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A Cloudification Methodology for High Performance Simulations

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Tesis Doctoral

A Cloudification Methodology for High Performance Simulations

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Firmas del Tribunal Calificador

	(Nombre y apellidos)	Firma
Presidente:		
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En Lega´nes, a de del 201

“I am prepared to go anywhere, provided it be forward.”

David Livingstone

Let us assure our readers that to the extent this article is imperfect, it is not a sin we have committed knowingly.

Justin Kruger and David Dunning

Take a look what you've started
In the world flashing from your eyes
And you know that you've got it
From the thunder you feel inside

I believe in the feeling
All the pain that you left to die
Believe in believing
In the life that you give to try

I've lost my fear to what appears
I do my best
You seem surprised and realize
That's in your eyes
The world is mine

The World is Mine by David Guetta

UNIVERSITY CARLOS III OF MADRID

Abstract

School of Engineering
Computer Science and Engineering Department

Ph.D. Program in Computer Science and Technology

A Cloudification Methodology for High Performance Simulations

by Alberto Garcia Fernandez

Many scientific areas make extensive use of computer simulations to study complex real-world processes. These computations are typically very resource-intensive and present scalability issues as experiments get larger, even in dedicated supercomputers since they are limited by their own hardware resources. Cloud computing raises as an option to move forward into the ideal unlimited scalability by providing virtually infinite resources, yet applications must be adapted to this paradigm.

The major goal of this thesis is to analyze the suitability of performing simulations in clouds by performing a paradigm shift, from classic parallel approaches to data-centric models, in those applications where that is possible. The aim is to maintain the scalability achieved in traditional HPC infrastructures, while taking advantage of Cloud Computing paradigm features. The thesis also explores the characteristics that make simulators suitable or unsuitable to be deployed on HPC or Cloud infrastructures, defining a generic architecture and extracting common elements present among the majority of simulators.

As result, we propose a generalist cloudification methodology based on the MapReduce paradigm to migrate high performance simulations into the cloud to provide greater scalability. We analysed its viability by applying it to a real engineering simulator and running the resulting implementation on HPC and cloud environments. Our evaluations will aim to show that the cloudified application is highly scalable and there is still a large margin to improve the theoretical model and its implementations, and also to extend it to a wider range of simulations.

UNIVERSIDAD CARLOS III DE MADRID

Resumen

Escuela Politécnica Superior
Departamento de Informática

Doctorado en Ciencia y Tecnología Informática

Una Metodología de "Cloudificación" para Simulaciones de Alto Rendimiento

por Alberto Garcia Fernandez

Muchas áreas de investigación hacen uso extensivo de simulaciones informáticas para estudiar procesos complejos del mundo real. Estas simulaciones suelen hacer uso intensivo de recursos, y presentan problemas de escalabilidad conforme los experimentos aumentan en tamaño incluso en clústeres, ya que estos están limitados por sus propios recursos hardware. *Cloud Computing* (computación en la nube) surge como alternativa para avanzar hacia el ideal de escalabilidad ilimitada mediante el aprovisionamiento de infinitos recursos (de forma virtual). No obstante, las aplicaciones deben ser adaptadas a este nuevo paradigma.

La principal meta de esta tesis es analizar la idoneidad de realizar simulaciones en la nube mediante un cambio de paradigma, de las clásicas aproximaciones paralelas a nuevos modelos centrados en los datos, en aquellas aplicaciones donde esto sea posible. El objetivo es mantener la escalabilidad alcanzada en las tradicionales infraestructuras HPC, mientras se explotan las ventajas del paradigma de computación en la nube. La tesis explora las características que hacen a los simuladores ser o no adecuados para ser desplegados en infraestructuras clúster o en la nube, definiendo una arquitectura genérica y extrayendo elementos comunes presentes en la mayoría de los simuladores.

