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A full stack simulator for HPC: Multi-level modelling of the BXI interconnect to predict the performance of MPI applications

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Julien EMMANUEL

**Un simulateur pour le calcul haute performance :
modélisation multi-niveau de l'interconnect BXI
pour prédire les performances d'applications MPI**

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Résumé

Pour obtenir les meilleures performances possibles dans les supercalculateurs, il est aujourd'hui nécessaire d'utiliser des réseaux d'interconnexion de plus en plus sophistiqués. C'est pour répondre à ce besoin qu'Atos produit le réseau BXI, composé de cartes réseau (NIC) et de commutateurs (switches). Le paramétrage optimal de ce matériel est une problématique complexe, en particulier parce que l'espace de paramètres que l'on souhaite explorer est grand, et qu'il n'est pas possible de faire des expériences réelles permettant d'explorer cet espace. Ainsi, on souhaite utiliser un simulateur pour évaluer les performances d'une application donnée pour un ensemble de paramètres.

La principale difficulté rencontrée lors du développement de tels simulateurs provient de la complexité de la pile logicielle utilisée sur les grappes de calcul que l'on souhaite simuler : les applications scientifiques sont souvent programmées à un haut niveau d'abstraction et leurs communications traversent plusieurs couches logicielles avant d'être exécutées par le matériel. Il faut donc choisir laquelle de ces couches logicielle intercepter en simulation, afin de garantir une bonne précision tout en conservant des performances acceptables.

Notre contribution prend la forme d'un simulateur du réseau BXI, qui propose un modèle simplifié du matériel, tout en permettant l'exécution d'applications complètes sur plusieurs machines simulées. Ce simulateur permet de prendre en compte les spécificités de toutes les couches logicielles intermédiaires entre le NIC et l'application simulée, moyennant des modifications mineures dans celles-ci. Nous validons ce modèle expérimentalement en comparant l'exécution de benchmarks sur une grappe de calcul équipée de matériel BXI et la simulation de ces benchmarks dans notre simulateur. Ce modèle bas niveau ayant un coût en performance non négligeable, nous présentons également une méthodologie pour alterner dynamiquement entre plusieurs modèles de précision différente au cours de l'exécution d'une simulation, afin de permettre à l'utilisateur de paramétrer au mieux quelles parties de l'application doivent être simulées avec le plus de précision.

Abstract

In order to obtain the best possible performance in supercomputers, it is necessary to use interconnection networks of ever-increasing complexity. In order to provide such networks, Atos designs the BXI interconnect, which is composed of network controllers (NIC) and switches. Optimal configuration of this hardware is a complex task, in particular because the parameter space to explore is very large, and it is not practically possible to run real-world experiments to explore this parameter space. For this reason, we wish to use a simulator to evaluate the performance of a given application for a set of parameters.

The main difficulty that arises when developing such simulators comes from the complexity of the software stack that is used on the clusters that we wish to model: scientific applications are often programmed at a high level of abstraction, and their communications go through several layers of software before they are executed by the hardware. Therefore, it is important to choose which software layer to intercept in simulation, in order to get a good accuracy of the model while keeping acceptable performance of the simulation.

Our contribution is a simulator of the BXI interconnect, which provides a simplified model of the hardware, while allowing the execution of complete applications of several simulated machines. This simulator accounts for the properties of all layers of the software stack between the NIC and the simulated application, thanks to minor modifications in these software libraries. We validate this model experimentally by comparing the execution of benchmarks on a cluster equipped with BXI hardware and the simulation of these benchmarks in our simulator. Because our low-level model has a significant cost in terms of performance, we also present a methodology to switch dynamically between several models of different accuracy during the execution of a simulation, in order to allow users to tune as well as possible which parts of the application should be modeled with the best accuracy.



Remerciements

Bien qu'il me semble impossible de remercier toutes les personnes qui m'ont aidé dans la réalisation de cette thèse, et qui m'ont soutenu durant ces trois années, je tiens à mentionner le rôle important de quelques personnes sans qui ces travaux n'auraient pas pu exister.

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Résumé détaillé

Pour obtenir les meilleures performances possibles dans les supercalculateurs, il est aujourd'hui nécessaire d'utiliser des réseaux d'interconnexion de plus en plus sophistiqués. C'est pour répondre à ce besoin qu'Atos produit le réseau BXI, composé de cartes réseau (NIC) et de commutateurs (switches). Le paramétrage optimal de ce matériel est une problématique complexe, en particulier parce que l'espace de paramètres que l'on souhaite explorer est grand, et qu'il n'est pas possible de faire des expériences réelles permettant d'explorer cet espace. Ainsi, on souhaite utiliser un simulateur pour évaluer les performances d'une application donnée pour un ensemble de paramètres.

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Chapitre 1

Ce chapitre introduit le contexte de nos travaux (décrit ci-dessus). Nous y présentons quelques informations sur le processus de développement qu'utilisent les équipes d'Atos pour créer le matériel BXI, qui sert de cas d'étude à nos travaux. Ce premier chapitre termine par une annonce nos contribution et du plan du document.

Chapitre 2

Le deuxième chapitre précise le contexte de nos travaux en présentant le domaine du calcul haute performance. Y sont présentées l'architecture d'une grappe de calcul (sujet

d'étude de nos expériences) ainsi que les caractéristiques du matériel réseau développé par Atos, que nous cherchons à modéliser. En particulier, nous présentons l'API Portals, qui est implémentée de manière matérielle par l'interconnect BXI d'Atos. Le chapitre se termine par une présentation des programmes informatiques que nous tâcherons de simuler par la suite, afin d'expliquer leur intérêt dans le cadre de la validation de notre simulateur.

Chapitre 3

Le troisième chapitre présente l'état de l'art existant dans le domaine de la simulation de systèmes HPC. Nous y présentons la principale difficulté auxquels tous les simulateurs font face : le compromis entre précision du modèle et performance de la simulation. Nous détaillons plus amplement les caractéristiques de quelques simulateurs qui se prêtent au type de travaux que nous entreprenons, en particulier SimGrid que nous avons choisi d'utiliser.

Chapitre 4

Le quatrième chapitre présente notre première contribution : un simulateur de l'API Portals, optimisé pour modéliser l'interconnect BXI d'Atos. Nous détaillons en particulier notre description de plateforme, qui modélise les différents composants matériels présents dans une grappe de calcul réelle, ainsi que notre implémentation de l'API Portals dans le monde simulé, en utilisant les briques de base offertes par SimGrid.

Nous présentons les outils qui ont été développés pour assister l'utilisateur du simulateur, et nous terminons avec des expériences de validation, qui comparent nos résultats de simulations avec des exécutions de benchmarks sur une grappe de calcul réelle (équipée de matériel BXI).

Chapitre 5

Le cinquième chapitre explique comment des bibliothèques logicielles abstraites peuvent être adaptées pour fonctionner au dessus de notre modèle bas niveau. Nous étudions en particulier l'API MPI, car c'est la plus couramment utilisée dans le domaine du calcul haute performance. Nous montrons que notre approche permet d'exécuter MPI en simulation avec très peu de modifications, ce qui nous permet de faire des simulations avec une pile logicielle beaucoup plus fidèle au fonctionnement réel par rapport aux modèles fluides pré-existant dans l'état de l'art.

Nous présentons une validation expérimentales, utilisant les programmes décrit dans le Chapitre 2. Nous comparons nos résultats à SMPI, simulateur pré-existant le plus proche de notre modèle. Nous en concluons que les deux modèles ont des forces et faiblesses complémentaires : là où notre approche (basée sur notre simulateur, S4BXI) offre un modèle plus précis, SMPI offre un modèle plus rapide d'exécution.

Après avoir étudié MPI, nous présentons des travaux préliminaires sur la simulation de l'API OpenSHMEM. Nous détaillons comment adapter cette bibliothèque à notre simulateur, et présentons des résultats expérimentaux.



Chapitre 6

Ce chapitre présente une nouvelle contribution : en se basant sur les forces et les faiblesses des deux simulateurs que nous avons étudiés, S4BXI et SMPI, nous développons une méthodologie de simulation permettant de coupler les deux modèles au sein d'une même simulation. Ainsi, les utilisateurs de notre simulateurs peuvent changer de modèle réseau dynamiquement, durant l'exécution de la simulation.

Nous présentons des résultats expérimentaux utilisant cette approche, sur deux programmes simulés. Nous proposons une conclusion qui met en avant les forces et les faiblesses de cette méthodologie de simulation.

Chapitre 7

Nous dédions un chapitre complet à la présentation des études futures qui pourraient être réalisées à partir de nos travaux. Nous présentons des exemples d'expériences sur lesquelles nous avons commencé à travailler, mais qui nécessiteraient plus de temps de travail. Nous détaillons en particulier une étude s'intéressant à la notion de contrôle de flux, dans le but de simplifier le processus de développement des prochaines générations de matériel BXI.

Chapitre 8

Dans ce dernier chapitre, nous présentons la conclusion de nos travaux : nous résumons nos contributions principales, ainsi que les portes que nos travaux ouvrent pour des études futures.

*À mon grand-père, qui n'aurait pas
compris un mot de ce qui va suivre,
mais qui aurait été très fier*

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Chapter 1

Introduction

1.1 HPC for simulation and simulation for HPC

Nowadays, many scientific domains rely on simulation in order to better understand the world around us, or to design systems that are difficult to prototype and test in the real world. There are many examples of such models, as can be seen on Figure 1.1 which shows an application of Computational Fluid Dynamics to model the airflow around a BAE-HAWK plane, or on Figure 1.2, which illustrates the Aevol model, a digital genetics platform designed to study the evolutionary process [LPRCB18].

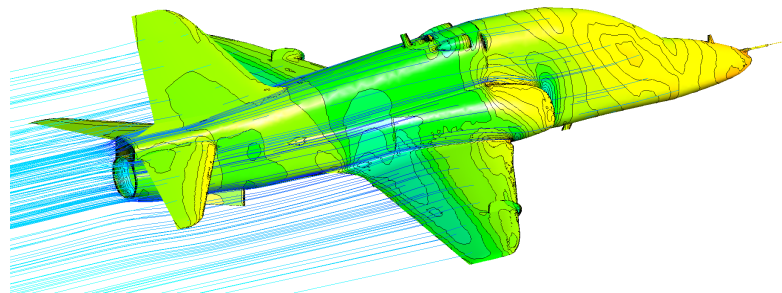


Figure 1.1: Fluid dynamics on a BAE-HAWK plane¹

As scientific models get more and more accurate, they also become increasingly complex, and they require an increasing amount of computing power to run. As a result, most scientific domains today require the use of High Performance Computing (HPC): clusters of an ever-growing number of machines which work together towards the same goal. HPC is such a powerful tool that it is used in most research fields, but also most industries, with applications as varied as healthcare, weather forecast, geology, every vehicle's design, etc. An example of such computing cluster is displayed on Figure 1.3, where we can see the supercomputing facility of the European Centre for Medium-Range Weather Forecasts (ECMWF) in Bologna, which is made up of Atos BullSequana XH2000 clusters and is used to run a global Earth system model, in order to get weather reports as accurate as possible. Additionally, as artificial intelligence takes an increasing space in our lives, through a huge diversity of algorithms, the amount of data that we need to process is growing at a very high rate, and the computing power required to train algorithms increases proportionally.

¹Image from <https://cfd2012.com/aircraft-design.html>

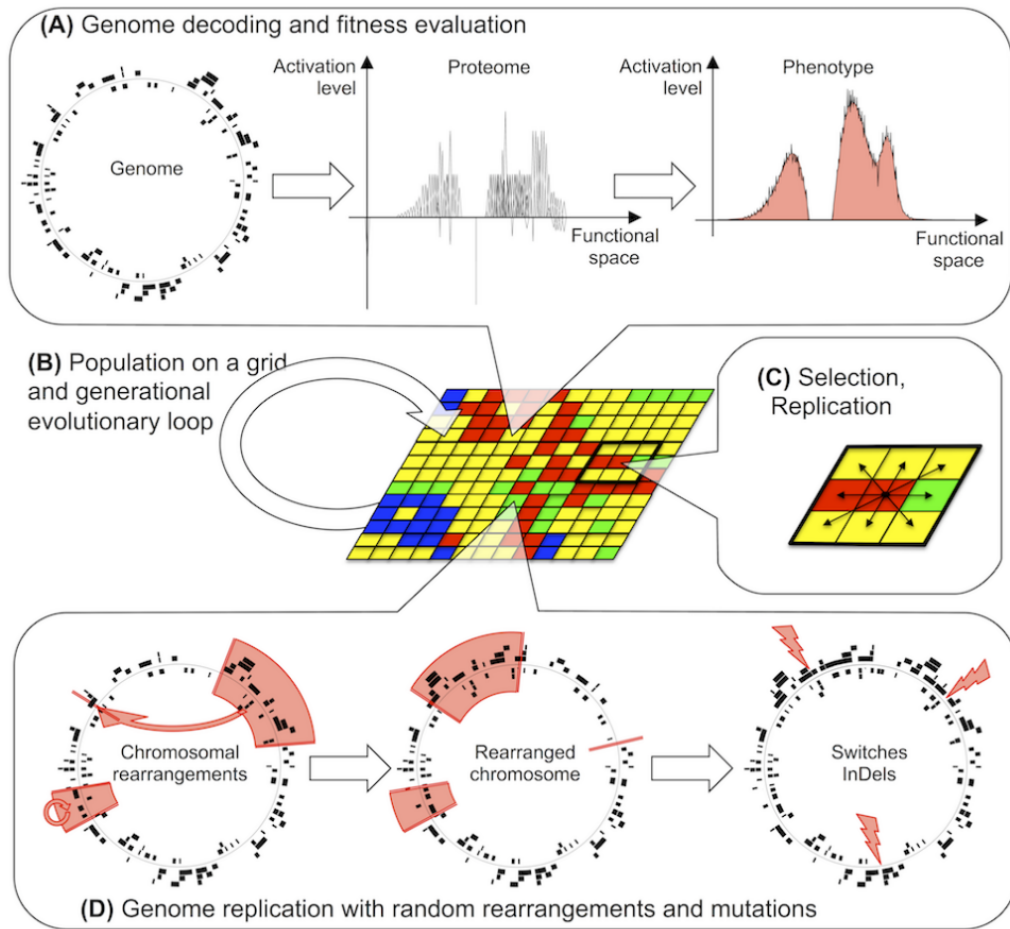


Figure 1.2: The Aevol model. Image from [LPRCB18].



Figure 1.3: HPC facility at ECMWF, made up of four Atos BullSequana XH2000 clusters²

²Image from <https://www.ecmwf.int/en/about/media-centre/focus/2022/fact-sheet-supercomputing-ecmwf>



As clusters get larger and larger, interconnection networks that connect the machines together need to handle huge quantities of communications, with the highest performance possible, in order not to slow down the scientific applications running on the cluster. In this context, Atos develops its own interconnection network, the Bull eXascale Interconnect (BXI), which is used in some of the most powerful European supercomputers, such as Tera-1000-2 [TOP17] which was the most powerful supercomputer in Europe at the time of its installation.

Because of the growing complexity of the hardware that is used to power supercomputers (CPUs, accelerators, interconnection network, etc.), predicting the execution time of a scientific application on a given cluster is a difficult task, although it is important for several reasons: for example to dimension new clusters, or to tune the parameters of the software stack and of the hardware to optimize performance. Additionally, designing next-generation hardware is increasingly hard, as we constantly aim for better performance, therefore conducting studies in simulation is a good tool to facilitate this design process. This is where simulation can help, by providing a model of the cluster which can be used to estimate its performance in various scenarios, even hypothetical ones that cannot be reproduced with the hardware currently available. This typically happens in the context of the co-design of next-generation hardware.

It is important to note that, since the application being run is usually itself a physical simulation, the word “simulation” can be used in this context to refer to two different objects: the simulation of a supercomputer, which uses the cluster as the object of its study, and the simulation that might run inside the cluster, which models a completely different system (as presented previously). In the context of our work, our contribution is the design of a simulator of HPC clusters (with a focus on the simulation of BXI), but in order to validate our model we will also manipulate physics models (presented in Chapter 2), which we will run in a virtual cluster in the simulated world. In order to differentiate both types of simulators, in this document we will refer to physics models as “scientific applications” or “user applications”, to avoid potential confusion with our model of BXI.

In the field of cluster simulation, many types of models are available, which are used to simulate various parts of a cluster with a high accuracy, or model the whole cluster, but with a more simplistic model. Our work is a collaboration between the “Laboratoire de l’Informatique du Parallélisme” (LIP) and Atos³. In this context, we focus on the communication aspect of supercomputers, and in particular on the BXI Interconnect made by Atos. Our model of this hardware is based on the SimGrid framework, which allows us to design a simulator modeling communications at message-level by leveraging SimGrid’s actor-based flow-model.

In the next section, we will present how BXI is designed at Atos, using our hands-on experience with this interconnect, the knowledge that we gained from working inside the low-level software team of this company, and our interactions with the hardware and high-level software teams. In particular, we will present the existing uses of simulation in this context, and illustrate the potential benefits of a more abstract simulator.

1.2 Design process of a NIC for HPC at Atos

The process of creating an Application Specific Integrated Circuit (ASIC), such as a Network Interface Controller (NIC) in the context of High Performance Computing, is very

³This PhD is funded by a “Convention industrielle de formation par la recherche” (Cifre)

costly: the full design and manufacturing process can cost millions of Euros. Every step of the process is complex, very time-consuming and expensive, from the design by an R&D team, to the prototyping, and then the actual production of the finished product. This is why this creation process (depicted in Figure 1.4) follows many steps that aim to facilitate and speed up the design, in order for manufacturers to remain competitive.

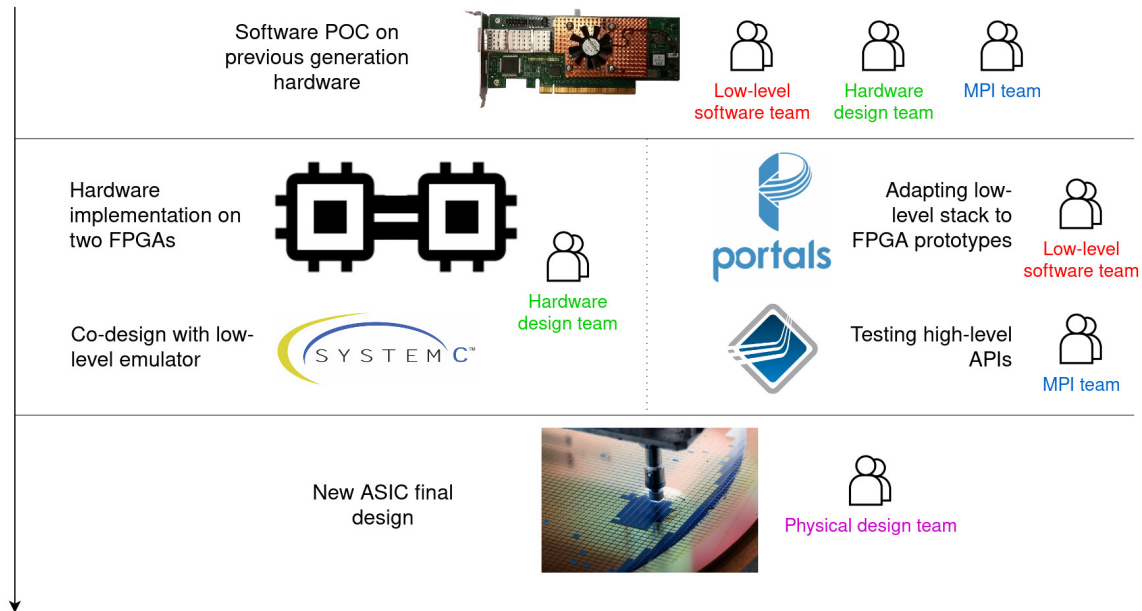


Figure 1.4: Design process of the BXI NIC at Atos

There are mainly four teams that are involved in the process: the hardware design is made by two teams, which are responsible for the prototyping on Field-Programmable Gate Arrays (FPGA) and the firmware development on one side, and the physical layout on the final ASIC on the other side. From the point of view of the software, there are also two different teams: one of them is specifically responsible for the tuning of Atos’s version of the Message Passing Interface (MPI), since this high-level API is the most commonly used in the field of HPC, therefore its maintenance and optimization are very important. The second team, BXI-LL, is responsible for the lower-levels of the software stack, which involves developing the driver for BXI NICs, as well as the user-level library for Portals, which is the network API implemented by the NIC. This API offers connectionless, reliable point-to-point communications, and since it is entirely implemented in hardware by the NIC, the user-level software library is a very thin wrapper that mainly formats commands and sends them to the NIC. Additionally, the BXI-LL team is responsible for the other high-level services that are supported by BXI, such as the Lustre distributed Filesystem, OpenSHMEM, etc.

As we can see on Figure 1.4, the design process of BXI NICs starts with an exploration of the possible features that could be implemented, either by emulating these features on hardware that is as similar as possible to the currently developed ASIC (for example by using old generation hardware to design the new generation), or using a high-level simulator to get a rough estimate of the functionality and performance of each option. Once this step is done and the least promising features have been abandoned, the remaining ones can be implemented in a first prototype. Because making a physical prototype would be extremely time-consuming and costly, this step is always done either on reconfigurable



hardware such as an FPGA, or in a very low-level simulation framework. Sometimes both are made, for example at Atos there is a SystemC model of the BXI switch, as well as an FPGA implementation. Additionally, in order to develop the driver and user library for the first generation of BXI, an emulator of the NIC was made using QEMU [Bel05], but it was not maintained for the later generation of BXI hardware. When the first prototype of the hardware is complete, software developers can start using it to design the driver that is going to power the hardware. Hardware and software developers then iterate over the prototype to improve both the circuit and the software stack, until both are ready for production use, which is assessed with manual tests, as well as the execution of a test suite designed by the BXI-LL team in order to test most use-cases of the hardware that need to be supported. At this point, the design on FPGA is passed to a dedicated team responsible for the layout of the different circuits on the final chip. Finally, the ASIC is ready to be manufactured at scale.

The issue with this workflow is that a prototype on an FPGA can be around two orders of magnitude slower than the final product, especially for large circuits where “artificial” bottlenecks can exist on FPGA but not on the final product: for example the BXI NIC made by Atos does not fit on a single FPGA, and therefore it is distributed across two FPGAs connected together. Even with this design, the NIC must be simplified to fit on two FPGAs: only two List Matching Engines (LMEs) can be implemented instead of four on the real ASIC for example. These engines are Application-Specific Instruction set Processors (ASIP), which implement most of the processing of incoming messages, with instructions optimized to sustain a message rate as high as possible (more details about the process of receiving messages will be presented in Section 4.2.1), therefore having only two on the FPGA platform instead of four on the final ASIC is a change that has a significant impact on the behavior of the NIC. With prototypes this slow, it is also impossible to generate enough traffic to cause meaningful congestion on the network, which is problematic because congestion is an important phenomenon to study, as it impacts greatly the performance of networks with real ASICs. Low-level simulators are even slower than FPGA prototypes, with speeds that are often several orders of magnitude slower than the final product. This means that during this development process, software teams can only test their code on very small scale tests (usually involving two machines at most in the case of NIC development). This is a problem because it makes it very difficult to evaluate the performance of the new hardware on a realistic application, which can exhibit unexpected behavior and performance because of the complex interaction between all the components of a modern cluster. For example, at a small scale an application might be CPU-bound, but at a larger scale communications might become more important and stress the memory, which could become the bottleneck since it is a shared resource between the CPUs and NICs. This problem becomes even more complex if a storage system or an accelerator uses the memory at the same time, or if the data that needs to be sent on the network is on the storage. All of these scenarios create interdependencies between the different resources, and their impact on performance at different scales can be unexpected.

This is why it would be beneficial for the different development teams to have a model of the new hardware at an intermediate level: more accurate than the initial rough approximations, but faster than low-level emulators, in order to study more realistic workloads. The hardware and low-level software team at Atos could use it to perform studies on specific properties of the hardware, for example evaluating the impact of different protocol design choices. The teams responsible for the development of Atos’s version of MPI could use it for higher-level studies, such as tuning the algorithms used by MPI to perform

complex operations between many machines, or testing their developments. Finally, Atos’s clients could use our simulator to evaluate the performance of their applications, and tune the configuration of their code before performing real-world executions. In particular, the main client of the BXI Interconnect, the “Commissariat à l’Énergie Atomique et aux Énergies Alternatives” (CEA) showed interest in our work, and could be a potential user of our simulator.

1.3 Contributions

In our work, we design a simulator of HPC clusters, that is focused on the simulation of the BXI interconnect made by Atos. As BXI NICs implement the Portals API in hardware, we propose an implementation of this API in simulation. To this end, we rely on the SimGrid framework, which provides a flow-model of communication, and allows us to implement a Discrete Event Simulator (DES) using cooperative Actors. Even though flow-models are typically used to simulate communication at message level, we use a novel approach that models transfer at a lower level of granularity than most state-of-the-art simulators. This design choice allows us to create a more accurate model of the hardware, without modeling each packet individually. To the best of our knowledge, this is the first time that a model of Portals has been made publicly available. We validate our model, using low-level experiments which rely on the Portals API.

We show that our simulation method is versatile, by running high-level network APIs on top of our low-level model. In this context, we study in detail the execution of Atos’s implementation of MPI in our simulator, and we also show preliminary work with OpenSHMEM. To validate our model in this context, and to compare it with the closest state-of-the-art MPI simulator, SMPI, we run unmodified scientific applications that are commonly used to assess the performance of HPC clusters. These experiments confirm our expectations, as we observe that our simulation method is more accurate than SMPI, but also slower, as our model is more detailed. Therefore, we explore a new method to tune the ratio between performance and accuracy of our simulation method, by combining our network model and SMPI’s, and enabling users to switch between them at runtime.

We conduct a study in order to assess the usefulness of potential evolutions of BXI NICs, by implementing flow-control mechanisms in simulation and testing this feature in different scenarios. This study shows the versatility of our simulator, as it demonstrates how low-level features of the hardware can be evaluated using high-level benchmarks, and we present a few other studies which could be conducted using a similar methodology (but which are left as future work).

1.4 Structure of this thesis

Our contributions are organized in seven chapters: Chapter 2 gives context regarding the field of HPC, by presenting the architecture of a typical HPC cluster and the most significant interconnection networks. It also details properties of the Portals API which will be important for the rest of our work, and describes a few scientific applications which will be used in our experiments.

Chapter 3 presents pre-existing simulators of HPC clusters, with a focus on SimGrid in order to illustrate the most important features which we leverage in our simulator.

Chapter 4 then focuses on our low-level model, by explaining how Portals is implemented in simulation, and which properties of the hardware are modeled by our approach.



It also shows validation results by relying on point-to-point benchmarks of Portals. Even though this work was published in [EMHP20], in this thesis we also present several features of our simulator which were added after the initial publication.

Chapter 5 explains how this model can be used to run high-level APIs, and in particular MPI. To this end, it details the modifications that need to be performed on the real-world implementations of MPI and OpenSHMEM in use at Atos, in order to make them compatible with our simulator. Part of this work was published in [EMHP21], but significant work has been added since: in particular, this publication does not mention our study on OpenSHMEM, and our benchmarks are now more complete.

Chapter 6 shows how we can combine two network models, and allow users to switch between them at runtime.

Chapter 7 discusses some ideas that are more experimental, in particular it details our study on flow-control in BXI (a very early version of this work was published in [EMHP21]), and it lists ideas that are left as future work.

Finally, Chapter 8 concludes this document by summarizing our work.



Chapter 2

Context: High Performance Computing

This chapter presents the context of our work. We will start with an overview of the architecture of a modern HPC cluster, and then showcase several benchmarks commonly used in HPC, which we will refer to later in this thesis (in the context of the validation of our simulator).

2.1 HPC clusters' architecture

Our work focuses on the network aspect of High Performance Computing. We will start with some context regarding HPC clusters, and then focus on the challenges that interconnection network face, both at the hardware and software level.

2.1.1 General overview

Because of the physical limitations that CPUs face, High Performance Computing (HPC) clusters use very specific hardware to get the most computing power possible from each machine that composes the cluster, and they also have an increasing number of machines connected together. This means that a typical machine (referred to as “node” in this document) is usually composed not only of one or more CPUs, but also one or more Network Interface Controller (NIC) and possibly one or more accelerator for fast parallel computation. These nodes are interconnected using switches of low-latency and usually high radix (i.e. a large number of ports allows connecting many nodes or other switches), which enables various topologies to be used. For example Figure 2.1 depicts a simple fat-tree, with wider links (higher bandwidth) closer to the “root” of the tree. On this example, we can see that the distance between two nodes is variable: two machines connected to the same switch will be able to communicate by traversing only two cables and one switch, whereas nodes on opposite sides of the tree will need to traverse four links and three switches to communicate, increasing the latency of network transfers.

While the diversity of hardware and increasing number of nodes makes clusters more performant, it also makes it more difficult to predict the performance of a cluster executing a given application, because of complex interactions between each type of hardware on each node. A second side effect is that clusters become increasingly more costly to build and run, which makes real-world experiments very costly. The increase of the number of nodes also makes the topology of the cluster more and more important: routers and cables

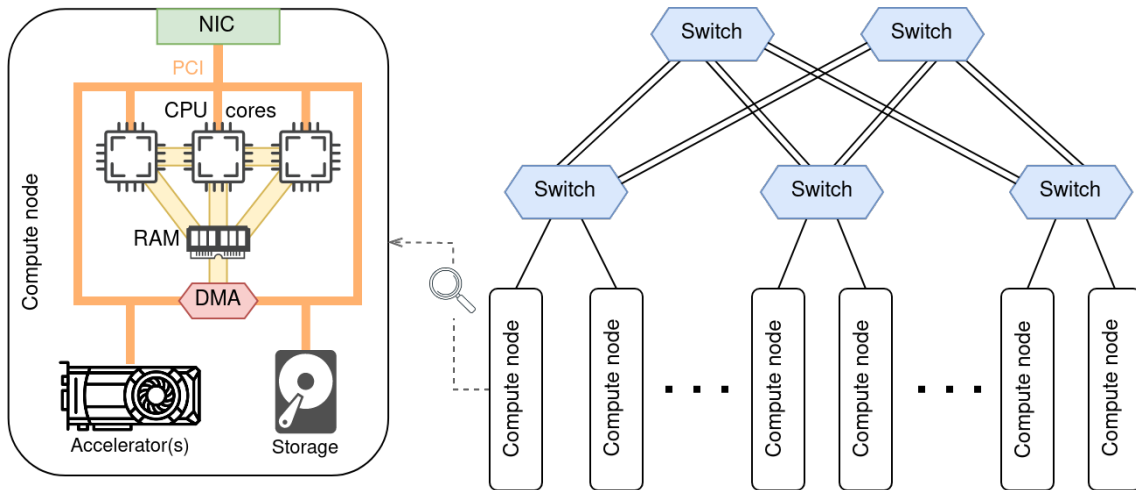


Figure 2.1: Simplified cluster representation, with a zoom on a compute node

are an expensive part of the cluster, but it is crucial that they have a good performance, so connecting all this hardware efficiently is very important. On Figure 2.1 we can see that while nodes are usually very similar to each other (a typical cluster will have many identical compute nodes, and a few service nodes for login, storage, management, etc.), the allocation of tasks on the cluster still matters, because of communications: nodes that are on different switches will have to go through more links and switches in order to exchange data, whereas nodes on the same switch will benefit from a very low latency. We can also see that messages can take several paths through the network when going from one node to another, which makes efficient routing important.

There has been many studies in the field of interconnection networks and routing algorithms, from which many topologies have emerged. To cite only the most commonly used, the Flattened Butterfly [KDA07] focuses on cost-efficiency, by relying on path diversity, which shows the best result when the routing algorithm used leverages adaptive routing, which means that switches can decide which path to choose on a message-per-message or packet-per-packet basis, instead of having a strict static route for each source-destination pair (which improves the load-balancing abilities of the network). Dragonfly [KDSA08] networks operate on the same idea, but they use groups of switches to emulate a “virtual router” of even higher radix than the underlying switches, which further reduces the cost of building the network, while still showing good performance. Torus [ASS09] topologies are more original since they do not use a traditional architecture with NICs on compute nodes and switches to connect them together: instead every node has an “interconnect controller”, which acts both as a NIC (with several “communication engines” to communicate with CPUs) and a small switch (with a dozen of ports typically). This allows nodes to be connected in small groups, and groups to be connected together along a variable number of dimension (up to 6D for the Tofu interconnect for example). Finally, the most common topology is probably the Fat-Tree [Lei85], which has been extensively studied, in order to improve routing [GGG⁺07], make accurate simulations [LHSJ15], etc. It relies on a hierarchy of switches, with compute nodes connected at the lowest level, and cables of increasing bandwidth as we get closer to the root of the tree, as depicted earlier in Figure 2.1. Several routing algorithms have been proposed on this topology, which rely on either static or adaptive routing [GGG⁺07], and which try to balance the load as well as possible between the different paths that are available in the tree. The most common



is D-Mod-K [Zah10] but others exist, such as node-type-based load-balancing [GQG18] which was proposed by Atos.

While our work could theoretically be used to study different topologies and compare their performance, it will not be discussed in detail in this thesis because the interconnect that we work on, BXI, is mostly used with Fat-Trees in production, therefore all our experiments will use this topology.

✿ 2.1.2 Networking hardware

In the world of High Performance Computing, there are several competitors when it comes to production interconnection networks: the most notable are Cray (acquired by HPE during this PhD), Mellanox (acquired by Nvidia during this PhD), Fujitsu and Atos. Another noteworthy interconnection network is OmniPath: while it has first been discontinued by Intel, it has since been bought by Cornelis Networks, and there are several interesting studies on its performance and modeling [RGI17].

Cray's interconnects support a wide range of topologies: from Dragonfly network in their latest Slingshot interconnect, to 3D-Torus in the Seastar interconnect [BPU05]. Torus networks have been shown to work in higher dimensions, for example in 6D with the Tofu interconnect [ASS09] made by Fujitsu, which is used in the Fugaku supercomputer (number two on the Top500 list as of the writing of this PhD). While early versions of Cray's interconnect were known to use Portals 3 as their lower-level network API, Slingshot is based on the Ethernet protocol [DDM⁺20]. On older generations of interconnect (as the Gemini and Aries which are still used in several clusters) the lowest software layer that is exposed to user code is composed of two APIs: uGNI and DMAPP [Cra10]. Cray's NICs typically support bandwidths up to 200Gbits/s.

Mellanox's interconnects are the most popular option for new clusters. They implement the standard Infiniband architecture [Pfi01], which is supported by most (if not all) higher-level APIs. They also feature a variety of hardware of different performance and price, such as the EDR and HDR series, which explains their popularity for clusters of all sizes. At the lowest level, users call the IB-verbs interface which is used to communicate with the NIC. High-end NICs from Mellanox typically support bandwidths up to 200Gbits/s, with the upcoming generation expected to support 400Gbits/s.

Atos's interconnect, BXI, will be our case study for this PhD. It implements in hardware the Portals 4 network API, and is used in some of the fastest European supercomputers. It is one of the youngest interconnect of the market, with NICs supporting bandwidths up to 100Gbits/s, but it has showed very good results so far, equipping supercomputers with a very good rank in the Top500 list: Tera-1000-2 was at the 14th place worldwide and n°1 in Europe at the time of its installation [TOP17], and currently Exa1-HF holds the 20th place worldwide [TOP21] (it was also 14th at the time of its installation in 2021).

All these interconnects share a few similarities: their main goal is to offload as much network processing from the CPU as possible. This is made possible using a few properties that differ from traditional networking hardware: first, OS-bypass allows user code to send commands to a NIC without any system call, which speeds up communications significantly. Most NICs also provide zero-copy processing, which implies that incoming messages can be processed fast enough so that the incoming data is routed to the correct location in memory without being copied in intermediate buffers. This is made possible either by pinning memory pages used for network communications (as Mellanox's hardware does), or by having a full Virtual-to-Physical (V2P) circuit on the NIC (as does Atos's BXI hardware).

While the simulation of other interconnects and network APIs have been studied in depth, for example the congestion on Infiniband networks by [Vie10][GR12], Intel OmniPath with OpaSim [CFAS18], or Cray’s interconnect [MCRC17], very few studies have been conducted on BXI, and the existing ones focus on very specific problems, such as the update of routing tables when the topology changes [VQ16]. In this thesis we will propose a model for Portals 4 and tune the simulator for accurate simulations of the BXI interconnect.

2.1.3 Networking Software Stack

While the typical software stack for HPC communications is very different from the traditional OSI layers, it features similar levels of abstraction (depicted on Figure 2.2). We will start by giving a global overview of these layers, before presenting Portals in more details in the next section, since it is the lowest-level software layer used at Atos, and it will be the most important from the point of view of our simulator.

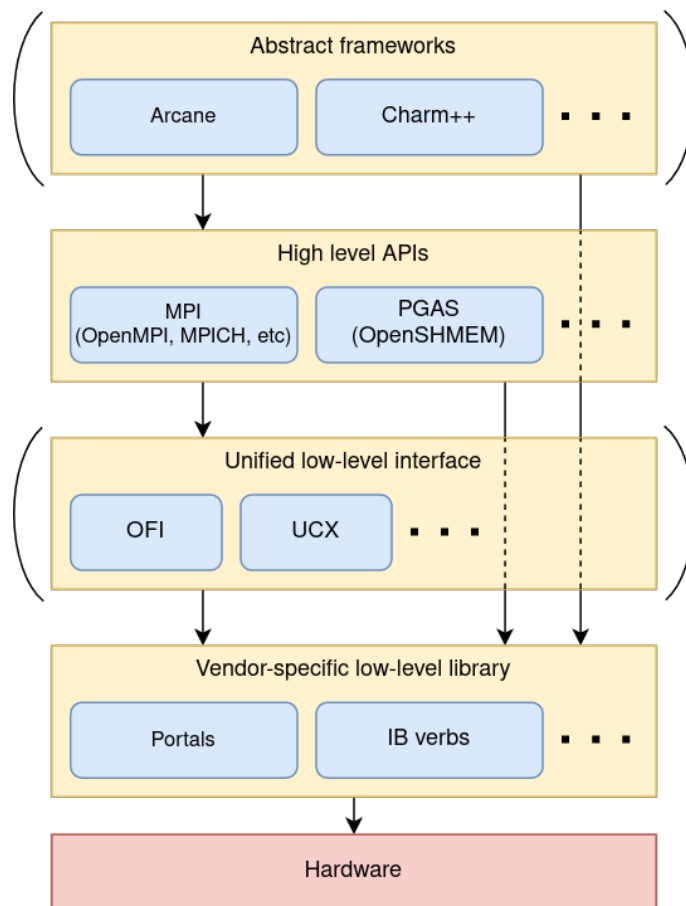


Figure 2.2: HPC software stack

At the lowest level, there is usually a very thin software library (potentially coupled with a kernel module), that directly interacts with the hardware, and exposes a few primitives with a very low level of abstraction to user code. It usually only performs point-to-point operations between two machines, and does not have any notion of collective operations involving several machines. For Infiniband this layer is called IB-verbs, and for Atos’s



BXI interconnect it is the Portals 4 API directly, as it is fully implemented by the NIC in hardware. It is this Portals 4 layer that our simulator will model, as it will provide a model of the behavior of the NIC.

Above this layer, high-level APIs provide more abstract features that allow programmers to write efficient code, focusing on the algorithmic aspects and abstracting away the implementation details of communications. In this category, several programming models exist: for example Partitioned global address space (PGAS), with implementations such as OpenSHMEM [CCP⁺10], allow user code to have a transparent representation of memory that is distributed on several machines. The most popular of these programming models is without a doubt the Message Passing Interface (MPI) [GWS06], which offers many ways of communicating: onesided, where a target machine exposes memory regions that other machines can query ; regular point-to-point operations where both machines are actively involved (using send and receive primitives) ; and finally collective operations which provide abstract communication primitives such as all-to-all pattern, gather (N to 1 communication), scatter (1 to N), and even simple data processing with reduce, allreduce, etc. primitives. These collective operations usually have several implementations, which can be chosen dynamically depending on the message sizes and the number of machines involved in the operation. There are many MPI implementations, such as OpenMPI, MPICH, IntelMPI, etc. We will study OpenMPI in particular, as it is the MPI implementation that is officially supported by our case study interconnect, BXI. It is worth noting that our version of OpenMPI is a fork optimized by Atos for BXI, which we will explain in more detail in Chapter 5. These high-level APIs are sometimes criticized for their cost in terms of performance, in particular MPI [RAO⁺17], but their compromise between ease of use and performance makes them the standard to write HPC applications. Some projects even try to replicate this type of programming model in hardware, as [MdFLBH19] does on Field Programmable Gate Arrays (FPGAs).

These two layers are the most important and will usually exist in any HPC software stack, but there can also be additional ones: in particular some APIs try to provide a unified interface between the low-level transport and the high-level abstract API. The goal of this added layer is to limit the number of implementations that need to be made in high-level APIs to accommodate for any possible low-level transport. This is similar to the intermediate representation compilers use, which allows them to have only N frontends and M backends to be able to compile N languages into M machine codes, instead of having $N \times M$ complete toolchains. These interfaces include the Open Fabric Interface (OFI) [GHS⁺15], of which Atos made an implementation built with Portals (in order to support BXI), as well as Unified Communication X (UCX) [SVL⁺15] or Nemesis [PGB11] for example.

Finally, while high-level APIs are already more user-friendly than low-level transports, they are still very general purpose and offer much control, which is why some frameworks can be used on top of them for even more abstraction. They can be domain-specific, as Arcane [GL09] for example, which is a tool made by the CEA to build physics simulators on top of MPI. Some libraries like SkePU [EK10] provide complete data-processing algorithms on distributed data, for example MapReduce, Stencils, etc. Some frameworks expose a unified API to execute algorithms on heterogeneous architectures (for example by exploiting local parallelism with OpenMP¹, inter-machine parallelism with MPI, etc.) like StarPU [ATNW11]. Some approaches even go as far as designing a full programming language for parallel processing, such as Chapel [PBCP⁺21], which implements a PGAS model

¹OpenMP is an API for parallel processing across CPU cores, which relies on compiler directives and a library

and uses low-level transports directly, or Charm++ [KK93], which provides automated load balancing and supports MPI as its transport mechanism.

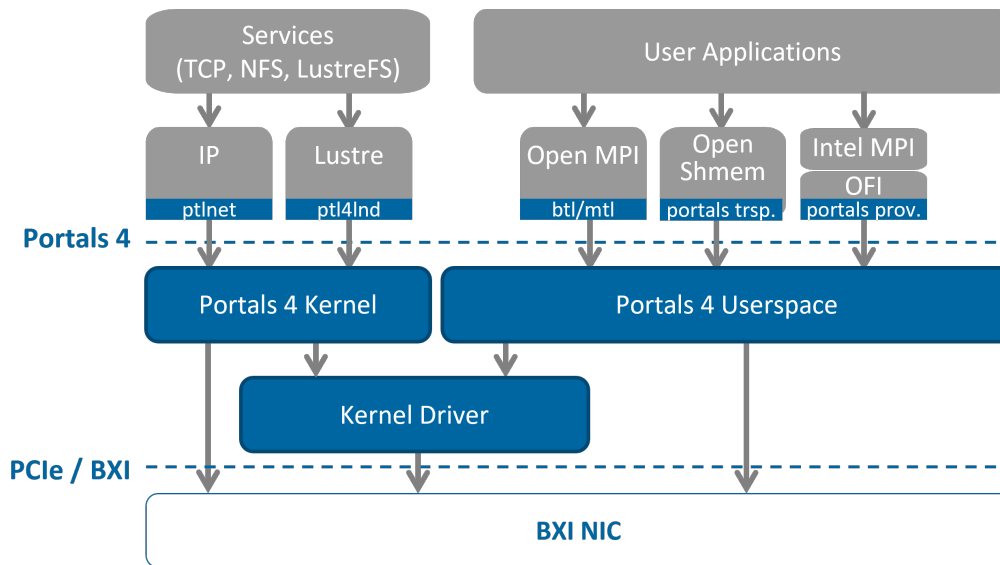


Figure 2.3: Atos’s software stack on top of BXI NICs

The software stack used at Atos, which is going to serve as a case study for this thesis, is depicted on Figure 2.3. It is based on Portals, which we will describe in more detail in the next section, and supports a wide range of higher level APIs and services: it can emulate the Ethernet protocol using a layer called Ptlnet, supports the Lustre distributed Filesystem, provides different APIs for fast computation such as OpenMPI, OpenSHMEM, and IntelMPI (on top of OFI), etc. In this thesis we will study in detail OpenMPI in particular, and we will discuss OpenSHMEM support.

2.2 The Portals API

Portals is a standard HPC API specified by Sandia National Laboratories [BSP+22]. It has been used in supercomputers for decades, with a few success stories like the ASCI Red supercomputer [MH98], which was the first to break the Teraflop barrier in 1996 using an early version of Portals. Since then Portals has been used mainly by Cray, and nowadays its main implementation is in the BXI interconnect made by Atos. This API provides connectionless, reliable communications using Remote Direct Memory Accesses (RDMA). While many details about the underlying protocol are left to the implementation, Portals is designed with OS-bypass in mind, and it should enable a “natural” implementation of MPI two-sided primitives, as well as PGAS one-sided operations.

2.2.1 Portals data structures

Portals features several data structures to interact with the hardware, which are defined in the Portals’s specification [BSP+22]. This section presents the most important ones in the context of our work.



General purpose structures

Network Interfaces (NI) act as an “entry” point, which represents the interface with the hardware. In Portals the addressing is analogue to IP addressing, since each physical NIC has a **Node Identifier (NID)**, which is the equivalent of IP addresses (although it is a simple number instead of a full address), and each NI (which usually corresponds to a single application process) has a unique **Process Identifier (PID)**. In those NIs, one or more **Portal Table (PT)** stores the data structures that will be used for the reception of messages. The pair $\{PID; PT\}$ is similar to ports in an IP-based stack.

Reception data structure

Matching Entries (ME) are used to configure the reception of incoming messages. A matching entry stores the address and length of the memory space where incoming messages’ data should be written, as well as match bits and ignore bits. Match bits are a set of 64 bits which allows an efficient routing of data at the receiver side: when an initiator sends a request, it includes match bits in the message, and the target uses these bits to identify which ME should be used to process the request, by testing each ME against the incoming message using the following criterion:

$$((incoming_bits \wedge match_bits) \& \sim ignore_bits) == 0$$

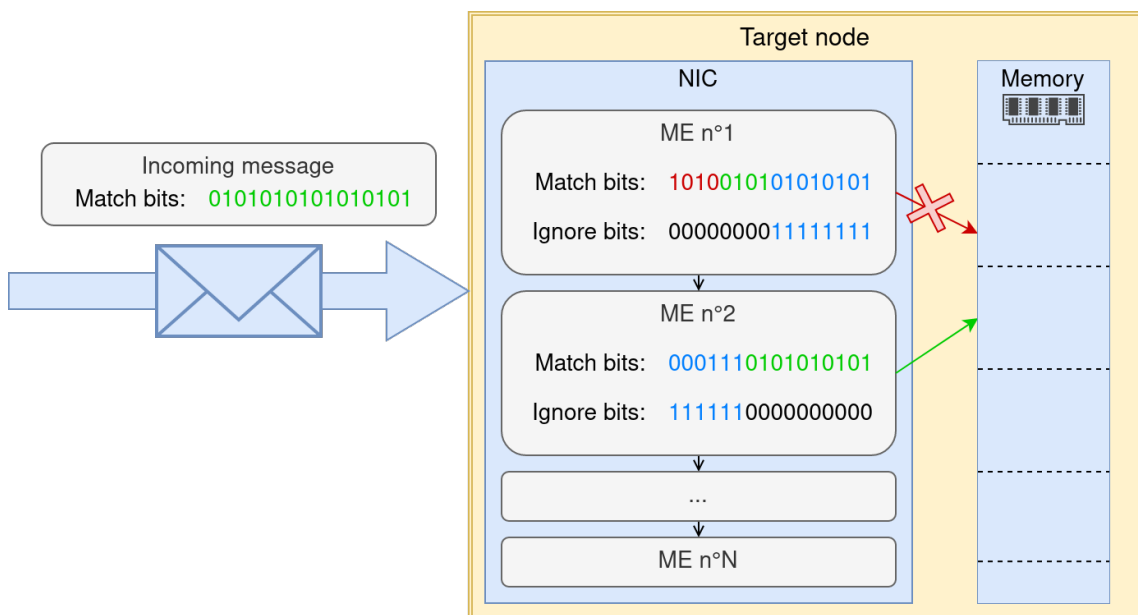


Figure 2.4: Example of matching between MEs and an incoming request

The first ME to match the incoming request is then used to determine on which memory region the requested operation needs to be performed. An example is shown on Figure 2.4, where we can see that nodes can have several MEs, which map to different locations in memory. To determine which ME needs to be used when processing an incoming request, Portals loops through the available MEs, and looks at match bits, using the opposite of the ignore bits as a mask (so the only match bits that are relevant are the positions where there is a 0 in the ignore bits). If those bits are the same as in the incoming message, the

ME is used to process the message (in order to determine the memory location where the incoming payload should be written). In the example, the first ME does not match, because the first bits are not ignored and they are different from the first bits of the incoming message, whereas the second ME matches because even though the first bits are different, they are ignored, and all the ending bits are identical to the bits of the incoming message. Therefore, the payload from the incoming message is stored in the memory location referenced by ME n°2.

MEs feature a variety of options that affect their behavior: they can have one or several uses, as well as locally manage the offset at which messages are written after each operation (by default this offset is specified on the sender side), etc. Portals also features more simple **List Entries (LE)**, which function exactly as MEs, but do not use match bits or ignore bits, which means that every incoming message will match the first LE posted in the Portal Table.

Transmission data structures

The data structure for transmission is more simple than the structures for reception: **Memory Descriptors (MD)** are simply used to represent the start and length of the memory zone that needs to be sent on the network. They also feature a few options, but which do not change drastically their behavior: these options mostly impact which events need to be emitted or not.

Event systems

Portals feature two distinct event systems, which allow users to be notified of the activity on the network by attaching data structures to a PT, an MD or an ME.

The first, more complete system involves **Event Queues (EQ)**, which record full events with detailed information on the corresponding operation, such as the type of event, an error code, and a variable number of fields depending on the type of the event (for example the NID of the remote peer who caused the event, or the amount of data that was impacted, etc.). EQs can be associated with PTs and MDs.

The second system is more lightweight: instead of EQs, it uses **Counting Events (CT)**, which do not record any information about the operations that is in progress. Instead, each CT features two counters that track successful operations and failed operations. CTs can either count by incrementing by one each time, or incrementing by the number of bytes that was manipulated in the corresponding operation (based on a flag at their creation). CTs can be associated with MEs and MDs.

Both systems can be queried through a variety of function, which can search for events (or a certain value in CTs) in a way that is either asynchronous or blocking, while looking at either one or several EQ/CT.

2.2.2 Communication primitives

Portals features several operation types to exchange and manipulate data. All these operations are strictly point-to-point, as Portals does not have a concept of collective operation.



PtlPut

Put operations are a very basic “send” operation, which corresponds to an RDMA write. As most operations, it can have match bits or not, and it will trigger various events that users can listen to: in particular a “SEND” event when the user buffer (which contains the data to be sent) can be safely re-used and an “ACK” event when an acknowledgement has been received from the remote node that was targeted. At the target, Put operations trigger a “PUT” event.

PtlGet

Get operations correspond to an RDMA read: making a Get request only sends a small message to ask the remote machine for a piece of memory, at which point the remote NIC will send back the requested data in a response. Unlike Put operations this means that the request is very lightweight (only a few bytes of metadata) and the payload which can have an arbitrary size is in the response instead. From a user perspective, the completion of the operation can be tracked by listening to a “REPLY” event. At the target, Get operations trigger a “GET” event.

PtlAtomic

Atomic operations operate in a way that is very similar to a Put, but the NIC also performs an arithmetic operation using two operands: the incoming payload and the data already present at the specified address in the remote node’s memory (which is also used to store the result). These operations can be a sum, product, etc. on various data types (integers, floating point numbers, etc.).

PtlFetchAtomic

FetchAtomic operations work in the same way as Atomics, but they also send a full response which contains the piece of data before it was modified by the Atomic operation. This means that FetchAtomic behaves as an Atomic and a Get at the same time: the request contains data to be used by the Atomic operation, but the response also contains data to be written at the initiator side as in a traditional Get. This also means that the operation involves two MDs at initiator side: one to describe the data to be sent and one to store the incoming response.

This operation has a variant, called PtlSwap, which operates very similarly to **PtlFetchAtomic** except that the permitted operation types are not arithmetic operations but different variations of swaps (conditional, with a mask, etc.).

🌿 2.2.3 Portals’s implementation in BXI

While Portals is a good specification for the API that should be exposed to users, at the lowest level significant freedom is left to the implementation. In this section we will present a few properties of BXI’s implementation of Portals which will be of interest when modeling Portals in our simulator.

End-to-End (E2E) Reliability

Since Portals is a reliable network API, it is the responsibility of BXI NICs to ensure that messages are delivered without errors. At packet-level the integrity of the data is enforced

using a Cyclic Redundancy Check (CRC): each network packet features a field in its header for CRC data, which allows the receiver of messages to check the integrity of the payload, and send an acknowledgement (ACK) with an error code if any packet was corrupted, which will trigger a retransmission of the message by the sender. At message-level, a system of timeouts and retries is implemented using a dedicated “E2E” circuit. This part of the NIC keeps track of all outgoing messages, and if no acknowledgement is received within a configurable delay, the NIC will retransmit it. This happens a tunable number of times until the message is eventually given up on. An interesting property to note is that since ACKs are important messages that need to be reliably transmitted to ensure all events are properly generated, BXI implements two levels of ACKs. We will call “Portals ACK” the messages that acknowledge the reception of a Put or Atomic operation (which can cause the emission of an ACK event for the user application), and “BXI ACK” the messages that acknowledge the reception of a Portals ACK (which is only used internally by the E2E logic to know that a Portals ACK message does not need to be retransmitted, in a way that is entirely transparent to the user application).

