a common task-oriented scheduler to all runtimes. Eventually, we have shown that by running in shared memory there were opportunities to improve MPI messaging performance. Going forward, we plan to further develop this work on the OpenMP side, seeking a practical way to define node-wide task stealing, which is currently not feasible between different parallel regions. This would enable OpenMP programs co-located in the same node (and virtualized in the same process) to dynamically balance their computations.

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