Como resultado, proponemos una metodología genérica de cloudificación, basada en el paradigma MapReduce, para migrar simulaciones de alto rendimiento a la nube con el fin de proveer mayor escalabilidad. Analizamos su viabilidad aplicándola a un simulador real de ingeniería, y ejecutando la implementación resultante en entornos clúster y en la nube. Nuestras evaluaciones pretenden mostrar que la aplicación cloudificada es altamente escalable, y que existe un amplio margen para mejorar el modelo teórico y sus implementaciones, y para extenderlo a un rango más amplio de simulaciones.

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Cuando empec la tesis doctoral, imaginé (supongo que como todo el mundo) que al acabarla sería la persona más feliz del mundo, y que gritaría y reiría dando saltos de alegría. Ahora, tras más de cinco años, resulta muy complicado describir el conjunto de sentimientos que tengo en mi interior. No ha sido fácil, no todo ha sido felicidad, y sinceramente, no sé si valdrá la pena. Pero sí sé que lo mejor de este viaje son las personas que me han acompañado por el camino.

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Abbreviations

ANOVA	**AN**alysis **O**f **VA**riance
ASCAC	**A**dvanced **S**cientific **C**omputing **A**dvisory **C**ommittee
BLAS	**B**asic **L**inear **A**lgebra **S**ubprograms
CFD	**C**omputational **F**luid **D**ynamics
DSM	**D**irect **S**tiffness **M**ethod
DSP	**D**igital **S**ignal **P**rocessors
FEM	**F**inite **E**lement **M**ethod
FPGA	**F**ield-**P**rogrammable **G**ate **A**rrays
FSM	**F**inite **S**tate **M**achine
GPGPU	**G**eneral **P**urpose **G**raphic **P**rocessing **U**nit
HPC	**H**igh **P**erformance **C**omputing
IaaS	**I**nfrastructure **as a** **S**ervice
ISO	**I**nternational **O**rganisation for **S**tandardisation
IT	**I**nformation **T**echnologies
I/O	**I**nput / **O**utput
LAPACK	**L**inear **A**lgebra **PACK**age
MNA	**M**odified **N**odal **A**nalysis
MPI	**M**essage **P**assing **I**nterface
MST	**M**inimum **S**panning **T**ree
NIST	**N**ational **I**nstitute of **S**tandards and **T**echnology
OpenMP	**Open** **M**ulti-**P**rocessing
PaaS	**P**latform **as a** **S**ervice
RPCS	**R**ailway **P**ower **C**onsumption **S**imulator
QoS	**Q**uality **o**f **S**ervice
SaaS	**S**oftware **as a** **S**ervice
ScaLAPACK	**Sca**lable **L**inear **A**lgebra **PACK**age
SLA	**S**ervice **L**evel **A**greement
TCO	**T**otal **C**ost of **O**wnership
UC3M	**U**niversity **C**arlos **III** of **M**adrid
XaaS	Anything (**X**) **as a** **S**ervice

Chapter 1

Introduction

This chapter introduces the context of the work presented in this thesis. The first section provides an overview on the main topics addressed in this thesis: simulation and Cloud Computing. The second section presents a brief description of the motivation, and of the limitations of current simulators to be addressed in this thesis. The next section discusses the specific goals of the thesis work. Finally, the chapter concludes providing an outline for the rest of this document.

1.1 Definition and Scope

During the last years, simulation has become the way to research and develop new scientific and engineering solutions in several areas [Ban98]. Simulation allows to reduce time and effort invested in testing new engineering structures, molecular designs, climatic conditions, etc. The ASCAC summary report [ABC+10] illustrates how simulation is used in leading science domains like aerospace industry, astrophysics, etc., and Maceri and Casciati [MC03] enumerate uses of simulation in civil engineering. Nevertheless, using simulators in developing science and engineering solutions requires to face several challenges. Some of these challenges are inherent to the simulation act: to develop a model that matches with the real system simulated, validate it, and extrapolate the results to the real world. Ho et al. [HMY+02] illustrates these challenges when developing simulation models for railway applications. However, some other challenges are related to the complexity and scalability of the simulators. These challenges go further than the simulator itself and impact on the relaying IT infrastructure.