Virtual Networks (VN)

According to the Portals specification, it is required for messages to be ordered. This means that commands issued to the NIC by the user should result in messages being sent on the network in the same order, and also that this order should match the order of receptions at the target (in case all messages target the same machine). This causes a practical issue in real-world scenarios, which can lead to a complete deadlock of a NIC in the worst case: for example if fetching the data that needs to be sent by a request triggers a page fault which can only be resolved with another Portals request (if this data is located on a Network File System for example). Such dependencies between requests are solved by allowing different VNs to progress independently: BXI supports a total of four VNs: a “COMPUTE” VN for requests, a “COMPUTE” VN for responses, a “SERVICE” VN for requests and a “SERVICE” VN for responses. In our previous example, the problem would be solved by starting the NFS in “SERVICE” mode while having the main application in “COMPUTE” mode.

This system also allows requests and responses to progress independently: for example a small ACK can progress even if a large request is in progress. This last property is to be taken with a grain of salt: even though the vast majority of the processing in the NIC allows all four VNs to progress independently, at the very end (writing the packets physically on the network cable) messages are once again sequential, and packets from different messages cannot be interleaved.

2.3 Benchmarks of interest

In HPC, there is a wide variety of benchmarks that are used to assess the performance of a cluster. The diversity of these applications comes from the need to evaluate performance at different scales, for example with low-level utilities to evaluate the speed of communications between a pair of machines, or at the opposite full scale applications which exhibit more complex behavior but which are also a more realistic use-case of an HPC cluster. Benchmarks can also have different goals in terms of workload: some are more network-intensive, others will focus on CPU usage, etc. The original use-case of most benchmarks is to evaluate the performance of real clusters. In contrast, this thesis focuses on simulation, and we will use the same benchmarks to assess the accuracy of our models.



We will therefore run these benchmarks both on real-life clusters and in simulation to compare the results.

Additionally, the applications in which execution flow does not depend on the manipulated data can be adapted in skeleton versions, where the execution flow and communication patterns are preserved but most of the expensive computation phases are removed. Skeleton versions of applications are especially useful to study the network's performance, in particular in simulation where the computational phases can be replaced by an increase of the simulated time, as we will see in more detail in Chapter 5.

This section will present the benchmarks we chose to use in this thesis, from the most simplistic low-level utilities to the most complete applications.

2.3.1 Network benchmarks

Ptlperf

Ptlperf (short for “**P**ortals **p**erformance”) is a tool developed at Atos, whose goal is to measure the network speed between two NICs using the Portals 4 API. It has various modes, which replicate more or less realistic scenarios:

- Fast mode sends as many messages on the network as possible without caring for acknowledgements or any other Portals event. It makes the resulting workload unrealistic, but it showcases the theoretical maximum transmission speed of the hardware.
- ACK mode counts completed requests by keeping track of acknowledgements from the target, a new message is sent each time the ACK event from the previous request is received.
- CT mode works in similarly, but it uses lightweight counters instead of full events to keep track of completed transfers, sending one message at a time.
- Reply mode implements a ping-pong instead of sending messages in one direction only.
- Match mode mimics a more realistic use case with several messages in flight, and a more realistic use of resources at the target side (MEs).

OSU Micro Benchmarks

Ohio State University (OSU) benchmarks are a set of dozens of “unit test” style benchmarks, made by the creators of the MPI implementation MVAPICH, targeted at MPI and OpenSHMEM: each benchmark calls a specific primitive in a short warm up loop and then a measurement loop, in order to determine its performance on increasingly large messages. While this creates highly artificial workloads, that do not correspond to a real-life scenario, it is an efficient and standard way to measure the performance of a specific primitive in a cluster. In essence, they are similar to Ptlperf in that they benchmark a specific primitive, even though the methodology is slightly different, since OSU benchmarks time a fixed number of calls, whereas Ptlperf tries to fit as many calls as possible in a fixed amount of time.

❁ 2.3.2 Realistic (proxy) applications

While low-level network benchmarks are a good entry point to evaluate the performance of an interconnection network, or the accuracy of a network simulator, they do not represent realistic workloads. Using more realistic applications is then important to evaluate the interactions between network operations, computations, I/O operations, etc., and we will use the following ones in our study.

LULESH

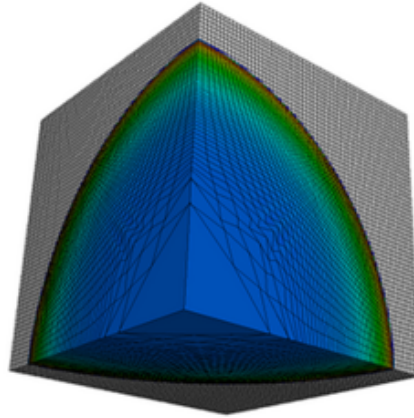


Figure 2.5: Visual representation of LULESH results²

Livermore Unstructured Lagrangian Explicit Shock Hydrodynamics (LULESH) is a very popular C++ proxy application that is commonly used to benchmark HPC clusters [KBK⁺13]. The underlying physics problem that it solves is a specific instance of a hydrodynamics problem, more specifically a Sedov blast wave problem, which studies the deformation of materials in 3D, as explained in [HKG11]. A graphical representation of an example result is displayed on Figure 2.5. As this application is very popular, implementations of LULESH exist for most parallel programming frameworks and hardware.

LULESH mainly uses point-to-point operations for its communications, along with more occasional Reduce and AllReduce calls. The execution flow of the application depends on the numerical results from computation, which is why it is difficult (if at all possible) to make a skeleton version of this application. It also has a constraint on the number of processes that need to be used to run it: because of the way work is distributed on the MPI ranks, the total number of process must be the cube of an integer (so 1, 8, 27 are valid numbers of ranks for example).

Quicksilver

Quicksilver is a C++ proxy application that uses a Monte Carlo algorithm [CC75] to solve a particle transport problem: it models a configurable number of particles, and their interactions in 3 dimensions with a predefined mesh. The possible interaction types are represented on Figure 2.6. Quicksilver has implementations both on CPU, with OpenMP and MPI, and on GPU with CUDA.

²Image from <https://asc.11nl.gov/codes/proxy-apps/lulesh>

³Image from <https://asc.11nl.gov/codes/proxy-apps/quicksilver>



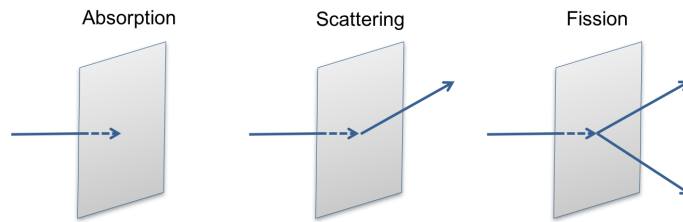


Figure 2.6: 3 possible interactions that a particle can have in the Quicksilver model³

It features a variety of point-to-point and collective operations, as well as custom datatypes, which makes it an interesting app to study. However, similarly to LULESH it is very hard to make a skeleton version for it as execution flow depends on the correctness of calculations.

HPL

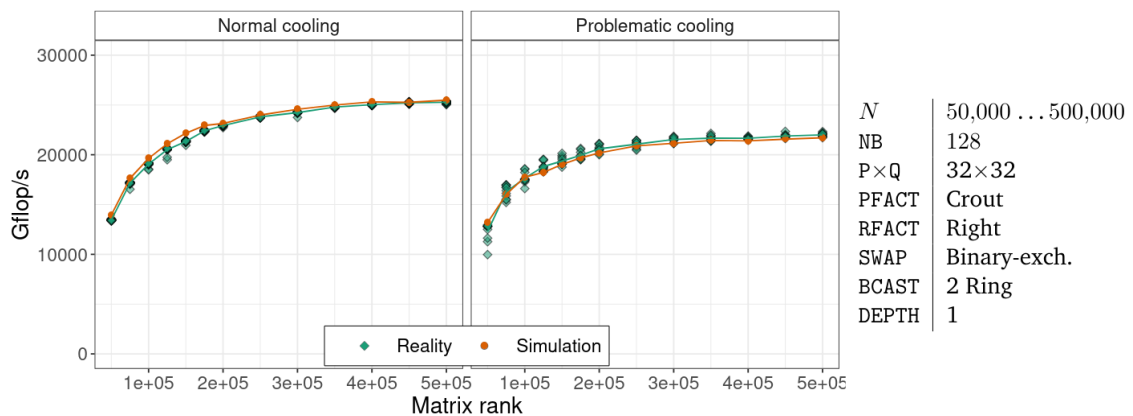


Figure 2.7: Results of HPL simulation in SMPI in two scenarios. Image from [Cor21]

High-Performance Linpack (HPL) is a very popular benchmark, famous for being used to rank supercomputers in the Top500 list [TOP22]. It solves a mathematical problem, more specifically a randomly generated dense linear system. The algorithm that is implemented is a lower-upper (LU) decomposition.

It relies on MPI for its communication, and on the Basic Linear Algebra Subprograms (BLAS) [LHKK79] for computation, which is a library that has many implementations, some generic and some vendor specific. For example, AMD provides its own version of BLIS [VvdG15], a framework that provides a fast BLAS implementation, which is optimized for AMD CPUs (in particular the Epyc and Ryzen architectures), and which is the version we will use in our experiments.

HPL does not use any collective operation from MPI directly, instead the application re-implements all collective primitives itself (using combinations of point-to-point operations), and allows users to tune the algorithm used for each type of operation in the input file that drives the execution.

What makes it an interesting application to study is that it has already been the subject of many studies, and therefore it already has existing skeleton versions: in this thesis we will be able to reuse a skeleton made for SMPI with no modifications. Simulation results obtained with SMPI in two scenarios (with or without a cooling incident on the cluster) are

shown on Figure 2.7. It also makes heavy use of user-made datatypes and communicators (by splitting the global “MPI_COMM_WORLD”), which is not very common, so it is a good way to test these features in simulation.



Chapter 3

Related work around simulation

As discussed in the previous section, an HPC software stack can be complex, and the hardware features many of optimizations and offloads that can have unpredictable effect on the performance on real-life applications. Because of this, it is very challenging to predict the execution time of an application on a given cluster, although it is an important problem to solve, in order to improve applications' code, optimize libraries, and design more performant hardware for the next generation. It is also important to be able to model the behavior of hardware before making physical prototypes, because it accelerates the development and reduces the costs of hardware design by orders of magnitude. For software developers, testing on real-life clusters, or hardware that is not available yet, can be difficult and costly (since clusters require a huge amount of power, and often have many users which need to share the resources). This is why simulators are a crucial tool for both hardware designers and software developers in HPC.

3.1 Tradeoff between performance and accuracy

We can categorize simulators in a few groups, depending on their use case: for hardware designers, most of the time simulators need to be a faithful emulator of real-world hardware, to be able to fine tune the behavior of the circuit to get the desired output. This type of simulation is called Cycle Accurate, Bit Accurate (CABA) when modeling processing units (like CPUs), and are often built with frameworks like SystemC [CMMC08] or gem5 [MCJW17] (sometimes both). When modeling networking hardware, this type of simulation is called packet-level (or flit-level), and is typically built with frameworks such as ns-3 [RH10], Omnet++ [Var01] or CODES [JBH⁺17]. The biggest advantage of this type of simulators is that they are very accurate and faithful to real-world hardware, but the downside is they are often very expensive to run in terms of performance, as the simulations are orders of magnitude slower than real-world executions.

At the other side of the spectrum, analytical models use abstract heuristics to estimate the execution time of an application, which allows users to get a rough but very fast approximation of the performance of a program on a specific cluster. The downside of these models is that to optimize performance they often ignore some properties of the real-world hardware that can have an important impact on the simulator's accuracy, such as congestion. In this category one of the most popular network simulators is LogGOPSim [HSL10], which is based on the LogP family of models. These models (LogP, LogGP and LogGPS) use different numbers of parameters to get a more or less accurate estimation of performance of network communications. They also need to be carefully calibrated [HLR07] in order to

get any meaningful prediction, and extended [FLPG18] to model high-level APIs such as MPI. For computational estimations, the closest equivalent is the study of the complexity of an algorithm [Coo83, Tur37], which similarly does not give an exact estimate of the performance to expect, but at least a good approximation of the order of magnitude.

3.2 Use cases and input formats

Not only do simulators choose different tradeoffs between accuracy and performance, but they also feature different methodologies, which translate into different inputs. The two main types of models are offline simulators and online simulators: while online simulators run the full application in a virtual world, offline simulators only replay a trace file, given as an input.

Trace files used by offline simulators describe the computation and communication phases of a given application, and they are obtained by instrumenting an application (or library such as MPI) and running it on a real-world cluster (ideally as similar as possible to the cluster the user wants to model). This makes traces potentially difficult to obtain, and for large applications the resulting file can be hard to handle because of its size. Offline simulators then replay traces with different settings to model different configurations (a faster network or a larger cluster for example). These simulators include BigSim [ZKK04], Dimemas [GLB00], and CODES [CLL⁺11]. While this methodology has a few downsides, it is still very widely used, because it allows simulators to be very fast, and models which are very abstract are often unable to run the full application anyway. This is why analytical models tend to use this method, and some simulators which support online simulation can have an option to generate or replay trace files (which is the case of SMPI [DLM⁺17] for example). This approach is also facilitated by the number of tools to analyze real world hardware's performance: indeed, regardless of simulation, several studies [JSGK17] and tools help analyze the performance of various workloads on a cluster, such as Netgauge [HMLR07], Vampir [KBD⁺08], Score-P [KRM⁺12], or Autoperf [CPB⁺19], most of which can be used to obtain traces of an application's execution.

In the case of online simulators, the full application is given as an input, with no prior real-world execution needed. With low-level models, the application's binary can usually be run as-is on top of emulated hardware, and function exactly as it would on real-world hardware. For more abstract models (flow models for example), this is not always possible, and running the application in simulation might require re-compiling it (which is what SMPI does), or at least intercepting function calls that are implemented by the simulator using `LD_PRELOAD` or syscall interception for example. These techniques were compared in more detail in [BQ15], and syscall interception was implemented in a tool called Simterpose. In our work, we will implement the method chosen by SMPI, which intercepts communication primitives using `#define` macros in C/C++, and requires re-compiling the application with specific flags. While this means that closed-source applications cannot be simulated with this methodology, we will see in Chapter 4 that re-compilation offers many other advantages which make this downside a small price to pay (especially since most commonly used benchmarks are open-source).

3.3 A few notable simulators

While we chose to use SimGrid for this thesis, which will be described in detail in the next section, there are several other projects with similar goals that could have been used.



This section will present SST and Shadow in particular, which are also commonly used for this type of work.

❖ 3.3.1 Structural Simulation Toolkit

The Structural Simulation Toolkit (SST) [HH11], developed by Sandia National Laboratories, is a very popular choice when picking a simulation framework, for both offline and online simulation. It is divided into two major components: the SST core, and SST/Macro. The core [RHB⁺11] implements the startup and configuration management required by the simulator; it is designed as a modular architecture, where models can then be plugged (using an XML configuration file). SST/Macro [JAC⁺10] is an extensible Parallel Discrete Event Simulator (PDES) implemented on top of MPI. It exposes several network models, including analytical and packet-level ones. Unfortunately flow models are no longer supported, in order to focus on the other two types of models. This is the main reason why we chose to use SimGrid instead. SST provides many low-level models [MUHD04] for commonly used components, such as CPUs, DRAM, memory controllers, simplistic NICs, etc. which makes it a good tool to run unmodified binaries on top of detailed hardware models, but this has an important cost in terms of performance. SST also supports the modeling of other properties of a cluster than the simulated time, as it integrates models of power consumption and temperature [HRT⁺12].

While SST has been used to model Portals 4 hardware before [GTK⁺19], this type of model is lower-level than what we intend to build in this thesis. This particular work is also unfortunately not open-source, which made it impossible to reuse, but the results show that SST is also a viable option for the co-design of HPC networking hardware.

❖ 3.3.2 Shadow

Shadow is a parallel discrete event network simulator. While it was originally made specifically to study the TOR network specifically [JH12], it has since demonstrated good results when modeling diverse applications, such as P2P networks [JNPW22]. We did not use it in this thesis, because it is still mainly an IP simulator, which is not widely known in the HPC community. It is still an interesting project because it tackles many issues that also arise in the type of HPC simulators that we will present in our work, and as such it is a good source of inspiration in many cases. In particular, Shadow executes unmodified applications, hooking into their code with a mixture of library preloading (using the `LD_PRELOAD` environment variable on Linux) and syscall interception. Then the simulator emulates a Linux kernel in order to make syscall interception transparent to the application, which involves reimplementing all logic that uses time, the filesystem, and the network (at TCP and UDP level). They also re-implement all features related to random generation (such as the content of the `/dev/random` file) in order to make simulations deterministic and easily reproducible. While this strategy is very efficient for Shadow's use cases, in our work we do not need to go as far as intercepting system calls. The reason is that in HPC, networking hardware uses OS bypass to optimize the performance of applications, and therefore software libraries operate mostly in user space, with little system calls.

3.4 SimGrid

We chose SimGrid to build our simulator because of its performant flow model and flexibility. SimGrid was first introduced in 2001 as “a simulation toolkit for the study of scheduling algorithms for distributed application” [Cas01], but it has since evolved to become a versatile simulation framework, with applications intended to cover “the cluster, grid, peer-to-peer, volunteer, or cloud computing domain” ([CGL⁺14]). While this goal seems ambitious (since many of these domains already have very specific simulators), many studies have shown that SimGrid is indeed a good fit for many of these use-cases. To name only a few, we can find existing work on domains as varied as HPL simulation [Cor17, CHLV17, Cor21] using the SMPI simulator, TCP networks [BDL⁺13] by leveraging a TCP-specific network model that was added to SimGrid in 2009 [VL09], Workflow Management Systems [CPO⁺19], and even P2P networks with millions of simulated machines [QRT12].

3.4.1 Architecture

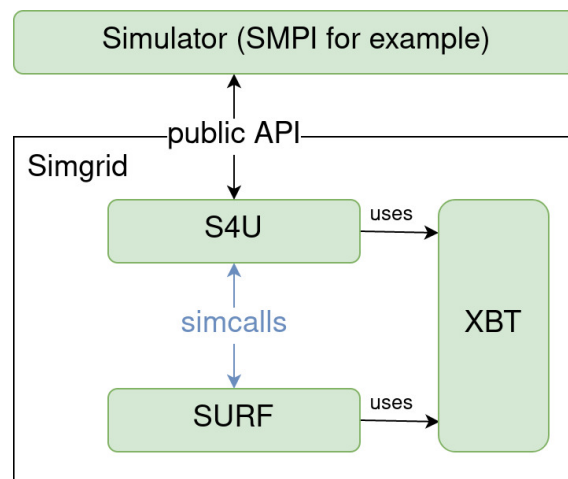


Figure 3.1: SimGrid’s architecture

Internally, SimGrid is made of three layers (as seen in Figure 3.1): at the lowest level, XBT (eXtended Bundle of Tools) is a collection of optimized C function to manipulate data structures, timers and other utilities. On top of it, the simulation kernel (called SURF) manages the virtual time and resources: it is in this layer that the duration of Activities (network, IO or compute) is computed in order to progress the virtual time and schedule the next piece of user code to be executed. The highest level is called S4U (Simgrid For You) and it implements the “public” API that is exposed to users. It provides abstractions for low-level concepts using C++ classes, representing the various resources that user code can interact with: Hosts represent simulated pieces of hardware (like a full machine, or a part of a machine) and Links represent any cable (usually network cables) that connects Hosts. Additionally, S4U provides classes to better abstract user code and communication, namely Actors and Mailboxes. Actors represent any piece of code that is to be scheduled asynchronously from other Actors’ code, in other terms it will often model a process in the simulated world (or some hardware’s logic that runs independently of other hardware). Actors need to be instantiated on a specific Host in the simulated platform in order for SURF to know at which speed computation phases need to be executed. Mailboxes on the



other hand, are a mechanism that allows Actors to communicate: traditionally, in SimGrid, data transfers will occur when two Actors issue a “send” and a “receive” call to the same Mailbox (which are identified by a unique name). By default, Mailboxes are not linked to a specific Host (they are not “located” anywhere on the simulated platform), which means that the Links used in a communication can only be decided when both the sender and the receiver have issued their call (`put` to send or `get` to receive) to the Mailbox. Indeed, this is only at this instant that SURF will be able to determine which Hosts are communicating. This means that Mailboxes effectively work as “rendezvous” points, although it is possible to set a specific Actor as a “permanent receiver” for a Mailbox, which allows the transfer to start as soon as a “send” is issued on the Mailbox (before any “receive”). This mechanic is depicted in Figure 3.2, and it will be used extensively in our simulator, which will be described in more detail in Chapter 4.

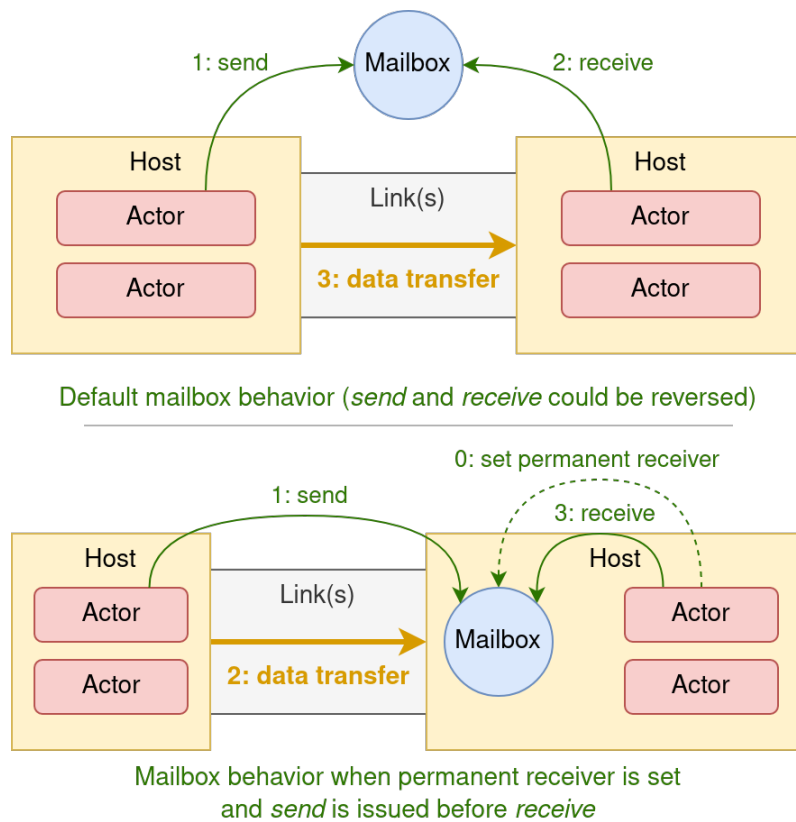


Figure 3.2: SimGrid’s mailbox system

SimGrid uses cooperative actors, and it is architected in a way that is heavily inspired by operating systems: indeed, the user-space interface (S4U) communicates with the simulation kernel (SURF) using a mechanism called “simcalls”, which are very similar to syscalls on Linux. A simcall is issued by an Actor each time it needs to perform an operation that might impact the simulated time (any computation, communication or IO). Effectively simcalls are a way for Actors to ask SURF to perform the desired operation and wake them up again either at the same date in the simulated world (in case of asynchronous operations), or whenever the operation is completed (in the case of synchronous operation), so each time an Actor performs a simcall it will yield to the kernel and trigger a new scheduling round. This only happens when Actors perform simcall, as SimGrid simulations

are cooperative, therefore it is the responsibility of Actors to yield (either using a `simcall` or by calling a dedicated primitive to do it explicitly).

✿ 3.4.2 Usage

While SimGrid is programmed with C++ 17, it offers bindings in C++ and Python. A Java interface also used to exist for the old MSG user API, but it has not been maintained when MSG was deprecated in favor of the S4U interface. During this thesis we use exclusively the C++ S4U interface. An example of a toy simulation using this interface is shown on Figure 3.3.

In this example, which implements a ping-pong with exponential message sizes, first our two Actor types are defined: `initiator` to start the “pings”, and `target` which will receive them and send “pongs” back. Their behaviors are simply a function, because that is sufficient for this simple example, but SimGrid supports making Actors from anything that is callable in C++, including objects (by overloading the `()` operator, which we will use extensively in this thesis). The initiator Actor simply sends “pings” of increasing size, attaching a sequence number to each message (`iteration`), and waits for “pongs”, checking that the “pong” sequence number is the same that was sent. The target “daemonizes” itself, which means that the simulation will end (and this Actor will be killed automatically) when all the other Actors are done executing their logic (which means that the end of the initiator will trigger the end of the simulation in this case). While this example is very simple, it already shows a few interesting things about SimGrid: First, we can see how the XBT layer can be used for several utility purposes, like an assertion API and a logging system. This logging system is very complete, and is used through C-style macros that mimic the `printf` API. Even though that is not showcased in this simplistic example, it supports a tree-like structure of categories and subcategories, which enables fine-tuning on the command line which level of log to display for each category. In the Actors’ code we can see the S4U API being used to interact with the Mailbox system in order to send and receive messages. As most resources in SimGrid, Mailboxes follow the RAII paradigm (Resource Acquisition Is Initialization), therefore we do not have to instantiate the Mailbox ourselves, we simply ask SimGrid to give us a Mailbox with that name, and internally S4U will either return it to us if it already exists or create it if it does not. This means that in our example, we do not know if the two mailboxes are going to be created from the `s4u::Mailbox::by_name` calls from initiator or the target (since all this code happens at $t = 0$ in the simulated world), but it does not matter since the result is going to be identical. It is worth noting that even if we managed to cause a potential race condition (because of two Actors executing code at the same simulated time), it is easier to debug in simulation compared to a real-world execution, because even though the order of operation happening at the same simulated time is random from a user perspective, it is deterministic, to ensure the reproducibility of SimGrid’s simulation. Finally, the `main` function sets up the simulation, declaring our Actors, and loading the platform and deployment from XML files before starting the simulation Engine. The output of this toy simulation is displayed on Figure 3.4. We can see that even though SimGrid provides methods to get the simulated time, we did not need to use them, as the logging system from XBT already prints the current Actor, simulated time, category and log level on each line.



```

1 #include <simgrid/s4u.hpp>
2
3 XBT_LOG_NEW_DEFAULT_CATEGORY(example, "Messages relative to the ping-pong");
4
5 using namespace simgrid; // Allows us to use s4u:: instead of simgrid::s4u::
6
7 static void initiator(std::vector<std::string> args) {
8     xbt_assert(args.size() > 1, "The initiator expects 1 argument");
9
10    int ping_pong_max_size = std::stol(args[1]);
11
12    s4u::Mailbox *target = s4u::Mailbox::by_name("target_mbx");
13    s4u::Mailbox *my_mailbox = s4u::Mailbox::by_name("initiator_mbx");
14
15    int iteration = 0;
16    for (int size = 1; size <= ping_pong_max_size; size *= 2) {
17        XBT_INFO("Sending ping of size %d", size);
18        target->put(new int(iteration), size); // Send ping
19        std::unique_ptr<int> pong = my_mailbox->get_unique<int>(); // Wait for pong
20        xbt_assert(*pong == iteration); // Check that the pong data is the current iteration
21        XBT_INFO("Pong (sequence = %d)", *pong);
22        iteration++;
23    }
24 }
25
26 static void target(std::vector<std::string> args) {
27     xbt_assert(args.size() > 1, "The target expects 1 argument");
28
29     s4u::Actor::self()->daemonize(); // Get killed automatically when initiator is done
30
31     int ping_pong_max_size = std::stol(args[1]);
32     s4u::Mailbox *my_mailbox = s4u::Mailbox::by_name("target_mbx");
33     s4u::Mailbox *initiator = s4u::Mailbox::by_name("initiator_mbx");
34
35     int size = 1;
36     for (;;) { // Safe endless loop because this Actor is a daemon
37         std::unique_ptr<int> ping_data = my_mailbox->get_unique<int>(); // Wait for ping
38         initiator->put(new int(*ping_data), size); // Send pong with the iteration number received
39         size *= 2;
40     }
41 }
42
43 int main(int argc, char* argv[])
44 {
45     s4u::Engine e(&argc, argv);
46     xbt_assert(argc > 2, "Usage: %s platform_file deployment_file\n", argv[0]);
47
48     /* Register the functions representing the Actors */
49     e.register_function("initiator", &initiator);
50     e.register_function("target", &target);
51
52     /* Load the platform description and then deploy the application */
53     e.load_platform(argv[1]);
54     e.load_deployment(argv[2]);
55
56     /* Run the simulation */
57     e.run();
58
59     XBT_INFO("Simulation is over");
60
61     return 0;
62 }

```

Figure 3.3: Simplistic ping-pong with SimGrid's S4U interface

```

1 [0.000000] [xbt_cfg/INFO] Configuration change: Set 'network/loopback-bw' to '99000000000'
2 [0.000000] [xbt_cfg/INFO] Configuration change: Set 'network/loopback-lat' to '0.000000001'
3 [0.000000] [xbt_cfg/INFO] Configuration change: Set 'network/model' to 'CM02'
4 [pm0-nod01:initiator:(1) 0.000000] [example/INFO] Sending ping of size 1
5 [pm0-nod01:initiator:(1) 0.000000] [example/INFO] Pong (sequence = 0)
6 [pm0-nod01:initiator:(1) 0.000000] [example/INFO] Sending ping of size 2
7 [pm0-nod01:initiator:(1) 0.000000] [example/INFO] Pong (sequence = 1)
8 [ ... 11 other ping pongs ... ]
9 [pm0-nod01:initiator:(1) 0.000000] [example/INFO] Sending ping of size 16384
10 [pm0-nod01:initiator:(1) 0.000001] [example/INFO] Pong (sequence = 14)
11 [pm0-nod01:initiator:(1) 0.000001] [example/INFO] Sending ping of size 32768
12 [pm0-nod01:initiator:(1) 0.000001] [example/INFO] Pong (sequence = 15)
13 [pm0-nod01:initiator:(1) 0.000001] [example/INFO] Sending ping of size 65536
14 [pm0-nod01:initiator:(1) 0.000003] [example/INFO] Pong (sequence = 16)
15 [pm0-nod01:initiator:(1) 0.000003] [example/INFO] Sending ping of size 131072
16 [pm0-nod01:initiator:(1) 0.000005] [example/INFO] Pong (sequence = 17)
17 [pm0-nod01:initiator:(1) 0.000005] [example/INFO] Sending ping of size 262144
18 [pm0-nod01:initiator:(1) 0.000011] [example/INFO] Pong (sequence = 18)
19 [pm0-nod01:initiator:(1) 0.000011] [example/INFO] Sending ping of size 524288
20 [pm0-nod01:initiator:(1) 0.000021] [example/INFO] Pong (sequence = 19)
21 [pm0-nod01:initiator:(1) 0.000021] [example/INFO] Sending ping of size 1048576
22 [pm0-nod01:initiator:(1) 0.000042] [example/INFO] Pong (sequence = 20)
23 [0.000042] [example/INFO] Simulation is over

```

Figure 3.4: Ping-pong’s output

❁ 3.4.3 Performance and isolation concerns

Despite being used to build single-threaded simulators, SimGrid has demonstrated a very good scalability thanks in particular to its platform representation [BLM⁺12] and the optimization of its sequential Discrete Event Simulation (DES) kernel [DLM⁺17]. This is because a DES requires many synchronizations, since there is a central value of the current simulated time that is shared by all Actors in the system, making parallelism very difficult. Some simulation frameworks try to use several threads regardless, or to work on top of MPI to distribute work on several machines (which is the case of the SST for example). The approach used varies, for example ROSS [CBP02] uses an optimistic scheduler to reduce the number of synchronizations required to the minimum, but this means that backtracking might be required when an inconsistency is detected. This makes simulators harder to write (since they need to implement rollback mechanisms), and it also limits the speedup that can be obtained from parallelization. Having a sequential DES also makes writing a simulator significantly easier: race conditions can still happen due to the asynchronous nature of the simulation, but most data structures can be used safely with no synchronization since Actors are executed one at a time, and therefore cannot access a piece of data at the same wallclock time.

The biggest issue that arises from having a single-threaded simulator is that all Actors share the same memory space. To work around this issue, and have a dedicated stack for each Actor, SimGrid allocates a tunable amount of memory to each Actor’s stack, and when switching context from one Actor to the other it provides different mechanisms: either using a full thread for each Actor, but with only one running at any given time (which is a very portable solution but very slow), `ucontext` from the System V API (which are faster but available only on Linux and FreeBSD), boost contexts (which are also reasonably fast but add a dependency), and finally “raw” contexts, which are implemented by SimGrid directly in x86 and amd64 assembly code. This last solution is extremely fast, as it requires only a few CPU cycles to switch contexts. Its only two downsides are that it is not portable



to other CPU architectures, and that this way of moving registers manually can make debugging much harder (in tools like GDB for example). For this reason, in this thesis we use “thread” context when debugging is needed (as it is very compatible with standard tools), and “raw” contexts when making full scale experiments.

To describe the simulated platform, on which Actors will be instantiated, SimGrid provides several interfaces. The most common one is through a static XML file, which is a list of Hosts, Links, and Routes to describe which Links are used to communicate between two Hosts. Additionally, some extra tags allow a more concise description of the platform, such as Router or Cluster to describe common topologies, but they are simply syntactic sugar and do not add any feature. This simulated hardware can also be grouped in NetZones that help describing heterogeneous platforms. Because a static platform can be very verbose (and the parsing of XML can have an important negative impact on performance for large platforms), SimGrid also exposes a programmatic API, which helps describe regular topologies with loops for example. At the beginning of this thesis this API used to be simplistic and required users to describe their platform in Lua, but it has since been deprecated in favor of a C++ API that is much more powerful. Although we started by using SimGrid with the XML description, we switched to the C++ API when it became available, therefore all our experiments will use this interface.

Finally, SimGrid offers a system of Plugins, which allows users to listen to events and extend the features natively offered by the framework. The most popular are the Energy and Filesystem plugins, which allow users to respectively estimate the power consumption of hardware, and model a complete Filesystem on top of the basic Storage features natively offered by SimGrid. We did not use the plugin system intensively in this thesis.

3.5 High-level models

While some specific parts of MPI have been studied in depth, such as the matching engine [LF19], it is very hard to fully model a complete MPI implementation. In HPC, there are two traditional approaches to model high-level APIs, such as MPI or OpenSHMEM for example. The offline approach requires obtaining a trace of the communications from a real-world execution, and then replaying it in simulation, potentially with different parameters, as we presented earlier. Such studies allow very fast simulation but require users to be able to obtain a realistic trace in the first place, which can be problematic. The online approach usually involves re-implementing the whole API on top of a simulation framework, in order to intercept communication primitives during the runtime of the application. While this requires a lot of work, it is the most commonly used, for example by SMPI [DLM⁺17], xSim [BE11] or SST/Macro [HH11], which all provide a complete MPI implementation in simulation (SMPI even goes as far as implementing several algorithms for each operation to mimic different real-world implementations of the MPI standard). Another approach would be to run a real-world API on top of a simulated low-level network library. While this makes the development of the simulator easier (since low-level libraries are usually more simplistic than high-level APIs), it proves very difficult to provide a simulated environment that is realistic enough to run the high-level API unmodified, which is why this approach is seldom used. We found an example of it in [KKW18], which manages to run the GASNet runtime on top of a simulated uGNI implementation (based on SST), although running more common APIs such as OpenMPI are left as future work. This last approach will be implemented for OpenMPI and OpenSHMEM over a simulated Portals implementation (using SimGrid) in this thesis, using different technical solutions than [KKW18] to overcome

the challenges that arise in the process (and which are described in detail in Chapter 5).

3.6 Multi-level modeling

Because the performance / accuracy tradeoff of simulators is their biggest limitation, some studies have tried to make it more dynamic. For example, Behavioral Emulation [RKN⁺18] tries to add this type of feature to the SST, by allowing users to write models of various granularity for each type of hardware. While this is an interesting project, it is very costly to use in terms of development time, because it is the responsibility of users to write each model at each granularity that they wish to study. Some simulators also feature options to make their low-level faster at the cost of some accuracy, for example by ignoring very short events, but from our experiments this type of configuration usually has a limited impact on performance and accuracy, as the underlying model is mostly the same in the end.



Chapter 4

S4BXI, a low-level Portals model

The goal of this thesis is to model applications that rely on the Portals API for their network transport. Although these applications are written using high-level communication libraries, we also want to take model low-level properties of the BXI hardware. This leads us to design a simulator that is abstract enough to be able to scale to hundreds of simulated processes, but which also features a model of the BXI NIC that is realistic enough to model the most significant optimizations of the hardware.

This chapter presents the simulator that we designed, S4BXI by focusing on the low-level model, whereas Chapter 5 will give more details on how it integrates with high-level APIs such as MPI. S4BXI is based on SimGrid, and as such it is a Discrete Event Simulator (DES) based on a cooperative actor model. It models the Portals 4 API, and as such it is by design a good model for BXI NICs, which implement this API in hardware. It is made in C/C++ from around 9 thousand lines of code¹. Finally, it is open-source under LGPLv2 license, and all the relevant links (source code, publications, related tools, etc.) can be found at <https://s4bxi.julien-emmanuel.com>.

We will start by describing how the real-world hardware is modeled using SimGrid's platform, as well as how we instantiate Actors on this platform, and then we will detail some technical aspects of our Portals implementation. Finally, we will present some validation experiments at a low level before moving on to higher-level experiments in the next chapter.

4.1 Platform model

As introduced in Chapter 3, SimGrid platforms are composed of Hosts, that represent simulated hardware, and Links, which represent cables (or buses). SimGrid allows any combination of Hosts and Links, but for the purpose of our simulators we add a few constraints on this representation.

Host types

In SimGrid, Hosts are supposed to be able to represent whole machines, and SimGrid natively allows to configure a Host as multicore (a virtual Host in the model can have several virtual cores). SimGrid does not have a fine model of scheduler inside each Host, and it does not model each core independently, which means that in practice, in the case of a multicore Host, every computation phase is evenly distributed across all cores.

¹Counted using cloc: <https://github.com/AlDanial/cloc>

In our case this proved to be problematic, as we wanted to be able to assign specific tasks to specific (virtual) cores, instead of having each computation phase distributed across all cores. For this reason, in S4BXI we use Hosts not to model full machines, but instead we define two types of Hosts, which represent hardware at a finer granularity: we have Hosts that represent a single CPU core, and Hosts that represent a NIC. This means that in practice, in our model each physical machine is represented by $N + 1$ virtual Hosts, where N is the number of cores in the CPU.

Link types

To connect these Hosts together, we have two types of Links: PCI Links and BXI Links. PCI Links model the PCIe bus inside each machine, which connects the NIC to the rest of the machine. This link is important because it is typically not modeled by other flow-level simulators, in particular SMPI, which usually models a whole machine with a single Host. We decided to do it because as interconnection networks get faster and faster, the transfer times across the PCI bus is of the same order of magnitude as network transfer times, which means that congestion on the PCI bus can happen and have an impact on the speed of inter-node communications. The second type of Links is the more traditional network cables that connect NICs to switches, and switches together.

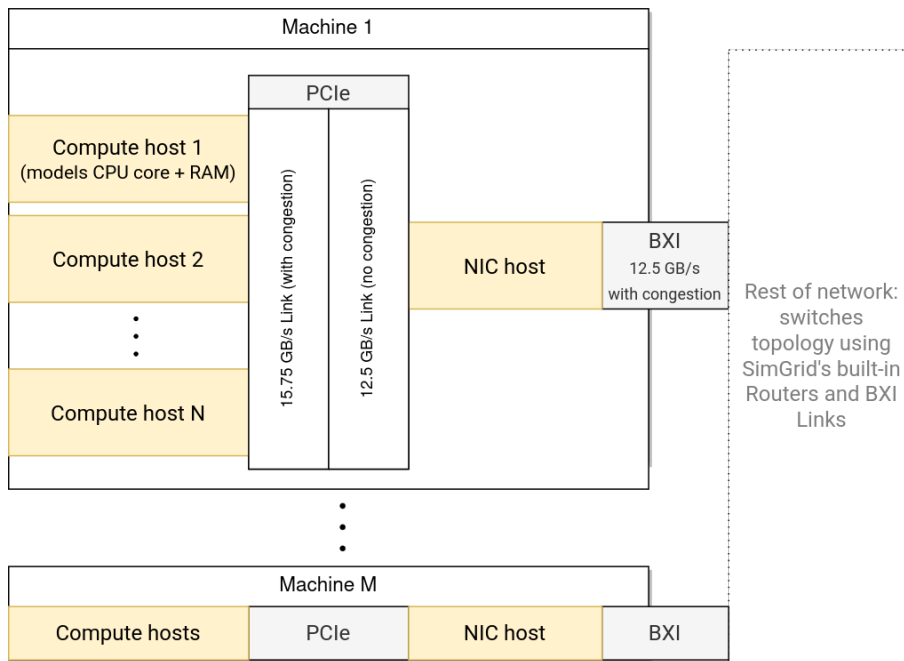


Figure 4.1: Platform model in S4BXI

One of the difficulties resides in the model of the PCI bus: while third generation PCIe x16 networks have a maximum theoretical bandwidth of 15.75 GB/s, most of our transfers (especially the transfers of consequent size) are going to flow from the PCI bus directly onto the BXI cable (which has a maximum bandwidth of 12.5 GB/s), with minimal processing in the middle. In real life this is handled with packetisation on each side of the NIC (across the PCI bus and then across the BXI cable), but because we use a flow model that operates at message-level, we cannot implement this level of granularity without losing a lot of performance. While we cannot model a total maximum bandwidth of 15.75 GB/s and



a per-message bandwidth of 12.5 GB/s in a single Link in SimGrid, we can model this behavior using two Links that each transfer has to go through: a 12.5 GB/s Link on which congestion is not considered, which limits the speed of each individual transfer, and a 15.75 GB/s Link on which congestion is considered, which limits the speed of all simultaneous transfers across the bus at any given time. We are allowed to connect these two Links back to back in simulation, even though it does not correspond to what can be done in real life. Indeed, SimGrid is very permissive in the description of platforms: every Host and Link has a Netpoint (in SimGrid vocabulary), which can be connected to any other Netpoint regardless of the type of hardware it is bound to, so it effectively allows users to connect Links together.

It is worth noting that there is no particular model for switches: indeed, we use native Router components provided by SimGrid to represent BXI switches, but even these components are just syntactic sugar to represent a Host with no Actors. These Routers work even though they do not implement any behavior, because the routing logic across the cluster (i.e. the set of Links to be used when communicating between two Hosts) is not performed at a high-level by Actors, but it is implemented at a low-level in the SURF layer of SimGrid. While making a more detailed model of switches at S4U-level using Actors would be an interesting subject of study, we chose to use the defaults routing algorithms offered by SimGrid in SURF because their fat-tree routing is faithful enough to what happens in real-world BXI fat-trees for our needs.

The platform model that results from our Links and Hosts is depicted on Figure 4.1, with a focus on one machine composed of N CPU cores.

4.2 Actor placement

Along with the platform description, a simulation needs to know which Actors to deploy on the simulated Hosts, which is done through a “deployment” in SimGrid. Similarly to the platform description, this can be done either statically in XML or dynamically in C++. Throughout this thesis we used a static XML deployment, since it is more concise than platform files, and therefore does not suffer the same performance issues (even though in some situations S4BXI may spawn a short-lived Actor to delay a specific task). Since the different types of Actors to be deployed are the same in each simulation, and only numerical parameters change (number of process to be deployed, number of nodes to be used, etc.), we made tools to automate the process of generating deployment files².

In order to implement the Portals API on top of the simulated hardware described earlier, S4BXI provides several types of Actors, each of which correspond to a different part of the communication logic. Their placement is represented on Figure 4.2 and will be detailed in the next sections.

²<https://framagit.org/s4bxi/s4bxi-config-generator>

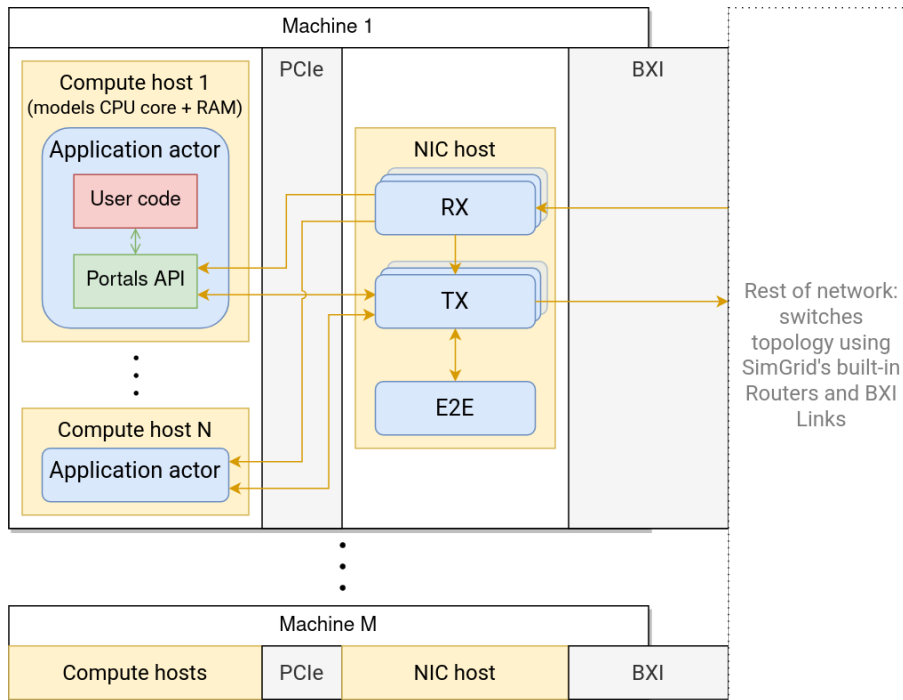


Figure 4.2: Actor placement in S4BXI

4.2.1 On-NIC Actors

Since the Portals API is implemented in hardware by the BXI NIC, most of the Portals implementation is done through three types of Actors that are instantiated on the “NIC Host” of each machine in our platform:

TX Actor

TX Actors model the “transmission” logic of the NIC. This means listening to command queues, processing message requests by doing any Direct Memory Access (DMA) and generating any event that might be required, and finally sending messages on the BXI Link to the rest of the network (through SimGrid’s Mailbox system). While the simulation works with only one TX Actor per NIC, users of S4BXI can choose to instantiate several, either to model parallel processing capabilities of the NIC, or to model different types of traffic. In BXI this last feature corresponds to the Virtual Networks that were presented in Section 2.2.3.

RX Actor

RX Actors model the “receive” logic of the NIC. To do this they listen to SimGrid Mailboxes, of which they are the permanent receiver (so that incoming messages can keep flowing in even if no Actor is available to process them yet, as described in Section 3.4). Then these actors process the request depending on its type, applying any Atomic operation, etc., and finally if an ACK or a Response is to be sent back it will be forwarded to the corresponding TX command queue (either *compute* or *service*). Similarly to TX Actors, RX Actors can be instantiated several times to model different VNs, or parallel processing capabilities of the hardware. For example, BXI NICs typically have four independent



Application-Specific Instruction set Processors (ASIP) for this purpose, which are called List Management Engines (LME).

E2E Actor

E2E Actors model the End-to-End reliability logic of the NIC which was described in Section 2.2.3. Since our simulator implements a flow model at message-level, it cannot model the CRC processing (encoding at sender, verification at receiver), since it is performed on each packet, but it models completely the timeout mechanism that is implemented in BXI, to retransmit messages which did not get acknowledged on time. The parameters (number of retransmissions and delay before retransmitting) are tunable using environment variables (`S4BXI_MAX_RETRIES` and `RETRY_TIMEOUT` respectively). In S4BXI, the E2E Actor of each machine receives a copy of each message that is issued by TX. The only exception is for BXI ACKs: in order not to have an infinite loop of acknowledgements (similar to the Two Generals' Problem³), these messages cannot have a further level of ACK, and they are therefore delivered unreliably. For each message, the E2E Actor then sleeps until the delay for retransmission is met. It then checks if an RX Actor has marked the message as “acknowledged” or not, and either drops the message if it is the case, or sends it back to the TX command queue for retransmission if the message seems to have been lost. This logic is represented on Figure 4.3: in this example only the first message sent is acknowledged in time, so the second one needs to be retransmitted.

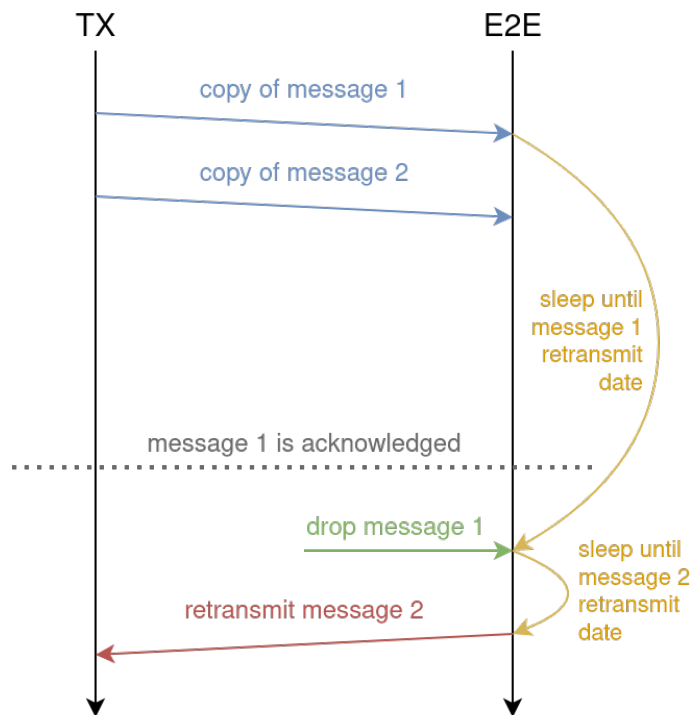


Figure 4.3: E2E logic in S4BXI

It is important to note that although several RX and TX Actors can be instantiated, every machine only requires one E2E Actor. This is because the delay before retransmitting a message is constant in BXI (as it is a parameter of the BXI kernel module), and therefore

³https://en.wikipedia.org/wiki/Two_Generals_Problem

if messages need to be retransmitted it will always be in the same order that they are received in by the E2E Actor. This means that this Actor can safely sleep until the next retransmission date when it processes a message, because even if another one is created in the meantime its retransmission date will necessarily occur later. Additionally, we can use a single “First In, First Out” (FIFO) data structure for all communications between TX Actors and the E2E Actors (in which TX Actors writes messages, which are read by the E2E Actor).

❁ 4.2.2 Actors on CPU cores

While the Actors instantiated on the NIC have a fixed behavior, Actors deployed on the simulated CPU cores must be more flexible in order to model any user application (as long as it uses the Portals API as its communication layer of course). This is done in a way that is strongly inspired by SMPI: S4BXI requires the user application to be compiled as a shared library, which allows the simulator to use the `dlopen` and `dlsym` C functions to load the `main` function from the program and run it in simulation. Since SimGrid uses cooperatives Actors, the user application simply yields automatically when any network operation is performed, through the Portals API which links with the implementation in S4BXI instead of a real-world one.

❁ 4.3 Portals model

❁ 4.3.1 Representation in S4BXI

In S4BXI, data exchanges are modeled using different Mailboxes, depicted in Figure 4.4. We can see that the event system translates to a variable number of mailboxes (one for each EQ) that are created through allocations by the user code (`PtEQAlloc` for EQs for example), and can then be queried through the Portals API. The mailboxes on the NIC do not directly map to Portals data structure, instead they are an approximate model of the hardware pipeline inside BXI NICs. We did not go for a faithful representation here, because the real-world components of the NIC are very complex, feature many more queues, and manipulate data at a different granularity in different places (for example packet size on the network is 72 bytes, while transfers across a PCI bus can range between 128 and 4096 bytes of packet size), whereas our simulator models traffic at message level, and therefore is not suited to model individual packets in the NIC. This design costs some accuracy, but greatly improves the performance of S4BXI.

In our model, TX Actors share **Commands Queues (CQ)**, one for each Virtual Network that is used by the simulation’s deployment (since inside each VN operations must be strictly ordered according to the Portals’s specification). They wait for commands from other Actors in an infinite loop and process them sequentially. These command queues are not directly Mailboxes: we added a layer of abstraction on top of it that we will call “S4BXI Queue”. These queues mimic the Mailbox interface, but they provide two implementations: they can either simply map to a Mailbox internally, or use a more performant implementation based on a C++ `std::queue` to store entries and a `simgrid::s4u::Semaphore` to allow processes to wait for a piece of data to be available (a standard C++ semaphore cannot be used because it needs to be blocking in the simulated world). This allows our queues to either model the time it takes to transfer data to them (using the Mailbox system), or to make operations instantaneous, which is often less accurate but will slightly improve the performance of the simulator. Similarly, RX Actors also poll on Mailboxes, one per VN, but which contain the incoming messages from the network. These Actors implement the



processing of these messages, including the matching logic of MEs, any memory operation that might be required, and if a response is needed, it is created in the RX Actor and forwarded to TX Actors through the corresponding S4BXI Queue. Finally, the E2E Actor has its own S4BXI Queue, which receives a copy of each message that TX Actors send on the network, except for BXI ACKs which do not have their own acknowledgement.