One way to classify simulators is according to the infrastructure required to run a simulation (i.e. how much resources and time are needed to run a simulation). In terms of computing power, or memory consumption, some simulators require no more than a desktop computer or workstation [SGG+12], while others require the use of hundreds of nodes [CHA+11]. Also, the most of the simulators are tied to a specific platform, so small simulators are generally desktop applications, while the most resource-demanding simulators are MPI programs, which need to be deployed in HPC environments like clusters or supercomputers. There are few simulators relaying on cloud environments [YCD+11].

Cloud computing is a relatively fresh term which has become in one of the most popular of those related with IT. Cloud computing is defined by the NIST [MG09] as "a model for enabling ubiquitous, convenient, on-demand network access to a shared pool of configurable computing resources (i.e., networks, servers, storage, applications, and services) that can be rapidly provisioned and released with minimal management effort or service provider interaction". In practice, an institution (e.g. an enterprise or university) could have its own datacenter to perform tasks, so it must carry with the respective management and maintenance. Other way is to outsource the IT infrastructure to cloud providers. Then, management and maintenance task are less demanding. A third option is the use of hybrid clouds, in which the institution has a private infrastructure and outsources more computing power to a cloud provider when the workload exceeds the available capacity.

With the explosion of cloud services and the Anything as a Service (XaaS) paradigm, cloud service providers have started to offer several HPC paradigms as cloud services [APK+12]. Examples of this are MapReduce [Ama], MPI implementations [RBA11], and GPGPU processing [ECW10]. In such cases, the client can resize the infrastructure according to the workload, and saves the costs associated to management and maintenance. On the other hand, the client must take a performance loss in comparison to bare metal executions. This loss comes from several factors: the virtualization layer, which adds a little overhead to the applications, but more importantly, the network latencies. Cloud infrastructures are associated to high network latencies due to the fact that virtual machines can be placed anywhere in the cloud data center (or even in different data centers). Besides, it is difficult for the applications to perform low level optimizations (e.g. topology optimizations) because the underlying infrastructure is hidden. Those simulators which run on HPC environments will likely benefit from these upcoming cloud paradigms, but this migration should be analysed carefully. In this thesis, the use of simulators both in HPC environments and the Cloud is addressed.

1.2 Motivation

The widespread use of simulators as a means of research and development in many fields has made it necessary to run the largest number of simulations in the lowest time possible [CBP00]. Moreover, the need of processing or storing data has been increased significantly as the simulations become more and more complex [LCL+09]. Furthermore, if it is desired to study variations of multiple variables involved in the experiment, a single simulation is not enough to get relevant results. Therefore, the use of simulators is limited by the availability of computing infrastructures (data centres, supercomputers, clusters, etc.) which have the required power to run the simulations. In this context the use of HPC, both infrastructures (clusters, supercomputers) and technologies (MPI, OpenMP, GPGPUs) is the major trend in simulation [ABC+10].

While these approaches have proved successful, they often rely on heavy hardware investment and they are tightly conditioned by its capabilities and, more importantly, its availability, which *de facto* limits actual scalability and the addressable simulation size. Since sharing resources across multiple clusters implies several limitations, cluster applications cannot be considered sustainable, because their scalability is strongly dependant on the cluster size. There are several issues that can be tackled in order to develop a sustainable application, such as:

- *Suitability*. The way an application uses computational resources, such as CPU, memory, and network, determines the performance of this application when it is executed on such different infrastructures like HPC clusters and clouds. Therefore, this usage should be analysed in order to establish under what kind of infrastructure an application will be sustainable. For instance, if a a particular problem's characteristics determine that it is necessary a huge amount of network communications, ultimately this resource determines the suitability of one kind of infrastructure (in this case a cluster) over the other (the cloud).This analysis should start from the applications problem domain, checking resource usage as the problem size becomes bigger and bigger.
- *Independence*. Making the application cloud/cluster independent, so that it can be deployed in either of them with minimal changes. In this way, computational resources, possibly located in different places, can be aggregated and local data center size would not be a limitation. Moreover, HPC and cloud resources could be exploited simultaneously following a hybrid scheme. Note that this issue clashes with the previous one.
- *Scalability*. Improving applications scalability by adapting them to the underlying infrastructure. In connection with the previous issue, clearly cloud infrastructures juxtapose several characteristics (flexibility and scalability) to traditional HPC environments (bare metal or topology optimizations, and low-latency networks), so the application should take the best from each kind of infrastructure. This would minimize the added overhead of working with more nodes, making a better use of the available resources.
- *Flexibility*. Making applications and infrastructures more flexible, bringing the possibility of scale up or down according to instantaneous user needs. This is an inherent characteristic of Cloud Computing infrastructures, and therefore it should be exploited by the applications. Computing resources could be fitted to specific simulation sizes and deadlines.

As the Cloud Computing paradigm gains more popularity, the more services are deployed in the cloud. The NIST definition of Cloud Computing also provides a description of three basic service models: IaaS, PaaS, and SaaS [MG09], but nowadays these service models have been extended to higher levels of abstraction (e.g. Database as a Service [HIM02, CJP+11], Network as a Service [CMPW12]) which as a whole provide an Anything as a Service vision (XaaS). Simulation is not aware of this trend, and there are current efforts to deploy simulation services on the cloud, like [AM13] and [Xia11].

Using Cloud Computing in simulation provides several advantages related with the elastic nature of the cloud. The infrastructure can be resized according to the number and complexity of the simulations, and there is a variety of platforms and services in which simulators could rely on. Along with its so-called pay-as-you-go model, allow to adjust the required instances to the particular test case size while cutting-down the resulting costs. It would enable the execution of large simulations with virtual hardware properly tailored to fit specific use cases like memory-bound simulations, CPU-dependant computations or data-intensive analysis.

But there is also a number of challenges that must be faced up. The Magellan Final Report [YCD+11] exposes these challenges, and some of them are stated here:

- There is an overhead for scientific applications executed on the cloud associated to the absence of high-bandwidth, low-latency interconnects in virtual instances located (possibly) on different places.
- The absence of high-performance file systems further impacts the productivity of running scientific applications which perform intensive I/O within the cloud environment.

Given the former, this thesis suggests a methodology to transform the applications making them both HPC and cloud suitable. The focus is on analysing the application problem domain, getting the dependences of the application input data. On those loosely coupled sets of data this thesis proposes a paradigm shift from classic parallel computations to a data-centric model that would distribute the simulation load across a set of independent instances in a cloud suitable manner. On those tightly coupled, backward compatibility is maintained on HPC programming paradigms, taking advantage of HPC features (if available).

This thesis focuses on resource-intensive parallel simulations which hold potential scalability issues on large cases, since cluster hardware may not satisfy simulation requirements under such stress circumstances, and therefore will likely benefit from Cloud Computing paradigm. A case study illustrating the whole methodology by means of a particular problem domain is provided: simulation of time-variant electric circuits using the modified nodal analysis (MNA) technique. The aim is to extend this problem to a general kind of scientific and engineering problems.

1.3 Objectives

The major goal of this thesis is to analyze the suitability of executing parallel simulations in clouds by performing a paradigm shift, from classic parallel approaches to data-centric models, in those applications where that is possible. The aim is to maintain the scalability achieved in traditional HPC infrastructures, while taking advantage of Cloud Computing paradigm features.