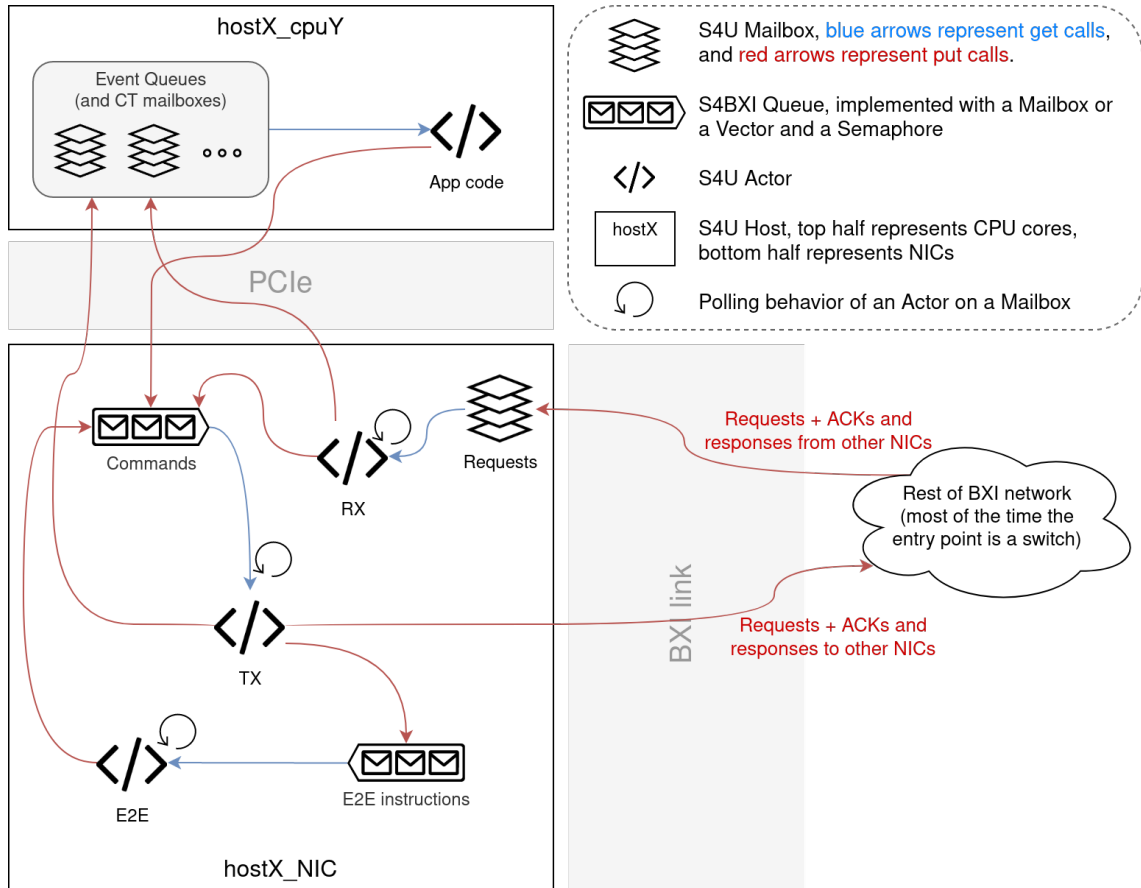


Figure 4.4: Mailbox usage in S4BXI

4.3.2 Tuning for the BXI interconnect

While Portals is a good specification for the API that should be exposed to users, at the lowest level significant freedom is left to the implementation. This results in many low-level design choices that need to be made in order to run this API on real-world hardware. Several of these characteristics cannot be modeled directly in S4BXI, because they are implemented at flit-level in BXI hardware. This is the case of low-level flow control for example, which is achieved using a credit-based mechanism in the real-world hardware. In this section we will present the specific properties of BXI which are modeled in S4BXI, because they operate at a level of granularity that is coherent with our flow model.

Virtual Networks

Virtual Networks in BXI were presented in Section 2.2.3. They are fully modeled in S4BXI, by assigning a VN number (from zero to three) to TX and RX Actors. Internally

this will result in the creation of several independent command queues that will receive requests for TX actors, and independent Mailboxes that will receive incoming messages for RX Actors (only one of each is represented on Figure 4.4). The difference between SERVICE and COMPUTE VNs is not the most important in simulation, since S4BXI does not support simulating any code that would typically run in SERVICE mode (such as a NFS). On the other hand, the difference between REQUEST and RESPONSE VNs is interesting to model so that ACKs and replies can progress independently from requests.

Command Queue depth

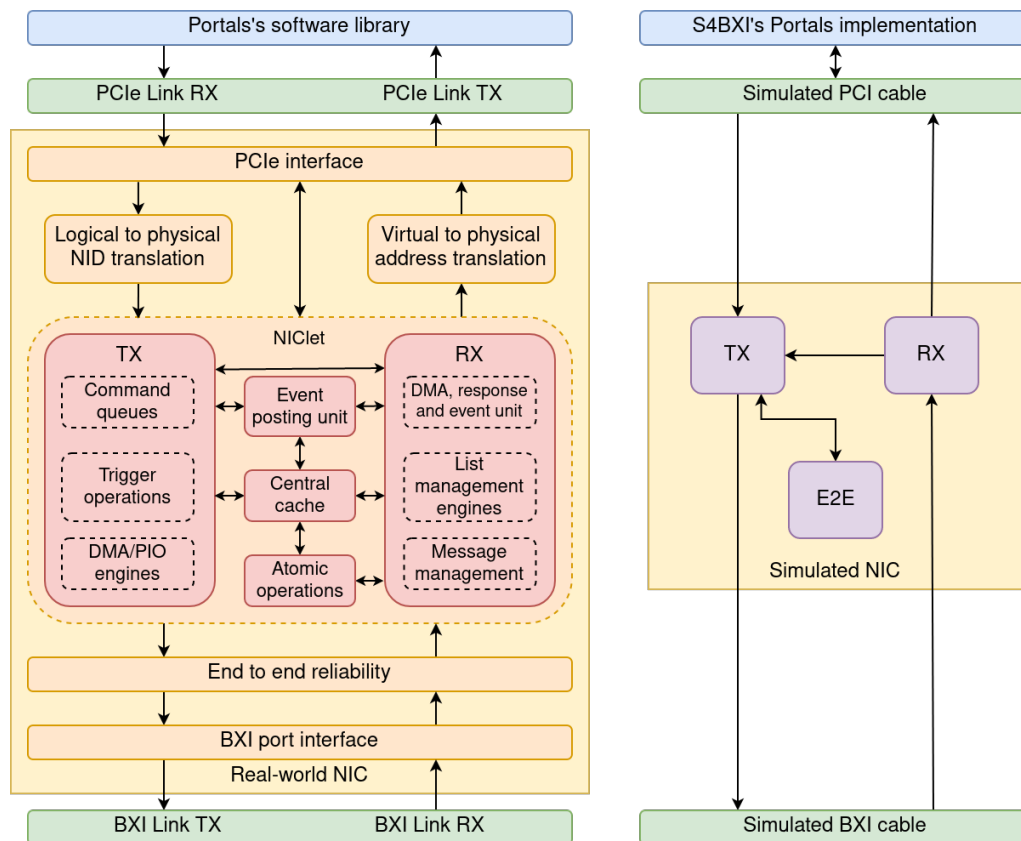


Figure 4.5: Internal pipeline of BXI NICs compared to S4BXI's implementation

Even though there is no particular restriction in Portals itself, in the real world limitations of the hardware imply that queues have a finite size, and therefore applications can only buffer a limited number of commands on the NIC before its command queues run out of space. This phenomenon is modeled in S4BXI, but in a slightly different way than in the real-world hardware: as explained earlier, the real-world NIC features many components that communicate together through internal queues. This means that the processing of commands goes through a pipeline, as shown in Figure 4.5. Thanks to this property, several commands can be in the pipeline at the same time (in different stages), which gives the software an illusion of parallel processing (although the vast majority of hardware components are strictly sequential). It also means that the first component in the pipeline is going to consume commands faster than we would expect in simulation: in S4BXI the whole processing of a command is implemented as a single sequential block



of code (usually in the TX Actor’s logic), which means that the internal NIC queues that operate on various packet sizes are not modeled in detail. Because of this, even though we know that the queues between the CPU and the NIC have 16 entries in them, we need to increase the queues’ size in simulation, in order to account for the depth of the whole pipeline. From our experimental tests we have determined that a depth of 89 entries in TX queues in S4BXI give the most accurate result, but it is important to note that this is only determined empirically, as we do not know in detail the depth and speed limitations of all intermediate queues inside the real-world NIC.

Reusing user buffers

With Portals, sending data usually triggers two events that are sent by the NIC to the user application: a SEND event and an ACK event (or REPLY if the targeted node sends data back, in the case of a FetchAtomic request for example). While ACK events simply inform the user that the message was successfully delivered and acknowledged, the SEND event is here to inform the user that the buffer from which data was sent can be re-used safely. What this last part means is different depending on the size of the payload: for large messages, the SEND event will be triggered at the same time as the corresponding ACK, because until the message is fully acknowledged the NIC could still need to access the payload in main memory in case of a retransmission by the E2E mechanism. For small messages (up to 64B), on the other hand, the NIC has enough internal cache storage to keep the full payload in what is called the “E2E context” of the message, which means that in the case of a retransmission the main memory will not be queried. For this reason, the transfer of small messages can be performed with a significantly lower latency, and achieve high message rates while having reliable transfers. This mechanism is fully modeled in the TX Actors of S4BXI, as we will be able to see in the experimental results of Section 4.6.

❧ 4.3.3 Streaming data from memory to memory across BXI

Real-world behavior

When sending data (through any request other than `Pt1Get` which performs a remote “read” operation), there are three different ways to move the payload from the memory to the NIC, which depends on the message size and options:

For the smallest messages, up to 8B for operations with match bits or 16B without match bits, the payload can be written “inline” in the command directly, since requests do not use the full memory size available for commands, according to the command format used to communicate with the NIC.

For larger messages, up to 408 or 416B (again depending on match bits), BXI uses what is called PIO (Programmed I/O). This method requires the CPU to write the payload (minus the first 8 or 16B) in a small space of “scratch” memory on the NIC, before sending the command with the remaining data (similarly to inline mode). This allows data to be accessible right away when the NIC processes the command, but it costs a small amount of time because it requires the CPU to perform two PCI writes as well as a memory fence between the two (in order to make sure data is written before the command).

For the biggest messages, DMA (Direct Memory Access) is used: the CPU simply sends a command containing the address and length of the memory to be transferred, and then the NIC reads the memory when it processes the command. Since the Portals library is mostly operating in userland (and not from a kernel driver), this means that the addresses sent to

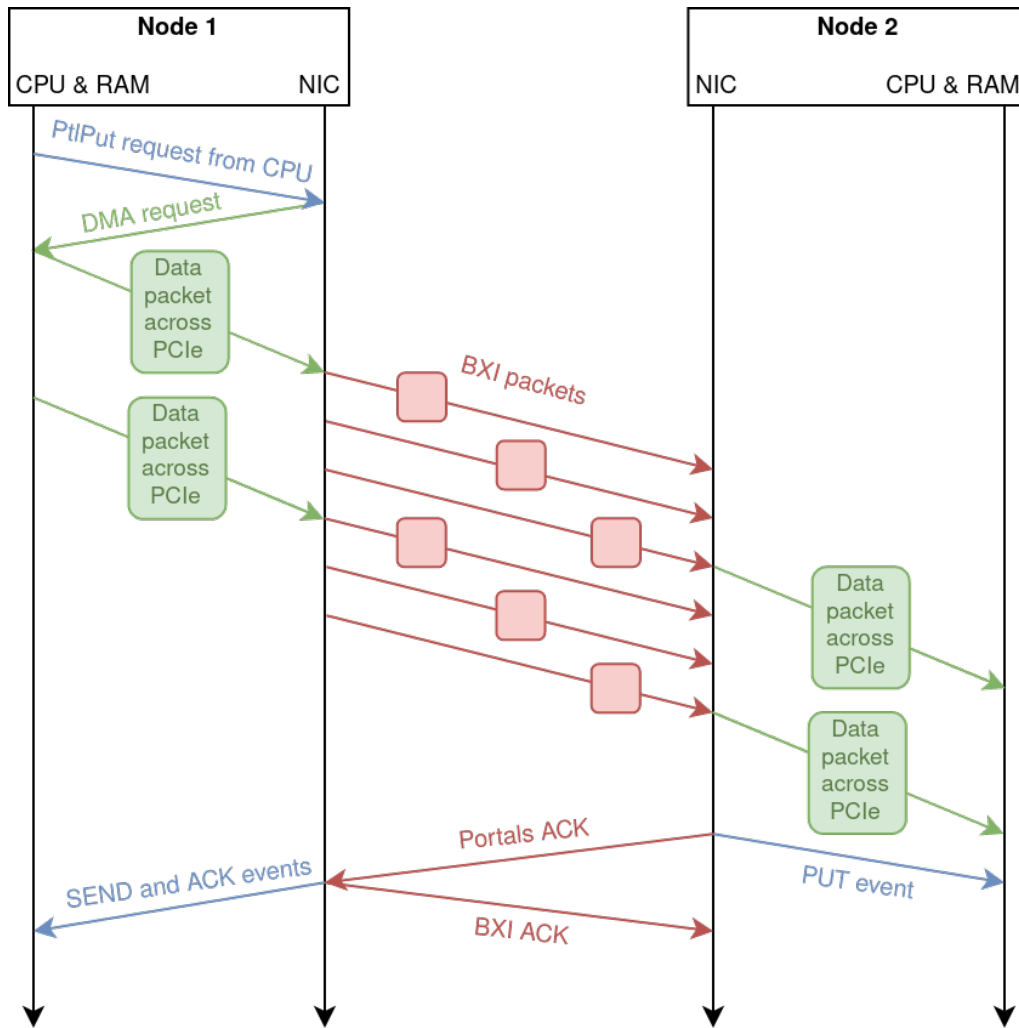


Figure 4.6: Data transfers when performing a DMA on real hardware

the NIC are virtual. This is why the NIC features a Virtual To Physical (V2P) component which implements the same page walk through the Memory Management Unit (MMU) as the CPU does, in order to request the physical memory address and send the data on the network. Additionally, it is important to note that during a communication using DMA, three transfers happen in total: a data read across PCI at the sender, the network transfer, and a data write across PCI at the receiver. Both the sender and the receiver of the payload synchronize on all three data transfers, which are dependent on each other: these transfers are all made of packets, and at the lowest level, flow control guarantees that the data progresses at a rhythm that is sustainable by both NICs using a flit-level credit system. This means that, as depicted in Figure 4.6, PCI packets (which are typically 512B, even though 256 and 1024B are also supported by BXI) are broken down into 32B flits, which are then packed into 72B BXI link-level packets (which contain two flits and 8B of header metadata), and then re-assembled into PCI packets to be written at the target side.

On the other hand, when sending data back in a response at target side (after a `Pt1Get` for example), the data transfer from memory to the NIC is always performed in the DMA style, since the targeted machine does not know which piece of memory might be requested



and when.

Model in S4BXI

In S4BXI, the inline and PIO transfers are modeled exactly as they happen in the BXI NIC (with easy to configure thresholds which allow testing different hypothetical scenarios). The DMA transfers, on the other hand, are by essence difficult to model because of the nature of our flow model. Indeed, as presented previously, in the event of a DMA we have three different transfers that are all dependent on each other, and this dependency can only be described accurately by modeling each packet. This section will present several ways to model these transfers, starting with the most naive and ending with the model that is currently implemented in our simulator.

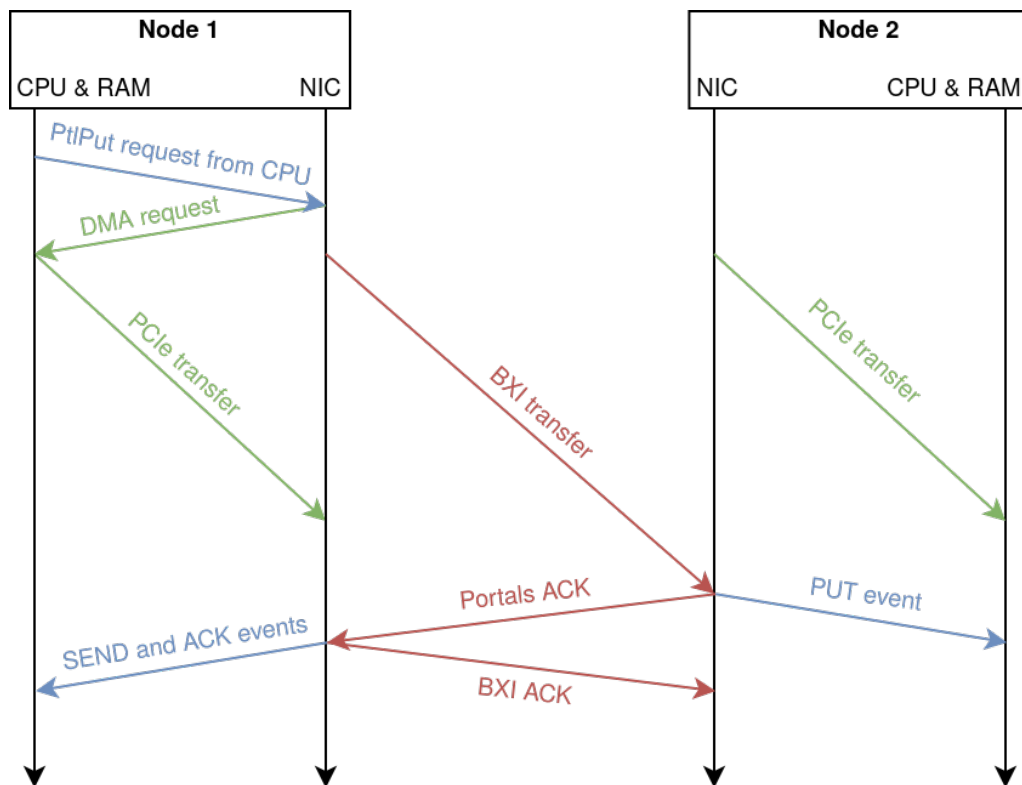


Figure 4.7: Naive flow model of data transfers when performing a DMA

A naive way to model this would be to start all three transfers at the same time in simulation (since they are very well pipelined in real life), as depicted in Figure 4.7. While this is a good approximation for moderate workloads, it loses significant accuracy if there is congestion on any of the transfers. In particular, the PCI write at the receiver will progress even if the BXI transfer gets slowed down by congestion. This results in an overly optimistic simulator in the case of communication-intensive workloads.

A different option to model this scenario is to perform the PCI write at target only when the network transfer across BXI is complete, as depicted in Figure 4.8. While this model accounts for congestion across the BXI network, it is very pessimistic in most cases, effectively reducing the maximum achievable bandwidth to half the bandwidth of the BXI cables, since the BXI transfer and the PCI write are performed sequentially.

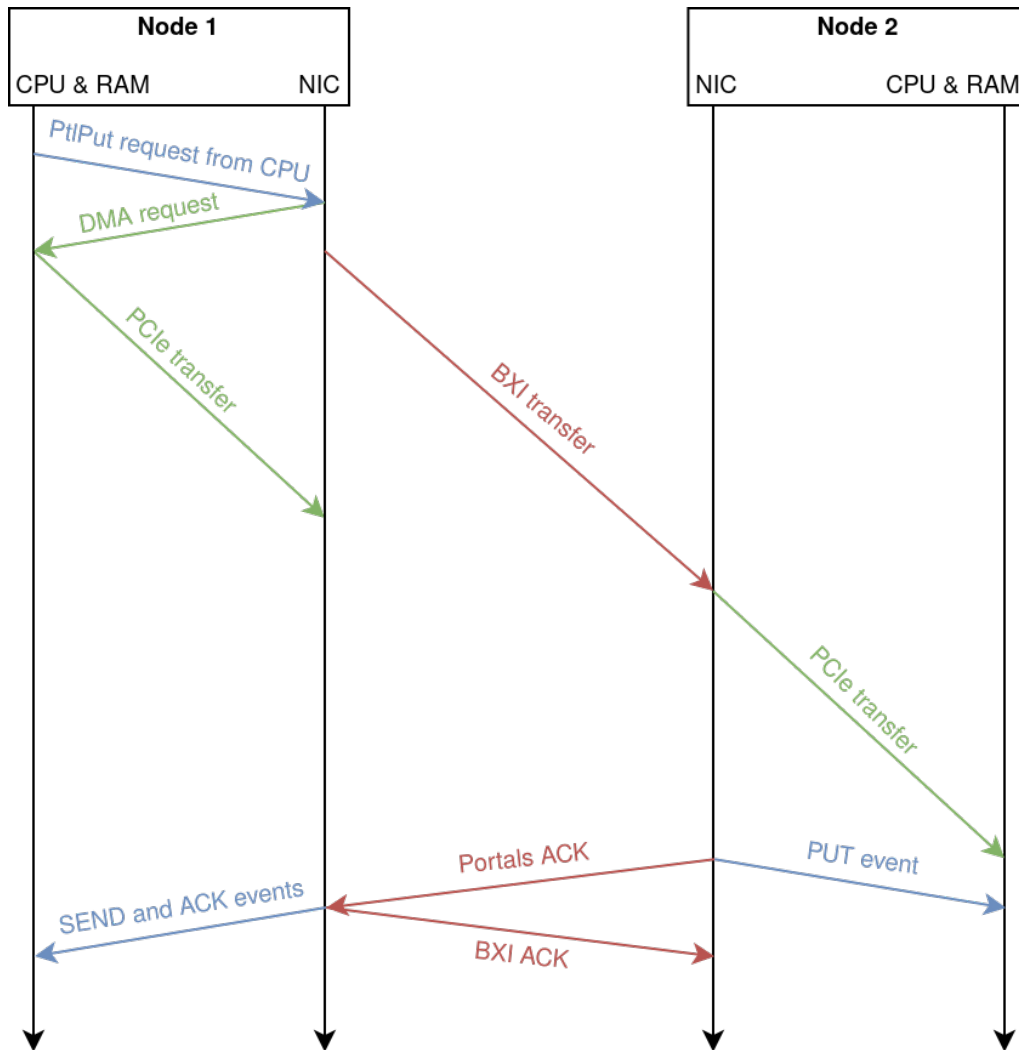


Figure 4.8: Flow model of data transfers when performing a DMA, accounting for network congestion

Finally, a solution to delay the PCI write while generating Portals events and acknowledgements faster is to perform the PCI write asynchronously in the background, as depicted in Figure 4.9. While this is still very far from a perfect model, it will generate a more realistic congestion on the PCI bus at receiver side, which will impact the generation of PUT events for example.

It is important to note that in any case, all these models are only realistic for large data transfers, in which the payload is composed of many PCI packets. Indeed, we can see on Figure 4.6 that even though the three types of transfers are very well pipelined, the first PCI packet at sender side needs to be fully received before initiating the transfer across BXI, and at receiver side, the BXI transfer needs to be fully completed before starting to write the last PCI packet. This means that for messages which can fit in a few PCI packets, the pipeline will not allow the transfers to overlap perfectly. The most pathologic case would be for messages that fit in a single PCI packet (so smaller than 512B), for which there is no pipelining at all, and the three transfers are essentially sequential. In S4BXI we account for this effect by adding a small sleep inside TX Actors before starting the transfer



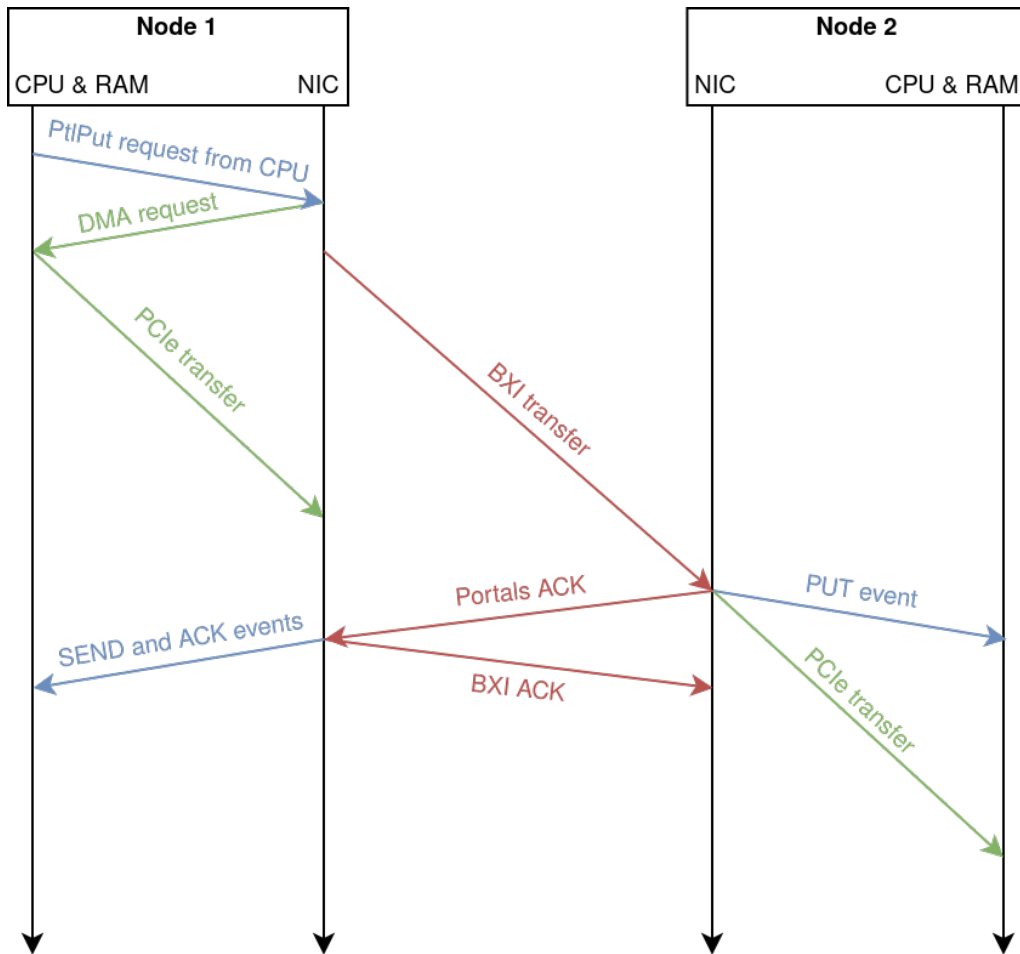


Figure 4.9: Flow model of data transfers when performing a DMA, with asynchronous PCI writes

across BXI, and another similar sleep in RX Actors before generating Portals events and any acknowledgement. Therefore, the final sequence of transfers that is implemented in S4BXI corresponds to Figure 4.10.

Finally, it is also important to mention that all transfers that are represented in each figure only model the time that operations take in our simulator: since our simulation is single-threaded, the data that is exchanged between two NICs is available at the target instantly by exchanging a C pointer. Therefore, it is not erroneous to issue a PUT event before the end of the PCI write at target side, as the RX side of our simulated NIC can access the payload at any point.

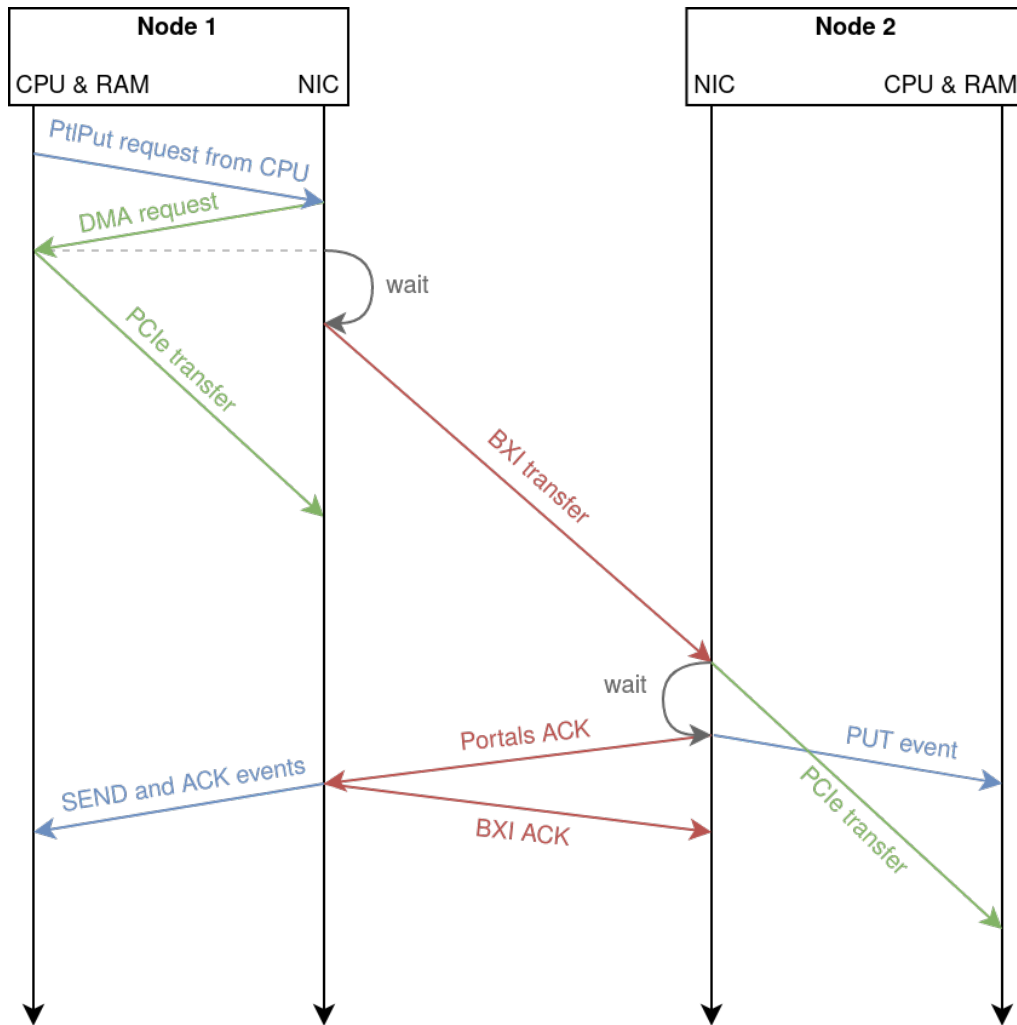


Figure 4.10: Flow model of data transfers when performing a DMA, as implemented in S4BXI

❁ 4.3.4 Performance options

In a first attempt to customize the performance/accuracy tradeoff of the simulator, we have implemented several options that can simplify the processing inside our simulated NICs:

Quick ACKs

Very often, messages containing data (`Pt1Put` requests for example) are much heavier than lightweight acknowledgements, and will account for the majority of the time spent performing network operations on a real-world cluster. Therefore, S4BXI allows generating ACK events instantaneously instead of creating a proper ACK message and sending it on the network. This means that in this case, ACK events at sender side are going to be generated from an RX Actor at the **receiver** side, which is obviously possible in simulation only (since it would require a network communication in the real world). If E2E processing is active, enabling this option saves not only one but two small ACK messages: the Portals ACK



used to generate the ACK event, and the BXI ACK used by E2E internally, as depicted in Figure 4.11

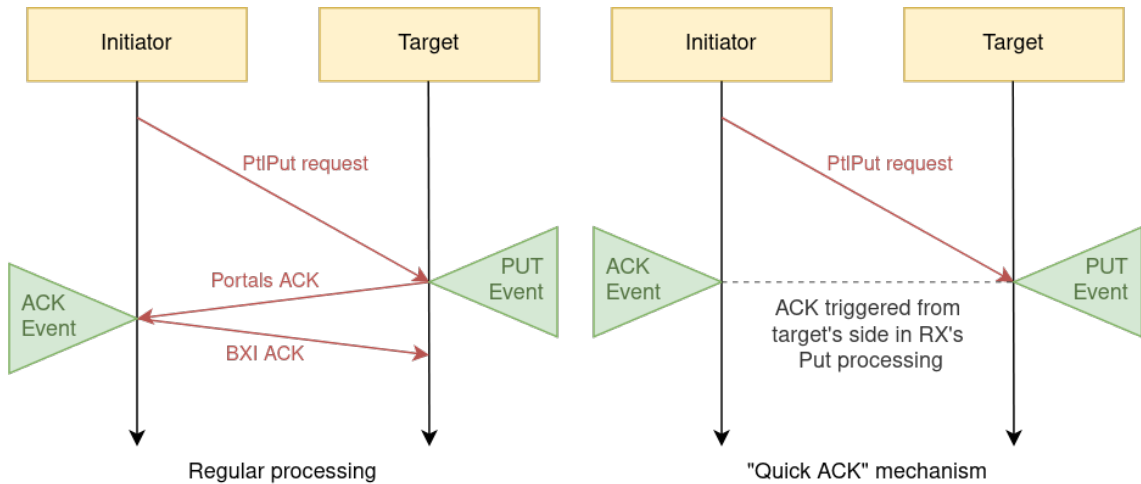


Figure 4.11: Quick ACK mechanism in S4BXI

Simplified PCI model

In the same spirit as Quick ACKs, S4BXI supports ignoring small PCI transfers: if messages of a consequent size are exchanged on the network, the time spent exchanging lightweight commands across the PCI bus in real world is usually negligible compared to data transfers (writes at target side or reads at initiator side). Therefore, S4BXI provides an option to ignore them and save a few operations in SimGrid's kernel, which is controlled either globally using the `S4BXI_MODEL_PCI_COMMANDS` environment variable, or on an Actor per Actor basis using the `model_pci_commands` property in the simulation's deployment. A more aggressive optimization consists in disabling every PCI transfer (including data transfers) completely. While this can increase performance a bit more, it is much less realistic. Similarly, this option can be enabled globally using the `S4BXI_MODEL_PCI` environment variable, or locally using the `model_pci` property on individual Actors.

4.4 Tracing and Visualization System

While SimGrid provides a low-level tracing system, which allows logging all activity on compute resources, links, etc., we felt the need to create our own too. Since it operates at Portals level, our system can add more metadata to operations: this provides a precise log of the different request and response types, whereas SimGrid's low-level system only provides the usage of each Link, without any information on the type of Portals operation.

Tracing in S4BXI is disabled by default. To enable it, one simply sets the environment variable `S4BXI_LOG_FOLDER` to a valid path. S4BXI will then write logs of all operation in CSV format (for easier parsing), splitting the log file every 10,000 lines. Additionally, the variable `S4BXI_LOG_COMPUTATION` controls whether CPU operations should be logged, or only network ones (since CPU operations can be very numerous, and not necessarily the main point of interest).


```

1 enum bxi_log_type {
2     // Messages types
3     S4BXILOG_E2E_ACK,
4     S4BXILOG_PTL_ACK,
5     S4BXILOG_PTL_GET_RESPONSE,
6     S4BXILOG_PTL_PUT,
7     S4BXILOG_PTL_GET,
8     S4BXILOG_PTL_ATOMIC,
9     S4BXILOG_PTL_FETCH_ATOMIC,
10    S4BXILOG_PTL_FETCH_ATOMIC_RESPONSE,
11
12    // PCI operations
13    S4BXILOG_PCI_PIO_PAYLOAD,
14    S4BXILOG_PCI_DMA_PAYLOAD,
15    S4BXILOG_PCI_DMA_REQUEST,
16    S4BXILOG_PCI_PAYLOAD_WRITE,
17    S4BXILOG_PCI_EVENT,
18    S4BXILOG_PCI_COMMAND,
19
20    // Compute operations
21    S4BXILOG_COMPUTE,
22 };

```

Figure 4.12: Event types in S4BXI's tracing system

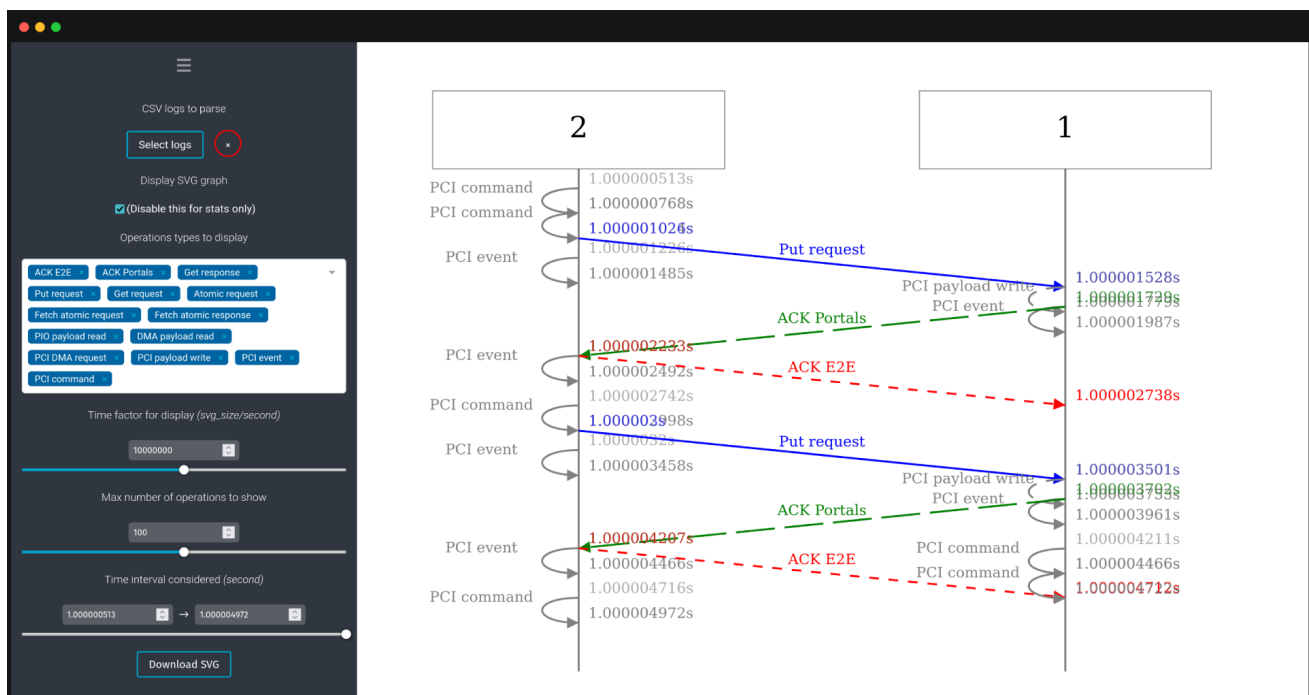


Figure 4.13: Example trace from S4BXI, two simple Put requests between NID 1 and 2

The different types of events logged by S4BXI is described in the enum `bxi_log_type`, which is shown in Figure 4.12. The output CSV files can be easily parsed, but to simplify their visualization we developed a small online tool⁴ to display operations in a sequence

⁴Hosted at <https://s4bxi.julien-emmanuel.com/log-viewer/>



graph. While it does not scale very well when the number of nodes involved is important, it is a useful tool to debug at a small scale, and its code⁵ gives a simple example of how to use the trace files. A screenshot of an example output of our tool is displayed on Figure 4.13.

4.5 Additional implementation considerations

4.5.1 Practical usage of S4BXI, and simulated process isolation

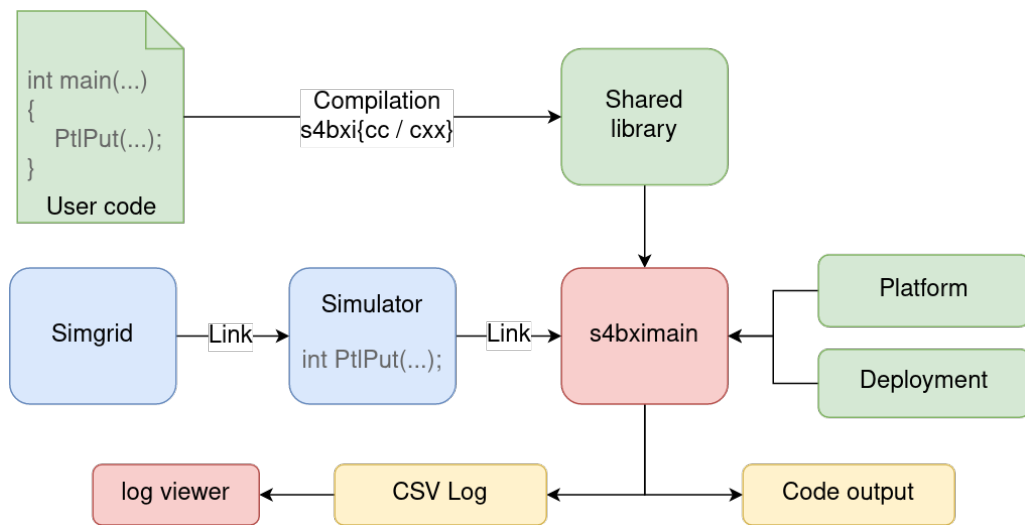


Figure 4.14: S4BXI components and usage

To facilitate the configuration of the compiler for S4BXI users we provide scripts that act as wrappers around compilers (namely `s4bxicc` and `s4bxicxx`) that have a very similar goal than the corresponding `smpicc` and `smpicxx`: make the compiled program a shared library, and include header files to redefine the symbols that we want to capture (using C macros). An overview of the methodology is shown on Figure 4.14: First the application’s code is compiled, either with our compiler wrappers directly or simply by adding the `-shared` flag manually. Then S4BXI is started (through the binary `s4bximain`) with three essential arguments: the simulated platform’s description, the associated deployment configuration, and finally the shared library which contains the application. Each Actor which runs the user application will then copy the application’s library on disk with a different name for each simulated process, and use the `dlopen` and `dlsym` function to extract the `main` symbol from the library and run it. The reason for copying the simulated application (instead of opening the same library from every simulated process) is that it allows us to trick the dynamic linker into thinking that all these copies are different libraries, which allows us to leverage the linker’s ability to isolate the global symbols (in particular global variables) of different libraries running in the same address space. This provides isolation between the different simulated processes even though they all run in a single thread in practice, without having to implement this feature ourselves.

⁵Open source at <https://framagit.org/s4bxi/s4bxi-log-viewer>

❖ 4.5.2 Platform implementation in S4BXI

At the beginning of this PhD, the most popular way of describing SimGrid platforms was using a static XML document⁶. Unfortunately, this wasn't a very flexible approach: there are XML tags that try to simplify the platform, such as `<cluster>` which creates the complete list of Hosts and Links for common topologies, but unfortunately when using these the “leaf” nodes of the cluster could only be simple Hosts (instead of the more complete model with PCI cables, etc. that we described above). For this reason we made some scripts to convert the output of real-world cluster management software (BXI-AFM in our case) into a SimGrid XML platform that comply with S4BXI's requirements. While this is a functional solution, it had the downside of generating potentially very heavy and verbose platforms, which could take a significant amount of time and memory to parse in SimGrid. Thankfully, since then the SimGrid team developed a C++ API (integrated in S4U) to describe platforms, which is significantly more performant and flexible. We added support for it in our simulator by checking the filetype of the platform at startup (either an XML file or a shared library compiled from a C++ platform), and in the case of a C++ platform our simulator looks for a specific symbol (`load_platform`) to call, which is responsible for generating the platform. While we kept the support for XML platforms, all our experiments will use the C++ API, which should become the standard way of using SimGrid in the future.

❖ 4.5.3 Portals's implementation in C/C++

On a real cluster, the user code (or a library such as MPI) includes the `portals4.h` header file, which provides the declarations for Portals's structures and primitives. In simulation, we simply reuse the `portals4.h` header provided by the real world implementation made by Atos (as well as a few BXI-specific helpers for an optimal compatibility, `portals4_bxiext.h` and `portals4_services.h`). These files allow us to have identical declarations, so that user code can use our simulated Portals or Atos's one transparently. The difference comes from the implementation: while the Portals primitives are implemented by Atos's library on a real cluster, in simulation S4BXI provides an implementation on top of SimGrid. This methodology is represented on Figure 4.15, in which we can see how the difference between real-world and simulation comes only from the implementation of primitives.

Internally all our Actors are implemented by C++ classes, as SimGrid is very flexible in this regard: Actors' behavior can be implemented either using a simple function, a class, or anything that is callable (our complete class hierarchy is represented in Appendix A. Therefore, the implementation behind the public interface is simply a small layer that retrieves the current S4BXI Actor instance (`BxiMainActor` in our class hierarchy) and calls a member function corresponding to the desired Portals primitive. This lookup of the current S4BXI Actor instance is optimized using a small plugin we wrote for SimGrid, which allows us to store this pointer in SimGrid's representation of Actors.

⁶The corresponding DTD is available at <https://simgrid.org/simgrid.dtd>



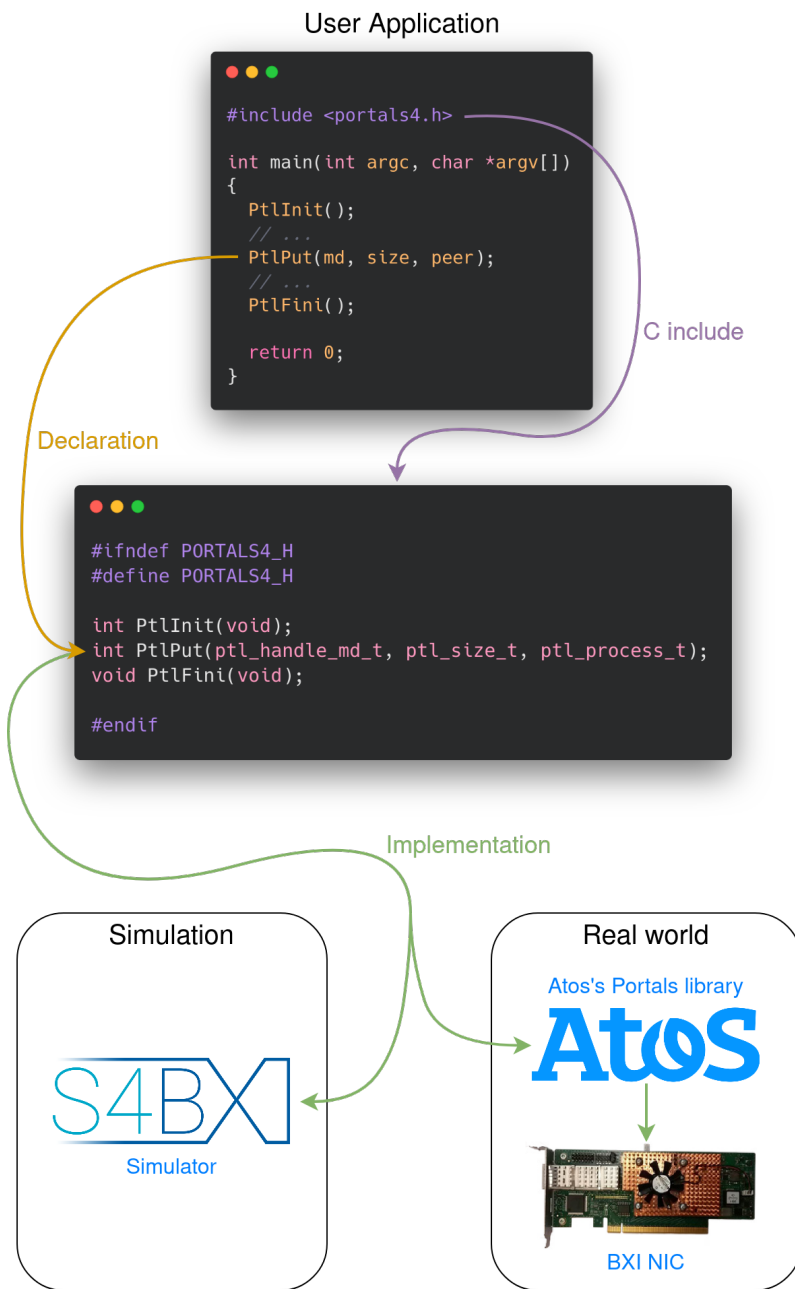


Figure 4.15: Declaration and implementation of Portals's primitives

4.5.4 Capturing function calls

While the Portals primitives naturally link with S4BXI's implementation in simulation, there are other function calls that need to be intercepted: all utilities that rely on time, such as `gettimeofday`, `sleep`, etc. must be re-implemented in simulation in order to use simulated time instead of wall-clock time. A traditional way to perform this interception is to preload a library using the `LD_PRELOAD` environment variable on Linux. While this is efficient, we chose a simpler approach (similar to SMPI) where the function calls that we re-implement are redirected to the simulator's implementation using `#define` C macros. This method is more intrusive since it requires re-compiling the simulated application, but in our

workflow it does not add any constraint since we already need to compile the application, in order to make a shared library (as explained in Subsection 4.2.2).

In S4BXI we implemented most functions that can be used to sleep with various precision (`sleep`, `nanosleep`, etc.), functions to query the current time (`gettimeofday`, `clock_gettime`, etc.) as well as a few other utilities such as `hostname`, `getpid`, etc. so that each simulated node returns a value from the simulated world instead of data from the machine running the simulation. We also support a subset of signal handlers that we encountered in low-level benchmarks: `sigaction` stores the handler for a given signal in a simulated-Actor specific structure, and this handler is then executed after a call to `setitimer` or `alarm` and the corresponding waiting time is elapsed in the simulated world. In order to wait for the desired amount of time, and call the appropriate handler when the timeout expires, we spawn a short-lived Actor so that the main application can continue to progress at the same time, as it would in real-life (since the timer runs in the background).

→ 4.5.5 Completeness

S4BXI was made with the end goal of simulating high-level APIs, in particular MPI, and therefore we only implemented the features that we needed for this purpose. This means that our Portals implementation is not complete, although the majority of Portals primitives are supported (and tested in our Continuous Integration). The main missing features are I/O Vectors (IOVEC), which are the ability to send several pieces of non-contiguous data at once, as well as triggered operations, which are the ability to send a message automatically when a specific event happens in Portals. We only left these features aside because of time constraints, and we believe that the current architecture of our simulator would make their implementation straightforward. Adding these features would only be a matter of investing some engineering time, if there was a need for it, since they would be very similar to the existing logic currently implemented in the simulator.

↻ 4.6 Experimental validation

In order to get a first validation of our Portals model (before moving on to higher-level APIs) we executed two types of benchmark on a BXI cluster and in S4BXI: first we started with custom-made tests, which are very simplistic, and then we ran `PtlPerf`, which is a pre-existing tool made at Atos to perform point-to-point performance measurements, as presented in Section 2.3.

→ 4.6.1 Custom made benchmarks

While we check that all request types are fonctionnally correct in our Continuous Integration, we studied in more detail `PtlPut` and `PtlGet` operations in order to validate their performance in simulated time against real-world executions on BXI hardware. Indeed, it is easy to write a test suite to ensure that all operations transfer data correctly, but evaluating the accuracy of the simulator is significantly harder to automate. We chose to study these primitives because they are the most commonly used, in particular they are the only request types that are used in the MPI implementation that we will study in the next chapter.



Benchmarks' behavior

Each benchmark that we made operates on the same principle: 10,000 requests (Put or Get) are sent from a machine A to a machine B, while both machines measure the total time. This workload is repeated for 64 different message sizes, which are chosen according to the following method: the first few message sizes are hardcoded and correspond to the sizes where we expect significant changes in the duration of the benchmark (because of the optimizations that we know exist in the real-world hardware and the S4BXI model), for example at 64B (and therefore 65B too in order to see the change clearly). Then, the next sizes are generated at random, using a distribution uniform on a log scale (in base two). We did not go for powers of two directly, to avoid testing only very particular values. We also did not go for a simple uniform distribution because we are more interested in small values, for which there are more variations in the performance of BXI.

We designed five types of benchmarks: three for the **Pt1Put** operation and two for **Pt1Get**. To make this section easier to read, we will name each of these variants, and illustrate them with sequence diagrams (which offer a simplified representation of the transfers involved, in particular they are a lot less detailed than figures 4.7 to 4.10):

Put-WaitAck performs Put operations. The benchmark waits for an ACK event before moving on to the next operation, which means that there is only one message inflight at all times. This corresponds to the sequence diagram on Figure 4.16a.

Get-WaitReply performs Get operations. The benchmark waits for a REPLY event before moving on to the next operation, so once again there is only one message inflight at all times. This corresponds to the sequence diagram on Figure 4.16b.

Put-NoWait performs Put operations as fast as possible, without waiting for any event. While this workload is not a very realistic use of BXI NICs, it allows us to benchmark the ability of the NIC to absorb and process many commands, and to see how the network performs when many messages are inflight at the same time. This corresponds to the sequence diagram on Figure 4.17a.

Get-NoWait performs Get operations as fast as possible, without waiting for any event. Once again this benchmark allows us to stress the NICs involved, in particular the target NIC which will receive many requests at a high rate. This corresponds to the sequence diagram on Figure 4.17b.

Put-WaitSend performs Put operations. The benchmark waits for a SEND event before moving on to the next operation. This is closer to a realistic use case of Portals, as this event indicates that the source buffer can be safely reused. In practice, it allows small messages to be processed in a pipelined way, while for large messages it is equivalent to waiting for the ACK event. This corresponds to the sequence diagram on Figure 4.18.

As illustrated on figure 4.16, the **Put-WaitAck** and **Get-WaitReply** benchmarks are very simplistic, as they evaluate the total latency of an operation, which includes an initial message and a response (either a full reply or a small ACK). On the other hand, Figure 4.17 shows that the **Put-NoWait** and **Get-NoWait** benchmarks stress both NICs involved much more, by requesting as many operations inflight as possible, which evaluates the capacity of the hardware to process commands and incoming messages in a pipelined way. Finally, **Put-WaitSend** corresponds to a more realistic usage of the hardware.