This allows us to perform simulations on the Cloud, resizing the infrastructure and dynamically balancing the workload according to the number and complexity of the simulations, but also keeping HPC technologies such as MPI, for those cases which getting data independence across the problem domain is not possible (i.e. they implement heavy communication patterns). By exploiting the data-centric paradigm, a virtually infinite scalability is achieved, so that large simulations can be executed independently of the underlying hardware resource, allowing us to spread simulation scenarios of different sizes in a more flexible way, using heterogeneous hardware, and taking advantage of shared inter-domain infrastructures. By maintaining HPC technologies those heavy-coupled problems not suitable to the data-centric approach can be tackled.

This goal can be split in the following ones:

O1 To explore the characteristics that make simulators suitable or unsuitable to be deployed on HPC or Cloud infrastructures.

O2 To propose a methodology to adapt scientific parallels simulations following a cloud-suitable data-centric scheme, while maintaining classic approaches to domain decomposition for those problems which cannot be split gracefully.

O3 To transform a memory-bound simulator into the proposed scheme, integrating the original application with both the MapReduce framework and MPI libraries.

O4 To demonstrate the feasibility of the resulting architecture comparing the behavior and efficiency of adapted vs. original applications in both HPC and cloud environments.

O5 To enhance the proposed methodology in order to include multivariate analysis simulations, as a particular case that can benefit from a cloud-suitable data-centric scheme.

With the study and analysis of the aforementioned objectives, the following contributions are foreseen:

C1 Classification of simulation problems according to its suitability to HPC and cloud infrastructures and the different ways of parallelizing such problems.

C2 Proposition of different mechanisms to split simulation domains in smaller sub-domains, with different degrees of data coupling, thus indicating the suitability of the simulator to different infrastructures, identifying architectural bottlenecks, and those aspects which limit the scalability of the application.

C3 Definition of a software framework suitable for both cloud and HPC systems, that makes use of data-centric schemes such as MapReduce.

C4 Implementation of the mechanisms and frameworks proposed in a simulator, and performance study when different computing resources (i.e. HPC and cloud) are used.

1.4 Structure and Contents

This document describes the work developed in this thesis. It has been organized into seven chapters, whose contents are summarized in the following paragraphs:

- Chapter 1 introduces the scope and the motivation for this thesis. Analyzing the suitability of performing simulations in Cloud by performing a paradigm shift is stated as the main goal.
- Chapter 2 describes the state of the art in HPC, Cloud Computing, MapReduce, and the current approaches to migrate scientific simulations to the Cloud.
- Chapter 3 contains the problem statement. A classification of simulation problems is proposed, and an illustrative example of a simulation problem is analysed and modelled, indicating all problem dimensions and their impact on the resource usage.

- Chapter 4 explores HPC-based approaches to decompose the problem, analysing their suitability and performance with regard to HPC and Cloud infrastructures.
- Chapter 5 describes the proposed methodology to migrate the application to the cloud, including all its phases, and providing an illustrative example of migration.
- Chapter 6 analyses the opportunities of the resulting architecture in multidimensional analysis of simulation problems, where there is a high degree of data decoupling.
- Chapter 7 presents the conclusions, describes the future research lines, and the contributions of this thesis.

Chapter 2

State of the Art

This chapter provides a detailed State of the Art in both High-Performance-Computing and Cloud Computing, which are the major trends used nowadays in simulation. In both cases current technologies and paradigms used are described, as well as current challenges which have to be tacked. Finally, a detailed analysis of the Hadoop MapReduce framework and its derived projects is also provided, indicating its architecture and components.

2.1 High-Performance Computing

The term High-Performance Computing refers to the application of aggregated computing resources and parallel processing algorithms and techniques to solve complex computational problems or analyse large amounts of data. Its applications are specially focused in scientific modelling, simulations and analysis, which tend to involve large amounts of data and sophisticated algorithms. Its main goal is to solve such problems in the minimum possible time, hence supercomputers tend to be composed of multiple interconnected nodes to increase concurrency.

2.1.1 HPC Infrastructure Elements

Supercomputers have many different architectures [Buy99], but share some common elements. Supercomputers are composed of hundred of thousands of compute nodes which perform the processing workload associated to a particular computational problem. A compute node is composed of one or several cores which share a main memory following a shared memory building blocks pattern [BKK+09]. The workload is distributed among as many as possible cores in order to increase the parallelism and reduce the total execution time. Compute nodes are linked with high-performance compute networks in order to share all data necessary to perform the calculations. Such networks are deployed following complex topologies, such as mesh, hypercube, or 3D torus [AK11]. The aim is to minimize communication delays between compute nodes maximizing the CPU usage.

I/O nodes conform the bridge between compute nodes (where the data is used) and file servers (where de data is stored). They are accountable for aggregating all I/O from the compute nodes, reading input data from the file servers, and writing output data to file servers. A separated network is deployed between compute and I/O (generally a tree topology) in order not to interfere with network traffic associated to computations. Finally, file servers are responsible for storing application data, balancing the storage workload as equally as possible between all servers. Figure 2.1, obtained from [LCL+09], shows an overview of the Blue Gene architecture, which contains all aforementioned elements.

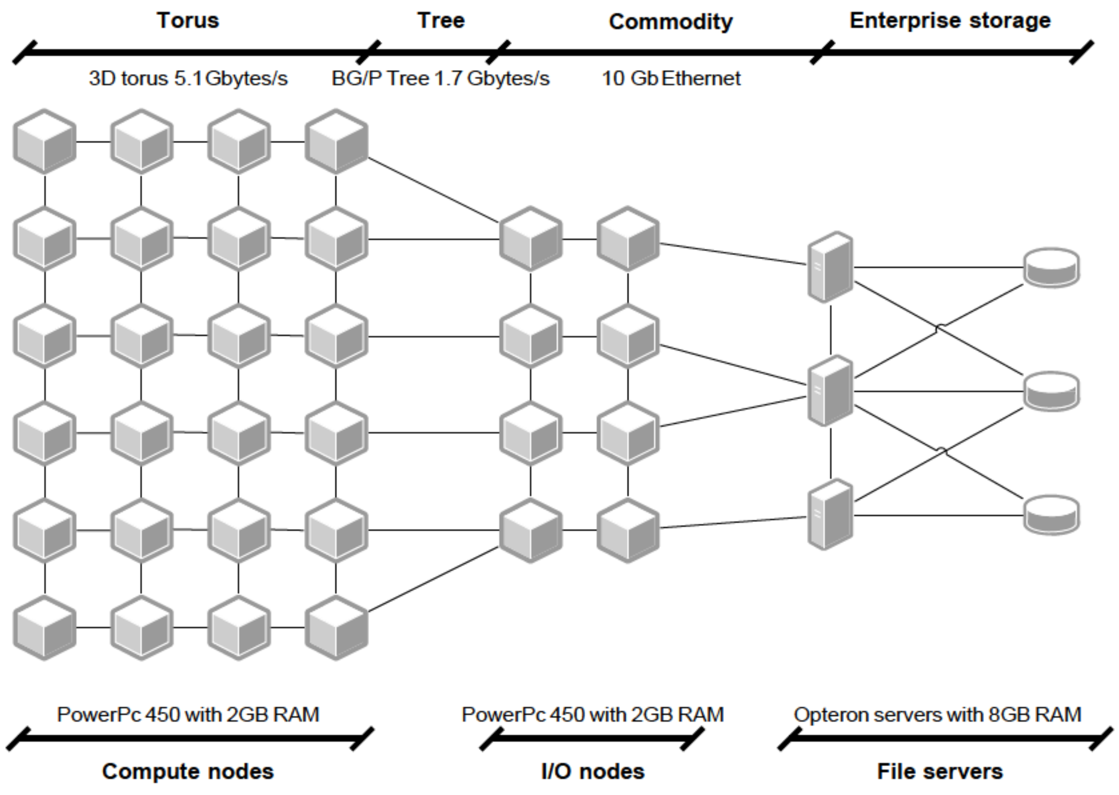


Figure 2.1: Blue Gene architecture overview.