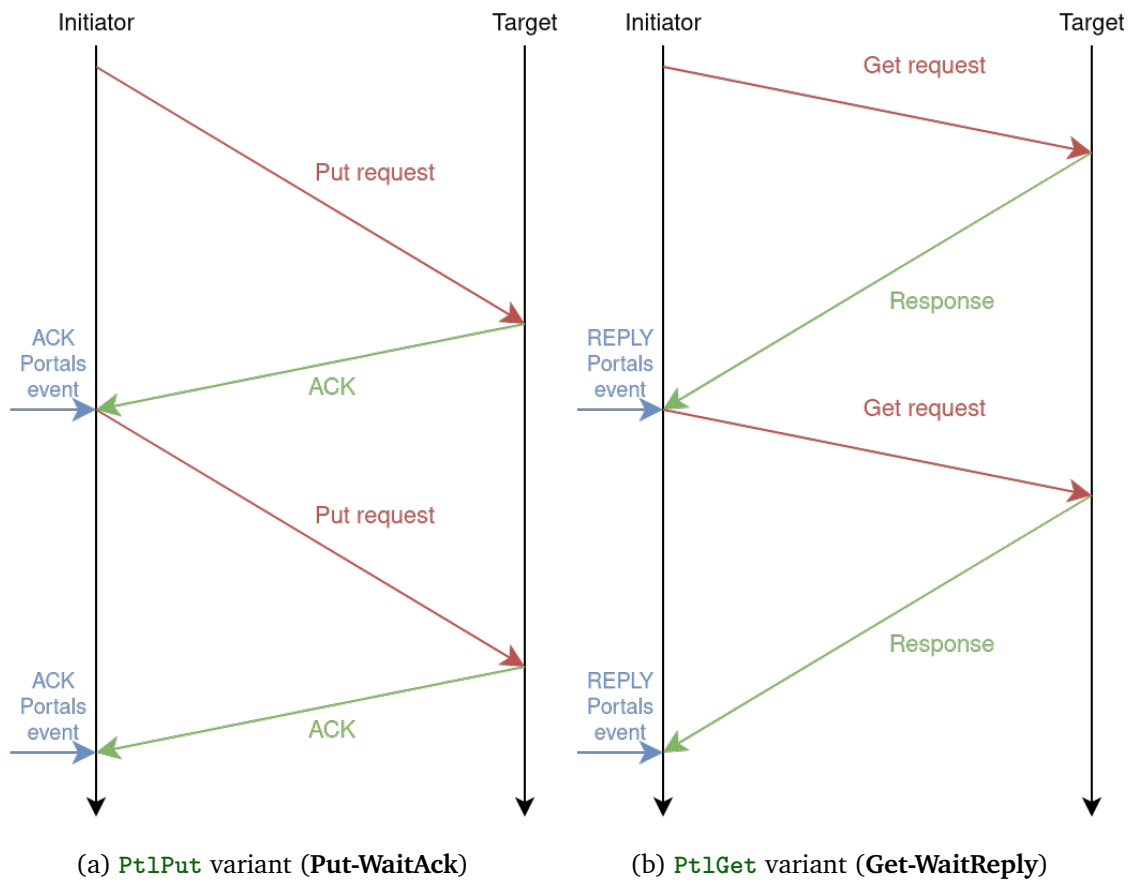


Figure 4.16: Portals experiment, one request at a time

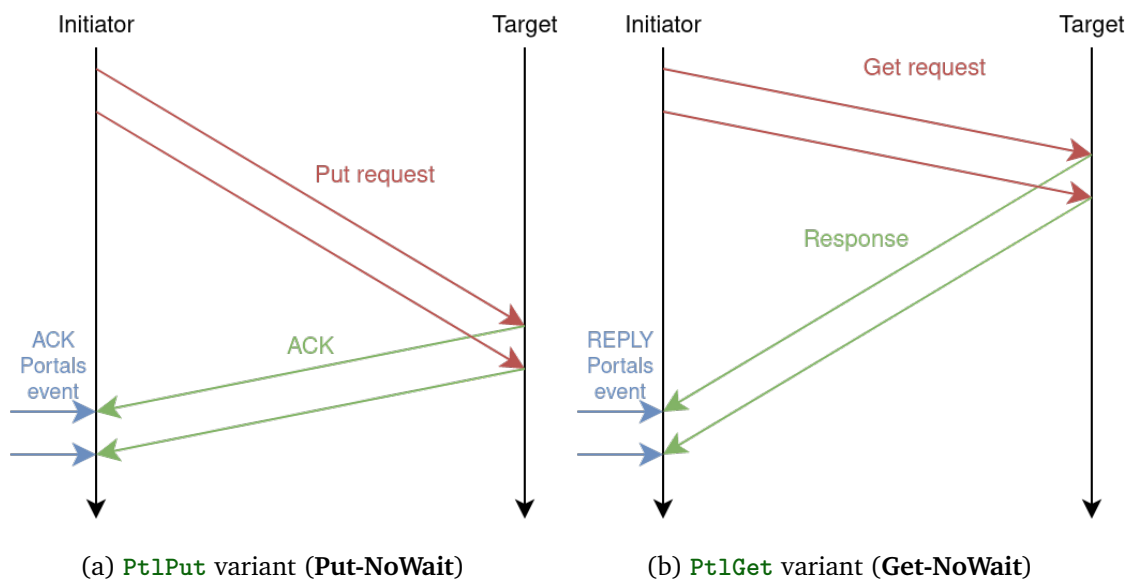


Figure 4.17: Portals experiment, sending requests as fast as possible



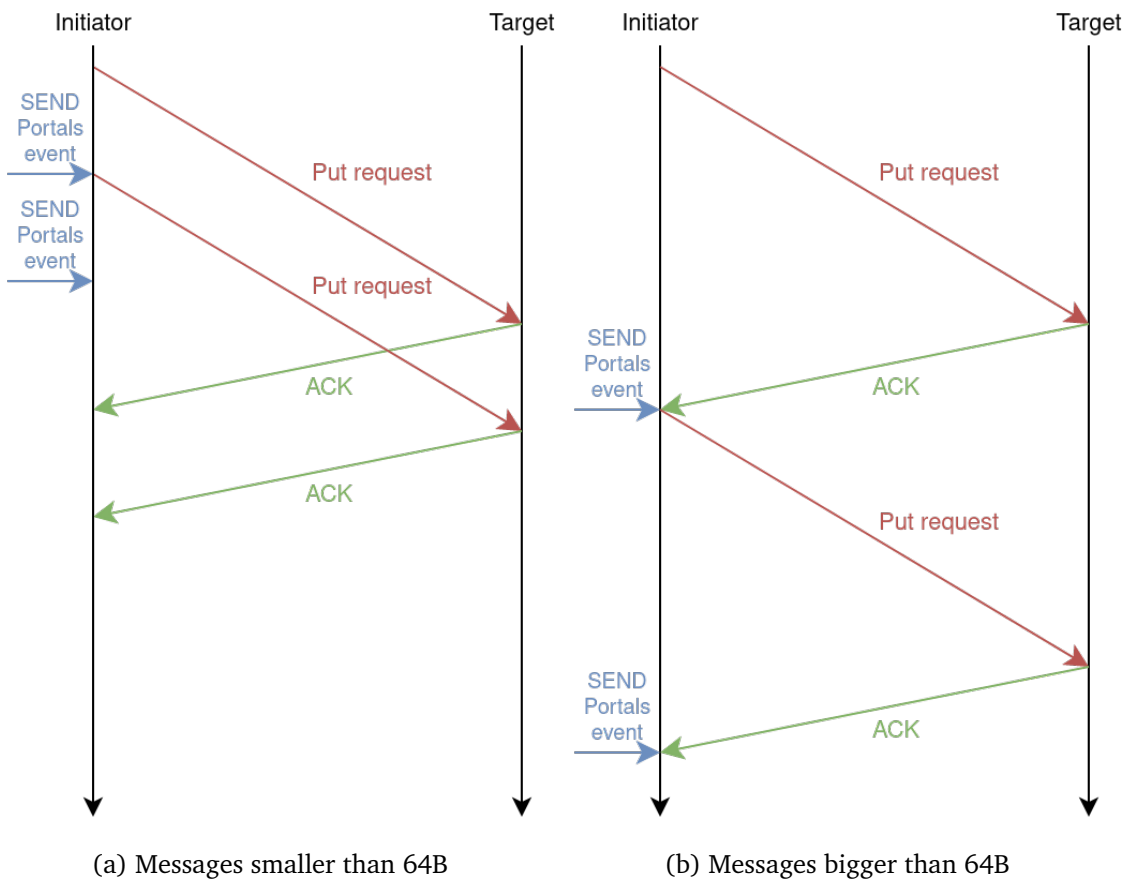


Figure 4.18: `PutWaitSend` experiment, waiting for SEND event between requests (`PutWaitSend`)

Experimental setup

When simulating these benchmarks, we observed that our simplistic CPU model caused the simulations to be overly pessimistic (to the point where putting a zero nanosecond latency on all Links of our simulated platform still gave pessimistic results). We concluded that since our benchmarks are focused on the network, the CPU sections between two network primitives are very short, and that the latency of starting and stopping our CPU timer impacted its measurements in a very significant way, resulting in pessimistic CPU times. To fix this problem, we can configure the CPU model to ignore computations that are shorter than a supplied threshold, therefore for these experiments we ignored all computations smaller than one microsecond, which effectively ignores all computation phases in this specific case (since the CPU time is only spent executing a `for` loop around the network primitives essentially).

From a technical point of view, in the real-world cluster the nodes we use are equipped with BXI v2 hardware and AMD EPYC™ 7763 64-Core processors. For the simulations we use a traditional desktop computer, which has an Intel® Core™ i9-10850K CPU and 32 GB of RAM. For each message size the experiment is executed five times on the real-world cluster in order to ensure that the results are consistent, and only once in simulation since it is fully deterministic and reproducible.

Results

The results of our benchmarks are displayed on the following figures:

- Figure 4.19 shows the result of the **Put-WaitAck** benchmark
- Figure 4.20 shows the result of the **Put-NoWait** benchmark
- Figure 4.21 shows the result of the **Put-WaitSend** benchmark
- Figure 4.22 shows the result of the **Get-WaitReply** benchmark
- Figure 4.23 shows the result of the **Get-NoWait** benchmark

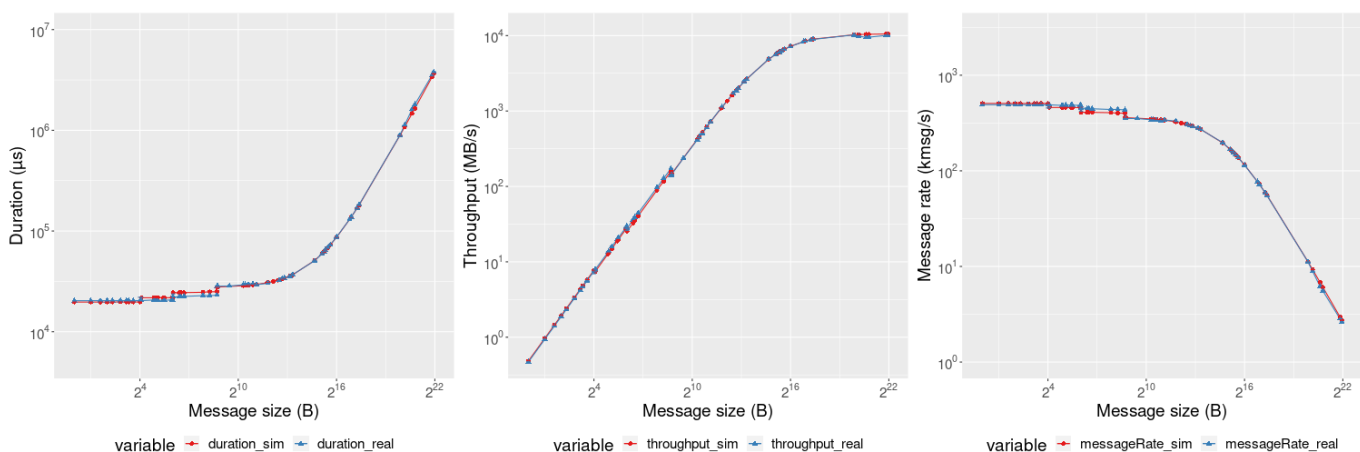


Figure 4.19: **Put-WaitAck** benchmark

Each graph shows the overall duration of the benchmark, the bandwidth, and the message rate, estimated by our simulator in red (with circular points) and as reported by



real-world runs on the BXI cluster in blue (with triangular points). It is important to note that all graphs use a log scale on both axes (a base two log on the x-axis and a base ten log

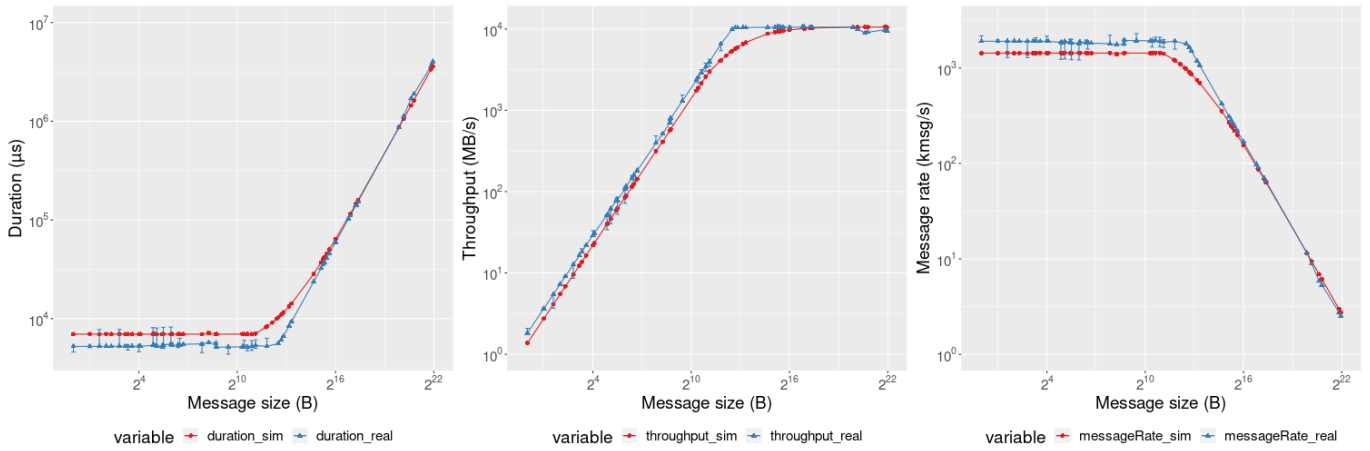


Figure 4.20: Put-NoWait benchmark

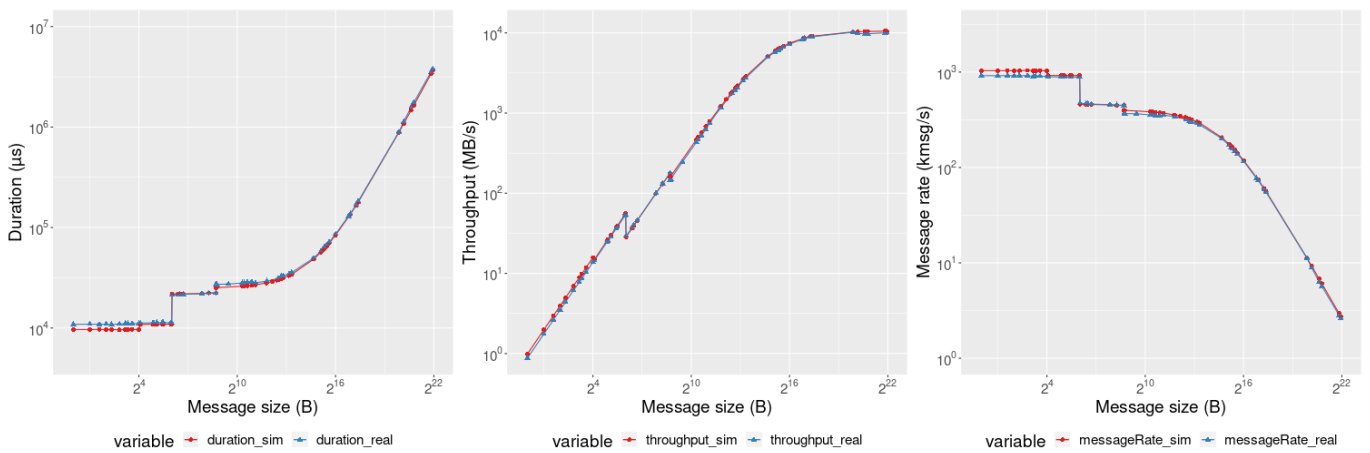


Figure 4.21: Put-WaitSend benchmark

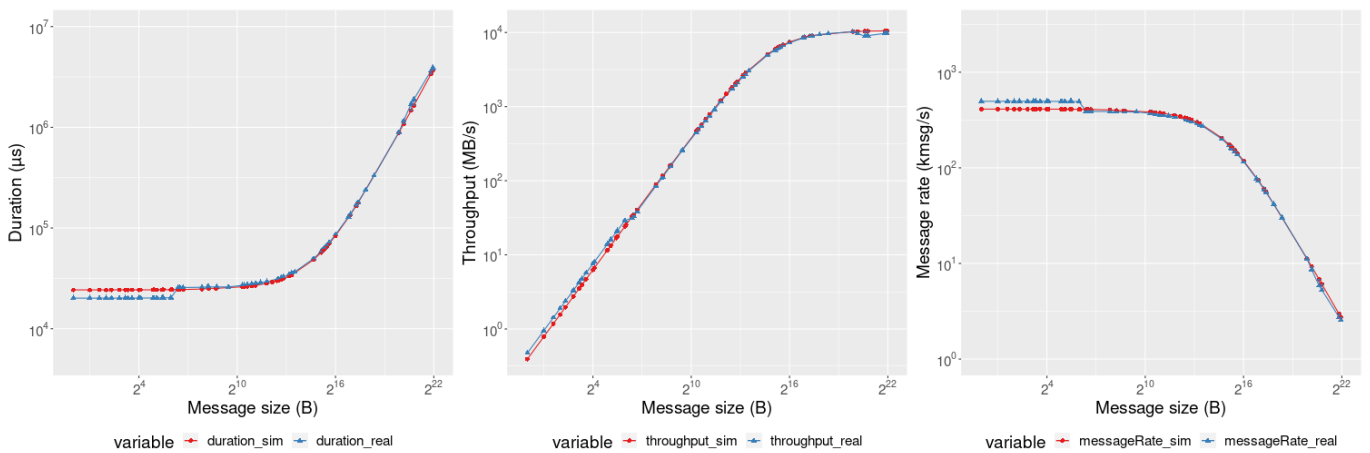


Figure 4.22: Get-WaitReply benchmark

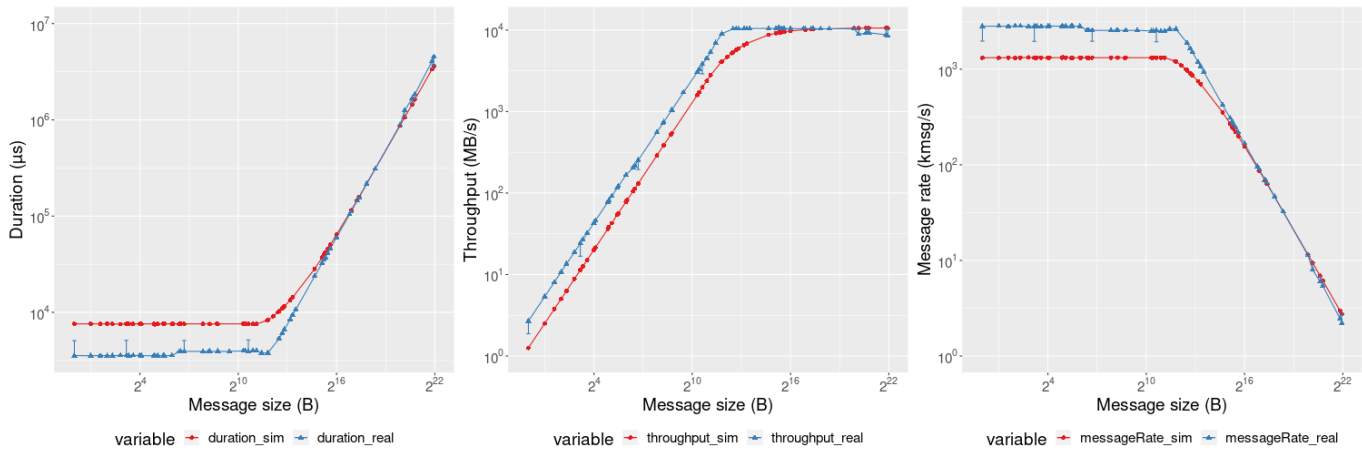


Figure 4.23: **Get-NoWait** benchmark

on the y-axis), in order to make results more readable. In particular, on all variants of our experiments, the left side shows experiments on small messages, therefore the duration of operations correspond to the latency of the hardware, whereas on the right side the duration of operations is dominated by the bandwidth of network cables. This explains why for large messages, all benchmarks exhibit the same behavior (which is perfectly captured by our simulator, as it is the easiest workload to model).

While most results given by our simulator are very good, there are a few notable things to see in these graphs: first, the benchmarks that perform one request at a time give excellent results in simulation. This is because these benchmarks mainly evaluate the latency of the network, which we can tune easily, without caring about the ability of the NIC to process requests in parallel (or at least in a pipelined way). On the other hand, benchmarks which send requests as fast as possible give results which are further from reality: it is harder to model these cases because the performance of the benchmark depends on the ability of the NIC to process requests quickly, and not only on the latency of the network. This is particularly difficult to estimate because of the tradeoff that we chose: since we use a flow model, and not a cycle accurate emulator of the NIC, the blocking time that the NIC needs to process requests can only be accounted for using approximate heuristics involving small `sleep()`s of a few hundred nanoseconds in the Actors of the NIC. This is a known limitation of this type of model, and we carefully tuned these delays, which shows very good results for **Pt1Put** operations (Figure 4.20), and acceptable results for **Pt1Get** requests (Figure 4.23).

For **Pt1Put** operations specifically, we can see that the graphs are very similar whether we wait for the full completion of requests (Figure 4.19), or just the SEND events (Figure 4.21). This is expected since for messages larger than 64B the SEND event is issued at the very end of the request's life. For small messages on the other hand, we can see that only waiting for the SEND event allows several requests to be processed in a pipelined way, resulting in lower latencies which are correctly modeled by S4BXI. Overall, the results of our simulators are excellent for these types of benchmarks, as they perfectly capture all the changes in performance that can be seen on the real-world experiment. This accuracy of S4BXI comes directly from our low-level model of the hardware, and in particular our model of PCI transfers, since different message sizes allow NICs to perform different optimizations on these transfers, which we were able to capture in S4BXI (without having



to use packet-level simulation).

For `PtlGet` operations, we can see that when sending them one at a time (Figure 4.22), there is a small performance gap around 64B. On one hand this is not very surprising, since we have already established that 64B is a specific value for BXI NICs, which is a usual threshold to be able to apply some optimizations (or not). The problem in this case is that for Get requests, there should not be any particular optimization of this sort as far as we are aware, which was confirmed by the hardware designers of the NIC (who were kind enough to answer all our questions to the best of their ability). Therefore, we did not model this performance gap in S4BXI, since its origin in the real world is unknown. While this is not the most satisfying conclusion, the performance gap is small enough that we do not expect it to cause a significant accuracy loss in the rest of our work, especially since the `PtlPut` primitive is more commonly used than `PtlGet`.

From a performance perspective, the simulation is slightly slower than the real-world experiment: regardless of the benchmark type, a simulation of 64 message sizes takes around 40 seconds of wall-clock time, while the real-world execution takes around 15 seconds. It is worth noting that the most time-consuming sections are different in simulation and in the real-world: on the BXI cluster, the larger the messages, the longer they will take to transfer, and therefore most of the time is spent in the transfer of large messages. In simulation on the other hand, the message size does not have a direct impact on the performance, because incrementing the simulated time has the same performance regardless of the size of the increment (whether it is one microsecond for a small message or 400 microseconds for a large message). What costs the most time in simulation is when many of transfers happen at the same time, because it causes many recomputations of the flow-model: each time a communication starts or ends, all transfers that use the same Link must have their ending date recomputed. It is therefore expected that our simulator is slower than the experiments that it models, since our random generation of message sizes favors small messages, which are transferred very quickly in the real world. Additionally, we expect simulation to be twice as slow regardless, because in the real world our two processes (the initiator and the target) run at the same time, on different machines, whereas in simulation they are executed sequentially (and asynchronously thanks to SimGrid's Actor scheduler).

Overall, these results are a good first step towards the validation of our model: the accuracy is acceptable on all benchmarks, and excellent on some of them. The performance is also acceptable, as it is of the order of magnitude we expected. Obviously the downside of our validation is that our benchmarks are very artificial, as we made them ourselves, which is why the next section will present results of the simulation of pre-existing Portals benchmarks.

4.6.2 PtlPerf

Unlike our previous tests, which measure the time needed to send a fixed number of messages, `PtlPerf` counts how many messages can be sent in a fixed amount of time (using the `PtlPut` primitive), and reports various statistics about the transmissions (as presented in Section 2.3.1). While it offers many modes and options, we ran it in CT (Figure 4.24), ACK (Figure 4.25), match (Figure 4.26) and reply (Figure 4.27) mode, for which the latency, throughput, message rate, and performance of the simulator (in wallclock time) compared to the real world execution are shown in the respective figures. CT, ACK and reply mode all use one message inflight, as they are only meaningful in this configuration, while for match mode we used the default limit on inflight messages, which is 256.

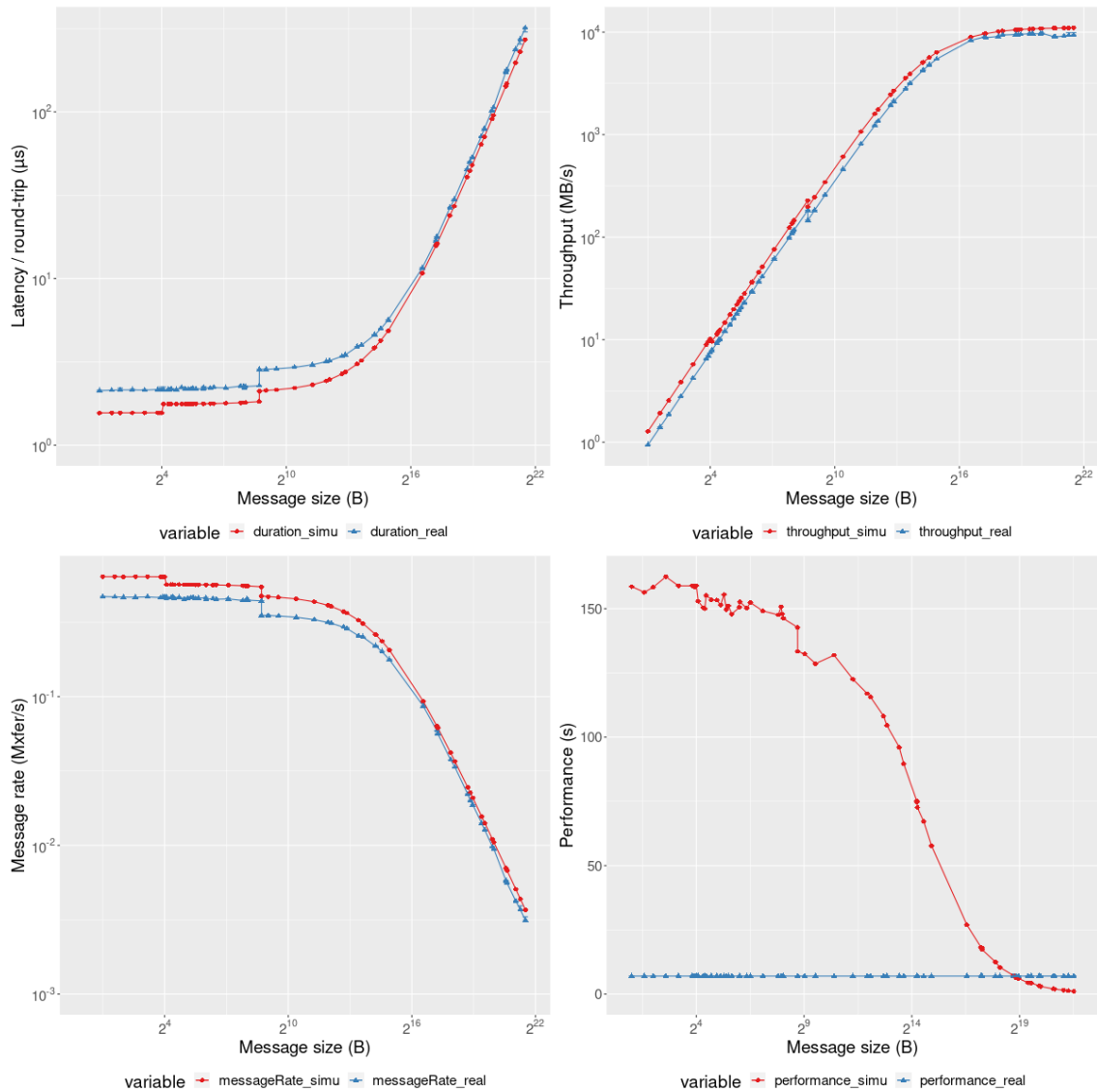


Figure 4.24: PtlPerf results for CT mode

We can see that ACK, match and reply modes have an excellent accuracy, and that CT mode is acceptable even though it is not as perfect. From a performance point of view, on all graphs we can see that larger messages cause the simulations to be faster. This observation is expected, since in simulation no data is actually transferred on a network, therefore modeling messages of all sizes has a similar performance (no matter by how much the simulated time is increased, the operation takes a constant amount of wall-clock time). Additionally, modeling larger messages has an advantage for ptlperf in particular: since this benchmark counts the number of messages sent in five seconds, instead of timing a fixed number of iterations, it is expected that fewer operations will be performed when larger messages are used, as each transfer takes more simulated time.

We can also see that the performance of CT mode is much better than the other ones, as it is the only benchmark which manages to be faster in simulation than the real execution (for the biggest message sizes that we tested). The explanation for this phenomenon comes from the way events are handled in PtlPerf's code: after sending a message, the CT



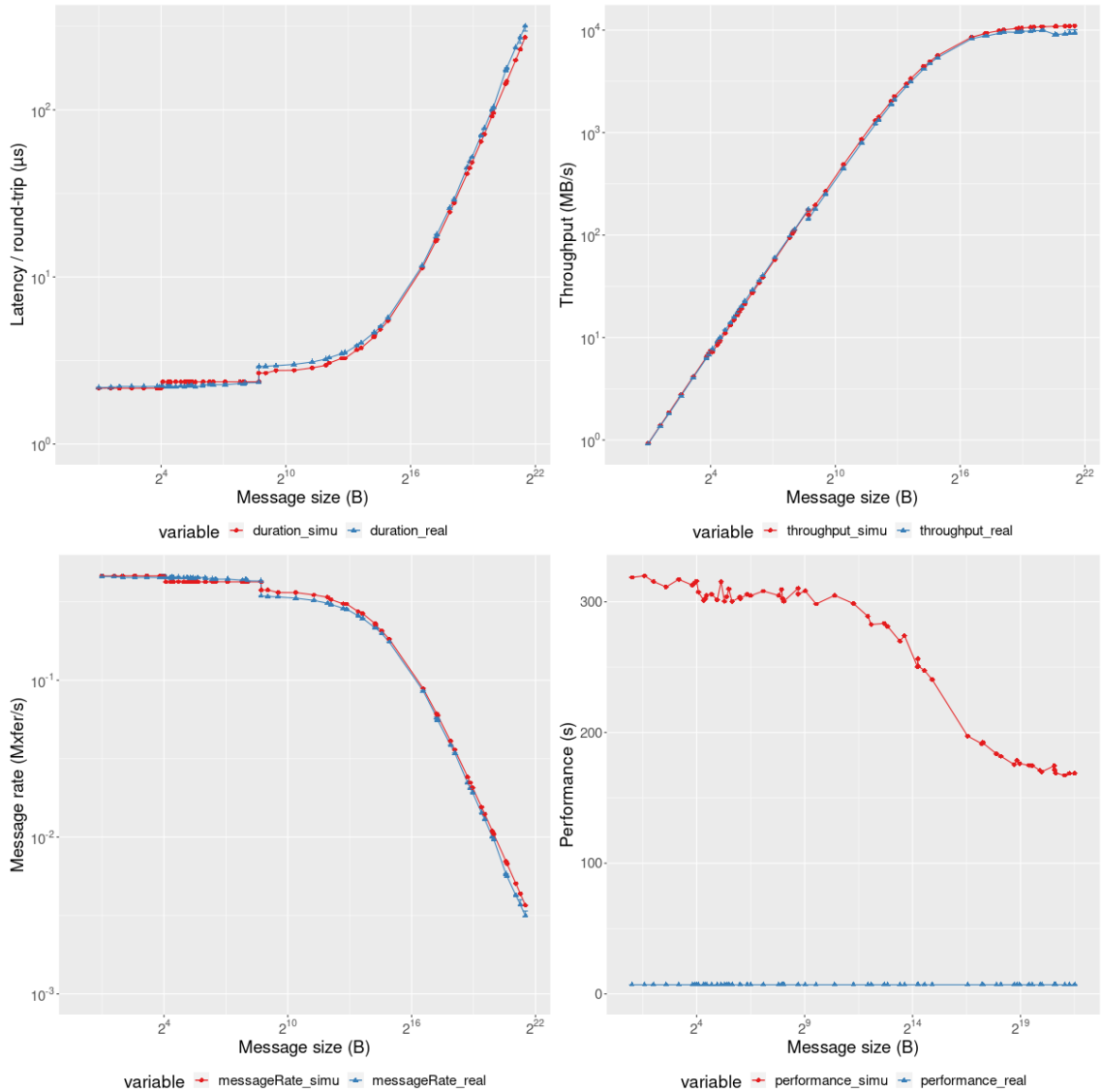


Figure 4.25: PtlPerf results for ACK mode

benchmark waits for the completion of the communication using the `PtlCTWait` primitive on a counter. In simulation, this has the effect of putting the corresponding Actor to sleep until the value of the counter is incremented, which is implemented in an optimized way in our simulator. On the other hand, the other modes use full events instead of counters, and instead of doing a `PtlEQWait` in order to wait for the completion of requests, they poll on the non-blocking `PtlEQGet` function between communications. In simulation, this has a very negative effect on performance, because each polling loop only progresses the simulated time by a very small amount, therefore the simulator will schedule the polling Actor thousands of times before anything meaningful happens (like receiving the event that is awaited), which is obviously very detrimental to performance. This is a fundamental issue that is common in most Discrete Event Simulators, and which we will discuss in more detail in the next chapter, because we will see that it is particularly problematic in MPI (in Section 5.3.5).

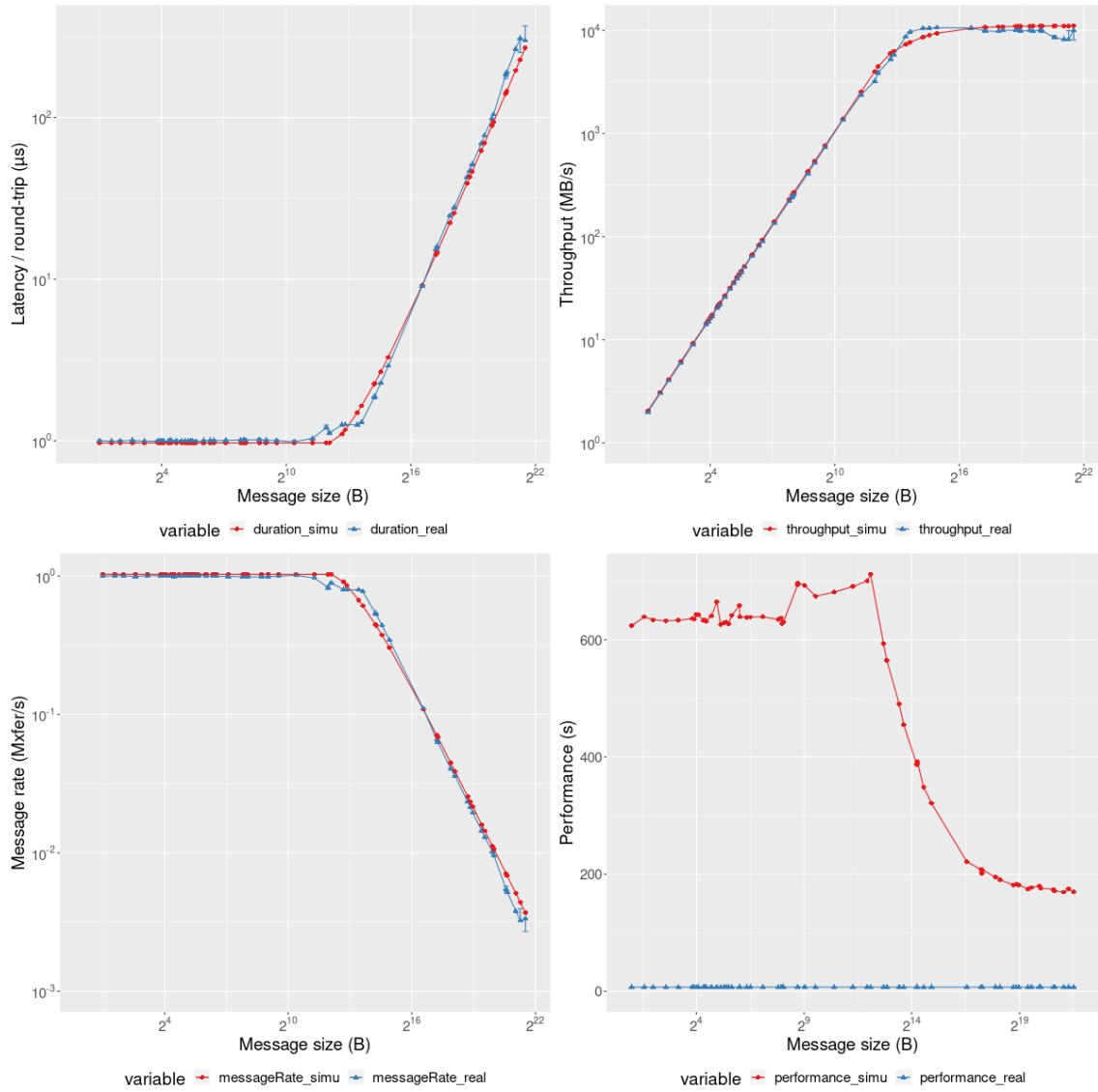


Figure 4.26: PtlPerf results for match mode



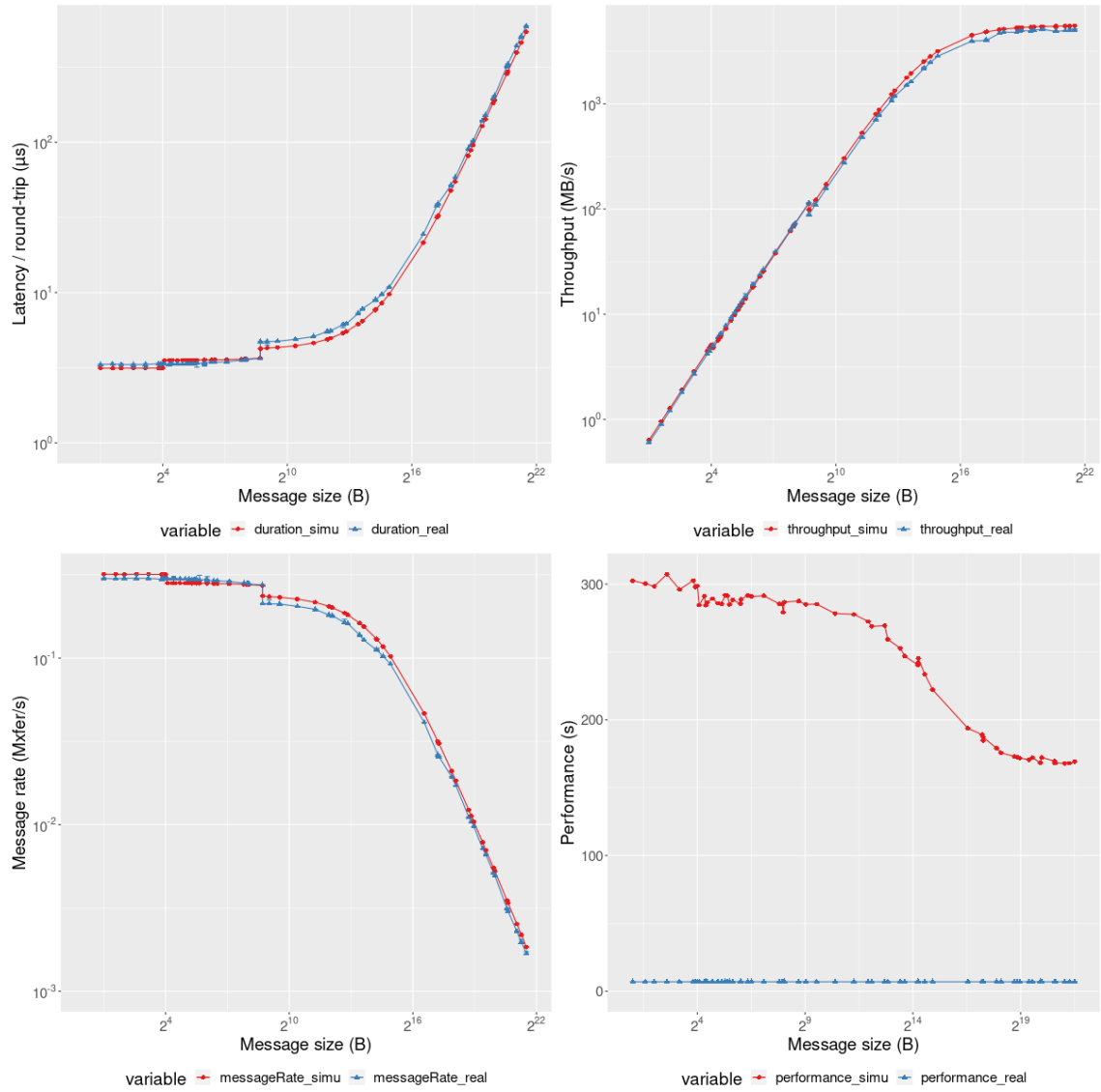


Figure 4.27: PtlPerf results for reply mode



Chapter 5

Usage with high-level APIs

In our journey towards accurate simulation of HPC applications, we now have a Portals simulator that we validated on point-to-point benchmarks. The next step is then to run high-level APIs (such as MPI or OpenSHMEM) on top of S4BXI, since real world applications and benchmarks are not usually written using low-level APIs directly. In this PhD we will focus on the study of MPI, and in particular Atos's implementation of this API, which is a fork based on OpenMPI which adds a transport (called BTL for Byte Transfer Layer) optimized for BXI. We will also show some results with OpenSHMEM on top of our simulator, even though we did not go as much in depth because MPI is more commonly used with BXI in real world scenarios.

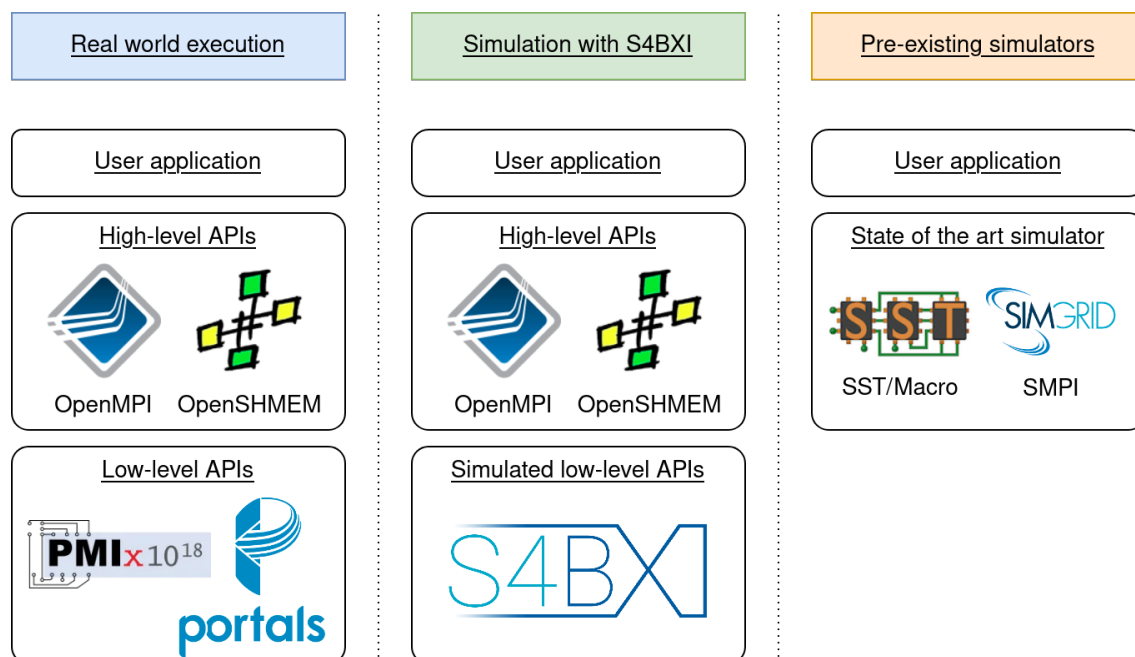


Figure 5.1: Software stack comparison: real world execution, S4BXI simulation and pre-existing state-of-the-art simulators

5.1 HPC software stack overview

As introduced in Section 2.1.3, a typical software stack in HPC is made of several layers. Even though we have seen that there are multiple possible combinations of these layers, in this section we will focus on applications that are written directly on top of a high-level API (in particular OpenMPI or OpenSHMEM), which uses Portals as a transport layer. It is important to note that even though Portals is the low-level API used for high-speed communications, high-level APIs also rely on communications across an out-of-band network in order to initialize: indeed, it is often more convenient to have access to a simple Ethernet network in order to exchange metadata that will be used to set up the high-speed network. This is why high-level APIs also use libraries such as the Process Management Interface (PMIx) for their initialization, as they make the exchange of metadata across an out-of-band network easier by providing primitives to perform barriers and basic data exchanges. This software stack is represented on the left side of Figure 5.1.

The way this type of software stack is traditionally modeled is by intercepting function calls at a high-level, and implementing full APIs such as MPI in simulation directly. This is the approach which is used by state-of-the-art simulators such as SST/Macro and SMPI, which is represented on the right side of Figure 5.1.

In comparison, our approach is to intercept communication primitives at Portals level, in order to run unmodified high-level APIs on top of S4BXI, as represented in the middle of Figure 5.1. There are several advantages to this approach: from a software development perspective, implementing Portals in simulation is faster than re-implementing all of MPI, since Portals only features point-to-point communications, whereas MPI offers a wide range of two-sided and one-sided (RDMA) primitives, both point-to-point and collective. Another advantage is that it allows running different high-level APIs with a reasonable development effort, instead of re-implementing fully every high-level API (as we will see with our OpenSHMEM experiments, even though the majority of our work is focused on MPI). On the other hand, there are also downsides to this approach: by running more software layers in simulation, we expect the performance of the simulator to be worse than higher-level models. There is also a more technical difficulty: in this case, our low-level simulator implements Portals but we do not have a model for PMIx (or the out-of-band network at all for that matters), which will complicate the initialization of the high-level APIs.

The principle of our approach is to intercept communication primitives at an unusually low level in the software stack. This method is not new and [KKW18] already implemented a similar concept, but it has never been applied to either OpenMPI or Portals. We will see in the upcoming sections that the technical solutions that we chose to work around the difficulties of this approach are different from the previous approach.

5.2 Atos's version of OpenMPI

As explained previously, the most common API used on top of the BXI interconnect is MPI, and in particular Atos's variant of OpenMPI, which we study in detail in this PhD. While OpenMPI is a very complex set of libraries with many features, we focus on the components that are used with BXI, which are represented in Figure 5.2.

The components can be categorized in two main groups: collective and point-to-point operations. Unlike Portals, MPI offers abstractions to perform complex operations involving many processes (called “ranks” in MPI vocabulary), without having the user worry about



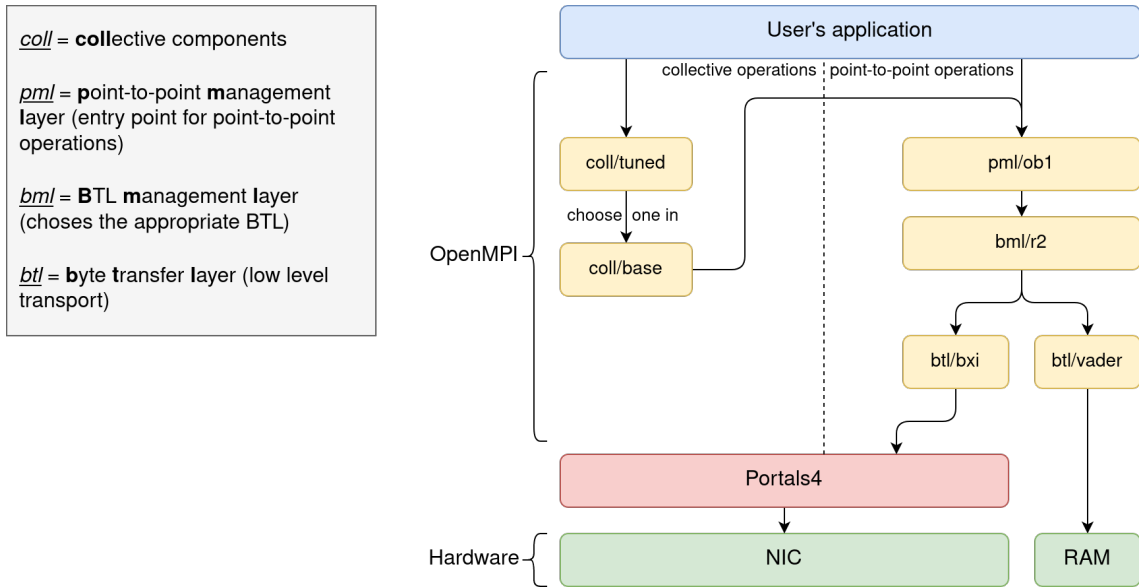


Figure 5.2: Relevant OpenMPI components when using BXI

implementation details. These operations are very diverse, such as “gather” (N to 1 communication), “broadcast” (1 to N), “alltoall”, “barrier”, etc. These operations all have a synchronous and asynchronous variant, to allow users’ application to perform computations while the operation is progressing. To achieve that, the **coll/base** component implements several algorithms that perform any given operation with a combination of point-to-point transfers (between only two processes). Examples of a few algorithms for the broadcast operations are displayed on Figure 5.3, where each arrow represents a point-to-point communication.

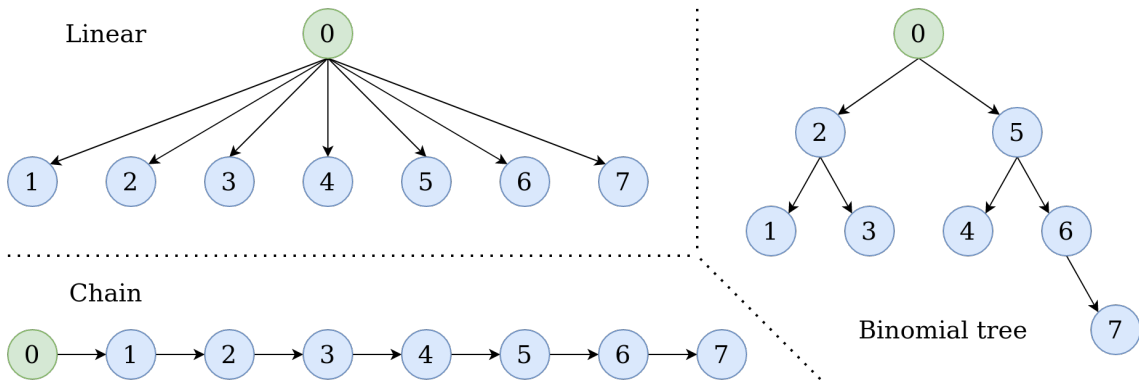


Figure 5.3: A few algorithm examples to perform a broadcast on 8 ranks from rank 0

The reason different algorithms exist for each operation is to improve performance: when the user calls a collective primitive, the **coll/tuned** component selects the algorithm to use in **coll/base** based on the number of ranks involved and the message size. It is important to note that in the community version of OpenMPI, this algorithm selection is based on benchmarks performed on old generation Infiniband hardware, which is why teams at Atos made their own benchmarking tools to optimize the algorithm choices for the BXI interconnect. Therefore, the algorithms used in Atos’s version of OpenMPI are not

the same as in the community version of OpenMPI, and still evolving (as this optimization work is not finished as of the writing of this PhD).

When performing point-to-point operations (either from user code or as part of a collective operation), there are three types of components that will be of interest to us: at the highest level, the PML (Point-to-point Management Layer) is responsible for any manipulation of the data that might be required, such as the fragmentation of large messages. In Atos's OpenMPI the PML that we use is called `ob1` and it is not modified from the community one. Then the BML (BTL management layer) chooses which BTL can perform the communication, based on the location of the two ranks involved (they could run on the same machine, or be on different nodes). The BML that we use is called `r2` and it is also identical to the community one. Finally, the BTL (Byte Transfer Layer) performs the low-level transfer. Usually several BTLs will be used, as we can see on Figure 5.2: for example, with the BXI interconnect the `btl/bxi` component will be used to perform communications across the high-speed network, but the `btl/vader` will be used to perform shared memory transfers for ranks that are on the same machine. Vader is a BTL that also comes unmodified from the community version of OpenMPI, and BXI is entirely made by teams at Atos.

5.3 Adapting OpenMPI for the simulated world

5.3.1 Simulation of out-of-band communications without PMIx

As introduced in the previous section, the main difficulty in running a real world MPI implementation in our simulator is the initialization: it requires either to implement the PMIx specification in simulation, or to modify MPI itself in order not to need this library. There are pros and cons to both options: implementing PMIx allows running MPI with very few modifications, and also facilitates running other high-level APIs (since PMIx is a tool commonly used by several libraries). On the other hand, developing and maintaining a PMIx simulator represents significant work, as it has many features. It is worth noting that regardless of the option we choose, the accuracy of the simulator will not be affected too much, since PMIx is only used briefly at the start and at the end of the execution of applications. In either case we will also likely need to rebuild MPI for simulation, since our simulator requires MPI to be built with a specific set of options (passed to the `configure` script) that are likely different from a production build for real world executions (in particular, we need to force OpenMPI to build into only three shared libraries, instead of one library for each component). In the case of running Atos's OpenMPI on top of S4BXI, we chose to add a small patch to MPI instead of implementing PMIx, for all the reasons mentioned above. In particular, we believe that this patch is easier to maintain than a full PMIx implementation, and we will see in the next sections that other small modifications to MPI's code will prove useful. A summary of the different software layers involved in the execution of an MPI application is depicted in Figure 5.4.

In total, our patch modifies 345 lines of code of OpenMPI: 41 lines are added, 224 are removed, and 80 are modified. This number is very small compared to the size of the OpenMPI codebase, which contains nearly 900 thousand lines of code. The detail of these statistics language by language are available in Appendix B. We also know from a year of maintaining our patch that the code that we modified is not updated very often, as we were able to rebase our modifications on top of the latest development to OpenMPI through seven versions (from version 4.0.4 to 4.1.4), without any major difficulty (the



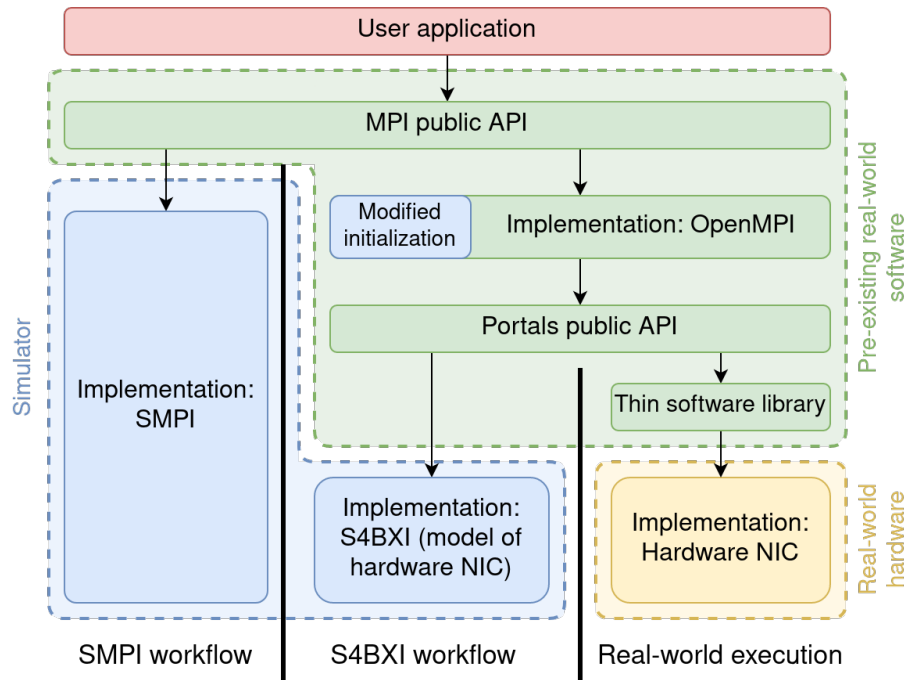


Figure 5.4: Software layers involved in state of the art simulation, S4BXI simulation, and real-world execution of MPI applications

rebase through git worked automatically in the vast majority of cases). The next sections give more detail about the components that are modified by this patch.

🌱 5.3.2 Adapting OpenMPI’s initialization for S4BXI

Our patch to OpenMPI affects two main components: the initialization of MPI itself (globally), and the initialization of the BTLs. The impacted components are shown in Figure 5.5.

In the initialization of OpenMPI, we mainly replace PMIx calls to functions native from our simulator in order to give all processes the knowledge of what their rank is, how many processes are involved in the current job, and which other ranks are local to the same machine. Additionally, there are a few barriers between all the ranks that are reimplemented with SimGrid’s built-in Barrier object instead of using PMIx. An example of such replacement is shown on Figure 5.6: below several layers of macros, `OPAL_MODEX_*` calls use PMIx to exchange data with other processes, so we replace them by simple function calls to our simulator which fetch the equivalent data in the simulated world. In this specific example, the call returns a Portals process structure (which includes a NID and a PID) for the requested MPI rank (which correspond to the `vpid` attribute internally in OpenMPI), which is used to initialize the `btl/bxi` component.

In the BXL BTL, the data that is exchanged at startup is mainly the Portals IDs of each process, in particular the NIDs of all the processes involved in the current job. At startup, the BTL also looks for all available NICs in Sysfs (in the `/sys/class/bxi` virtual folder), in order to use the closest one (in the case of a NUMA machine). This processing had to be removed for simulation at first, since on the host running the simulation, any BXL NIC physically present on the machine does not correspond to the hardware simulated by our model in the virtual world. Since then, the MPI team at Atos has been kind enough to add

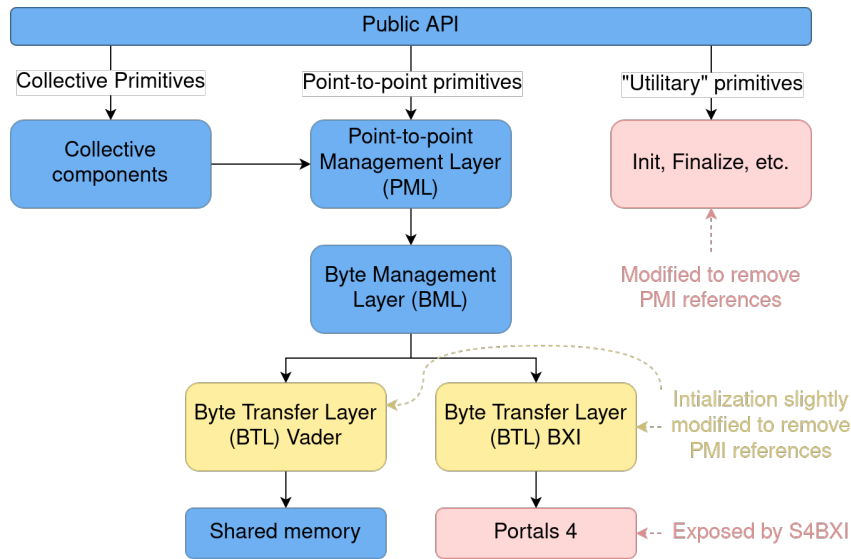


Figure 5.5: MPI components impacted by our patch (dark blue is unmodified, medium yellow corresponds to minor modifications, and light red is heavily modified)

```

1 - OPAL_MODEX_RECV(ret, &mca_btl_bxi_component.super.btl_version,
2 -                   &proc->proc_name, (void**) id, &size);
3 + ret = s4bxi_get_ptl_process_from_rank(proc->proc_name.vpid, *id);
4 + size = sizeof(ptl_process_t);

```

Figure 5.6: Example section of our patch to OpenMPI

an option in MPI to disable this optimization (and therefore use any available NIC without asking for a particular location), which allows our patch to be even lighter since we do not need to hardcode the removal of this feature.

5.3.3 Shared memory support

As presented in Section 5.2, MPI supports using several BTLs for point-to-point communications. In the case of BXI clusters, most of the time two BTLs will be used: BXI for communications on the high-speed network, and Vader for intra-node communications using shared memory (when several MPI ranks are executed on the same machine).

In order to support Vader in simulation, we also modified its initialization. It is not strictly necessary in order to perform simulations of MPI (we could have simply disabled Vader altogether), since communications between two ranks on the same machine can still be performed through BXI: in that case messages just go back and forth on the PCIe bus without being sent on the network (both in a real execution and in simulation). Nevertheless, we added support for Vader in order to allow users to replicate their real-world scenario as closely as possible in simulation. In theory this BTL is easy to initialize, and does not require any data from the simulator, but in practice there is a different kind of issue with the modeling of this BTL in simulation: by default, the name given to the files which hold data in shared memory (in the `/dev/shm` folder) can be identical on different machines. In a real-world execution this does not matter, as each machine will hold its own set of files, but in simulation all ranks run on the same physical machine (which executes



the simulation), which means that different simulated processes could overwrite the data of processes on different simulated nodes. Therefore, we had to make the name of these files unique across the whole simulation, which required a small modification of Vader’s initialization. It is worth noting that this modification is not related to PMIx, and therefore it further justifies our choice to patch MPI instead of reimplementing PMIx in simulation, as this part of the patch would have been required in any case.

❧ 5.3.4 Handling copies of MPI libraries in S4BXI

Up to this point, the simple applications that we modeled did not have any dependencies on external libraries, except Portals which is directly provided by our simulator. Now that we try to model MPI, we face a new difficulty: as explained in Section 4.5.1, we rely heavily on the linker to isolate the global symbols of the user application in each simulated process, but we do not have a way of isolating different copies of external libraries (such as OpenMPI) yet. This is problematic because OpenMPI relies heavily on global variables, which need to be “private” to each simulated process. In order to tackle this issue, we can take inspiration from SMPI: the same way that it copies the user application N times (for N simulated processes) in order to isolate them, it also has an option to make multiple copies of any linked library, and then “re-link” the copies of the user application and the libraries together (the current proof-of-concept implementation uses a somewhat brutal `sed` command in the copied user applications directly). In the end, each simulated process has its own copy of the user application, which is linked with its own copy of any library that needs to be “privatized”, as depicted in Figure 5.7.

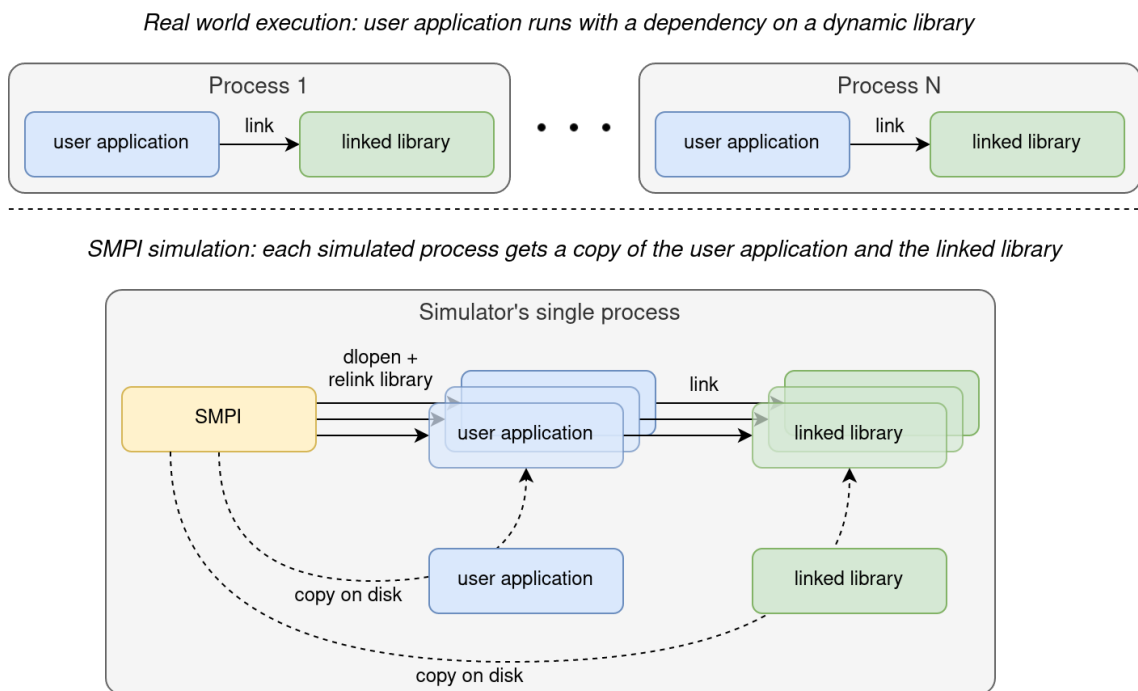


Figure 5.7: Methodology to “privatize” libraries in SMPI, compared to the real-world execution

While this works well for libraries that are self-contained, we encountered an issue when trying this methodology with MPI: OpenMPI does not consist of just one library, but of

three libraries (called OMPI, OPAL and ORTE), which are all linked to the user application, but also linked to each other. Therefore, in order for this “privatization” to work, we had to extend it in order to relink not just the user application to each library, but also the copies of each library together. This extended approach that we implemented in S4BXI is depicted in Figure 5.8.

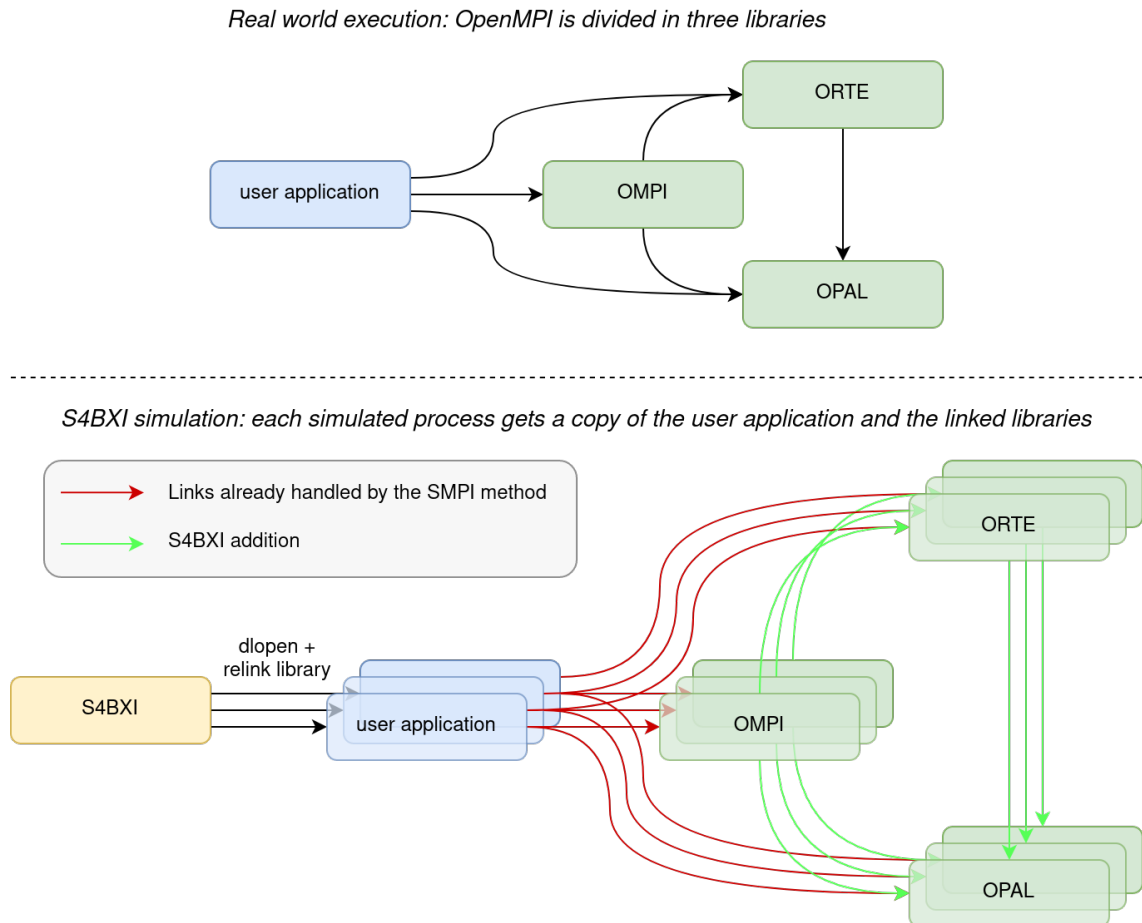


Figure 5.8: Methodology to “privatize” OpenMPI libraries in S4BXI, compared to the real-world execution (the “copy on disk” step is still present but not depicted for clarity)

❁ 5.3.5 A word on performance regarding polling

Thanks to our patch to OpenMPI, we can run simulations of real-world applications on top of our simulator. However, we still face an issue when it comes to performance, because of a fundamental problem with discrete event simulators: polling. This issue was already mentioned in Section 4.6.2, as we observed that it impacted greatly the performance of Ptlperf’s simulations, but it is really with MPI that this problem is the most noticeable.

In simulation, we have two different “times”: “wall-clock time”, during which the user waits for the simulation to finish, and “virtual time”, which is a variable inside SimGrid used to keep track of the time in the simulated world. On the other hand, on a real cluster executing a scientific application, there is only one time: the makespan of the application. This difference becomes very important if an application performs polling, i.e. loops over



<pre> 1 ptl_handle_eq_t event_queue_handle; 2 // ... 3 int ret; 4 ptl_event_t event; 5 do { 6 ret = PtlEQGet(event_queue_handle, &event); 7 } while (ret == PTL_EQ_EMPTY); </pre>	<pre> 1 ptl_handle_eq_t event_queue_handle; 2 // ... 3 int ret; 4 ptl_event_t event; 5 6 ret = PtlEQWait(event_queue_handle, &event); 7 </pre>
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(a) Polling around EQ Get

(b) Passive wait with EQ Wait

Figure 5.9: Two ways of waiting for an event in Portals

a check until it completes. In the real world, performing polling or a “passive” wait is equivalent if nothing else is running on the same CPU core. An example is depicted on Figure 5.9: while both solutions would take the same amount of time in a real-world execution, these two programs have a very different simulation performance.

The explanation is that `PtlEQWait` is cleverly implemented in our simulator, i.e. the Actor who calls the primitives is put to sleep until the arrival of the awaited event. On the other hand, the active polling loop of Figure 5.9a causes an issue, because `PtlEQGet` takes a small amount of wall-clock time to simulate, but it doesn’t allow the virtual simulated time to progress. This means that when an Actor runs such a polling loop, it will be continuously scheduled to run by SimGrid’s scheduler, but the simulated time will never progress, effectively resulting in a deadlock of the simulation (with respect to wall-clock time).

This is a significant issue, because OpenMPI relies on polling mechanisms every time an application asks to wait for the completion of a request (in this context a “request” is to be taken in a very broad way: it could represent a message transmission, a message reception, a collective operation, etc.). It is worth noting that this problem is not specific to OpenMPI over Portals, but is a common problem in discrete event simulation: if we look at simulators which operate one level of abstraction higher in the software stack, we can see the same problems. For example, if an application calls the `MPI_Test` primitive in a loop (which is not uncommon), SMPI will suffer the same issue. The way SMPI handles the problem is by injecting increasing amounts of delay in the simulated time, in the form of a small CPU execution (which is purely artificial and does not correspond to real computation).

Algorithm 1 OpenMPI’s algorithm to wait for the completion of a request

Input *request* a pending request, *BTL* the list of BTLs in use, *N* the number of BTLs

```

1: while request is not complete do
2:     for  $i \leftarrow 0$  to  $N - 1$  do
3:         progress_btl_number( $i$ )
4:     end for
5: end while

```

Initially, we resolved this issue in our simulation with a better approach: by analyzing the code of OpenMPI, we were able to find a heuristic to determine when it was safe to perform a Portals EQ Wait (i.e. blocking wait) instead of a loop over an EQ Get. This allowed us to keep an accurate simulation while speeding it up by orders of magnitude. Unfortunately, this solution only worked well at the time when we supported only the BXI BTL in simulation. Indeed, internally the algorithm used to wait for the completion of a request roughly follows Algorithm 1, where the PML will loop over each BTL and call its

Algorithm 2 Algorithm 1 applied to our specific case

Input *request* a pending request

- 1: **while** *request* is not complete **do**
- 2: progress_btl_BXI()
- 3: progress_btl_vader()
- 4: **end while**

“progress” function until the request is complete. The “progress” function of a BTL typically runs every callback that is ready in the context of asynchronous operations, and checks for new events coming from the underlying transport. When we supported only one BTL, it was easy to replace the progress function by a blocking wait. Unfortunately, when we added support for shared memory transfers using the vader BTL, this optimization stopped working, because the completion of a request could now come from any of the two BTLs, as depicted in Algorithm 2. In the general case it is not possible to know from which BTL the completion of a request will come, because of how generic a request is in this part of a code. Additionally, our problem was further complicated by the fact that some options of OpenMPI require progress functions to run as often as possible: for example, it is possible to turn on flow control for the BXI BTL of OpenMPI, in which case if too many messages are already in flight, new ones will wait in a queue (in order not to flood a target). It is then in the progress function of the BXI BTL that a check will be performed to see if pending messages can be sent. Therefore, having a blocking wait in this function stops this check from working properly, since it might get scheduled too late, or not at all in the worst situations.

This problem further reduces the number of cases in which our heuristic to improve performance works, and therefore we abandoned it completely: in the latest versions of our simulator, we implement the same mechanism as SMPI in S4BXI, i.e. injecting growing amounts of delay inside `PtLEQGet` to make sure that a polling loop can still allow the simulated time to progress at a reasonable rate (this small delay is configurable using the environment variable `S4BXI_ACTIVE_POLLING_DELAY`).

5.4 Compatibility with SMPI sampling

When running applications in simulation, one of the biggest concern is the memory usage and the performance of the simulator: indeed, most simulators built with SimGrid are single-threaded, which means that all processes of the application end up being executed sequentially on one CPU core. To mitigate this issue, SMPI offers a set of macros in order to replace some heavy computation parts with increments in the simulated time. The amount of computation time to inject can be statically provided by the user, or determined automatically at runtime, thanks to macros which replace `for` loops. These macros allow SMPI to execute the first iterations of the loop in order to measure their duration, and to replace the later ones with artificial computation time. For memory usage, SMPI allows users to mark some memory allocation as “shared”, which means that all simulated process will use the same physical memory region instead of all doing a new allocation. Of course this generally makes the result of computations functionally wrong, but for applications in which the control flow does not depend on the input data it is a good solution to run full size applications in simulation and get good performance estimations. These macros effectively allow users to make skeleton version of their application, in order to speed up



simulation and allow it to run on a single CPU.

In S4BXI, we are able to re-use all these SMPI macros transparently, since both simulators are based on SimGrid. This allows us to re-use studies that have been conducted on specific applications in order to create optimized skeleton versions. For example, Tom CORNEBIZE’s thesis [Cor21] studied HPL extensively, and we re-used his model of HPL’s computation phases in order to speed up S4BXI simulations by orders of magnitude. This will be demonstrated in our validation experiments in Section 5.5.

5.5 Experimental validation

While most applications can be run using both MPI and OpenMP parallelization (sometimes even CUDA), in our experiments we will distribute them using MPI only, as our simulator does not support arbitrary OpenMP (nor CUDA) code. This is a common limitation which is present in similar simulators as well (such as SMPI for example). There is a priori no fundamental limitation that would prevent us from developing a model for OpenMP or CUDA, but such a development is way beyond the scope of this thesis.

We will start with OSU micro-benchmarks, which are a set of very simplistic “unit-style” tests that benchmark a single primitive in a loop. While the resulting workload is completely unrealistic, it is a common tool to assess the performance of a cluster on a specific MPI primitive, and it is also a good validation that all collective and point-to-point operations work without errors in simulation. We will then study realistic applications that we presented in Chapter 3: LULESH, Quicksilver and HPL.

From a technical perspective, all our benchmarks will be executed on a real-world cluster composed of nodes equipped with BXI v2 hardware and AMD EPYC™ 7763 64-Core processors. In simulation, we will run each application both in our model (with OpenMPI on top of S4BXI), and in SMPI, in order to compare our approach to the closest state-of-the-art simulator.

5.5.1 OSU micro-benchmarks

For these experiments, we will run point-to-point benchmarks on two machines, and collective operations on 16 machines, with only one process on each machine in order to maximize the network load. Experiments were also performed on 32 MPI ranks (8 nodes and 4 processes per node), but the conclusions were very similar, therefore this data is only shown in Appendix C to keep this section more readable. The simulations are performed on one of the machines from the real-world cluster, with an AMD EPYC™ 7763 64-Core processor (even though only one core of the processor is used in each simulation). Since OSU micro-benchmarks cover many MPI primitives, it is impractical to analyze the result of each simulation exhaustively. Instead, we present a few significant experiments, but we also show global statistics about all the simulations.

Across all benchmarks, we get mainly two types of results. In some cases, both SMPI and OpenMPI over S4BXI give very good results (i.e. latencies reported by the benchmark at the end of its execution). We can see an example of such a behavior with the AllGather benchmark, depicted on Figure 5.10 (AllGather allows all processes to send chunks from a local buffer to all the other processes in the job).

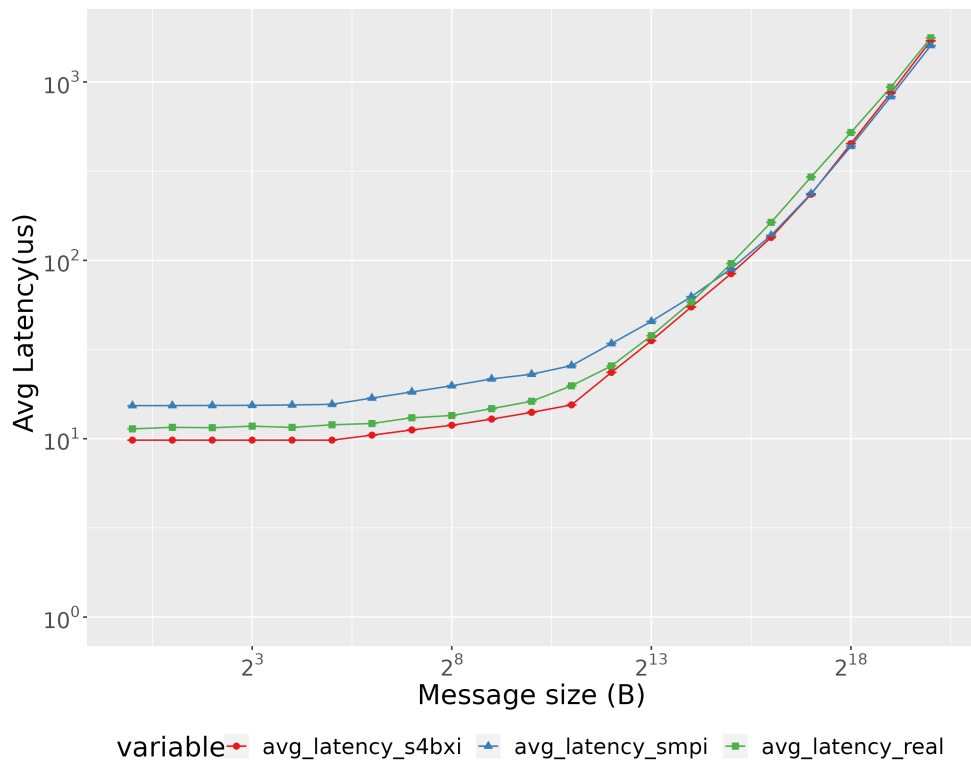


Figure 5.10: OSU AllGather benchmark: comparison between the real-world run, an SMPI simulation, and an OpenMPI over S4BXI simulation

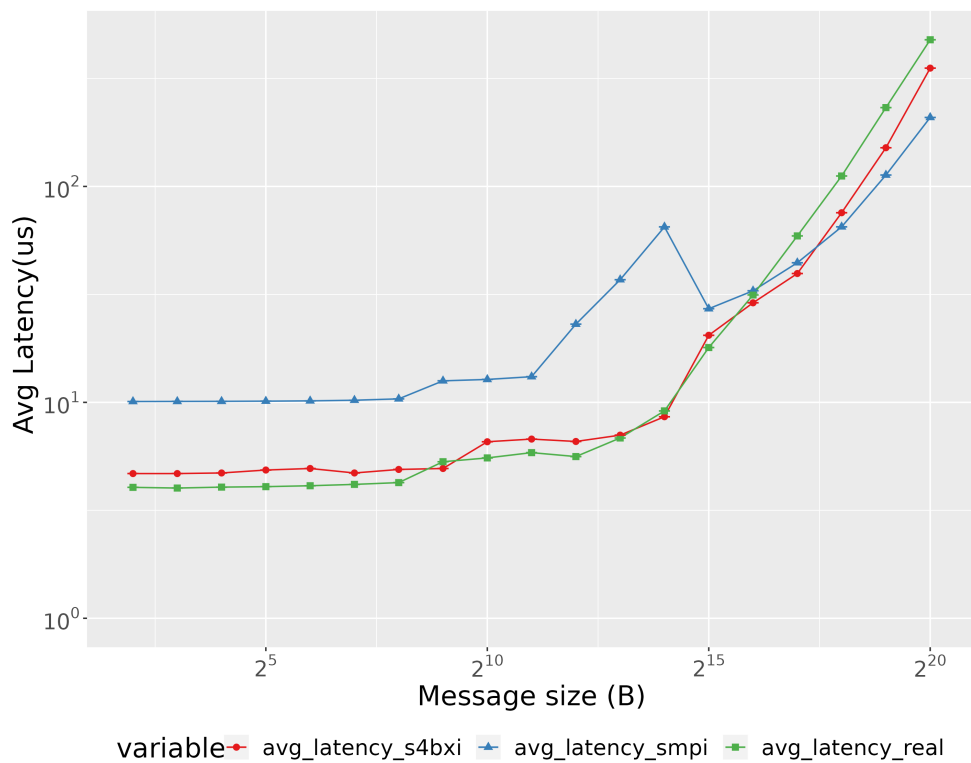


Figure 5.11: OSU Reduce benchmark: comparison between the real-world run, an SMPI simulation, and an OpenMPI over S4BXI simulation

In other cases, we can see a significant loss of accuracy for SMPI, usually for specific message size. We can see an example of such a behaviour with the Reduce benchmark, depicted on Figure 5.11. Reduce allows a “root” process to synthesize values from all processes into a single value, by applying an arithmetic operation (for example a sum, taking the maximum, etc.). In these cases, SMPI lacks accuracy because its implementation of the collective operation does not match the algorithm used in Atos’s version of OpenMPI. Therefore, the sequence of point-to-point transfers that are simulated is not an accurate model for the real-world benchmark, whereas in S4BXI we run the real-world MPI implementation in our simulator. Consequently, we get a realistic model of collective algorithms because of our simulation method.

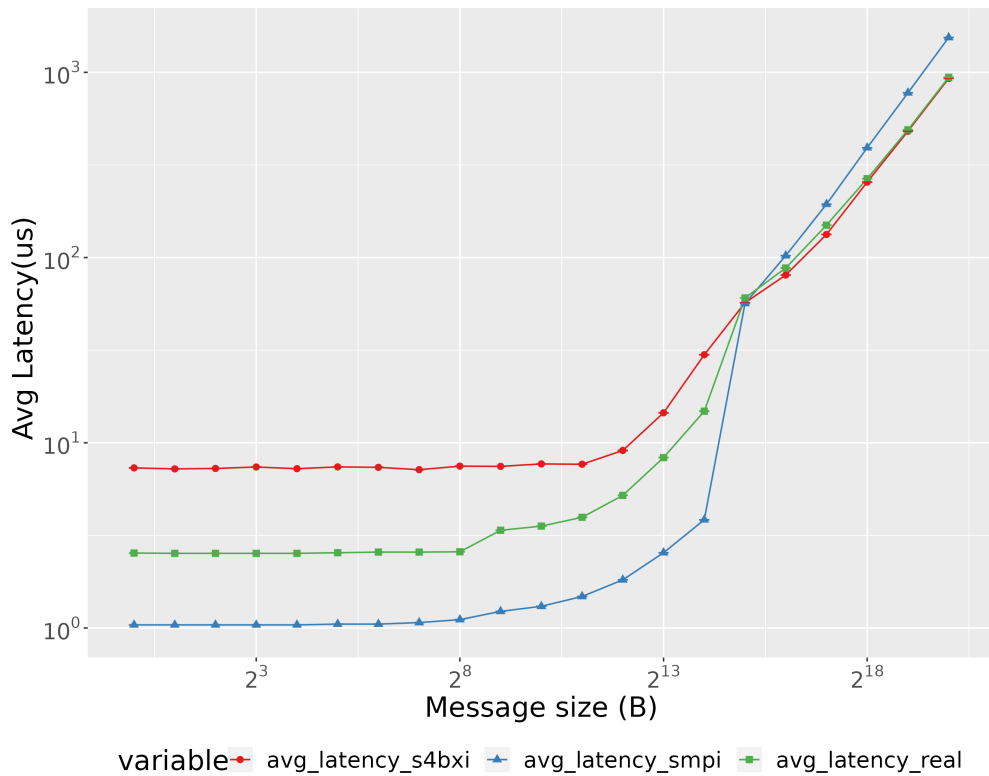


Figure 5.12: OSU GatherV benchmark: comparison between the real-world run, an SMPI simulation, and an OpenMPI over S4BXI simulation

Finally, there is one benchmark in particular that is particularly pathologic for our simulation method: GatherV, which is depicted on Figure 5.12. GatherV allows a “root” process to fetch values from all processes, using non-continuous buffers. In this experiment, OpenMPI over S4BXI is too pessimistic, while SMPI is too optimistic but to a lesser degree. These results are very similar with the asynchronous variant of this collective operation, IGatherV. These results are unusual compared to the majority of our simulations, but we did not investigate them in depth for two reasons. First, because of a lack of time, but also because we did not encounter these operations in any of the applications that we executed in simulation.

In order to get a more general view of our results compared to SMPI, we plotted the average error of each simulation, by computing the absolute difference between our simulation result and the value from the real-world experiment, and averaging these values

across all message sizes. The resulting graph is shown on Figure 5.13.

We can see the three different patterns that we presented. First, most simulations are of a similar accuracy in both approaches. In several other cases simulations are significantly more precise in OpenMPI over S4BXI. Finally, there are still a few operations for which both simulators have a high error, in some of these cases our simulation method has an even larger error than SMPI, but these cases are rare.

From a performance perspective, we can see on Figure 5.14 the slowdown of running a simulation compared to performing an execution on a real-world cluster. Most of the time, simulators are two orders of magnitude slower than real-world executions (around 100 times slower). This result is expected, as OSU benchmarks are extremely communication-intensive, and therefore they stress our simulators to the maximum. This figure also shows that S4BXI is generally slower than SMPI, which comes from our architecture with more software layers, but the slowdown of our approach is still of the same order of magnitude as state-of-the-art simulators. In some rare cases, our approach even manages to be slightly faster, for operations that are particularly costly to model in SMPI.

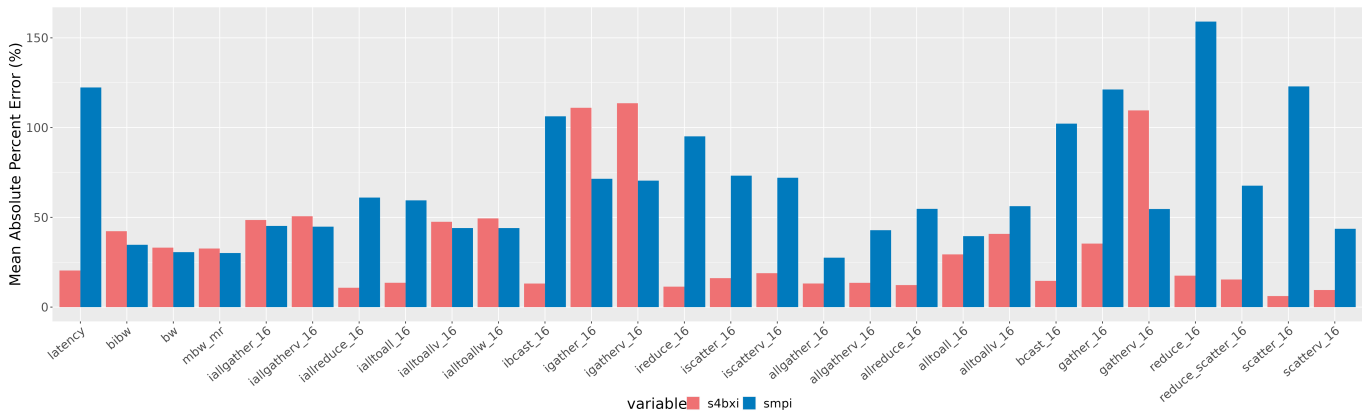


Figure 5.13: Average error of both simulators: SMPI compared to OpenMPI over S4BXI

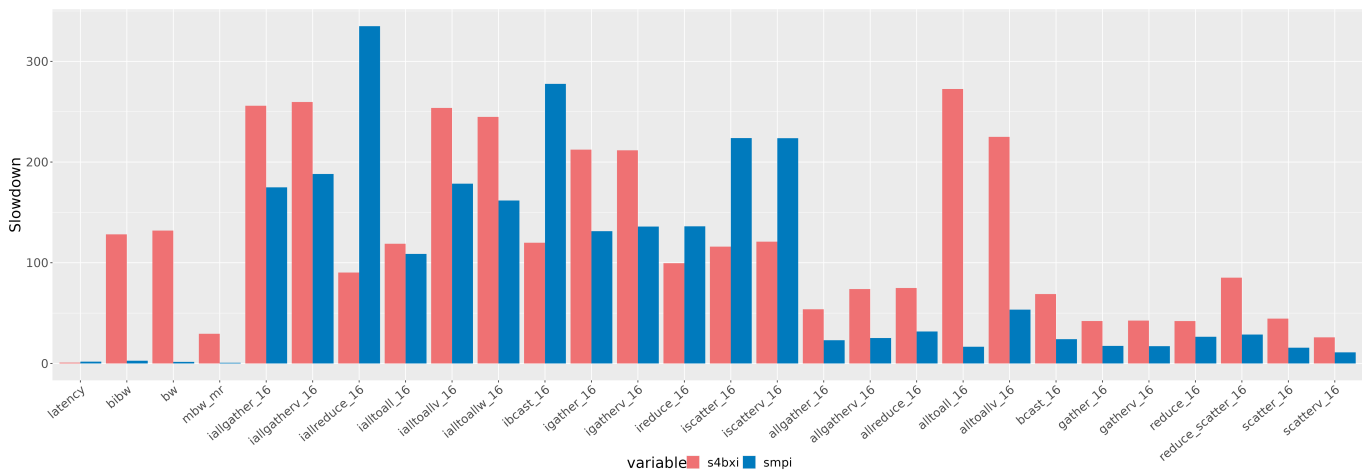


Figure 5.14: Average slowdown of both simulators compared to the real-world execution



5.5.2 LULESH

LULESH is a proxy application that is commonly used to assess the performance of a cluster. In particular, it is frequently used to benchmark BXL, which is why it is an interesting application to run in our model. As presented in Section 2.3.2, LULESH has a few requirements: it can only run on a number of MPI ranks that is the cube of an integer, for example 1, 8, 27, 64, etc. processes. In our case, we are going to run this application with 1 rank, 8 ranks on 8 machines (1 rank per machine), and 27 ranks on 9 machines (3 ranks per machine).

Each real-world experiment and each simulation is executed five times in order to check the consistency of our results. LULESH is also executed for eleven different problem sizes, which gives us executions that range from 0.15 seconds up to a bit over a minute on the real-world cluster.

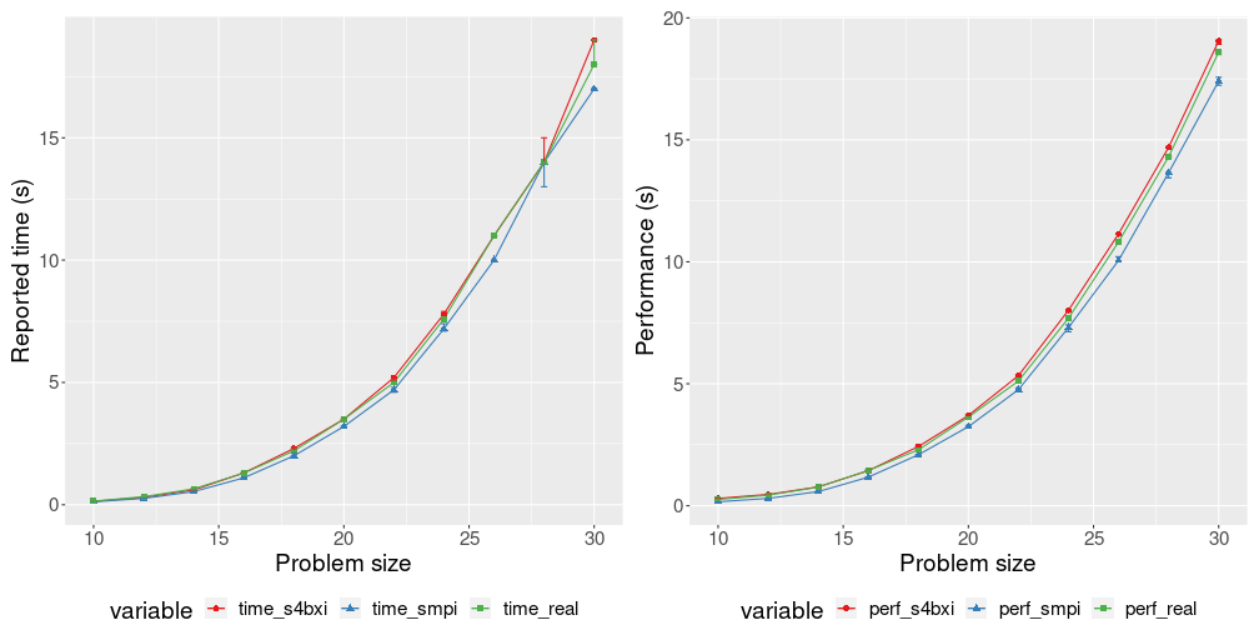


Figure 5.15: LULESH results on one MPI rank, comparing our simulator, SMPI, and a real-world execution (left graph shows accuracy, right graph shows performance)

Results are displayed for 1 MPI rank on Figure 5.15, for 8 MPI ranks on Figure 5.16, and for 27 MPI ranks on Figure 5.17. The simulation for only one process does not give us any information on the validity of our network model, as there is no network communication, but it is a good reference point to validate two things: first, that our model of computations gives us accurate results, and second, that the performance of the simulators in this scenario is good (that the overhead of running the application in simulation is small). We can see on Figure 5.15 that these two properties are indeed correct for both S4BXI and SMPI: on the left side, we can see the time reported by LULESH at the end of its execution, which allows us to assess the accuracy of the simulators. On the right side, we can see the performance of the simulators compared to the execution time of the real-world run. Both graphs show that the simulators are very close to the real-world run.

On the other hand, on Figure 5.16, we can see the result of an execution on 8 nodes (with 1 process per node), and the corresponding simulations. We can see that the accuracy of both simulators is still excellent, as they are very close to our reference values from the

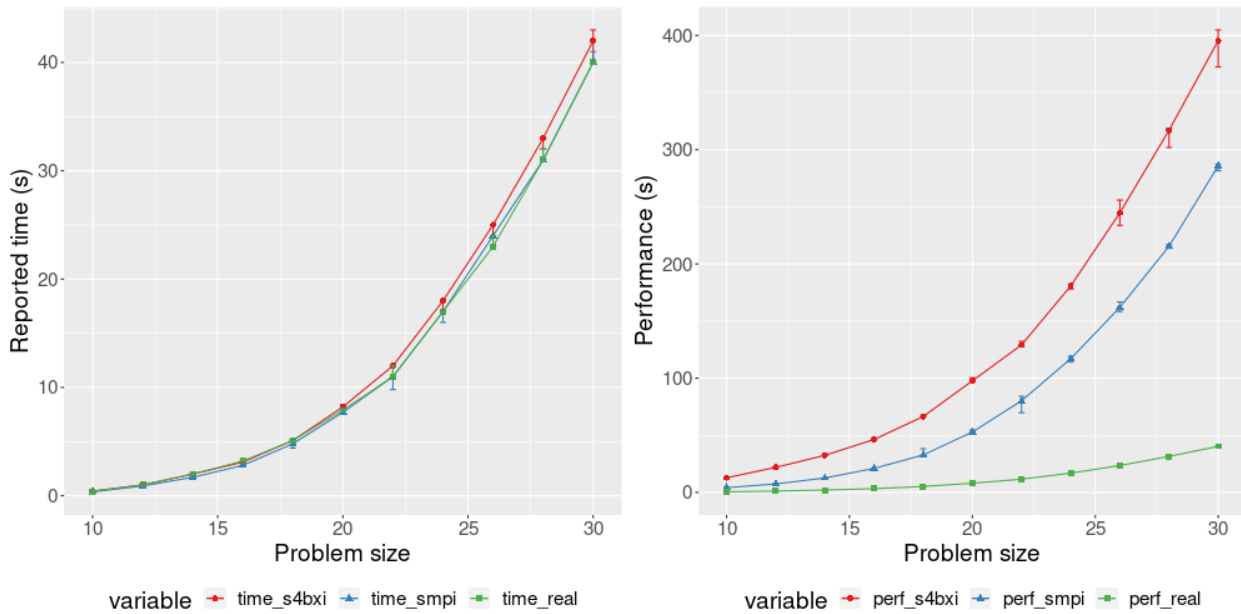


Figure 5.16: LULESH results on 8 MPI ranks (8 nodes, 1 ranks per node), comparing our simulator, SMPI, and a real-world execution (left graph shows accuracy, right graph shows performance)

real-world on all problem sizes. From a performance point of view, both simulators are significantly slower than the real-world execution. This result is expected, since all eight simulated processes are executed sequentially in these single-threaded simulators (and therefore we expect a slowdown of at least a factor of eight). We can also see that the S4BXI approach is slower than SMPI, which once again is expected, since running a full OpenMPI implementation on top of Portals is slower than running an MPI implementation that was specifically optimized to run in SimGrid.

Finally, the execution on 27 ranks (with 9 nodes and 3 processes per node) allows us to test further the network model of each simulator, and also to make sure that intra-node communications give accurate results. As presented in Section 5.3.3, intra-node communications can be performed in two different ways: either using the Vader BTL, or simply by going through Portals. Of course, enabling Vader to perform communications across shared memory is irrelevant in SMPI, as it does not feature such low-level configuration options. The results are displayed on Figure 5.17 with Vader disabled on the real-world execution and OpenMPI over S4BXI, and on Figure 5.18 with Vader enabled. We can see that the results are very similar in both cases, and that our two simulators perform well regardless of whether we use Vader or not. The reason why the performance of LULESH is identical whether we use Vader or not, comes from the efficiency of BXI NICs. Indeed, when Portals is used to transfer data between two processes on the same machine, the NIC effectively acts as a DMA controller, which copy the payload from the source buffer of the sender process to the reception buffer of the target process. This is very similar to how Vader operates, using shared memory to copy data between processes, therefore it is expected to observe a similar performance. Once again, we see a considerable loss of performance compared to the execution on 8 processes, which corresponds to what we expected (as we now run 27 MPI ranks in a single thread in our simulators).

The conclusion of this experiment is that while both simulators have a very good



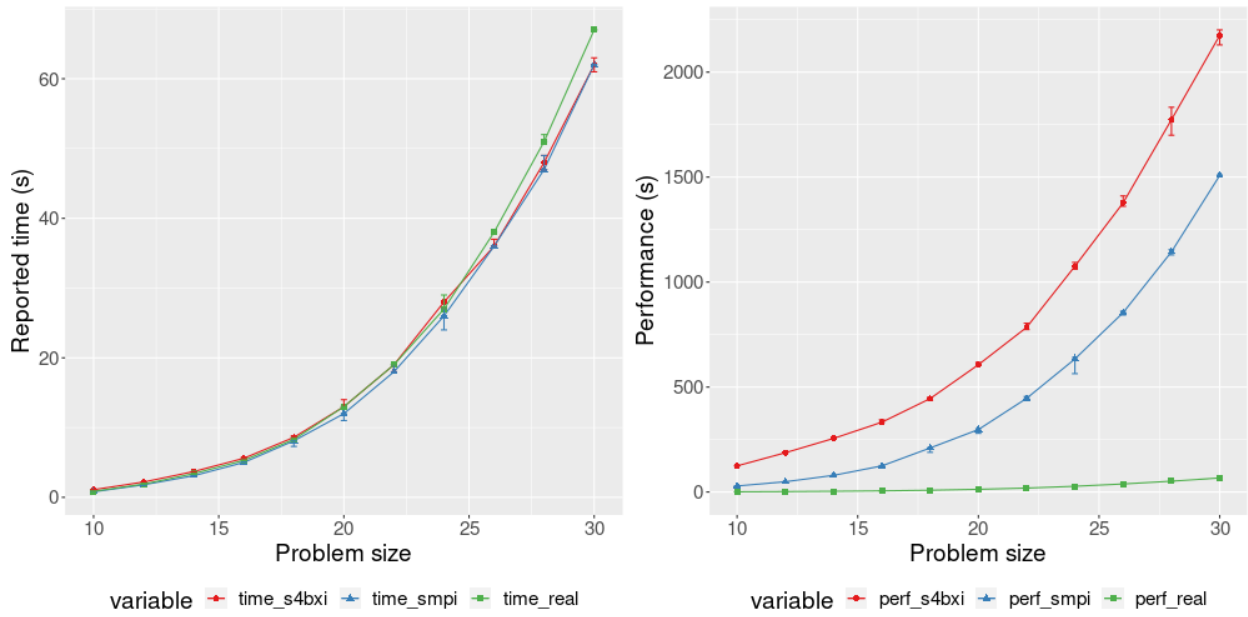


Figure 5.17: LULESH results on 27 MPI ranks (9 nodes, 3 ranks per node), comparing our simulator, SMPI, and a real-world execution. Vader is disabled in real-world OpenMPI and OpenMPI over S4BXI

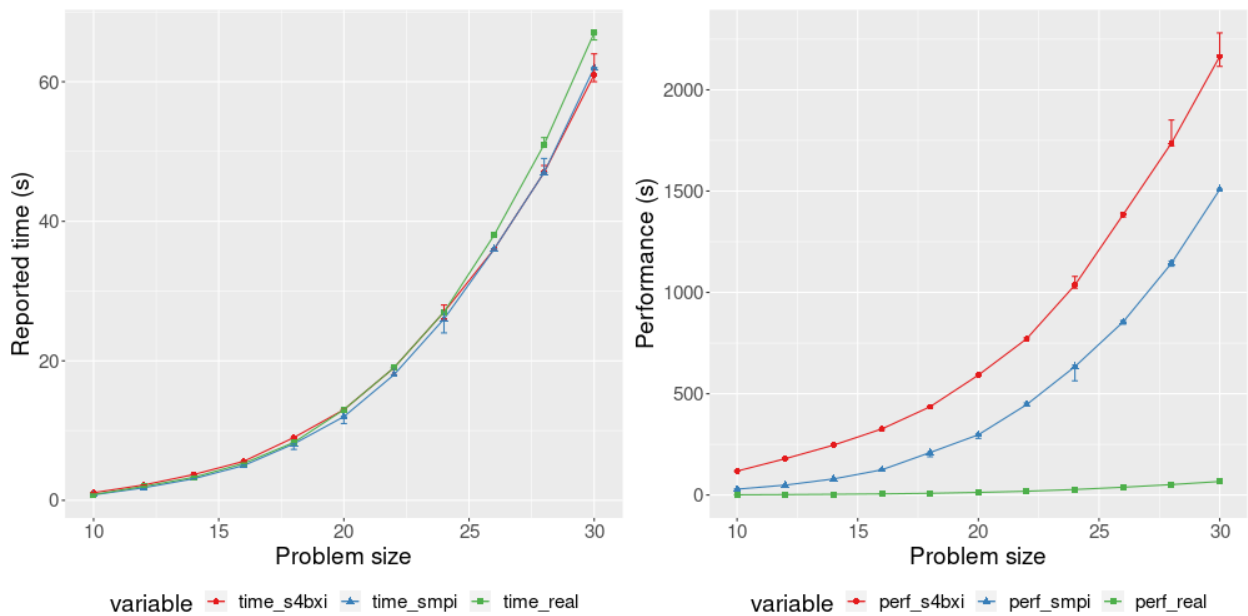


Figure 5.18: LULESH results on 27 MPI ranks (9 nodes, 3 ranks per node), comparing our simulator, SMPI, and a real-world execution. Vader enabled in real-world OpenMPI and OpenMPI over S4BXI

accuracy when running LULESH, our approach does not offer any benefit over SMPI, as the accuracy is similar, and the performance inferior. This result is not very surprising, as LULESH relies heavily on point-to-point communication (with little collective operations). Since SMPI is calibrated specifically on these point-to-point primitives, it is expected to

get very good results, and these experiments validate that our calibration of the network parameters of SMPI is accurate too.

5.5.3 Quicksilver

Quicksilver is an application that performs ten independent cycles of computations on a configurable number of particles. At the end of the execution, Quicksilver reports three performance values for each cycle of computations: the time taken by the initialization, the “tracking” phase (where most computations happen), and the finalization of the cycle. In practice, we have observed that the initialization and finalization phase of each cycle have a duration which is negligible compared to the “tracking” phase, therefore we will only show the tracking times of each cycle in our graphs, for more clarity. We have run Quicksilver for different particle numbers, ranging from 10,000 up to 1,000,000, and many cluster configurations: we used platforms with all combinations of 1, 2, 4, 8 and 16 nodes with 1, 2 and 4 processes per node. Since the resulting graphs are very numerous, in this section we will present a few representative cases of the types of results we obtained.

From a technical point of view, the simulations were performed on one of the machines from the real-world cluster, with an AMD EPYC™ 7763 64-Core processor. Every real-world execution was executed five times, and each simulation was executed twice (because of a lack of time towards the end of this thesis). Additionally, once again we had the choice of enabling Vader or not when using several processes per node. We observed little difference with and without Vader in our results (both in simulation and the real world experiments), therefore we will only present experiments performed without Vader, in order to reduce the number of variables to analyze in this section.

We will start by analyzing small problem sizes, with only 10,000 particles. First, as with LULESH, we can see that both simulators give a very good result when running Quicksilver on only one node with only one process, which is depicted on Figure 5.19. This is expected of course, since the simulators are running the application with no communications, but it allows us to confirm that both simulators work and that we get the same output in

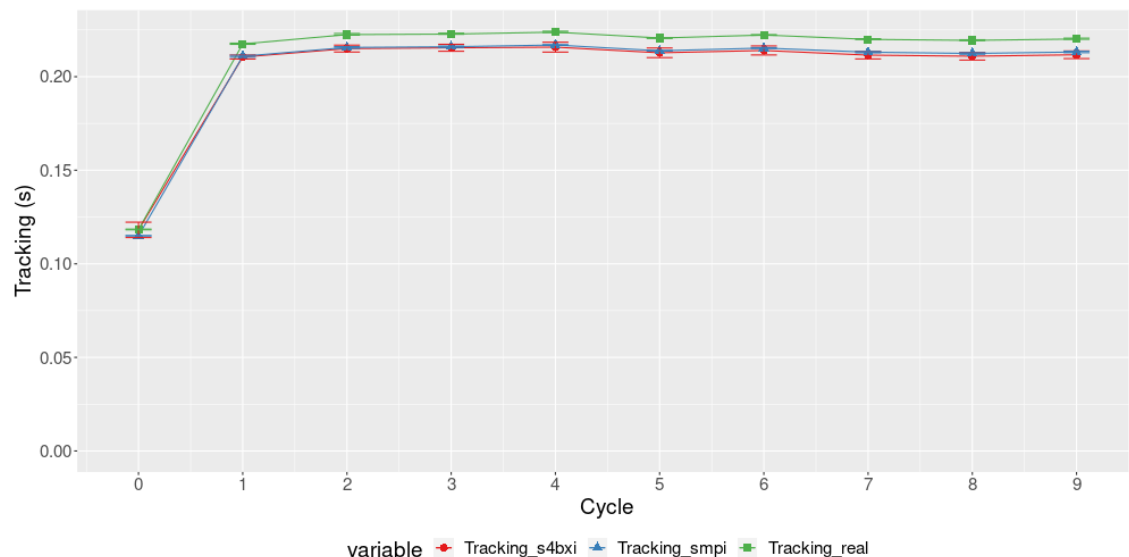


Figure 5.19: Quicksilver experiment on 10,000 particles, with 1 node and 1 process per node



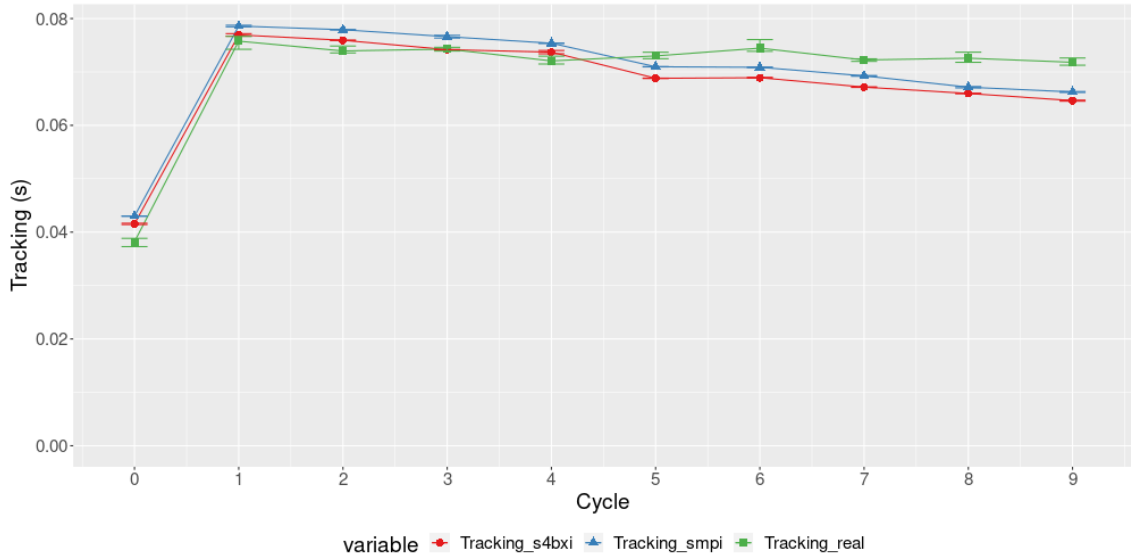


Figure 5.20: Quiksilver experiment on 10,000 particles, with 4 nodes and 1 process per node

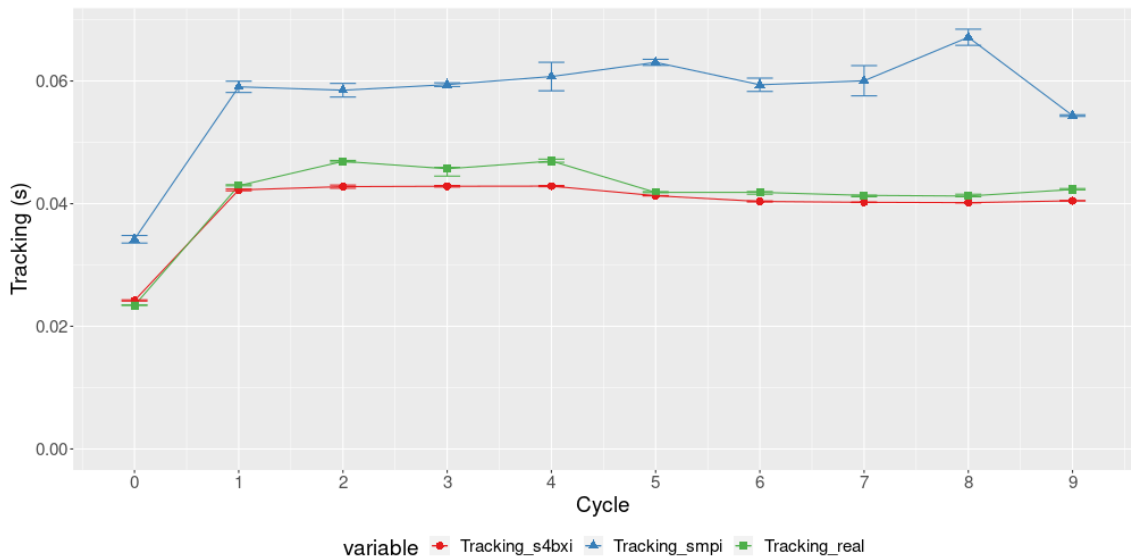


Figure 5.21: Quiksilver experiment on 10,000 particles, with 8 nodes and 1 process per node

simulation and the real-world experiment.

With very small cluster sizes, we can see that both simulators continue to have a good accuracy. For example, Figure 5.20 shows the result of executing Quiksilver on four nodes, with one process per node, and still 10,000 input particles.

On the other hand, as soon as we use more than 8 MPI ranks (regardless of the number of nodes), we observe a quick degradation of the accuracy of SMPI, while OpenMPI over S4BXI keeps a good accuracy. We can see the start of this trend with an execution on eight nodes and one process per node on Figure 5.21. It only gets worse for larger numbers of MPI ranks, as we can see on Figure 5.22 for 16 nodes and one process per node, or

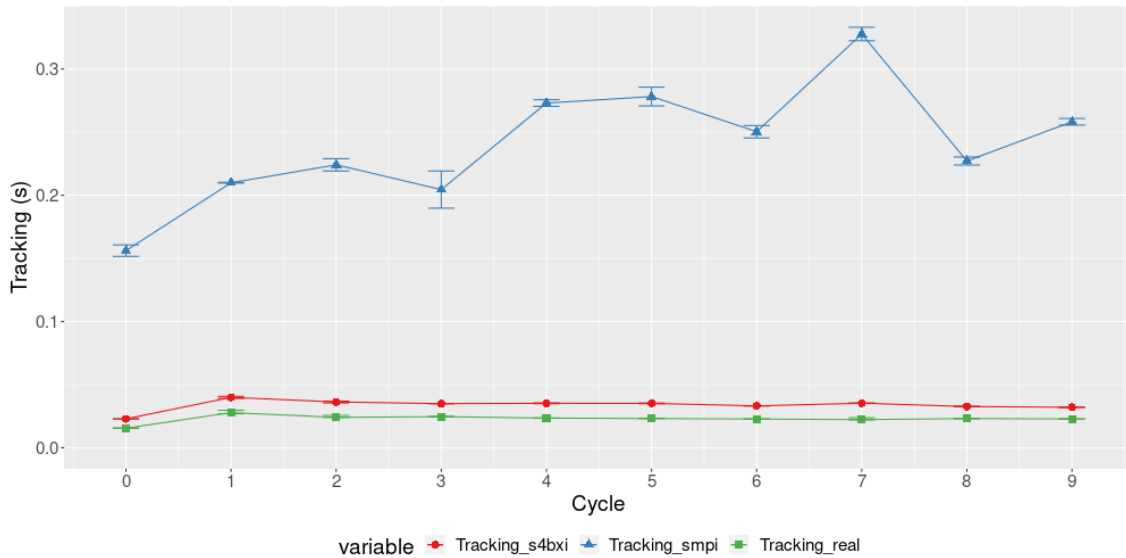


Figure 5.22: Quicksilver experiment on 10,000 particles, with 16 nodes and 1 process per node

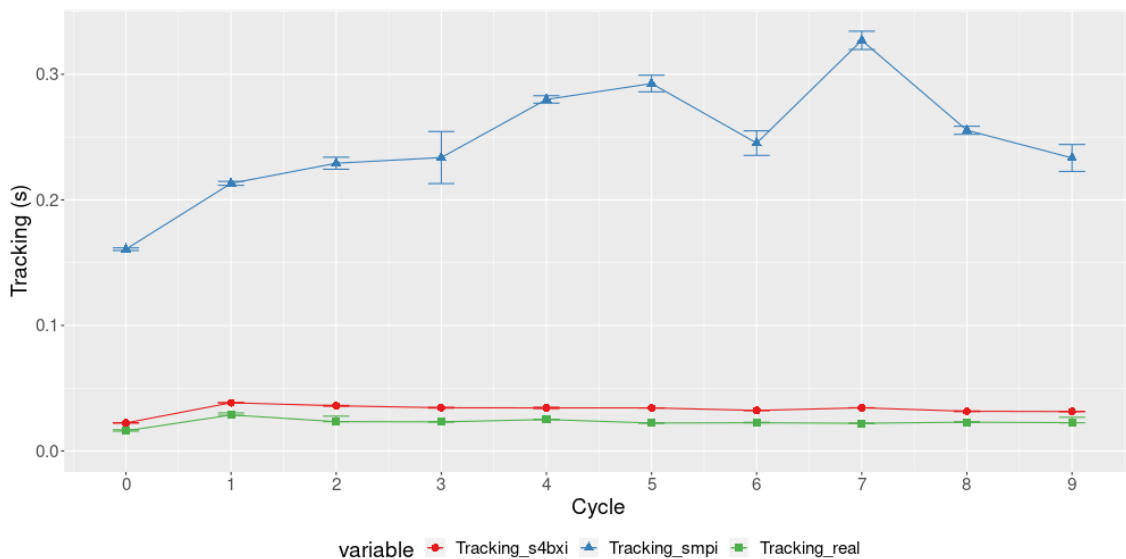


Figure 5.23: Quicksilver experiment on 10,000 particles, with 4 nodes and 4 processes per node

Figure 5.23 for four nodes and four processes per node (so 16 processes in total again).

As we increase the number of particles given as an input to Quicksilver, we can observe the same phenomenon. The only difference is that as we increase the problem size, SMPI remains accurate for larger cluster sizes, but we always observe a point where SMPI's accuracy drops dramatically. For example, with 1,000,000 particles, we conserve a good accuracy of both simulators up to 16 MPI ranks, as we can see on Figure 5.24 (with eight nodes and two process per node). Starting from 32 MPI ranks, we can see the accuracy of SMPI drops, for example on Figure 5.25.

This lack of accuracy from SMPI is highly unexpected, as we never obtained results so



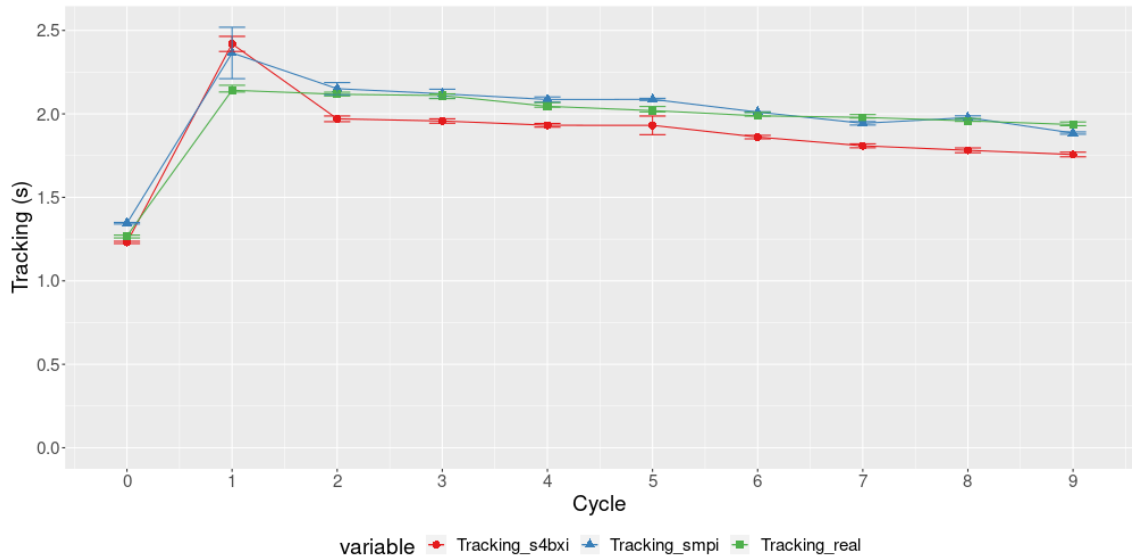


Figure 5.24: Quicksilver experiment on 1,000,000 particles, with 8 nodes and 2 processes per node

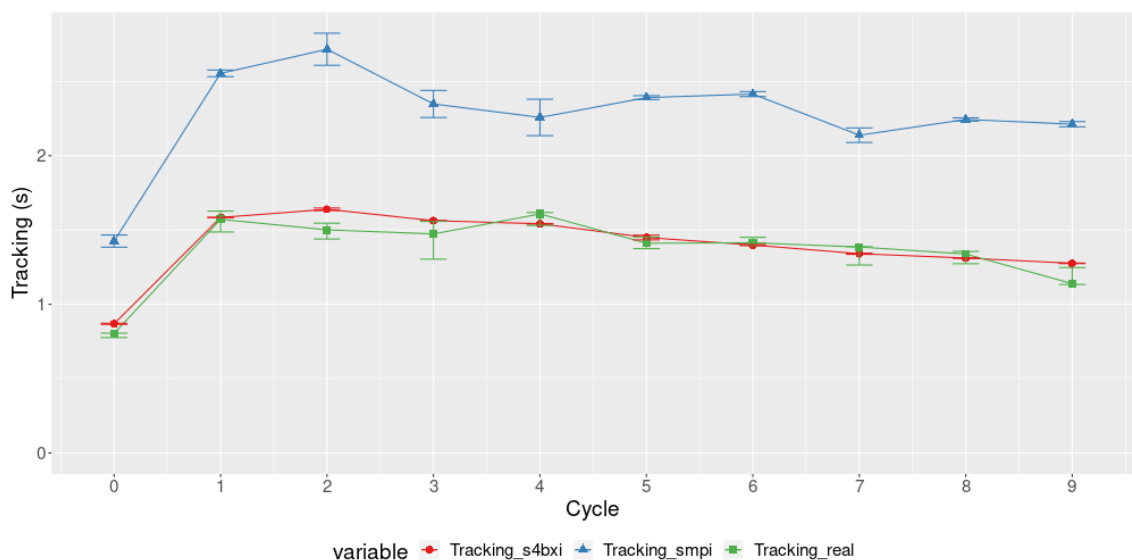


Figure 5.25: Quicksilver experiment on 1,000,000 particles, with 16 nodes and 2 processes per node

far away from the real-world experiment in OSU benchmarks or LULESH. We were not able to identify what could be so detrimental to the SMPI model in Quicksilver, only that the accuracy drop is very consistent, and depends on the problem size and the number of MPI ranks, regardless of the number of nodes they are distributed on.

🌿 5.5.4 High-Performance Linpack (HPL)

Finally, we tested our simulator on HPL. This application is particularly interesting to study because we can use two different versions: in addition to the “regular” version

of HPL, we can use a skeleton version of the application, made by Tom CORNEBIZE during his PhD [Cor21]. The idea behind this version of HPL is that it performs the same communications as the full application, but it replaces the most costly computation phases with a delay that estimates the corresponding CPU time and which is simulated instantaneously. The skeleton version does not compute the same result as the original application but its simulated execution time is approximately the same. In practice, the vast majority of the CPU time of the benchmark is spent in one function (`HPL_dgemm`), which performs a Double precision GEneral Matrix Multiply (DGEMM). Therefore, we can save a lot of time in simulation by removing the code of this function, and by replacing it with a function call to our simulator in order to inject an artificial amount of computation time in the model directly. Of course, this skeleton version of HPL does not perform accurate computations, as many CPU operations were removed, but the timing of HPL in simulated time is preserved because the operations that we removed do not affect the execution flow of HPL.

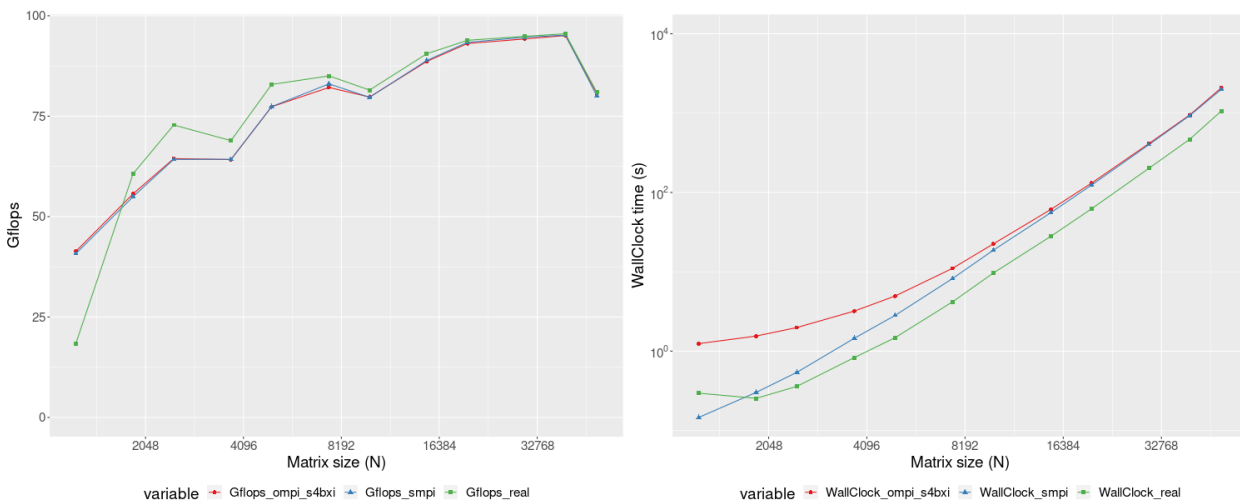


Figure 5.26: HPL experiment on 2 nodes with 1 process per node

We will start by presenting our results for the full version of the application: Figure 5.26 shows data from both simulators (SMPI and OpenMPI over S4BXI) compared to real-world executions, for a very small number of MPI ranks: two nodes with only one process per node. The left graph shows the precision of the simulators, by plotting the performance reported by HPL (in GFlops), whereas the right graph plots the performance of the simulators (with respect to wall-clock time), compared to the duration of the real-world experiment. We can see that even though the real-world experiments show a surprising evolution of the computing power (in Gflops) when the problem size increases, both simulators manage to model these effects accurately. As the number of processes is very small, we can see that the performance of both simulators is reasonably good, and that for large problem sizes they perform very similarly.

Executions with more MPI ranks are displayed on Figure 5.27 for 50 MPI ranks (ten nodes and five processes per node) and on Figure 5.28 for 128 MPI ranks (16 nodes and eight processes per node). On both figures we can see that the accuracy of the simulators is comparable, with a slight advantage for SMPI. This result is not surprising, because of how HPL uses MPI: even though the benchmark needs to be able to perform collective communications, it does not use the collective primitives offered by MPI. Instead, all



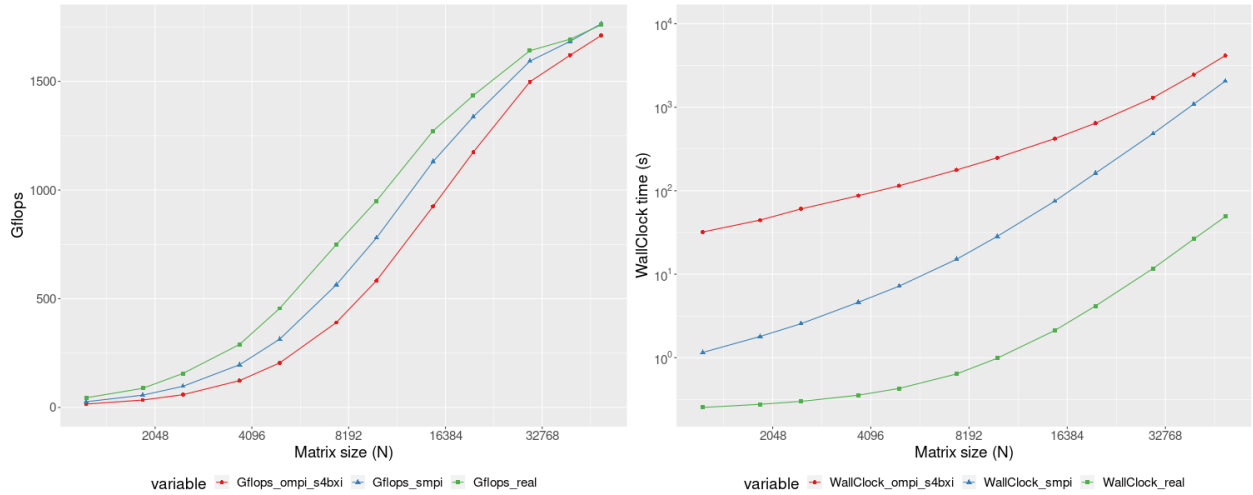


Figure 5.27: HPL experiment on 50 MPI ranks (10 nodes with 5 processes per node)

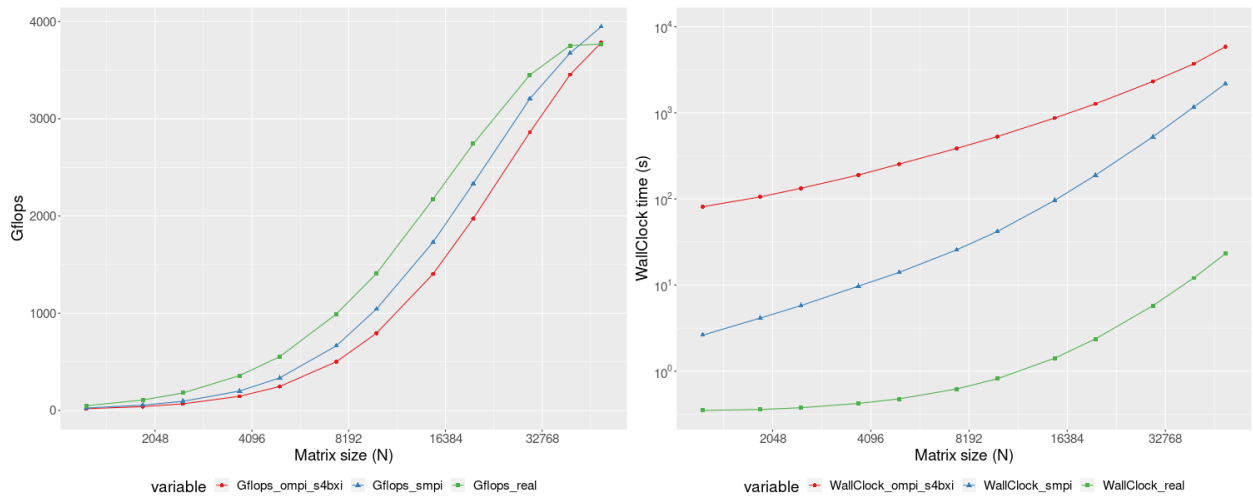


Figure 5.28: HPL experiment on 128 MPI ranks (16 nodes with 8 processes per node)

operations are re-implemented in HPL with a combination of basic “send” and “receive” point-to-point primitives. Since SMPI’s network model is specifically tuned to perform well on these point-to-point operations (using coefficients on the latency and bandwidth of Links), it is expected to get good results in this context. In comparison, OpenMPI over S4BXI models low-level network operations, which also gives good results. Nevertheless, in order to surpass the accuracy of SMPI on this type of workload, our approach would require a finer tuning of very low-level parameters inside our simulator. From a performance perspective, as expected the duration of simulation increases with the number of simulated MPI ranks. We can see that the gap between the performance of SMPI and OpenMPI over S4BXI increases when we simulate more MPI ranks, as we can see in Figure 5.26 where both simulators are extremely close, whereas the gap is a lot more important on figures 5.27 and 5.28. This different in scaling is expected, since the proportion of network operations (compared to the computational phases) increases as well, and modelling communications is more costly with our approach than SMPI (which has a more simplistic network model).

In order to improve the performance of the simulators, we can use the skeleton version

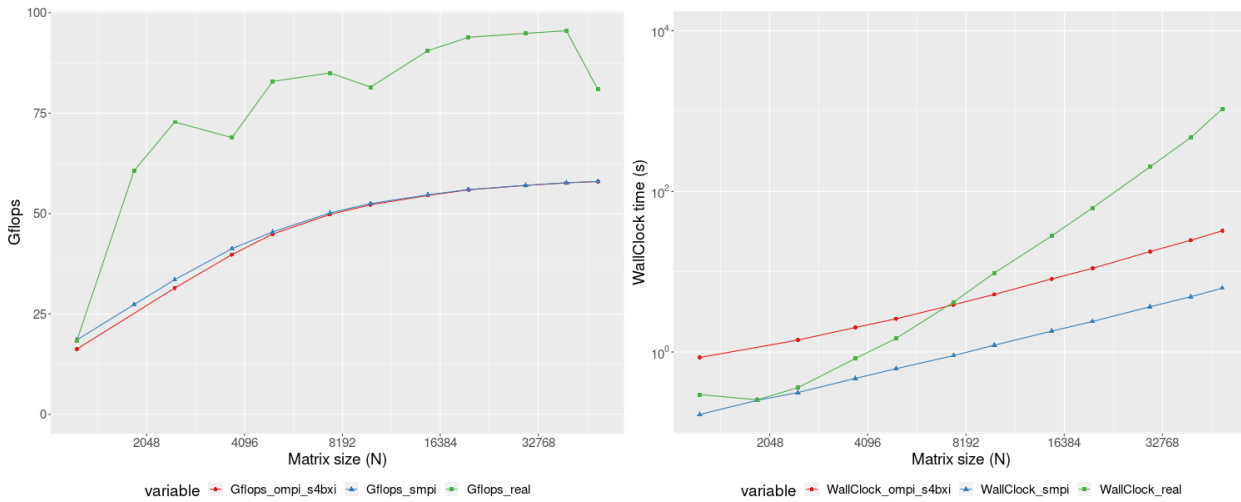


Figure 5.29: HPL skeleton experiment on 2 nodes with 1 process per node

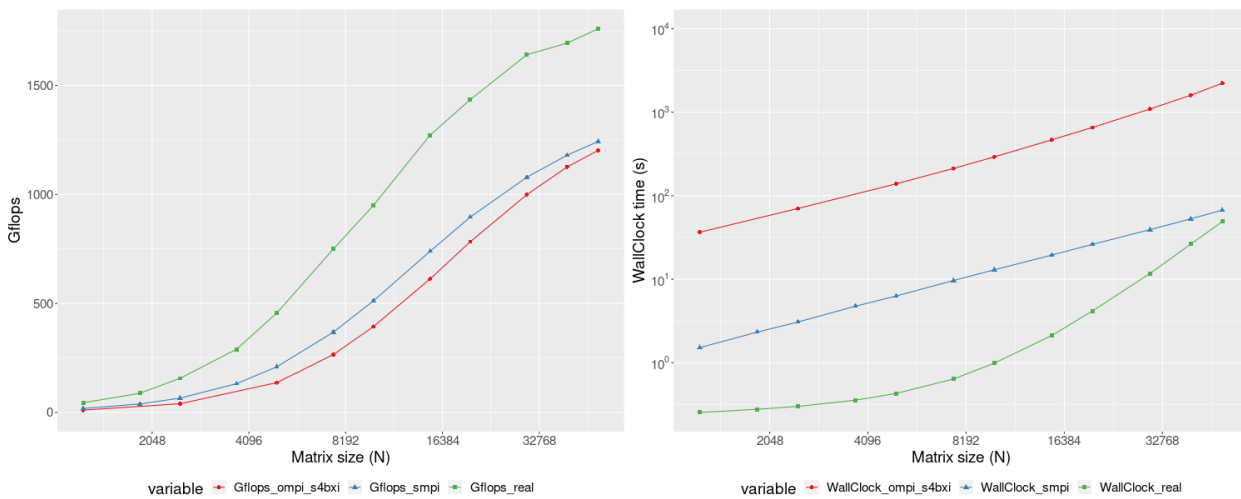


Figure 5.30: HPL skeleton experiment on 50 MPI ranks (10 nodes with 5 processes per node)

at our disposal. However, the main difficulty is to tune the artificial computation time to inject in SimGrid (in the `HPL_dgemm` function). In his PhD, Tom CORNEBIZE uses machines from the Grid5000 testbed, and we re-used his tuning without any modifications at first. Results are depicted on Figure 5.29 for two MPI ranks (two nodes and one process per node) and on Figure 5.30 for 50 MPI ranks (ten nodes and five processes per node). From a performance perspective, we can see that both simulators are sped up significantly (the SMPI simulation on two MPI ranks is even faster than the real world experiment for all problem sizes). Of course, the gap between the execution time of the simulators stays significant, as the network model of our approach is still costly on the skeleton version (as the number of communications is identical). Regarding accuracy, we can see that this version of HPL (with this tuning) made both simulators very pessimistic, which shows that the CPUs on our clusters are much more efficient at running DGEMM operations than Grid5000's ones.

To get a better tuning of our DGEMM model, we instrumented the real-world version



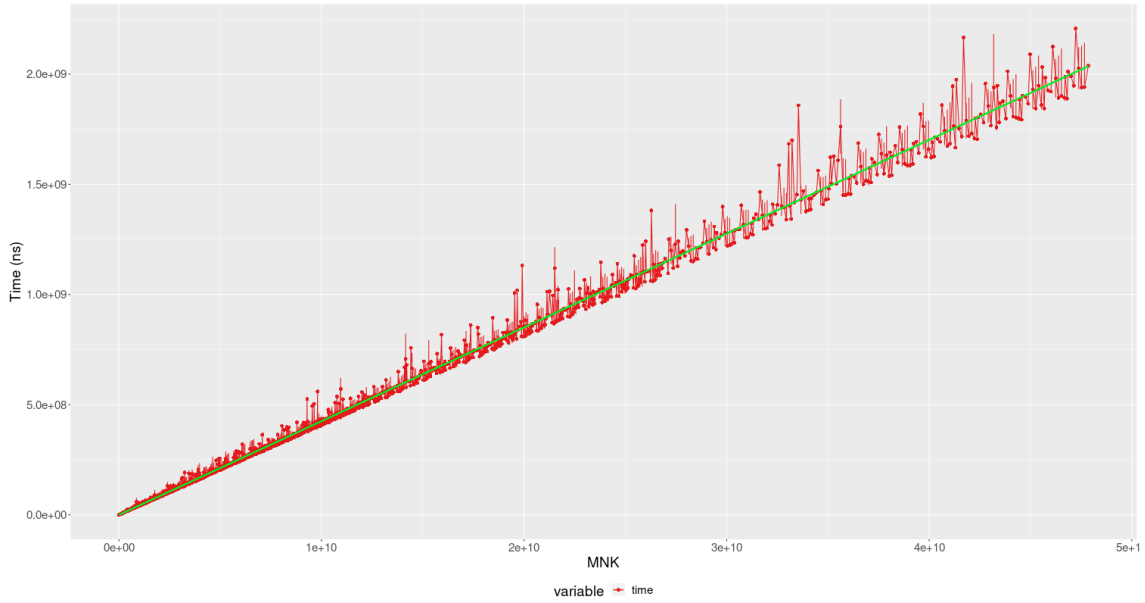


Figure 5.31: Duration of `HPL_dgemm` as a function of $M \times N \times K$

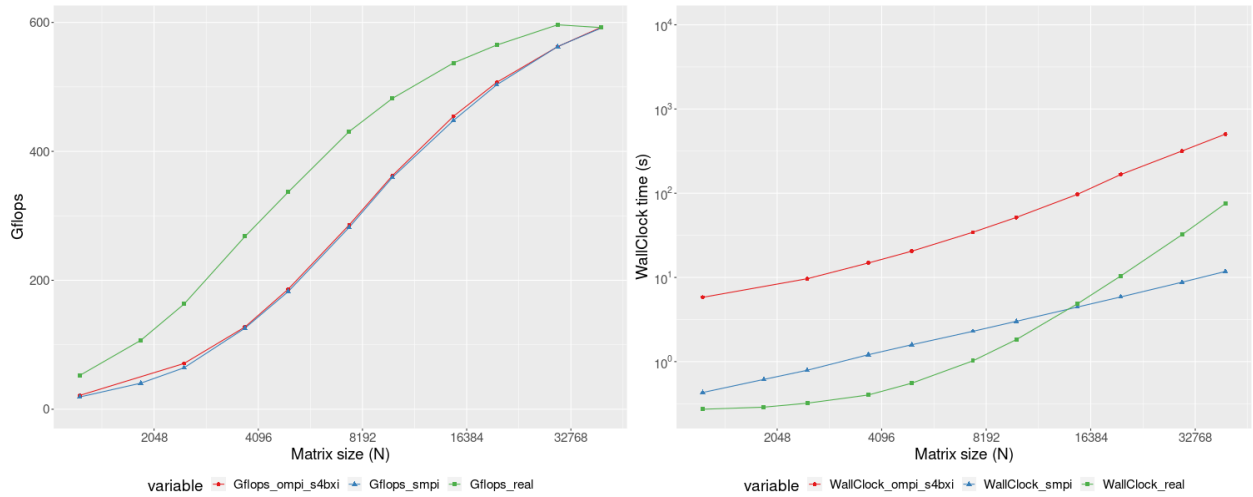


Figure 5.32: HPL skeleton experiment on 16 MPI ranks (4 nodes with 4 processes per node), with our tuning

of HPL to measure the duration of the `HPL_dgemm` primitive as a function of its numerical parameters (which are called M , N and K). By plotting the performance of `HPL_dgemm` as a function of each combination of the parameters (M , N , K , $M \times N$, $M \times K$, $N \times K$ and $M \times N \times K$), we identified that the execution time of `HPL_dgemm` seems close to a linear function of $M \times N \times K$ (with a significant amount of noise): Figure 5.31 shows this data, depicted along with the corresponding linear regression. Consequently, we managed to tune the estimation of the computation time; this allowed us to get the results depicted on Figure 5.32. The corresponding run of the full benchmark (on 16 MPI ranks) is shown on Figure 5.33. As we can see, even if our heuristic to estimate the duration of `HPL_dgemm` is better adapted to our cluster, it is still far from perfect. This is expected since our tuning is more simplistic than the study conducted by Tom CORNEBIZE.

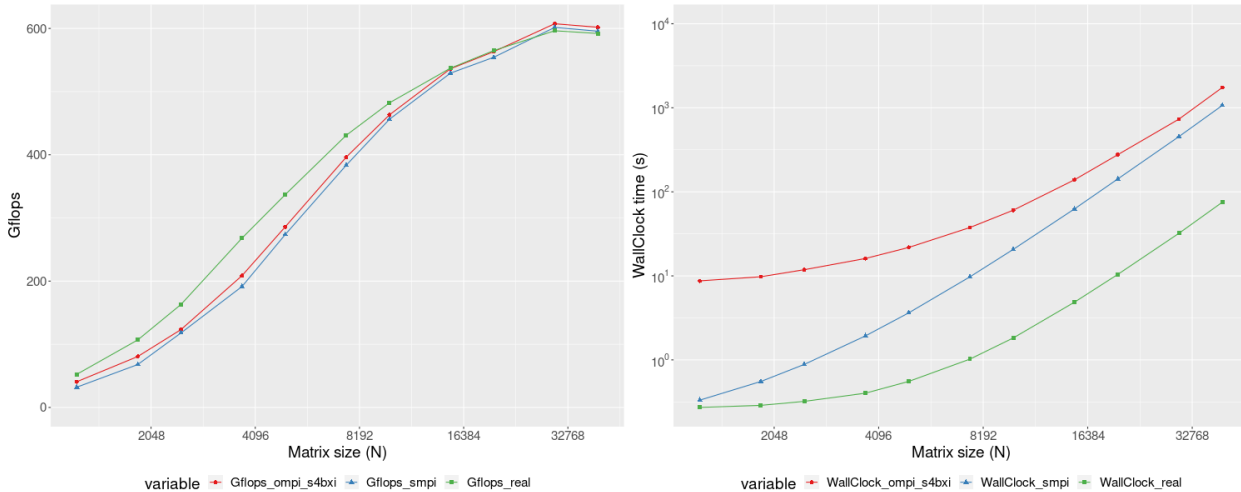


Figure 5.33: Full HPL experiment on 16 MPI ranks (4 nodes with 4 processes per node)

The most important takeaway from these experiments is that this type of skeleton application, originally designed for SMPI, is fully compatible with S4BXI simulations out of the box. Even though the improvement in performance is not as important with our model as it is with SMPI, we showed that this type of patch to an application works in an identical way in S4BXI and SMPI, as we can see from the accuracy graphs.

5.6 OpenSHMEM

While modeling MPI is the main usage of our simulator, one of the strengths of S4BXI is its adaptability: since it is modeling a low-level API, it can be used to run a variety of higher-level APIs. To demonstrate that, we have worked on the simulation of the OpenSHMEM library.

5.6.1 Running OpenSHMEM in S4BXI

OpenSHMEM follows a Partitioned global address space (PGAS) model, which means that, compared to MPI, it focuses less on message passing. Instead, it gives every process in the job a transparent view of a “global memory pool”, which in practice is distributed across several nodes. For our study we adapted Atos’s version of OpenSHMEM to support running on S4BXI. The Atos version is very similar to Sandia’s implementation of OpenSHMEM (<https://github.com/Sandia-OpenSHMEM/SOS>), with only minor modifications to support execution over BXI.

Similarly to OpenMPI, we chose to add support for OpenSHMEM simulation over S4BXI by adding a small patch to OpenSHMEM. The architecture of OpenSHMEM’s code proved to be easier to work with for our purpose, because the project’s scale is significantly smaller, therefore making a preliminary patch to run this library in simulation was much easier than the same developments in OpenMPI. In the end, our patch simply adds a new file to OpenSHMEM, and the only modifications we made to existing code was in the build scripts to include our new file. Internally, OpenSHMEM uses a concept of a “runtime” that should be initialized. The project natively provides four runtimes: one over MPI, and three over various versions of PMI (PMI, PMI2 and PMIx). Therefore, to add support for



S4BXI we only need a new runtime, which implements basic utilities (like a barrier, basic metadata exchange), and we are ready to perform simulations. This runtime only consists of 11 functions, most of which are trivially implemented using S4BXI: the vast majority are implemented in one line of code, and the largest one only has five lines of code. The full runtime is given in Appendix D.

Because of time constraints, and because our main goal was simulating MPI accurately, we did not study OpenSHMEM benchmarks with as much detail as MPI ones. The validation we performed focused on two aspects: the unit test suite provided with OpenSHMEM, and the OSU-microbenchmarks (which also have an OpenSHMEM variant even though the MPI benchmarks are more notorious).

🌿 5.6.2 Experimental validation

In order to test our simulations of OpenSHMEM, we first ran the unit test suite provided by OpenSHMEM in our simulator, on a desktop computer. Every test was executed four times: with 2, 4, 8 and 16 nodes and always one process per node, this amounts to 392 runs in total. We used a fairly low value for the timeout, of one minute, because we observed that most successful tests ran in a few seconds only. The results are mixed: while the majority of tests pass – 228 executions succeed – we still have 154 errors, and 10 timeouts. Indeed, we expected some tests to fail, as they perform operations that are not supported by our simulators, such as using `pthread` mutexes which are not properly intercepted by S4BXI. However, the amount of errors is still a lot more important than what we expected, and too large to reliably run OpenSHMEM in simulation. Nevertheless, these results show that with few efforts we are already close to having a functional OpenSHMEM simulator, as most basic tests work as expected.

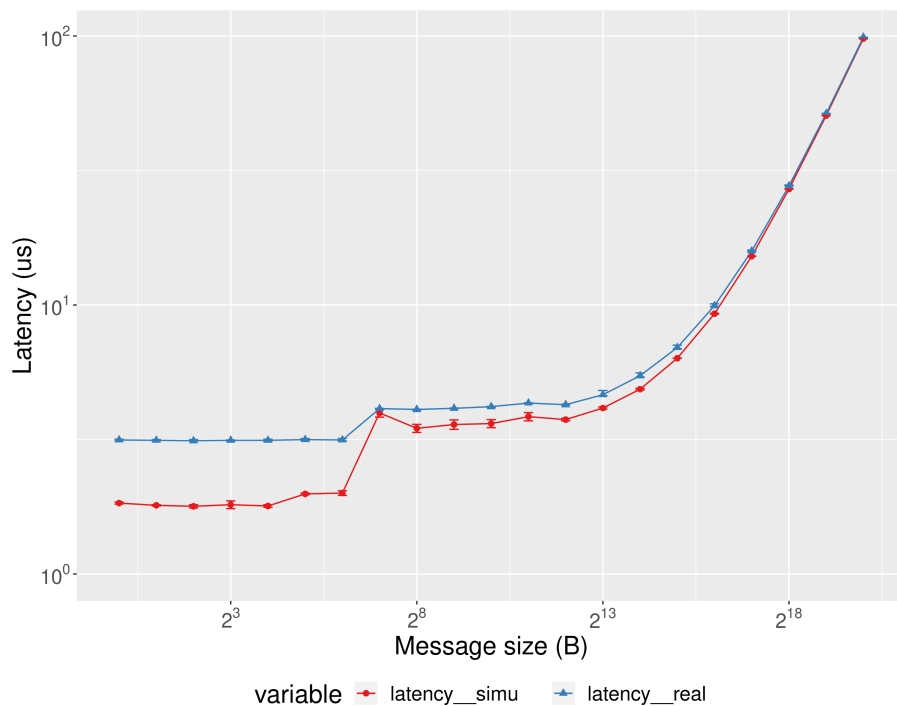


Figure 5.34: Benchmark of the “put” operation of OpenSHMEM between 2 nodes

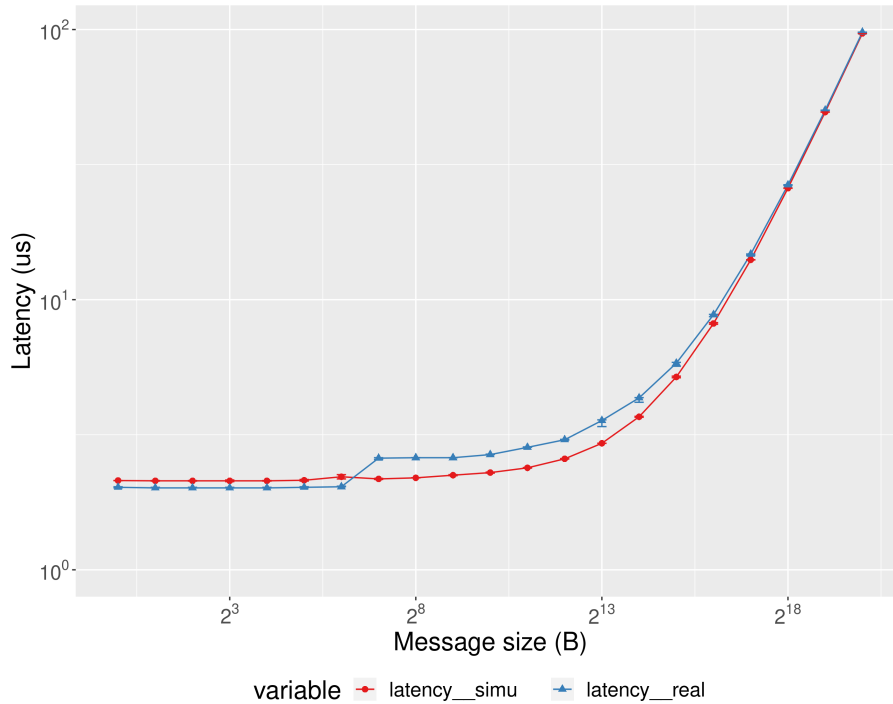


Figure 5.35: Benchmark of the “get” operation of OpenSHMEM between 2 nodes

Running OpenSHMEM was only a side experiment in this thesis, and we did not invest the time required to fully debug the problems. The only hypothesis that we have is that OpenSHMEM tries to locate memory regions inside the current binary at startup, which might cause problems in simulation since we do not execute applications directly from their binary, but instead we run them from a shared library which is opened by our entry point, `s4bximain`. In the real-world, each process would be isolated by the operating system and deployed on several machines, but in simulation OpenSHMEM might locate the same memory region for all processes (by looking directly in `s4bximain`) with no isolation. This could cause issues but would require further investigations.

After running unit tests, we tried the OpenSHMEM variant of OSU benchmarks. Once again, some tests do not terminate properly, therefore we only present a few of those which work correctly, in order to give an idea of the precision that we can expect out of OpenSHMEM simulation. For point to point operations, we can see on Figure 5.34 the result of the “put” benchmark between two nodes (which correspond to a remote write), and on Figure 5.35 we have a similar benchmark for the “get” operation (remote read). We can see that the accuracy is not perfect, especially for “put” operations of a small size, but overall it is already acceptable, even though we did not perform any particular tuning to make OpenSHMEM simulations more accurate.

For collective operations, we can see on Figure 5.36 the result of the “fcollect” benchmark on eight nodes, which concatenates data from multiple processes into a buffer on every process of the job. Finally, Figure 5.37 shows the result of the “reduce” benchmark on 16 nodes, which performs various reduction operations (min, max and sum) using data from all processes (similarly to MPI’s reduce operation). We can see that the conclusion is the same on collective operation than with point-to-point ones: overall the accuracy is acceptable, even though in this case we can see some unexpected performance jumps, that



we did not investigate because of a lack of time.

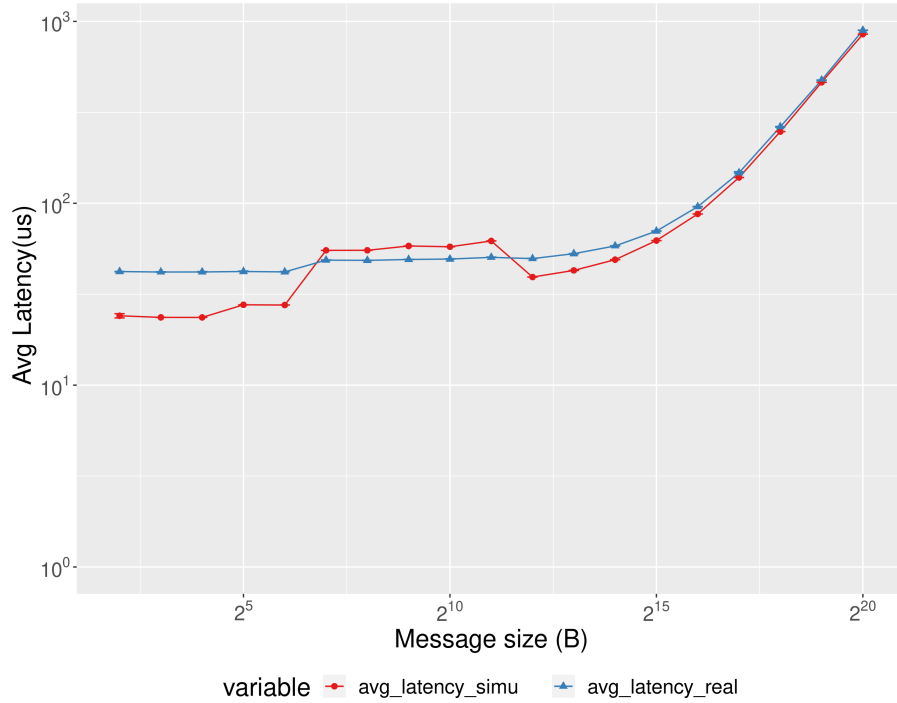


Figure 5.36: Benchmark of the “fcollect” operation of OpenSHMEM using 8 nodes

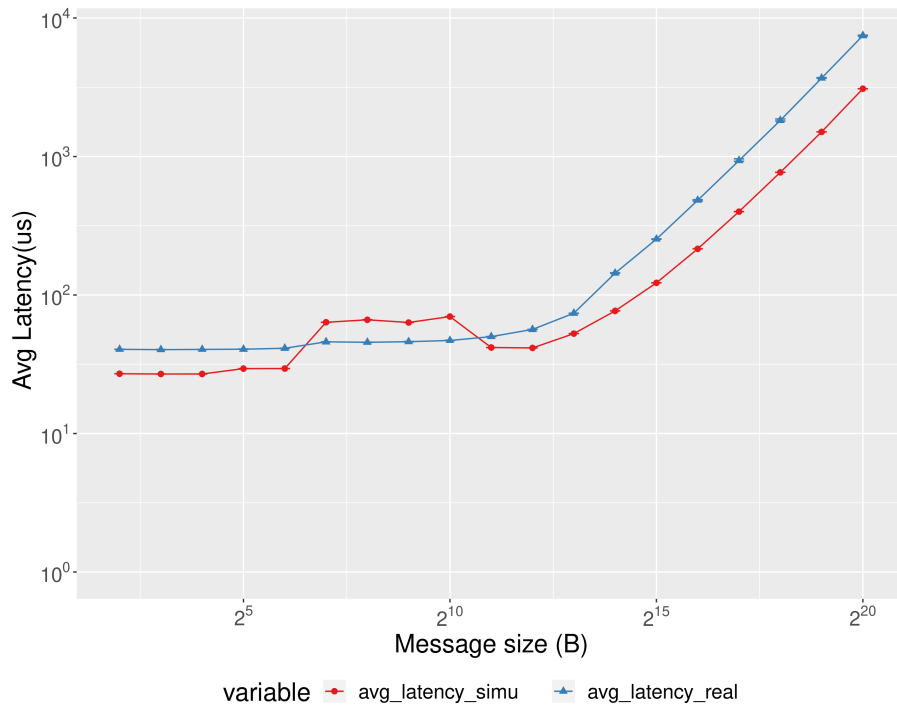


Figure 5.37: “Reduce” OSU benchmark using 16 nodes

5.7 Summary

Simulating high-level APIs with our method has proved perfectly achievable, even if some development time has been required. Even though our simulations are slower than real-world experiments, they have other advantages: they only use one CPU core, therefore exploring a vast parameter space can be done in parallel with many simulations on one or several machines. Additionally, our simulations can be used to test many scenarios, as high-level APIs are modeled with a high fidelity (since we run them with few modifications).

Even though our results concern mainly MPI, our preliminary results with OpenSHMEM show that our method can be adapted to other high-level API, making S4BXI more versatile than most state-of-the-art simulators.



Chapter 6

A more flexible accuracy/performance tradeoff

In the previous chapter, we have shown how S4BXI can be used to run high-level APIs, and therefore run realistic applications in simulation. While our validation experiments show a good accuracy of our method, the biggest drawback of our model compared to state-of-the-art simulators is its performance. This was even more noticeable in earlier versions of S4BXI: we managed to optimize our model during the development of this chapter's work, allowing our performance to get closer to SMPI's. In this chapter, we will explore ways to improve the speed of simulation, using several network models, which will allow us to dynamically switch at runtime between a slow and accurate model, and a fast but less accurate one. This is useful to model precisely a region of interest of the simulation, while modeling other parts coarsely.

We will start by motivating our choice of models in Section 6.1.1, and show how these two models are used in Section 6.1.2. Then we will detail the technical developments that are required to implement model changes in sections 6.2, 6.3 and 6.4. Additionally, we will explain how we can make model changes more flexible by tracking asynchronous operations in Section 6.5. Finally, we will present our experimental results in Section 6.6, and conclude in Section 6.7.

6.1 Design choices

6.1.1 Two network models over SimGrid

Since S4BXI is based on SimGrid, we chose to support the following network models: Atos's implementation of OpenMPI on top of S4BXI, and SMPI. Using SMPI as a second model is very convenient from a technical perspective: since both models rely on SimGrid, they naturally share a common source of truth for the simulated time, they both use SimGrid's Actor system. If we wanted to support different state-of-the-art models, for example SystemC emulators or abstract LogGOPS simulators, most of our methodology would work the same way, except that a significant development effort would be required to make the architecture of the simulators compatible. For example, it would require synchronizing the simulated time in all models, making sure the scheduling of actors performed by SimGrid is compatible with the other simulators, etc.

6.1.2 Different ideas to share the network loads

Before we explain how SMPI is used in an otherwise “S4BXI” simulation, we need to discuss the way our two models are going to be used. There are essentially two ways of dividing our usage of the simulators: either “spatially” or “temporally”.

A spatial division is pertinent when some nodes of the cluster are more interesting to study than others (for example the “root” node in a collective operation with a “tree” implementation). In this case, the other nodes would use SMPI to have a better performance, and the selected node(s) would use OpenMPI over S4BXI to have a better accuracy. Such an execution is depicted on Figure 6.1, with a simplistic cluster of three nodes connected to a single switch.

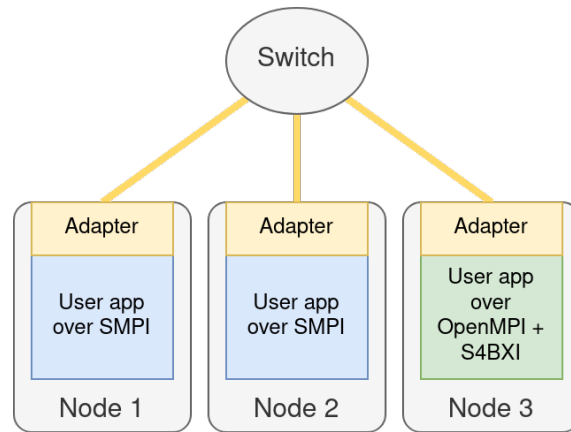


Figure 6.1: Spatial distribution of the network models

This approach has two main downsides: first, it is not always trivial to select which nodes should be modeled with high accuracy, and which ones should be modeled in a more performant way. It would be particularly hard and impractical to express it manually in user applications’ code, and making the decision automatically would require having a very good knowledge of the different algorithms for collective operations used in MPI, in order to make a heuristic more efficient than deciding at random. Second, allowing nodes that run different models to communicate together is a significant challenge, which would require intrusive modifications in each model’s code (S4BXI and SMPI) in order to have “adapters” between the two models (which are shown on Figure 6.1). Indeed, while both models rely on SimGrid’s Mailbox system to communicate, these Mailboxes currently use different names, and the format of data exchanged through them is very different. Additionally, collective operations use different algorithms when performed in SMPI and OpenMPI over S4BXI, which results in a different set of point-to-point communications. Reconciling these two implementations of collectives would be a very significant challenge if we wanted to use different models on different machines at the same simulated time.

On the other hand, a temporal division means that instead of focusing our study on a specific set of nodes, we focus on certain “phases” of users’ applications. This idea leverages the fact that HPC applications typically have long execution times, with different workloads in different phases of the application. For example, an application could have an initialization phase, then intense computation, and finally a phase to collect the results and make statistics about the execution. In such a scenario, having a precise model of the first and last phases is usually not very important, and it would be desirable to focus on the computational phase with our precise model. An example of this idea is depicted



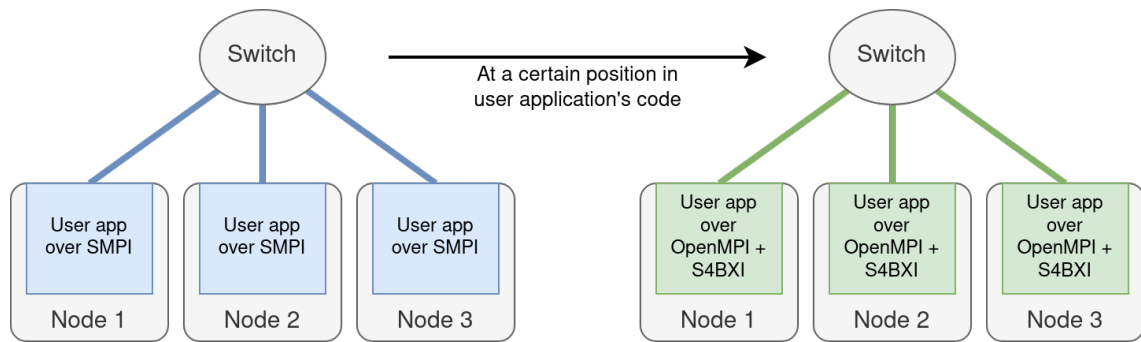


Figure 6.2: Temporal distribution of the network models

on Figure 6.2, with the same three-nodes cluster, and two different phases: a first one which we simulate quickly, in order to focus on the second one with our more accurate model. This solution has the advantage that at every moment all nodes use the same model, therefore there is no need for “adapters” between models. It is also easier to decide when to switch models: a superficial knowledge of applications is usually enough to have a good idea of the different phases they go through. Therefore, it is relatively easy to manually add a line of code in the application in the places where a model change should occur.

For this reason, in our study we will only implement a temporal division of the usage of our two models.

🌿 6.2 Architecture changes in S4BXI to support SMPI

Separation of S4BXI components

In order to enable dynamic model changes during a simulation, we added a component to S4BXI, called “MPI middleware”, which manages our two MPI models (OpenMPI over S4BXI and SMPI). It is important to note that even though our MPI middleware is part of S4BXI, its function is very different from our Portals implementation in S4BXI. Indeed, even though our simulator consists of only one codebase, three functions must be distinguished:

1. S4BXI exposes the Portals API to any code that links against it, implementing Portals using SimGrid’s Mailbox system to exchange data, as presented in Chapter 4.
2. It also provides a set of utilities to run unmodified user code, using a method heavily inspired by SMPI (with on-disk copies of libraries and “dlopen” calls), which was also presented in Chapter 4 (and extended in Chapter 5 to support MPI simulation).
3. Finally, it features an MPI middleware, which exposes the MPI API, and implements mechanisms to manage two underlying implementations of MPI, which we detail in this chapter.

A note regarding software design

For our purpose, having all three features in the same codebase allowed us to prototype a working simulator quickly, but in order to make a full product out of this simulator it would be advisable to split the code into well-defined modules with proper interfaces. In particular, features 1 and 2 are also part of a single codebase in SMPI: while our

Feature 1 is completely different from SMPI’s counterpart, since SMPI implements MPI instead of Portals, there are many similarities between S4BXI’s and SMPI’s Feature 2. Having this feature better isolated from the rest of SMPI would have allowed us to re-use it instead of re-implementing most of it. Indeed, the mechanisms used to isolate simulated processes are independent of the API that is implemented by the simulator. Consequently, it would be beneficial to make it a re-usable component of SimGrid (instead of being a part of SMPI). Better decoupling would thus be desirable, as discussed informally with SimGrid’s development team, but it has not been done during this PhD. It could also be a good occasion to evaluate different techniques to isolate simulated processes: for example the project Remote SimGrid¹ proposes an experimental methodology which uses distinct processes that communicate with a central SimGrid “server” using a custom BTL in OpenMPI. This type of approach could be used in a shared component by both S4BXI and SMPI.

6.3 Redirecting MPI calls using S4BXI’s middleware

In order to switch dynamically between two MPI implementations, we need to be able to intercept calls to the MPI API. In order to do this, we re-use the same method that we presented in Chapter 4 in order to intercept calls to `sleep`, `gettimeofday`, etc.: we inject an additional header in users’ applications, which uses C-style macros (`#define`) to redirect MPI calls to our functions. A few examples of these macros are given on Figure 6.3 (passing the file and line of the MPI call to our function is only useful to our logging system, which helped us debug our middleware more easily).

```
1 #define MPI_Init(...) S4BXI_MPI_Init(__FILE__, __LINE__, ##__VA_ARGS__)
2 #define MPI_Send(...) S4BXI_MPI_Send(__FILE__, __LINE__, ##__VA_ARGS__)
3 #define MPI_Recv(...) S4BXI_MPI_Recv(__FILE__, __LINE__, ##__VA_ARGS__)
4 // ...
```

Figure 6.3: Example macros to intercept MPI calls

Now that calls are redirected to our middleware, we need a way to forward them to the correct implementation (OpenMPI over S4BXI or SMPI). To achieve this, we need our middleware to store pointers to every symbol of both MPI implementations, so that we can

¹<https://framagit.org/simgrid/remote-simgrid/>

```
1 // Interception in the header file that's injected in user code
2 MPI_Request S4BXI_MPI_REQUEST_NULL();
3 #define MPI_REQUEST_NULL (S4BXI_MPI_REQUEST_NULL())
4
5 // Implementation in our simulator
6 MPI_Request S4BXI_MPI_REQUEST_NULL()
7 {
8     BxiMainActor* main_actor = GET_CURRENT_MAIN_ACTOR;
9     return (main_actor->use_smpi_implem ? NULL : main_actor->bull_mpi_ops->REQUEST_NULL);
10    //
11    //           SMPI value      OpenMPI value
12 }
```

Figure 6.4: Example implementation of a “constant” in our middleware



decide which one to use at runtime. Of course, we cannot rely on functions' names since they are the same in both libraries. To get these pointers, we use the `dlopen` and `dlsym` functions on both SMPI and OpenMPI at the start of the simulation. It is important to note that even though SMPI is instantiated only once, each simulated process has its own copy of OpenMPI (as presented in Section 5.3.4), which means that the pointers to MPI symbols must be specific to each simulated process (at least the OpenMPI ones). It is also worth mentioning that even though most symbols we need to intercept are functions, we also need to support constants which can have different values in different implementations, such as `MPI_REQUEST_NULL` for example. This means that even though these symbols need to appear constant to each MPI implementation, from our middleware's perspective they must be implemented as functions which can return two different values, as illustrated for `S4BXI_MPI_REQUEST_NULL` on Figure 6.4.

Finally, we need to be able to instantiate SMPI from S4BXI. While this does not seem to be the most difficult part, it still required some development effort: indeed, SMPI expects to be started from the `smpirun` or `smpireplay` binaries, and there is no out-of-box way of setting it up programmatically. In particular, a few symbols we need were not originally public in the SimGrid library, which made it impossible to link against them in S4BXI.

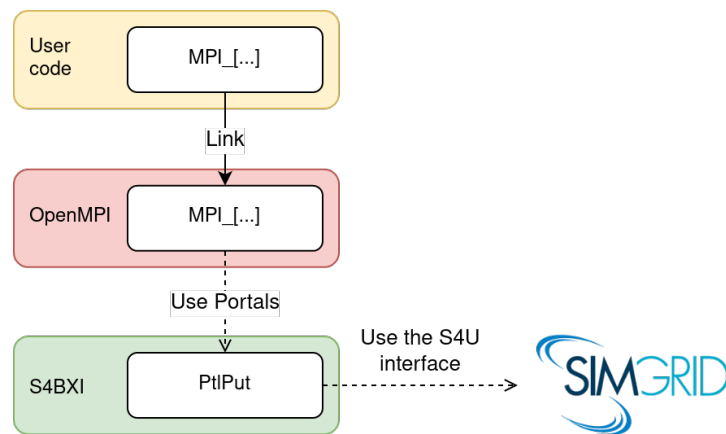


Figure 6.5: Execution of an MPI call, before adding our middleware

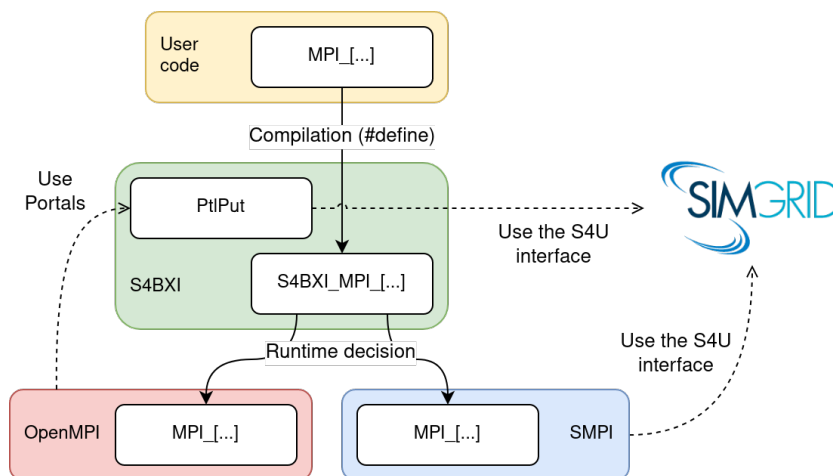


Figure 6.6: Execution of an MPI call, after adding our middleware

Thankfully, SimGrid’s development team was kind enough to make a patch to SMPI to allow us to use these symbols. Additionally, to use some of the functions that are needed to set up SMPI, we have to import a few header files directly from SimGrid’s sources, because they are not part of the public headers that are installed with each release of SimGrid. In the end, thanks to the cooperation of SimGrid’s development team, and thanks to the clean architecture of SMPI’s code, we are able to instantiate SMPI’s model programmatically from S4BXI, without having to patch SimGrid (even though it is not an officially supported use-case of SMPI).

Thanks to these three steps, our middleware is able to instantiate SMPI and extract symbols from both SMPI implementations at the start of simulations, which allows us to intercept functions calls at runtime and forward them to either implementation, based on a configuration parameter of S4BXI. From a practical standpoint, switching from one MPI implementation to the other is achieved through a call to S4BXI’s `s4bxi_use_smpi_implem` function, which needs to be performed by all simulated processes. Therefore, it is the responsibility of the application’s developer to ensure that all MPI ranks change their MPI model at the same point in the application. In particular, it is important for all sides of each communication to be performed in the same model: for example, a “send” and a “receive” must be performed with the same MPI implementation on both processes involved. The initial implementation to use when the simulation starts can be configured using the environment variable `S4BXI_SMPI_IMPLM`. The resulting control flow of an MPI call is depicted on Figure 6.6. This figure can be compared to the method of Chapter 5 which does not involve a middleware, and is depicted on Figure 6.5.

6.4 Maintaining MPI’s internal coherency

In the development of our middleware, there is a difficulty that needs to be considered: we cannot simply redirect MPI calls to the currently used implementation, otherwise any switch between the MPI models would cause crashes in our simulation. The reason is that some function calls must be forwarded to both implementations instead of just one, in order to maintain a consistent state in both implementations of MPI: the most obvious examples are `MPI_Init` and `MPI_Finalize`, which need to be called in both implementations in order to set them up correctly. Furthermore, the state of both implementations needs to be kept in sync in other places too: in MPI, users can create their own communicators, by splitting the global communicator (`MPI_COMM_WORLD`, which holds every process of the current job), which is useful to perform collective operations on a subset of the MPI ranks in the current job. Similarly, users can create their own datatypes, from combinations of the basic types that MPI provides, in order to simplify the transmission of message containing custom data structures. These communicators and datatypes are opaque types from the point of view of the user’s application: they are only manipulated through MPI calls, and therefore their internal structure is left to the implementation. As a consequence, the internal data structure created in one MPI implementation cannot be used in the other, but we still need the datatypes and communicators that are created in one model to be usable in the other.

The simplest way to achieve this is again to call both implementations regardless of the current model: when an application creates or modifies a communicator or a datatype, we forward these modifications to both implementations. To appropriately dispatch these modifications, we add wrappers around communicators and datatypes, called respectively `BxiMpiComm` and `BxiMpiDatatype`. Their function will be explained by using communicators as an example, even though datatypes work in a very similar way.



The declaration of `BxiMpiComm` is shown on Figure 6.7.

As we can see on the figure, our wrapper holds a reference to the implementation of the current communicator in both models (Atos's OpenMPI and SMPI). The three utility functions are used to either fetch a specific implementation (`bull_comm` and `smpi_comm`), or get the correct one according to the current configuration (which model is currently being used), with `implem_comm`. This last function also needs to handle specific communicators, such as `MPI_COMM_WORLD` and `MPI_COMM_SELF`. Indeed, these communicators are not user-created: `MPI_COMM_WORLD` automatically holds all MPI ranks of the current job, and `MPI_COMM_SELF` only contains the current process. It is worth noting that even though C and C++ are statically typed languages, we can manipulate SMPI communicators, Atos communicators, and S4BXI communicator wrappers using the type `MPI_Comm` every time,

```

1 class BxiMpiComm {
2   public:
3     MPI_Comm bull;
4     MPI_Comm smpi;
5
6     static MPI_Comm implem_comm(MPI_Comm original);
7     static MPI_Comm bull_comm(MPI_Comm original);
8     static MPI_Comm smpi_comm(MPI_Comm original);
9 };

```

Figure 6.7: `BxiMpiComm`'s class declaration

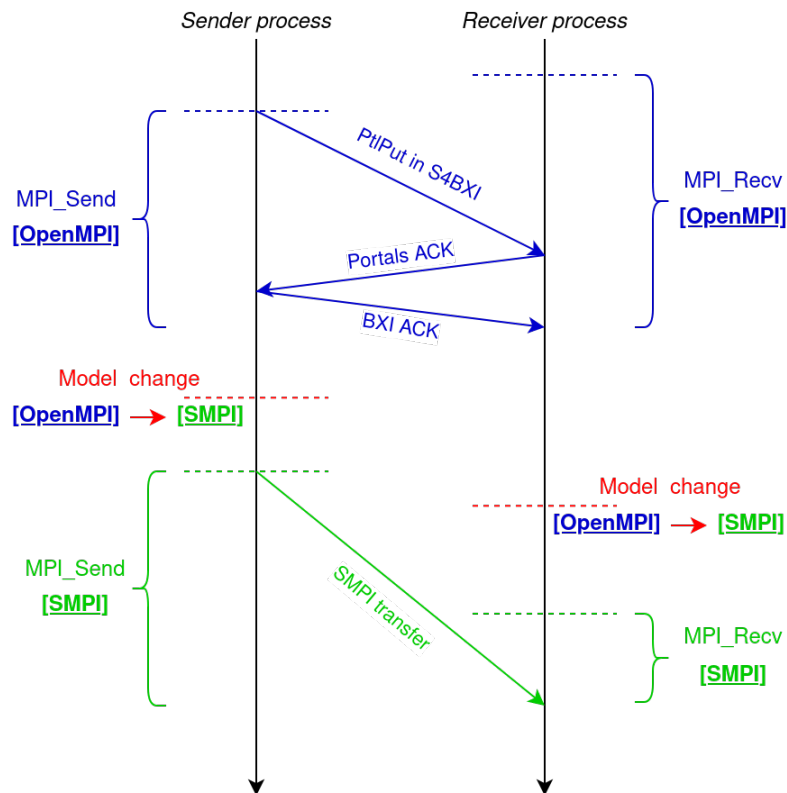


Figure 6.8: Sequence diagram for two MPI data exchanges, after adding our middleware

because in all three cases an `MPI_Comm` is an opaque type corresponding to a pointer, and therefore it always has the same size. Unfortunately, we do not have any way to keep type safety here without making many modifications in SMPI or Atos's MPI, because both models implement the same specification (MPI), and therefore they have to use the same names for communicators and datatypes. As a consequence, we have to be very careful when casting an `MPI_Comm` to any of the three implementations (two models plus our wrappers), since we are losing type safety by using one general type to store pointers to more specific structures. Thankfully this is completely transparent to user applications, as casts only appear in our middleware where extra care has to be taken to avoid errors when casting types. For example, in `implem_comm`, the parameter `original` comes from the application, and therefore it hides a pointer to a `BxiMpiComm`, whereas the return value will hide a pointer to an `MPI_Comm` from either Atos's implementation or SMPI. `bull_comm` and `smpi_comm` also take the same parameter, but they always return the same kind of `MPI_Comm`.

An example of communications using our middleware is depicted on Figure 6.8, where a sender process will first transmit a message to the receiver process in the OpenMPI over S4BXI implementation of MPI, and then a second message in the SMPI implementation. The associated code is shown on Figure 6.9 We can see that the first transfer uses Portals, which is implemented by S4BXI, whereas the second one is simply handled by SMPI with a more simple model. We can also see that it does not matter if model changes do not occur at the exact same simulated time in all MPI ranks, as long as both sides of each communication (a synchronous send and receive here) are performed in the same model.



```

1 #include "mpi.h"
2
3 #define SENDER 0
4 #define RECEIVER 1
5
6 int my_rank, data;
7
8 void exchange_data() {
9     if (my_rank == SENDER)
10        MPI_Send(&data, 1, MPI_INT, RECEIVER, 0, MPI_COMM_WORLD);
11     else if (my_rank == RECEIVER)
12        MPI_Recv(&data, 1, MPI_INT, SENDER, 0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
13 }
14
15 int main(int argc, char *argv[]) {
16     MPI_Init(&argc, &argv);
17
18     // Fetch the rank of current process (it's the same in
19     // both MPI implementations, either one can be used)
20     MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
21
22     // Start with OpenMPI (could be configured using the
23     // S4BXI_SMPI_IMPLM=0 environment variable instead)
24     s4bxi_use_smpi_implem(0);
25
26     // Exchange data using OpenMPI: SENDER will send "42" to RECEIVER
27     if (my_rank == SENDER)
28         data = 42;
29     exchange_data();
30
31     // Switch to SMPI
32     s4bxi_use_smpi_implem(1);
33
34     // Exchange data using SMPI: SENDER will send "43" to RECEIVER
35     if (my_rank == SENDER)
36         data = 43;
37     exchange_data();
38
39     MPI_Finalize();
40     return 0;
41 }

```

Figure 6.9: Code for two MPI data exchanges, after adding our middleware

6.5 Making model changes more lenient

At this point, our method to switch models dynamically works in most cases, but there are conditions under which model changes could cause a crash: asynchronous operations. For example, if an application starts an operation in Atos’s MPI, then switches to SMPI, and finally waits for the completion of the request, an error would occur at runtime. Indeed, calling SMPI’s `MPI_Wait` primitive with an `MPI_Request` created by Atos’s implementation is obviously erroneous (as requests are also an opaque type with very different underlying implementations). This specific example is depicted on Figure 6.10.

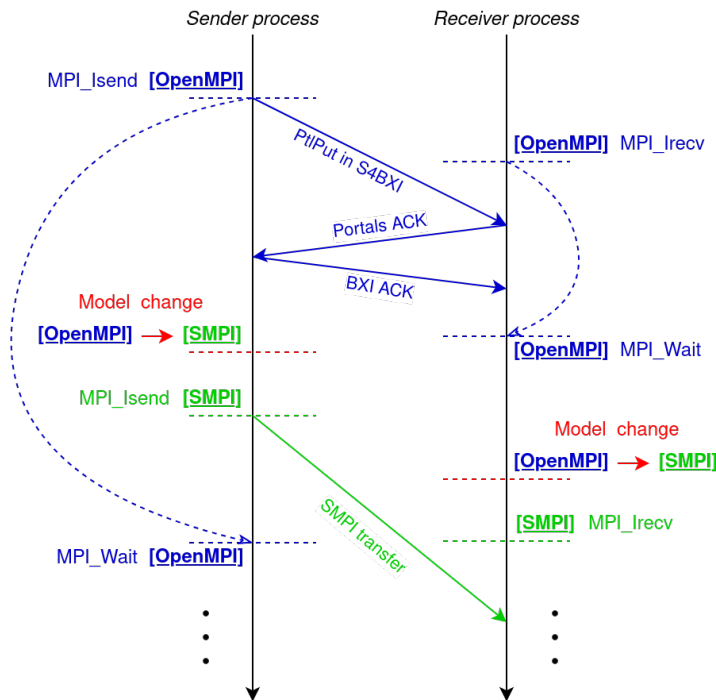


Figure 6.10: Illustration of problematic asynchronous operations: sender process waits on an OpenMPI request after switching to the SMPI model

In order to handle this issue, and allow users to switch models at nearly any point in the execution of their application, we keep track of asynchronous requests created by the user. In this context a request is a broad concept, as it could represent any asynchronous operation: a “send”, a “receive”, a full collective communication, etc. We keep track of all asynchronous requests created in the SMPI implementation of MPI and to complete an asynchronous request we check the model in which the request was created, i.e. whether it is tracked as an SMPI request or not, and switch to the adequate model to handle the completion event.

The way we implement it is with a C++ `unordered_set`, in which we store a pointer to every `MPI_Request` that is created in the SMPI implementation of MPI. Then, each time a request is queried (by `MPI_Wait`, `MPI_Test`, etc.), instead of checking the model in use for the current Actor globally, we look for the request in our `unordered_set`: if we find it, then it is an SMPI one, and therefore we must use the SMPI variant of the requested primitive, even if the user switched to OpenMPI in the meantime. Conversely, if the request is not found, then it is an OpenMPI one, and we must use Atos’s primitive. If we go back to



our example on Figure 6.10, with our asynchronous request tracking, the sender process will use OpenMPI's `MPI_Wait` on the request created by the first `MPI_Isend` even though the application switched to SMPI in the meantime.

This new addition to the middleware implies that the change of model is no longer happening all in one go, when the user requests it, since a few communications are still on their way and will be handled in the model previously in use. This could be perceived as a problem for the interpretation of the simulation result, as the two models are mixed, but events that are interpreted in the “previous” model are not causing any communication: they are only primitives that test the completion of requests. Consequently, these events interpreted in the “wrong model” are not going to cause major discrepancy in the accuracy or speed of the simulation. Additionally, in realistic cases it is likely that users will switch model in places where few asynchronous requests are pending, therefore very few MPI calls will use the “previous” model.

Finally, a concern we had while implementing this feature regards performance: when using SMPI, each time a primitive takes a request as a parameter, our `unordered_set` of pointer will be traversed to determine the model to use (in the case of Atos's OpenMPI, the `unordered_set` would be empty most of the time so the problem is not as significant). We feared that this might be costly in terms of CPU time, which is why we tested different structures to keep track of requests, and concluded that the `unordered_set` is the most performant. In the end, across the applications we tested, the difference in performance between keeping track of SMPI requests or not ends up being negligible, therefore we did not add an option to turn off this feature when using S4BXI's MPI middleware.

6.6 Experimental results

In order to test our model changes, we used three applications: OSU micro-benchmarks, Quicksilver, and HPL. Since HPL gives very similar results in simulations that are completely in SMPI or completely in OpenMPI over S4BXI, we did not obtain any noticeable difference in performance by adding model changes, and therefore this section will only present our results with OSU micro-benchmarks and Quicksilver.

6.6.1 OSU micro-benchmarks

In order to change models in OSU micro-benchmarks, we set the number of iterations over the benchmarked primitive to 110 (10 warmup ones and 100 measure ones), using the benchmarks' configuration parameters. Then we added a check in the code of each benchmark in order to switch model after a configurable number of iterations. Each time we started with SMPI, and we switched to OpenMPI over S4BXI after either 0 iterations (so instantly at startup), or 10, 20, 30, etc. all the way to 110 (in which case OpenMPI over S4BXI is not used at all). Plotting the results of our simulations is not trivial: there are 31 benchmarks, 11 different points at which we change models, and many message sizes. The resulting data ends up spanning over four dimensions, therefore we had to make choices about what to depict. We started by performing the same calculations that we presented in Section 5.5.1, in which we showed the average error and the slowdown of simulators. However, in this section, we compare 11 different models (with a variable proportion of each implementation) instead of just two, therefore it was not convenient to plot all 31 benchmarks side-by-side. For this reason, we will plot the average of the 31 average errors, and the average of the 31 slowdowns, as a function of when we switch our network model.

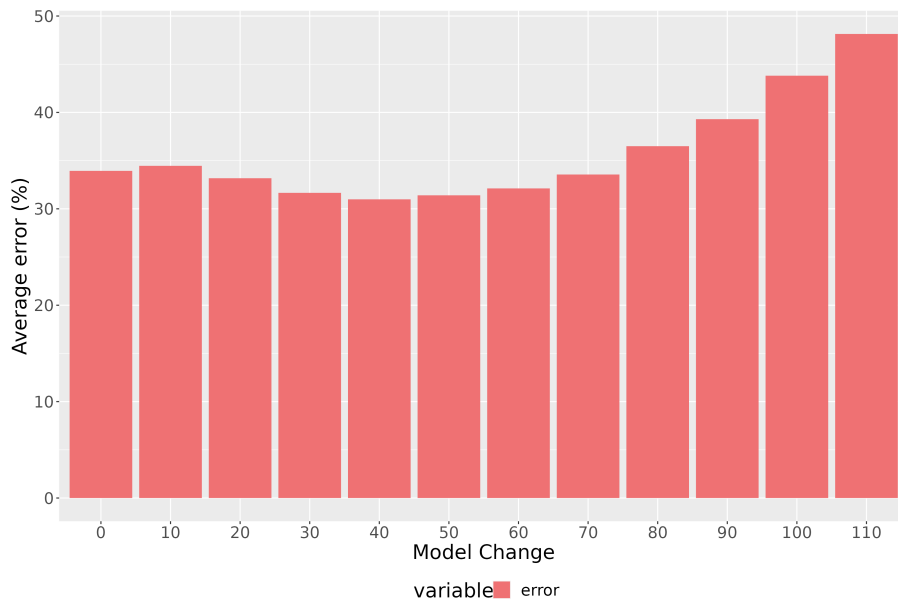


Figure 6.11: Average error across all OSU benchmarks, as a function of when we switch our network model (16 processes)

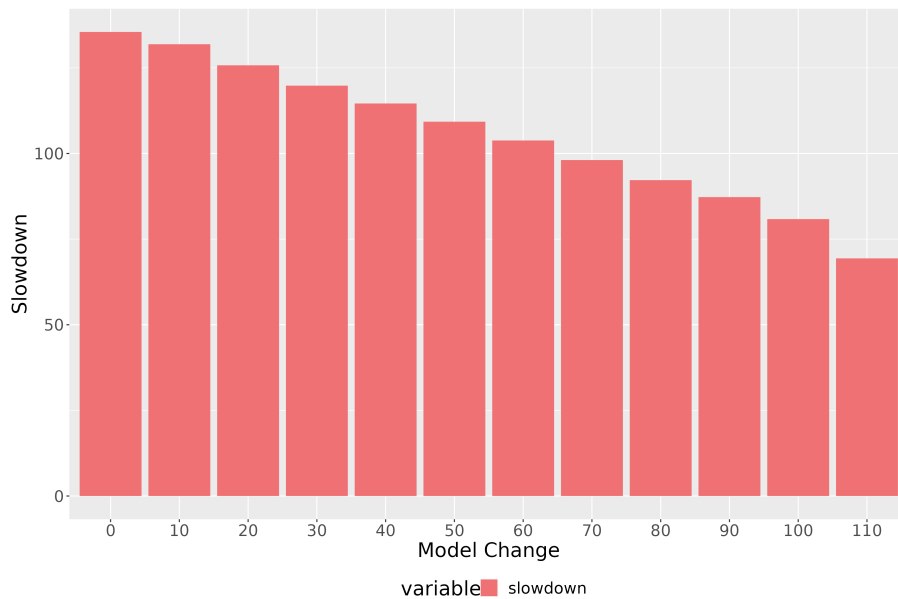


Figure 6.12: Average slowdown across all OSU benchmarks, as a function of when we switch our network model (16 processes)

From a technical point of view, we used similar settings as we did in Chapter 5: executions on 16 nodes with one process per node, as well as eight nodes with four processes per node, and simulations on one of the machines from our real-world cluster.

For 16 MPI ranks, the accuracy of our simulation method is shown on Figure 6.11. As expected, an execution using only OpenMPI over S4BXI (on the left) is more accurate than using only SMPI (on the right). We can also see that there is little difference in accuracy if we change models instantly or after ten iterations. This is also expected since the first



ten iterations are just warmup, and are not timed by the benchmark. In the middle, we can see that, in this particular case, the errors of both network models cancel out for some benchmarks (in the case where one model is too optimistic and the other too pessimistic), which gives us an even slightly lower error than with only OpenMPI over S4BXI.

From a performance perspective, we can see on Figure 6.12 that the more we use SMPI, the smaller the slowdown is, as expected.



Figure 6.13: Average error across synchronous OSU benchmarks, as a function of when we switch our network model (32 processes)

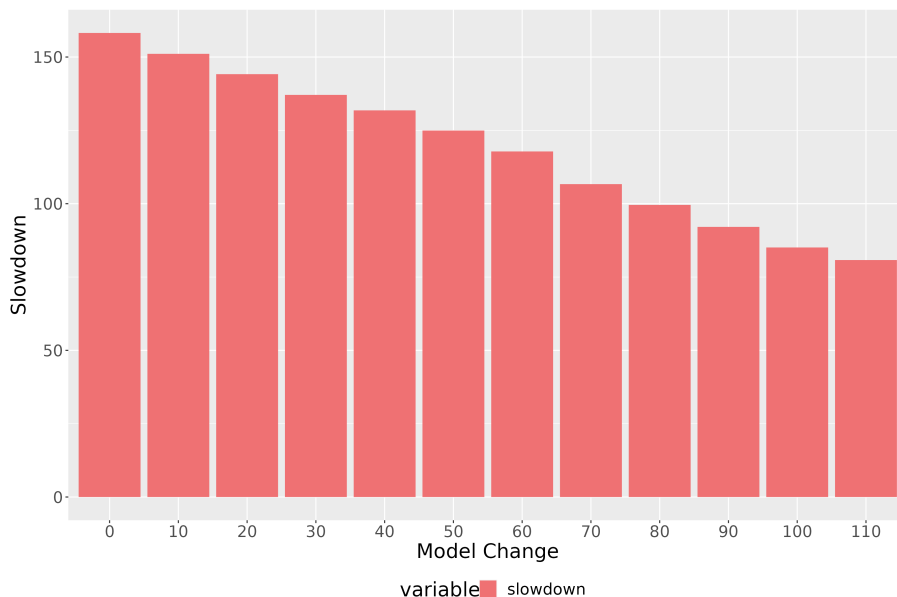


Figure 6.14: Average slowdown across synchronous OSU benchmarks, as a function of when we switch our network model (32 processes)

For 32 MPI ranks on the other hand (8 nodes and 4 processes per node), the results are a bit different. We need to differentiate two cases, which give us very different results: synchronous and asynchronous operations. In the case of synchronous operations, we get the similar results as with 16 MPI ranks, as depicted in Figure 6.13 for the accuracy, and Figure 6.14 for the performance of our simulations.



Figure 6.15: Average error across asynchronous OSU benchmarks, as a function of when we switch our network model (32 processes)

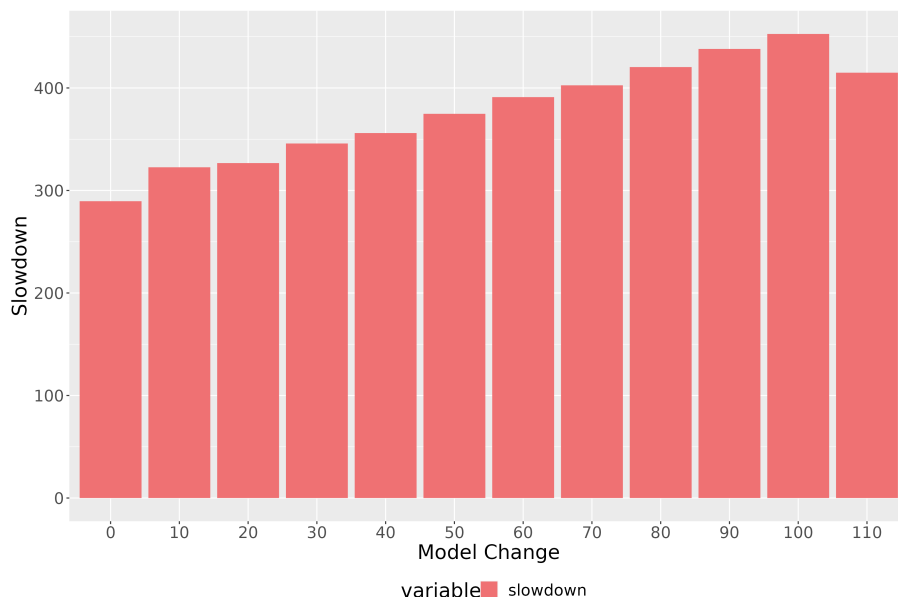


Figure 6.16: Average slowdown across asynchronous OSU benchmarks, as a function of when we switch our network model (32 processes)

For asynchronous operations, the results are way more variable between the different



operations (in particular the IAllGather primitive is very pathologic in SMPI), and therefore looking at averages is not as meaningful. For accuracy, we can see on Figure 6.15 that the results are similar to everything we have seen so far: our approach performs better than SMPI in average, and if we change models around the middle of each benchmark we get an even better accuracy because errors from both models cancel out (luckily). From a performance perspective on the other hand, Figure 6.16 shows that our approach is faster than SMPI, even though our model is more detailed. This is unexpected, but after discussing asynchronous collectives with SimGrid’s development team, it seems that these operations are rarely used in real applications (indeed, we never encountered them in our studies), and therefore there has been less work put into optimizing them. This is why we did not spend more time studying them in more detail. Instead, we decided to benchmark more realistic applications.

6.6.2 Quicksilver

After testing our approach for model changes on OSU benchmarks, we tried it on Quicksilver: since this application performs ten cycles of computation, that are relatively independent, it was easy to add model changes between cycles in the code. Therefore, we executed Quicksilver in simulation for 11 different configurations: we always started with SMPI, and then we switched to our approach after a variable number of cycles. As a result, we have eleven simulations for 100% SMPI usage, 90% SMPI usage, 80%, etc. all the way to 0%, if we switch to OpenMPI over S4BXI immediately at startup. From a technical perspective, simulations are executed on a desktop computer, which has an Intel® Core™ i9-10850K CPU and 32 GB of RAM. Once again, the resulting data is very large, as these model changes add a new variable to our simulations, along with the existing ones: number of nodes used, number of processes per node and number of initial particles fed to Quicksilver (which correspond to the problem size). As a result, we will not study every graph, but instead we will explain the trends that we observed when each variable changes.

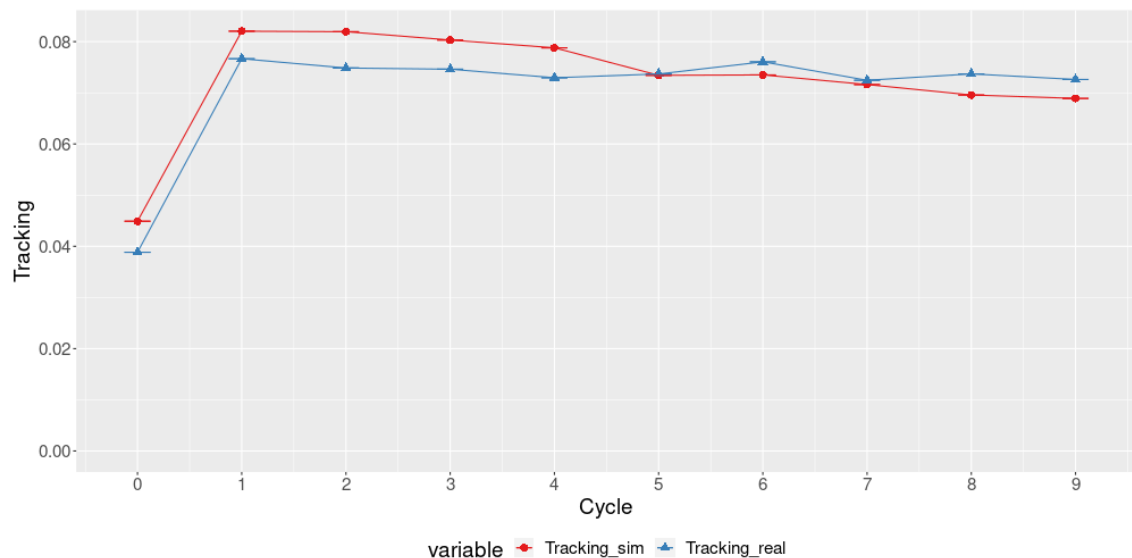


Figure 6.17: Accuracy of Quicksilver’s simulation on 4 MPI ranks, with a model change from SMPI to our approach after cycle n°4, with 10,000 input particles

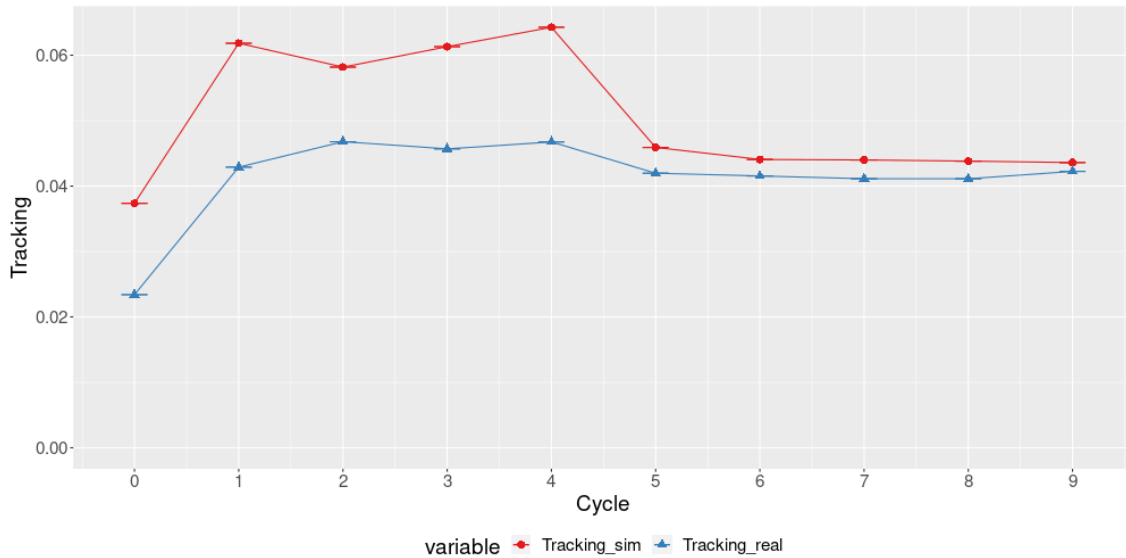


Figure 6.18: Accuracy of Quicksilver’s simulation on 8 MPI ranks, with a model change from SMPI to our approach after cycle $n^{\circ}4$, with 10,000 input particles

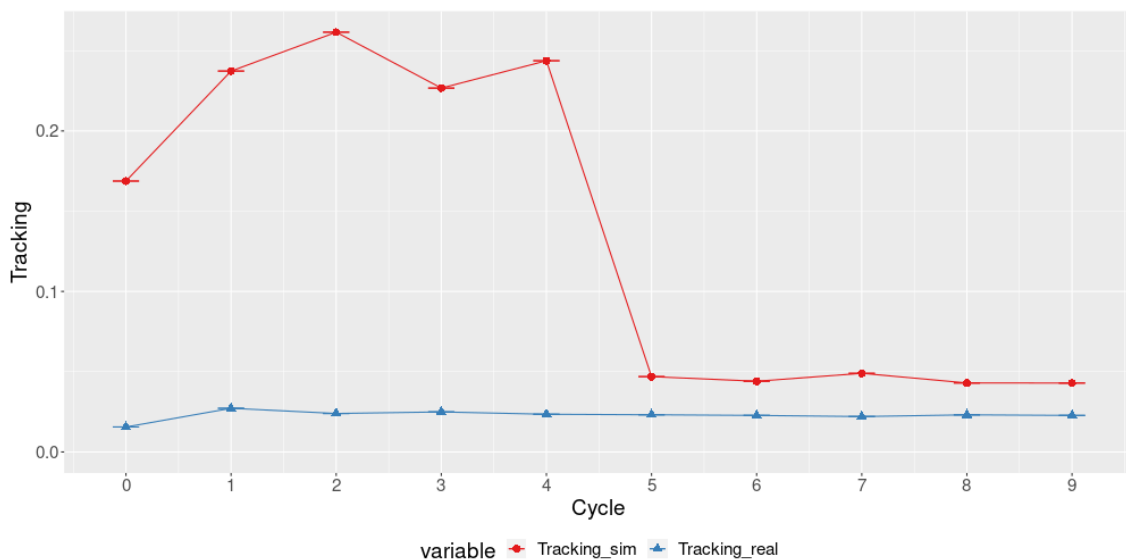


Figure 6.19: Accuracy of Quicksilver’s simulation on 16 MPI ranks, with a model change from SMPI to our approach after cycle $n^{\circ}4$, with 10,000 input particles

Regarding accuracy, the simulations behave as we expect based on the results of Chapter 5: as we have seen in Section 5.5.3, SMPI shows a good accuracy as long as we model a small number of MPI ranks. To visualize this, we plotted the result of three different simulations: all of them use 10,000 input particles, and they switch from SMPI to OpenMPI between the iterations four and five, therefore the left part of each figure shows SMPI’s accuracy, and the right part shows our approach’s accuracy. Figure 6.17 shows that the accuracy remains good during the whole simulation if we run Quicksilver on four MPI ranks (four nodes and one process per node). On the other hand, Figure 6.18 shows a lack of accuracy at the start of the simulation when we use eight MPI ranks (eight nodes and



one process per node). Finally, Figure 6.19 shows that this lack of accuracy of the SMPI part of the simulation only increases with the number of MPI ranks, as we have seen previously, since the figure depicts a run on 16 MPI ranks (16 nodes and one process per node). In all cases, when we switch to the OpenMPI model, the accuracy improves, as expected.

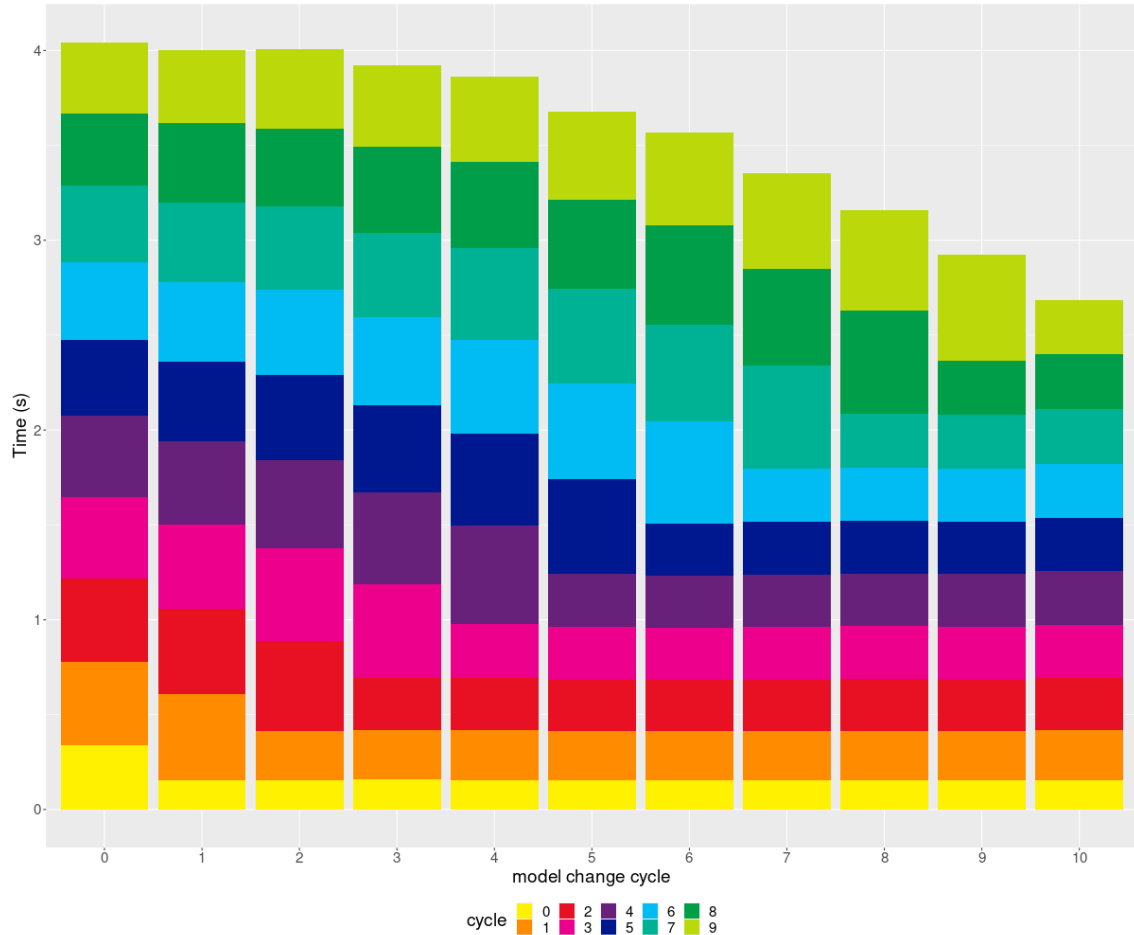


Figure 6.20: Performance of Quicksilver’s simulation on 4 MPI ranks, with 10,000 input particles

From a performance perspective, the results that we obtain are more surprising. In an attempt to better understand our data, we plot the performance of the simulation for each model change position, therefore we have 11 bars that each represent a simulation. However, inside each bar, we also display the performance of each cycle individually, with the first cycle at the bottom, and the last one at the top. Figure 6.20 shows the performance of simulations on four MPI ranks, and we can see that our model changes behave as expected: the simulation using only our approach (highest bar on the left) is slower than a fully SMPI simulation (lowest bar on the right), and in between the performance improves (lower and lower bars) as we increase the proportion of SMPI use.

However, for simulations of more than eight MPI ranks, the performance follows a very unexpected pattern. This is depicted on Figure 6.21, with simulations on eight nodes and one process per node: we can see that the performance of the simulation is the worst when we switch models after cycle number five. In other words, it is faster to perform a simulation exclusively with our approach, rather than using SMPI for the first half. If we

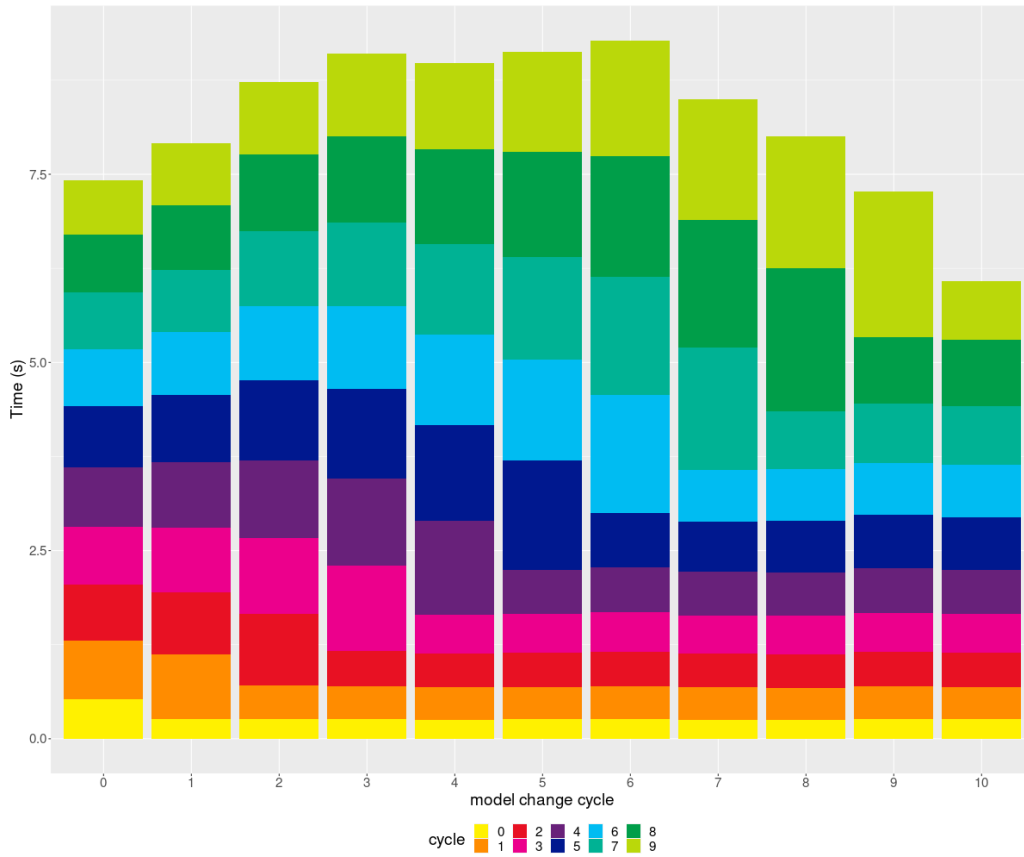


Figure 6.21: Performance of Quicksilver's simulation on 8 MPI ranks, 10,000 input particles

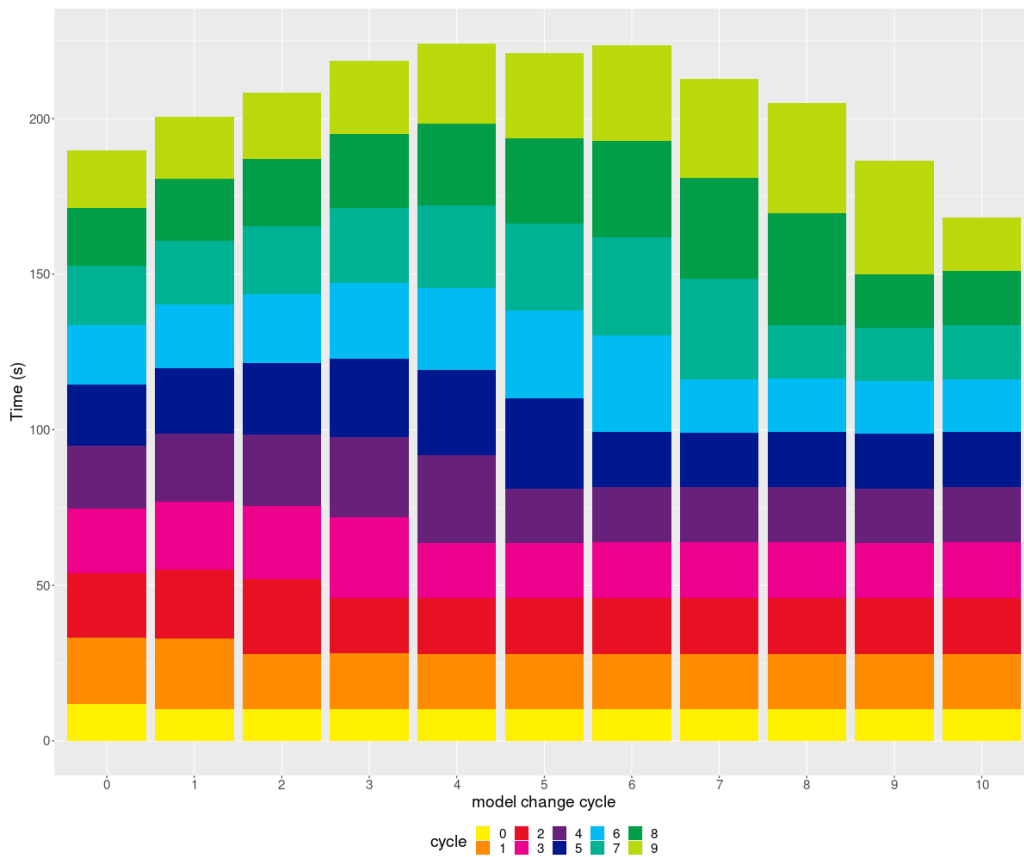


Figure 6.22: Performance of Quicksilver's simulation on 8 MPI ranks, 1,000,000 input particles



look at the performance of each cycle individually, we can see that the first cycles (lower on the bars) always have the expected duration: they are slow when performed with OpenMPI over S4BXI, and quicker when performed with SMPI. On the other hand, later cycles have a completely unexpected performance, as it seems that running SMPI at first slows down the later cycles (although each cycle should be independent, at least from the point of view of communications). Although this change in behavior reminds us of the performance loss of SMPI as the number of MPI ranks increases, it is a distinct phenomenon: indeed, it always happens around the same number of MPI ranks, and it does not vary with the problem size. We can confirm this on Figure 6.22, where the same simulations are executed, but with 1,000,000 input particles.

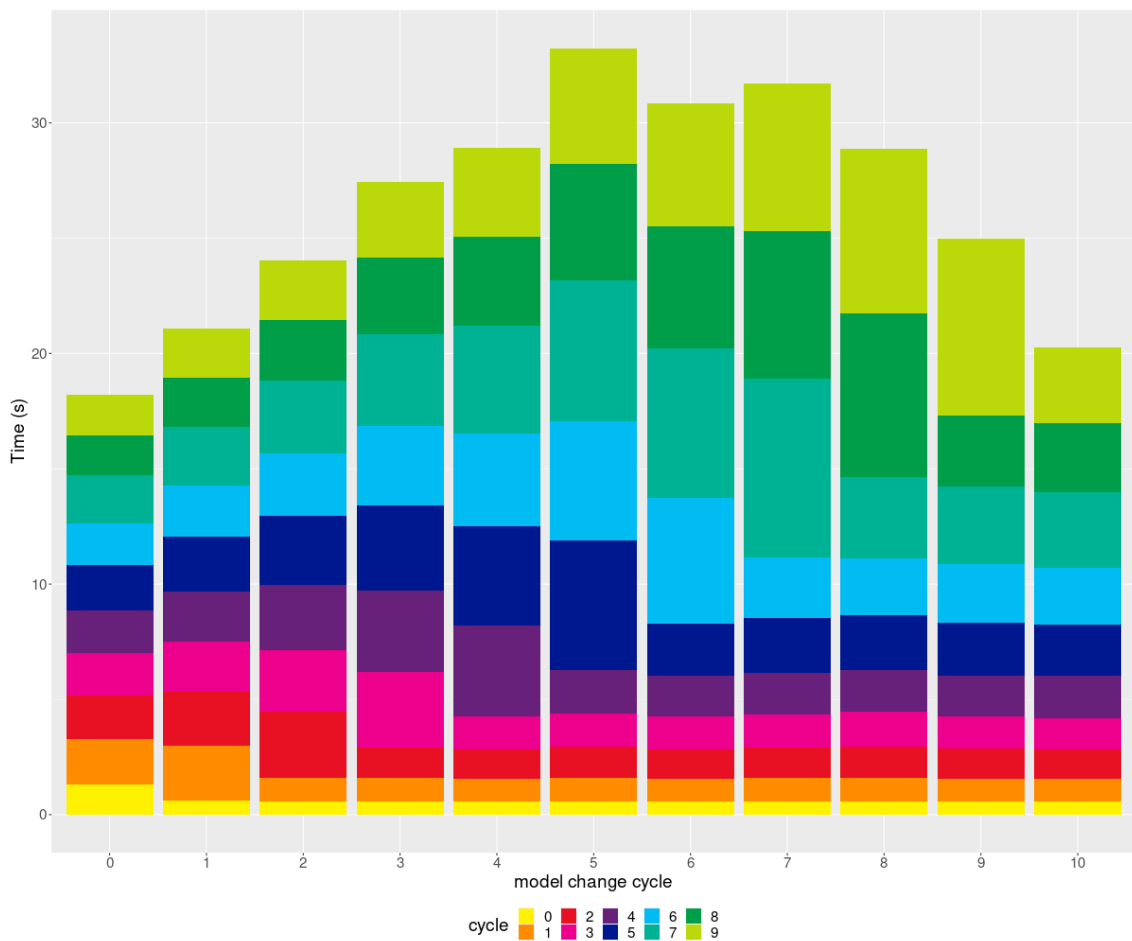


Figure 6.23: Performance of Quicksilver’s simulation on 16 MPI ranks, with 10,000 input particles

Finally, we can see on Figure 6.23 that this oddity in our performance measurements only gets worse as we increase the number of MPI ranks: the figure depicts runs on 16 nodes and one process per node. It gets even worse since we can see that a simulation which uses only our approach is faster than a simulation with only SMPI. This confirms that Quicksilver is particularly pathologic for SMPI, for a reason that we still do not know, even after running thousands of simulations. Indeed, our analysis of performance (using

Linux’s `perf` tool²) reveals that a large amount of time is spent in SimGrid’s code, but it is not trivial to retrace the calls that might have caused this behavior in SMPI, S4BXI or users’ applications, since Actors issue “simcalls” that are then executed in an entirely different context by SimGrid.

6.7 Concluding remarks

All of these experiments, on OSU micro-benchmarks and Quicksilver, show several results: first, our model changes behave as expected in many situations. However, as we have seen, there are several configurations in which our results are unexpected, and model changes do not help performance at all (in the worst case it can even lower the performance of simulations). This shows that making our simulation method more and more complex also makes it more unpredictable, which is what we wanted to avoid in the first place, by making simulations instead of real-world experiments. Additionally, we can see that even in favorable cases, the difference in performance between an experiment fully on SMPI and fully on OpenMPI is not large enough to make model changes really useful. Even though switching models can speed up simulations, the order of magnitude of the execution time is similar, and therefore it will not be sufficient to model clusters of a very different scale, at least in the current state of our development.

Overall, our work shows that dynamic model changes are achievable without modifying any of the two MPI implementations involved. However, to make them more useful it would be beneficial to use two models with a more important difference in performance. For example, we could use an MPI implementation more simplistic than SMPI, or a very detailed emulator instead of OpenMPI over S4BXI. Therefore, we believe that our work provides a good framework, which could be built upon to create simulators with a flexible performance / accuracy tradeoff.

²<https://github.com/torvalds/linux/tree/master/tools/perf>



Chapter 7

Ongoing and future work

Through chapters 4 and 5, we have shown that our simulation method is flexible, as it models low-level properties of the hardware, but still allows the simulation of full applications on top of high-level APIs. This opens the door to many potential studies using our simulator. In this chapter, we present some ongoing work and ideas. Some are already implemented, but require additional work to be considered as fully completed, while others are only ideas that can be explored in future work. In particular, we will present a study on flow-control, which is a feature being investigated as part of the design process for the next-generation BXI hardware. We also present a few ideas of how S4BXI could be used in the future.

7.1 Flow control in BXI

In networking, flow-control consists in limiting the amount of data that can be sent on a given channel, typically to avoid saturating a shared link. The flow-control currently available in Portals only covers a very specific issue: a “flow control situation” happens when a node receiving messages runs out of resources to handle the incoming traffic (for example when there is no ME or LE to process a request). When this happens, the target NIC completely disables the corresponding Portals Table entry (PT), which will cause the initiator NIC to receive ACKs with an error status, and it notifies the user application. It is then the responsibility of the application to fix the problem which triggered flow-control, and enable the PT again. This mechanism is designed to handle extreme cases of resource exhaustion, and leaves a lot of responsibility to the application. The hypothesis we want to test is whether it would be beneficial to implement a different version of flow control, where the NICs would limit the number of messages inflight to another node, which would lower the congestion on the cluster, and avoid situations of resource exhaustion. In particular, we want to test two cases: limiting the number of messages inflight between two NICs, and limiting the number of messages inflight between two processes. As it turns out, these two options are already implemented in software in OpenMPI. Therefore, it would be interesting to compare the performance of the network when this type of flow control is enabled in software, in OpenMPI, and when it is implemented in hardware directly. To test this last scenario, a real-life experiment would require the design and manufacturing of several NICs, while we can estimate the effect of this change with a few modifications of our simulator.

In order to check the efficiency of the different flow control implementations, we designed the experiment depicted on Figure 7.1: our simulated platform consists of two

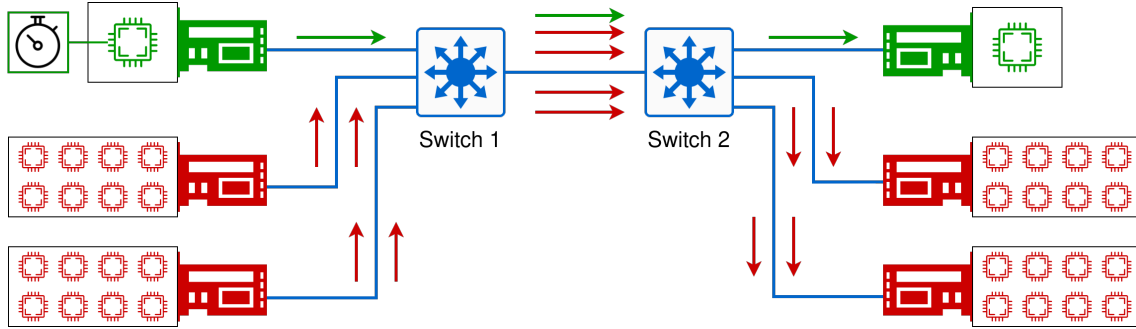


Figure 7.1: Our flow control experiment

switches connected together, with the same number of machines connected to each switch. This way machines connected to *Switch 1* that communicate with machines connected to *Switch 2* will share a common BXI Link. While this is a very simple topology, it is representative of real-world scenarios as pruning is very common in HPC clusters, which means that most of the time there will be shared links of this sort between switches (this is especially common in fat-tree topologies). The workload that we simulate is simple: pairs of machines (two in the figure) run several processes each (eight in the figure), which will flood the network by sending as many 16MB messages as possible to each other. While this is not what a realistic application would do, it does emulate realistic situations where an application running on many nodes would have an intense communication phase. On the other hand, the remaining pair of machines simply runs one process each, which sends a fixed amount of 16MB messages sequentially. We measure the latency between the second pair of machines (top pair of Figure 7.1), which gives us an estimate of the congestion on the shared BXI link.

As this experiment was conducted in parallel with the rest of our work (in particular in parallel with the simulation of MPI), it evolved along with our simulation method. Initially, we implemented this small benchmark with Portals directly, and measured the latency of sequential messages for different values for our flow control: how many messages are allowed inflight between pairs of nodes or pairs of processes. The result of our simulations at that time is depicted on Figure 7.2, which was obtained for messages of one megabyte and only one pair of machines flooding the network (with eight processes on each machine). On this figure, the lowest horizontal line corresponds to the latency of messages when no machine is flooding the network (which correspond to a simple point-to-point sequential transfer). The top dotted line corresponds to the latency of sequential messages when flooding machines are at their full speed, with no flow control at all (which is what the current BXI hardware would do). The two curves correspond to the latency of messages for different values of process-level flow control, and node-level flow control. The two curves are very similar except one is a translation of a factor eight along the x-axis of the other one; this is expected since flooding machines run eight processes each, therefore node-level flow-control is roughly eight times stricter than process-level flow-control. We can also see that if we limit the number of messages inflight to the extreme, the latency of messages gets very close to the scenario when no one is flooding the network. Even though our experiment is quite artificial, it gives us an idea of the effect that flow-control implemented in BXI hardware could have on the congestion on a cluster.

As we progressed in our work, we did our flow-control experiment again, but in more realistic conditions, using MPI instead of Portals. Therefore, we re-implemented



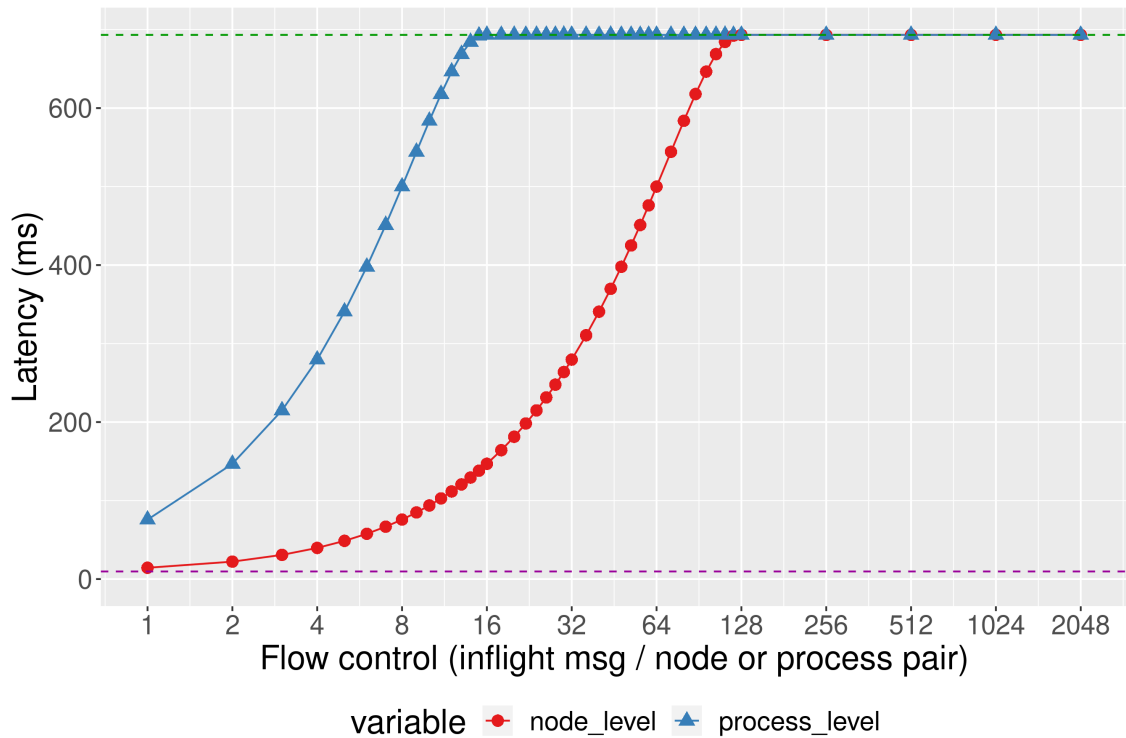


Figure 7.2: Results of our flow control experiment with Portals, 1MB messages, 1 pair of nodes flooding the network with 8 processes per node

our benchmark, as close as possible to the original one, but using OpenMPI instead of directly Portals for our communications. Running the experiment in the same conditions as previously gave us the results depicted on Figure 7.3. We can see that even though flow-control still affects the congestion on the network, the difference between a strict flow-control and no flow-control at all is much smaller. From this experiment, it seems that when messages are not slowed down by congestion, they can go nearly as fast with MPI as they were going with Portals directly. On the other hand, when we try to add congestion to the network, the nodes flooding the network do not manage to send as many messages inflight as previously. Therefore, the sequential transfers that we measure are not slowed down as much, and flow-control does not have an impact as important as previously. The conclusion we can draw from this experiment is that even though flow-control seems like an interesting feature to have in theory, in a real-world scenario there are many factors which can affect the amount of congestion on the network, which is why this type of simulation is a good tool to measure the expected performance of this type of feature.

Finally, we tried re-creating our experiment in a setting that is comparable with a real-world experiment, in order to increase our confidence in our simulation results. Of course, it is impossible to re-create our experiments on a real-world cluster, since the flow-control that we propose is not implemented in BXI v2 hardware. What we can compare in simulation and in the real world, however, is flow-control implemented in software. In particular, Atos’s version of OpenMPI offers two parameters to control the number of messages inflight in the BXI BTL: one to configure the limit of messages inflight, and one to control whether the “inflight message counter” should be shared between all processes of a node or not. By combining these two options, we can emulate in software an experiment which is quite

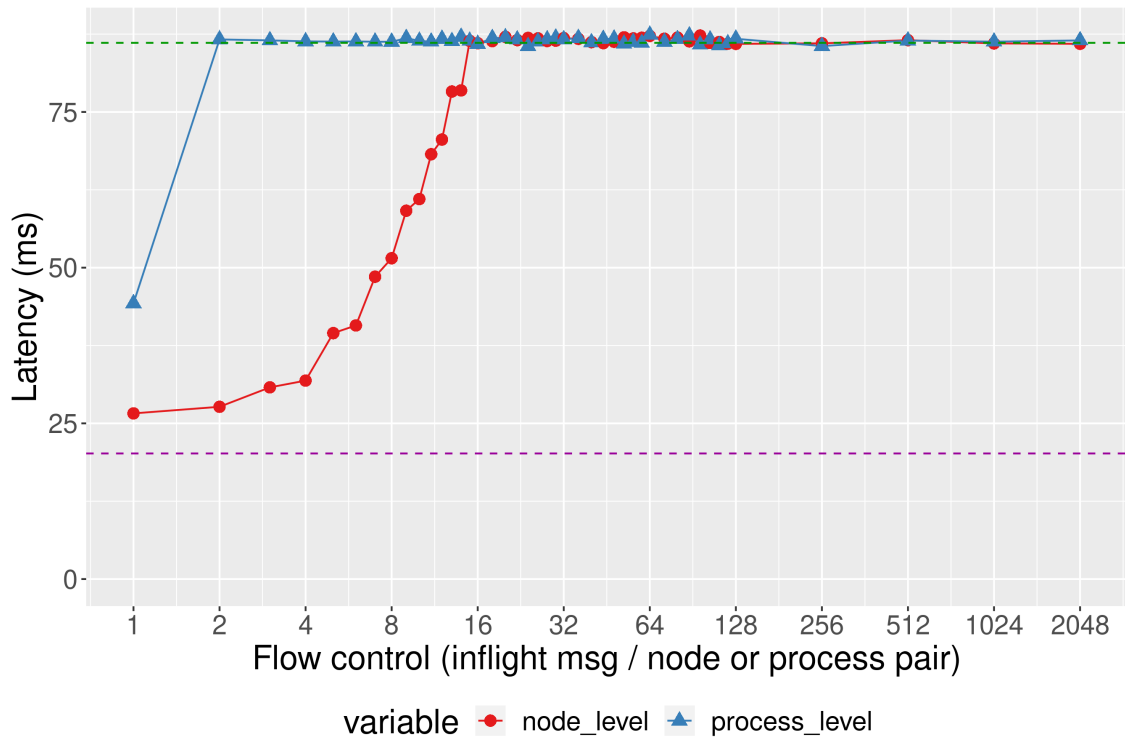


Figure 7.3: Results of our flow control experiment with MPI, 1MB messages, 1 pair of nodes flooding the network with 8 processes per node

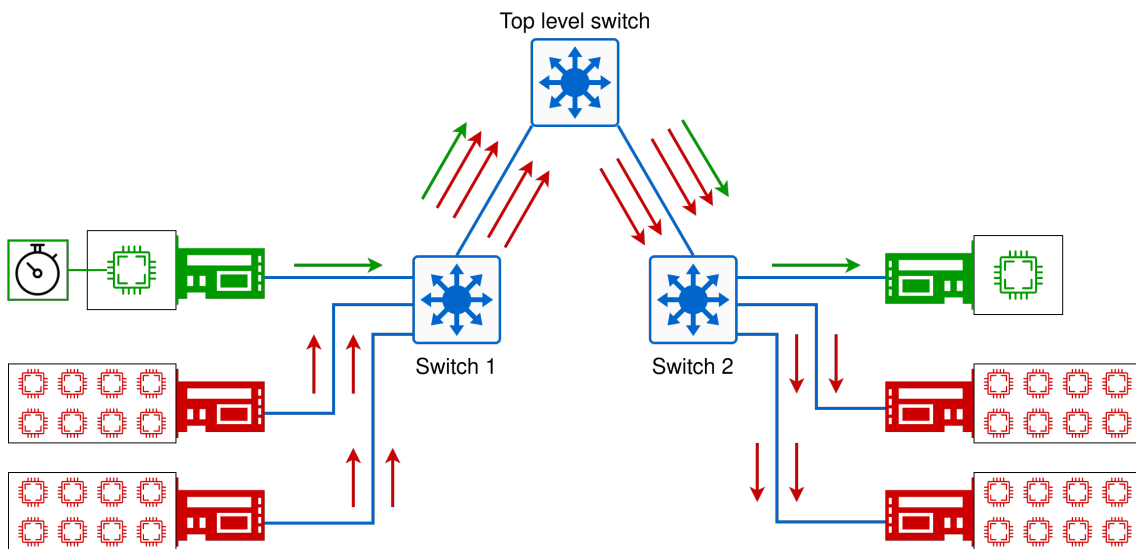


Figure 7.4: Flow control experiment compatible with our real-world cluster

close to the scenarios that we explored in simulation previously. Unfortunately, we realized that running the real-world experiment would also require changing our cluster's topology slightly: indeed, we did not have any machines available which were connected in the configuration depicted on Figure 7.1 (as it is very rare to have machines connected to switches connected to compute nodes and also directly together). Indeed, while this type of platform exists in Torus networks, in BXI we only have access to fat trees, where switches with compute



nodes are not directly connected to each other, but instead they are connected to a higher level of switches (closer to the root of the fat tree) . Therefore, we changed our experiment slightly, to the configuration depicted on Figure 7.4.

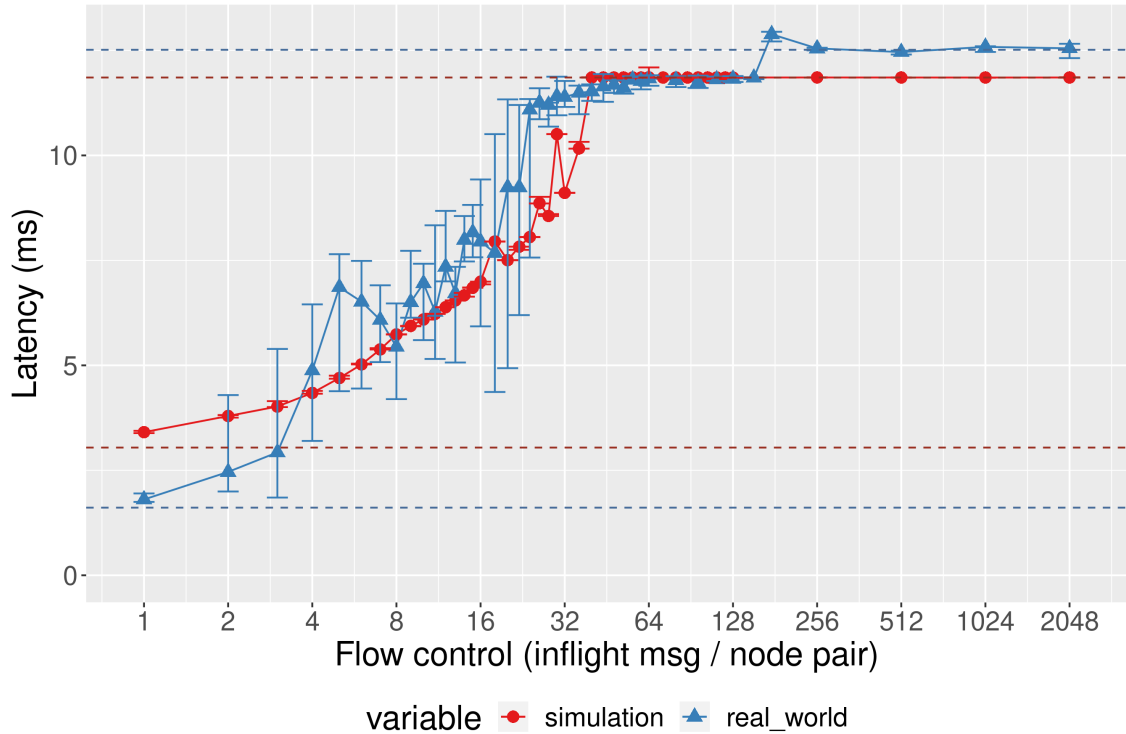


Figure 7.5: Node-level software flow control in OpenMPI, 16MB messages, 4 pairs of nodes flooding the network with 8 processes per node

For this experiment, both the simulation and the real-world cluster use the software flow-control implemented in MPI. The results are displayed on Figure 7.5 for node-level flow-control, and on Figure 7.6 for process-level flow-control.

It is important to note that in this configuration, we had difficulties obtaining meaningful results on the real-world cluster for two reasons. First, the machines used were quite slow, and we did not manage to create any significant congestion on the network, therefore we had to increase the message size to 16 megabytes, and to use four pairs of machines flooding the network (instead of just one previously). Second, we observed a lot of variations in our data, which made it very difficult to analyze. In an attempt to improve this point, we ran each real-world experiment ten times, and we removed the two biggest and two smallest values for each point, as we often saw “extreme” data-points with unrealistic values, which we believe must have been affected by phenomena outside of our control.

Regardless, we can see on both figures that even though our simulator is far from perfect, it captures well the order of magnitude that we can expect for the latency of messages when software flow-control varies. This is especially true for node-level flow-control (on Figure 7.5), where our results are close to the real-world data. For process-level flow-control, we can see on Figure 7.6 that setting the limit of inflight messages to one gives an extremely short latency for the flow of sequential messages, which we do not capture in simulation. Although this behavior is unexpected from the real-world run, we can see that it is a lot more consistent than other data points, as it has a very small variation

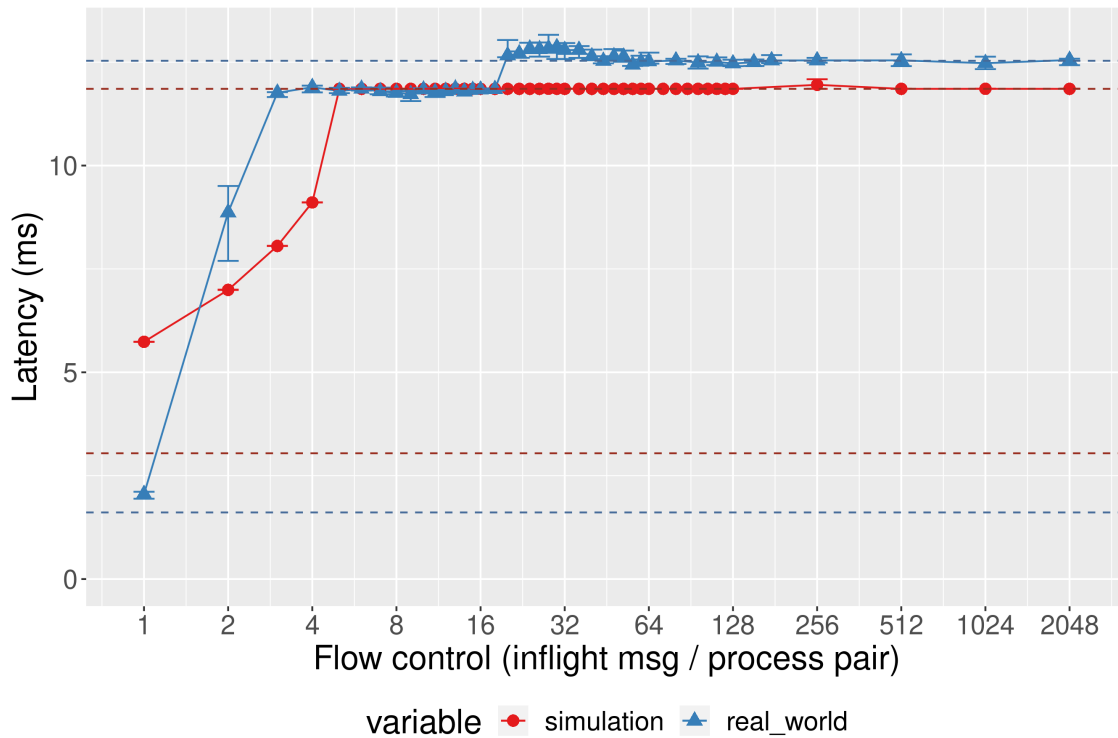


Figure 7.6: Process-level software flow control in OpenMPI, 16MB messages, 4 pairs of nodes flooding the network with 8 processes per node

across several runs (depicted by the error bar). Another unexpected result that we can see on both figures is the result for very lenient flow-control values: in both cases we can see a “jump” in latency, around 16 messages inflight on Figure 7.6 and around 128 messages inflight on Figure 7.5. Once again, this behavior is unexpected from the real-world, as we do not believe that there should be any special condition in OpenMPI’s code to operate any differently before or after this value. At a lower-level, in BXI, to the best of our knowledge the only instance where this value could appear is in the size of the command queues between the CPU and the NIC: each process can use 16 “slots” on the NIC’s memory to post commands. Therefore, it is possible that having to wait for a free slot in Portals’ library impacts the latency of flooder nodes differently than restricting the number of messages inflight in OpenMPI, one layer higher in the software stack. Unfortunately we lacked time to study precisely these unexpected behaviors of real-world hardware, therefore we did not test our hypotheses. Indeed, setting up experiments allowing us to validate or not these experiments is not trivial.

To conclude, we can see that even though our model of congestion in the context of software flow-control is not perfect, and does not take into account all the properties of the real-world experiment, it still gives us a decent estimation of the congestion that we can expect in such a scenario. These results give us confidence that the data we obtained when modeling flow-control in hardware shows the correct order of magnitude that we can expect for the congestion on a cluster, if flow-control was implemented in hardware in the next-generation of BXI NICs. Additionally, it is important to detail a few things about our workflow during the writing of this PhD: for every single experiment (real-world or simulation, S4BXI or SMPI) in chapters 4, 5 and 6, our figures depict data that was



obtained in the last weeks of this PhD, in parallel with the writing of this document, in order to ensure that all our experiments were reproducible with the latest version of OpenMPI, SimGrid, SMPI and S4BXI (no matter how old the original developments were). However, because of a lack of time and because of technical difficulties, we were not able to reproduce the results regarding flow control. Therefore, all the data of this chapter has been obtained a few months earlier, using the versions of SimGrid, OpenMPI and S4BXI available on 16th March 2022.

7.2 Future work

In addition to flow control experiments, our simulator and methodology are versatile enough to open the door to many potential studies. This section presents a few ideas that we did not have time to conduct ourselves.

OpenSHMEM: even though our work on OpenSHMEM already gave us promising results, our study using this API is very preliminary. Indeed, in order to make this type of simulation more robust, some bugs need to be fixed, and some function calls that are not currently supported by S4BXI need to be intercepted (and reimplemented in simulation), such as a few `pthread` utilities (mutexes for example, which would be easy to implement using SimGrid’s Mutexes). This would allow the simulation of larger scale OpenSHMEM applications, such as the “OpenSHMEM Benchmark suite” (OSB) [NAB⁺]. OpenSHMEM is a particularly interesting API to study because it leverages the full capabilities of the Portals API, whereas Atos’s OpenMPI uses a more limited number of primitives offered by Portals.

In order to improve OpenSHMEM support, a first idea would be to reference all function calls that should be intercepted by our simulator, but are currently not supported, to evaluate the difficulty of implementing them in simulation. It would also be important to check the address of symbols that are located by OpenSHMEM at startup, to see if the memory regions that are involved are different on each simulated process or not. If the addresses are identical, a modification to OpenSHMEM’s initialization would probably be necessary to use unique regions in each process, and better isolate them.

Additional low-level studies: it is important to note that even though our simulator offers a fairly low-level model, it is not suited to study effects that are visible at packet-level in the real-world. Nevertheless, our flow-control experiments show that S4BXI can be used to study the protocol implemented by BXI NICs in interesting ways. We believe that more experiments of this type could be performed, to test the different ways that Portals can be implemented.

As an example, the latest BXI hardware has a feature to disable end-to-end reliability, which is also supported in S4BXI, but we do not believe that the impact of this option on the performance of application has been studied in great detail. In this context, S4BXI could be used to evaluate the implications of making Portals unreliable, both in terms of functionality (how user application could handle the loss of a message), and in terms of performance (how big of a latency is saved by reducing the number of ACKs).

Additional MPI studies: one of the strengths of S4BXI is that it allows users to replicate how the real-world Atos’s MPI implementation works, in particular regarding the algorithms used for collective operations. This means that it would be a good tool to tune the collective algorithm to be used for different message sizes and cluster sizes. Indeed, this precise tuning is currently done on real machines, which is very time-consuming on a limited

amount of computing resources. In particular, it is very difficult to tune operations for more than 32 nodes, as the development clusters at Atos are small. This usage of the simulator has been discussed with the MPI development team at Atos, but it has not been done yet, because we chose to focus on the simulation of larger scale application. Nevertheless, tuning this type of algorithms would be a very good use case of S4BXI, as we have already seen in our benchmark that our approach models this selection accurately.

Further Vader tuning: currently all operations regarding shared memory in MPI (using the Vader BTL) are considered as “CPU time” by S4BXI, as all of MPI is considered as “user code” from the point of view of our low-level model. This means that copies of data in memory are simply benchmarked and then injected in the simulated time, similarly to how all computation time is accounted for. We believe that it would be more accurate to stop the benchmark of CPU time when entering the Vader BTL, and inject a set amount of time, that would be carefully calibrated as a function of the size of data to be transferred between MPI ranks. Indeed, the performance of memory accesses might exhibit a different performance when simulated processes run one at a time (in our single-threaded simulator), or all in parallel (in a real-world execution), therefore modeling these operations using a well-calibrated model could give better results. This approach would require patching OpenMPI further, and designing a way to calibrate the time that Vader operations take, but we believe that it would make the simulations more reproducible, as it would reduce the amount of benchmarked CPU time. This work would be very similar to the study that Tom CORNEBIZE conducted on HPL by benchmarking the `HPL_dgemm` function, therefore an efficient methodology to conduct this type of study is already available.

Perturbations on the network: in the simulated world, communications always complete gracefully, with no error. However, we know that in the real world a cluster can suffer from perturbations, for example data corruption (detected at the target side by a CRC check), or transient failures of some cables. In these cases, it is the responsibility of the E2E component of the NIC to retransmit messages, which has a huge impact on performance. These types of issues were not studied in depth in S4BXI, but it would be a good use case of our simulator. Indeed, S4BXI fully implements the E2E reliability of BXI, and SimGrid provides options to specify a “profile” for each Link, in order to disable it at specific times in the simulation. Such experiments could help improve the configuration of the E2E component of BXI, in particular the delay used before retransmitting messages.

Support for a wider range of parallelization techniques: currently S4BXI only supports Portals, MPI and to a degree OpenSHMEM, although in a realistic scenario many applications support running computations in parallel using both MPI and OpenMP. Currently, any OpenMP primitive would not be intercepted in S4BXI (or SMPI for that matters), and therefore it would spawn actual threads in our otherwise single-threaded simulation. As long as parallel sections in OpenMP do not perform any network operation (or any operation that could yield to SimGrid’s scheduler), the application should run properly, and probably give a result that is close to what the user expects. However, this methodology is very fragile: it would be much safer to find a way to intercept the creation of threads by OpenMP, and reimplement them in simulation using SimGrid Actors. This study is very ambitious, as it would probably be complex enough for a full PhD of its own. Additionally, this work could be generalized to a wider scope than S4BXI simulations, and be performed in the context of any SimGrid simulation directly. This would allow several simulators (for example SMPI and S4BXI) to benefit from the results of this study.



More robust interception of symbols: S4BXI intercepts function calls to MPI and parts of the C library (`gettimeofday`, `sleep`, etc.) using C-style `#define` macros, similarly to how SMPI operates. While this method is efficient, it requires injecting an additional header in all files of the user application's code. Several other approaches exist, such as preloading a library using the `LD_PRELOAD` environment variable for example, which does not require any modification of user's code. Therefore, it could be interesting to explore other methods of interception in S4BXI, for example by re-using studies that have been conducted in this domain in SimGrid, such as [BQ15].

Many of the ideas presented above result from either the studies we have conducted, or the discussions we had with the SimGrid team and Atos's development teams. More generally, we believe that we illustrated the versatility of our simulation methodology, and that our simulator is a good tool to experiment with several features, assuming they can be expressed at the level of detail provided by S4BXI.



Chapter 8

Conclusion

In this PhD, we have presented a new simulator, S4BXI. After validating our model of Portals, we have used it to run high-level APIs, which is rarely done in other state-of-the-art simulators. This allowed us to execute complete applications which rely on MPI, and validate the accuracy of our simulator in a wide range of scenarios. We have compared our model with the closest existing simulator, SMPI, and shown the strengths and weaknesses of both approaches. In particular, we have seen that in the majority of cases, S4BXI has a higher accuracy and a lower performance compared to SMPI, which is expected from our lower-level model.

We have leveraged both models' strengths in order to design a more flexible simulation method, which allows users to switch between different models of MPI at runtime. Even though it performed as we expected in most simulations, we also found several cases in which the performance of our approach followed unexpected patterns. Even in favorable cases, the execution time of simulations with different proportions of each model is always of a similar order of magnitude, therefore it is debatable whether it is desirable to add a layer of complexity for a small performance gain. Overall, this approach would probably give better results with different network models (lower-level or more performant). Finally, our approach and its unexpected results raise a question regarding simulation in general: since our models approximate very complex real-world behaviors, it is important to contain the complexity of the model itself to be able to interpret the results with confidence (except in the case of emulators of course, which are complete mirrors of real-world hardware). Overall, being able to switch between network models made more sense when S4BXI's performance was worse than it is today, since we managed to optimize it in parallel with our "model-change" study. This confirms that this idea would only be useful if we implemented it with very different models, such as an emulator and an analytical model for example.

Lessons learnt about SimGrid: Throughout this work, we have used SimGrid extensively. Its Actor model proved very efficient to describe the behavior of independent simulated hardware components (CPU cores and different components of BXI NICs). In particular, this paradigm allows developers of simulators to structure their code, usually with one Actor for each piece of simulated hardware, and explicit communications between these Actors. Nevertheless, this paradigm also allows scheduling one-time asynchronous activities using anonymous short-lived Actors, which makes this approach very flexible. Furthermore, the flexibility of SimGrid's Actors allowed us to test different scenarios quickly, for example by implementing the processing of the NIC once, and testing different deployments of the Actors on our platform.

Additionally, SimGrid's asynchronous cooperative Actors executed in a single-threaded simulation simplify greatly the development of simulators, because there is little potential for race-conditions: since the Actors are executed sequentially on the "host" machine that runs the simulator, race-conditions can only happen when Actors perform operations that yield to SimGrid's scheduler (and all race conditions are only with respect to the simulated time). Therefore, it is usually safe to access any data structure in between these operations, as there is always only one Actor running. Obviously, the fact that SimGrid's simulators are single-threaded raises the issue of performance, but this problem is not as important as it seems for two reasons: first, multi-threaded simulators require many synchronizations, which limits their scaling. Second, the fact that our simulation run on one thread means that many simulations can be executed in parallel (either on different cores, or on different machines). For example, for our OSU benchmarks, we were able to run all 31 benchmarks at the same time, so even if the slowdown of each simulation compared to a real-world experiment is significant, the total time of our experiments ends up being divided by 31, which makes it more reasonable. Obviously, it is not always useful to run several simulations in parallel (for example when running a large application to dimension a cluster), but it is still a common use case of this type of model, for example when exploring a large parameter space (in order to optimize the configuration of a piece of hardware or software). Therefore, it is important to keep in mind what the strengths of our model are: it is not a good fit for all studies on HPC clusters, but we believe that it is an efficient tool for many experiments.

Finally, we believe that SimGrid's flow model is a good tool to create simulators at an intermediate level of abstraction (by modeling communications at message-level). Nevertheless, with S4BXI we reach the limit of this type of model: we believe that any simulator that attempts to model hardware at a lower level should rely on a packet-level model instead. Indeed, our model of CPU cores, NICs, and PCIe buses already add a significant amount of complexity compared to simpler models, for example SMPI which models a full machine a single Host. Therefore, modeling transfers at a lower level, for example to better represent the interdependency between several communications, would benefit from a packet-level model. On the other hand, such a model would probably be pathologic for the performance of a flow-model, as it would cause require SimGrid to handle a large number of transfers each time a communication is performed by the user application.

Long term plans: The flexibility of our model opens the door to many studies, for example with other high-level APIs, or different "what-if" scenarios to help the co-design of next-generation hardware. In the context of this PhD we experimented with OpenSHMEM, and designed experiments to evaluate the usefulness of flow-control in BXI NICs, but many other studies could be conducted with the tools that we provide.

In this PhD, we presented a few studies that could be performed in the short term using S4BXI, but in the longer term several ideas could be worked on. As presented previously, it would be interesting to design network models that are either very simplistic, and therefore very fast, or very detailed, in order to better leverage the framework that we created to switch between different MPI models. A different approach to improve the performance of simulations would be to make them parallel: even if this would cause many difficulties, which we already detailed, being able to execute simulated processes in parallel is an active research topic, with many simulators attempting it. Overall, whether it is through parallelization or model changes, the performance improvement that would be desirable is



of several order of magnitudes, because it would allow this type of simulation to be used in completely different use case: for example dimensioning clusters composed of thousands of nodes, which is unrealistic with the current version of S4BXI. While it is unreasonable to expect a low-level model to run at this scale, a combination of parallelization and different network models could allow us to reach this performance in the most favorable cases, and maybe occasionally switch to a slower but more accurate model.

From a functionality perspective, it would be valuable to support the use of OpenMP and CUDA code within applications in S4BXI. This is a very ambitious task, but it could benefit other simulators as well if it was implemented in SimGrid directly, which would make both S4BXI and SMPI more flexible. Even though supporting this type of API would be very complex, SimGrid's development team has showed interest in studying it: in particular, there has been preliminary work on the support of the `pthread` library¹, which is a first step towards OpenMP support.

¹<https://framagit.org/simgrid/simgrid/-/issues/112>



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Appendix A

S4BXI class hierarchy

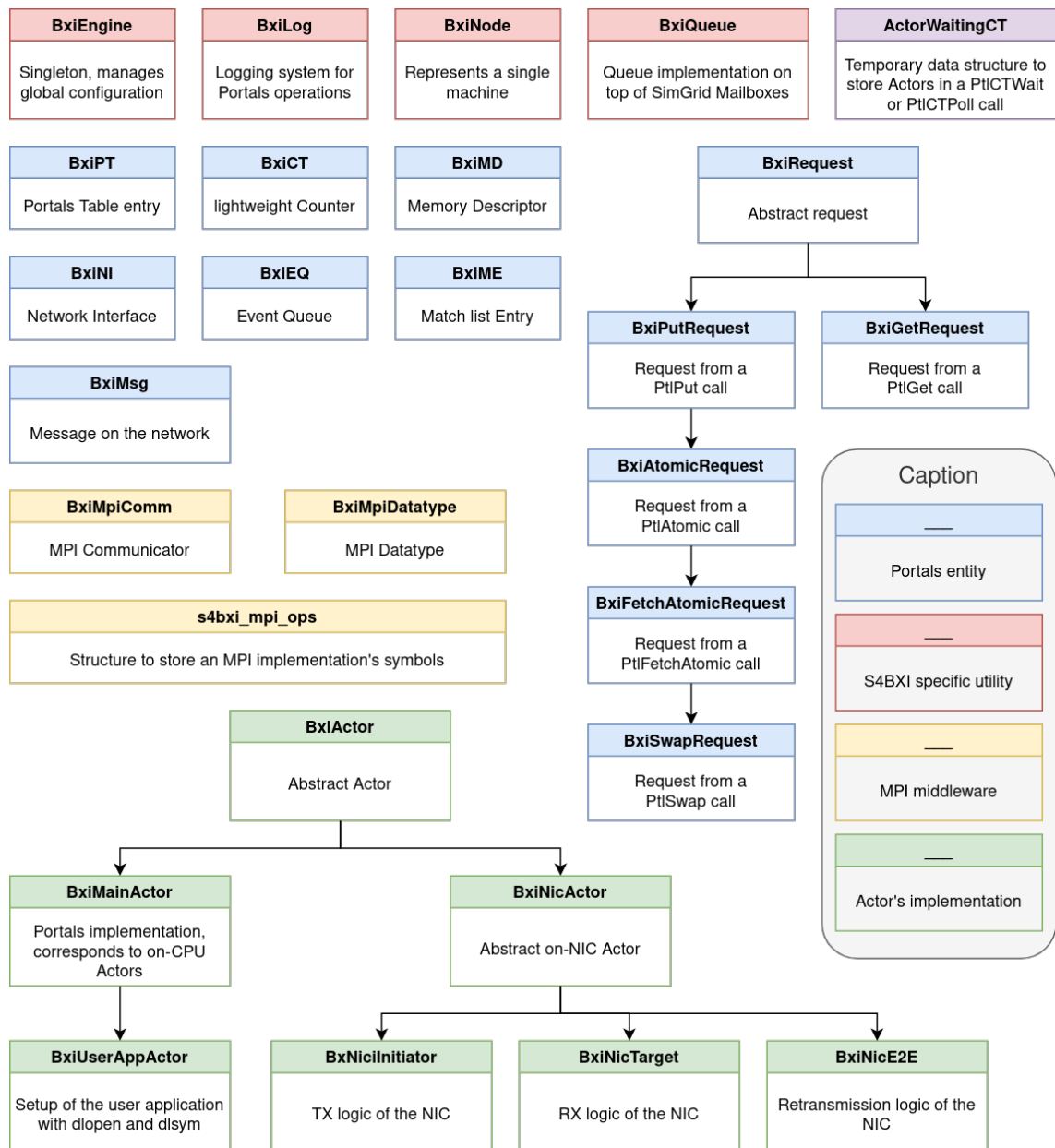


Figure A.1: Full class hierarchy of our simulator

Appendix B

OpenMPI patch

The following statistics were computed using cloc (<https://github.com/AlDanial/cloc>):

Language	files	blank	comment	code
C				
same	0	0	4412	18200
modified	43	0	46	36
added	0	52	290	74
removed	0	0	1	149
C/C++ Header				
same	0	0	848	626
modified	3	0	5	5
added	0	7	90	6
removed	0	0	0	75
make				
same	0	0	14	38
modified	1	0	0	0
added	0	0	0	0
removed	0	0	0	0
Bourne Shell				
same	0	0	0	0
modified	0	0	0	0
added	4	19	7	34
removed	0	0	0	0
SUM:				
same	0	0	5274	18864
modified	47	0	51	41
added	4	78	387	114
removed	0	0	1	224

Figure B.1: Full statistics of our patch on OpenMPI to make it compatible with S4BXI (the Bourne Shell additions are simply small scripts we added to simplify the compilation, they are not meaningful modifications of the source code)



Language	files	blank	comment	code
C	3659	122710	161263	668491
C/C++ Header	1304	33020	78829	116212
m4	404	5947	5590	46664
Fortran 90	781	3535	8066	19540
make	622	4024	11923	16190
Bourne Shell	69	1084	1904	7397
Perl	53	1624	2027	7091
Java	38	1507	5674	6360
TeX	5	485	60	2947
Python	11	698	846	2348
YAML	17	96	141	800
C++	9	170	416	791
lex	7	191	249	549
diff	3	53	325	368
INI	1	66	0	294
Bourne Again Shell	7	49	46	216
zsh	1	26	25	196
Markdown	6	54	0	133
DTD	3	23	21	113
D	4	17	59	67
C Shell	2	15	35	61
Puppet	1	5	2	59
Fortran 77	2	21	35	52
Gencat NLS	1	0	0	51
reStructuredText	2	28	17	49
sed	2	8	15	41
Tcl/Tk	2	19	45	39
Dockerfile	1	2	0	3
JSON	1	0	0	3
SUM:	7018	175477	277613	897125

Figure B.2: Full statistics of OpenMPI after our patch

Appendix C

OSU micro-benchmarks

Aggregated statistics of our OSU micro-benchmarks runs on 32 MPI ranks are shown on Figure C.1 for the accuracy of simulators, and Figure C.2 for the slowdown compared to the real-world run. The full data, for each MPI primitive, is available in the following git repository: <https://framagit.org/Webcretaire/phd-benchmark-data>.

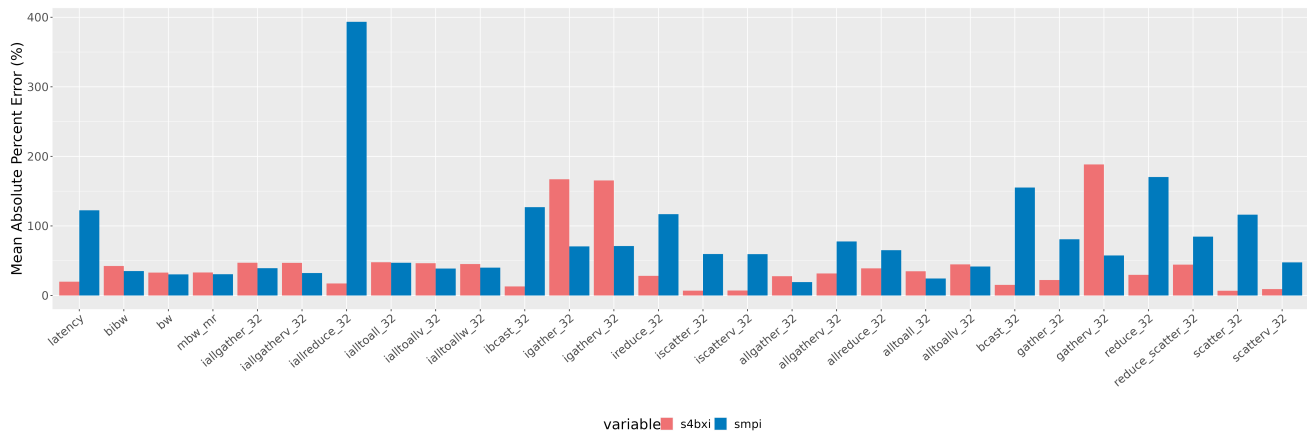


Figure C.1: Accuracy of SMPI and OpenMPI over S4BXI

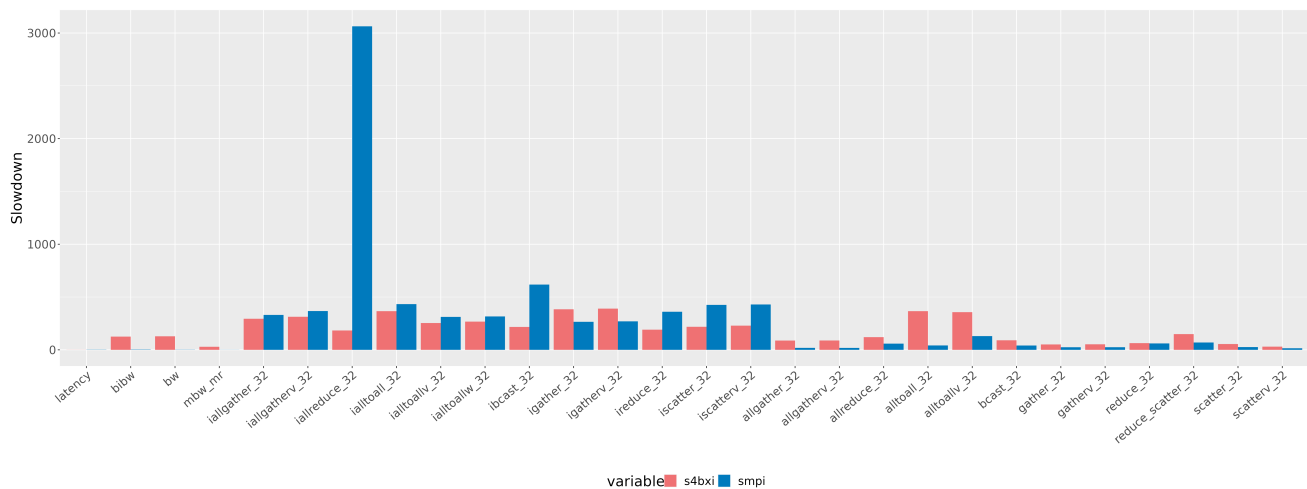


Figure C.2: Slowdown of SMPI and OpenMPI over S4BXI



We can see that the IAllReduce benchmark is particularly pathologic for SMPI, as it has a huge error and a very bad performance. The real-world experiment is surprisingly quick for large message sizes (see https://framagit.org/Webcretaire/phd-benchmark-data/-/raw/master/5_high_level/OSU/32ranks/iallreduce_32.png), but our simulation method manages to model it accurately. These results seem to indicate that the default algorithm used for this IAllReduce at this cluster size is particularly bad for BXI in the community version of OpenMPI (which is implemented in SMPI), and that it was optimized particularly well by Atos's teams.

Appendix D

S4BXI runtime for OpenSHMEM

```
1 #include "config.h"
2 #include <s4bxi/s4bxi_c_util.h>
3 #include "runtime.h"
4 #include "shmem_internal.h"
5 #include "uthash.h"
6
7 struct keyval_entry
8 {
9     size_t length;
10    void* value;
11 };
12 typedef struct keyval_entry keyval_entry_t;
13
14 int shmem_runtime_init(int enable_node_ranks)
15 {
16     return 0;
17 }
18
19 int shmem_runtime_fini(void)
20 {
21     return 0;
22 }
23
24 void shmem_runtime_abort(int exit_code, const
25     char msg[])
26 {
27     s4bxi_fprintf(stderr, "%s\n", msg);
28     s4bxi_exit(exit_code);
29 }
30
31 int shmem_runtime_get_rank(void)
32 {
33     return s4bxi_get_my_rank();
34 }
35
36 int shmem_runtime_get_size(void)
37 {
38     return s4bxi_get_rank_number();
39 }
40
41 int shmem_runtime_get_node_rank(int pe)
42 {
43     shmem_internal_assert(pe <
44         s4bxi_get_rank_number() && pe >= 0);
45     return pe;
46 }
47
48 int shmem_runtime_get_node_size(void)
49 {
50     return 1;
51 }
52
53 int shmem_runtime_exchange(void)
54 {
55     return 0;
56 }
57
58 int shmem_runtime_put(char *key, void *value,
59     size_t valuelen)
60 {
61     keyval_entry_t *v = (keyval_entry_t *)
62         malloc(sizeof(keyval_entry_t));
63     v->length = valuelen;
64     v->value = value;
65
66     s4bxi_keyval_store_pointer(key, v);
67
68     return 0;
69 }
70
71 int shmem_runtime_get(int pe, char *key, void *
72     value, size_t valuelen)
73 {
74     keyval_entry_t *v = (keyval_entry_t *)
75         s4bxi_keyval_fetch_pointer(pe, key);
76
77     if (!v || valuelen < v->length)
78         return 1;
79     memcpy(value, v->value, v->length);
80
81     return 0;
82 }
83
84 void shmem_runtime_barrier(void)
85 {
86     s4bxi_barrier();
87 }
```