2.1.2 HPC Programming Models

In order to be executed on massively parallel supercomputers, applications have to be specifically tailored. Several programming models, runtimes, and libraries are currently used in order to do so:

MPI The *Message Passing Interface* is a specification which describes syntax and semantics when, in distributed memory applications, multiple processes want to cooperate by means of exchanging messages. MPI represents a standard ***de facto*** when developing HPC applications which are going to be executed across multiple compute nodes. Currently the latest version of MPI is 3.1 [For15], and indicates the function prototypes for C and Fortran implementations, as well as message formats and expected behaviours. Currently the most important implementations of this standard are MPICH [MPI03], developed by Argonne

National Laboratory, and Open MPI [GFB$^+$04] developed by a consortium of academic, research, and industry partners.

OpenMP *Open Multi-Processing* is an extension to the programming languages C/C++ and Fortran, based on compiler directives [Boa13]. OpenMP provides automatic parallelization of loops by adding compiler directives to the loop declaration. The compiler interprets the directive and divides the loop task between several threads, so that the computational effort is divided among multiple cores. The main advantage of OpenMP is the reduced impact on the application source code, thus allowing to parallelize an application just adding a few lines of code. Due to the fact that MPI provides distributed memory parallelism, and OpenMP provides shared memory parallelism, they are used together frequently when programming massively parallel applications [RHJ09, SJF$^+$10]. MPI distributes the effort between compute nodes, while OpenMP distributes the effort between cores of the same node.

GPGPUs During the last years the use of *General-Purpose-Graphic-Processing-Units* as a means to perform compute work offloading the CPUs have become widespread. GPGPUs evolve from the traditional video games graphic cards to generic devices capable of performing a huge number of parallel arithmetical operations. The main advantage is the high level of parallelism achieved by these devices, but as main drawback, these devices are difficult to handle by programmers, requiring specific libraries and code for each concrete kind of device [OHL$^+$08]. The following list describes current technologies used to program GPGPUs

CUDA Platform developed by Nvida with the aim of exploiting processing power of its GPUs [NVI11]. CUDA provides C and C++ extensions, plus a mathematical library specifically optimized to be executed on Nvida cards. While Nvida are the most popular GPGPUs in supercomputing, AMD and Intel have developed its own alternatives to Nvida GPGPUS: AMD APP, and Xeon Phi respectively.

OpenCL OpenCL is the open counterpart of proprietary GPGPU programming platforms [TNI$^+$10]. OpenCL provides a programming language and API which creates data-level parallelism thus allowing to offload compute tasks onto heterogeneous platforms like CPUs, GPUs, digital signal processors (DSPs) and field-programmable gate arrays (FPGAs). Currently, all GPGPU developers support OpenCL on its devices.

OpenACC OpenACC [Ope11] is a collection of compiler directives, similar to those utilized in OpenMP, which can be used to perform parallel calculations on the CPU as well as to offload compute task onto GPGPU devices. As OpenMP, OpenACC allows to parallelize applications using these hardware devices with a minimum impact on the source code. Besides, OpenACC provides portability across multiple GPGPUs from differentproviders.

2.1.3 Current Supercomputers and Petascale Systems

Complex resource-intensive applications have traditionally found in high performance infrastructures the necessary hardware to fit their high-end needs. Supercomputers constitute a canonical sample of systems that are designed to achieve the highest number of floating-point operations per second (*FLOPS*)[KT11]. HPC clusters and grids result from the association of a set of supercomputers under the same local network or across several administratively distributed systems, respectively; they can also be heterogeneous and, as previously mentioned, gather both CPU and GPU nodes [KES+09, FQKYS04].

Current leading systems in the Top500 rank [DMS+97] are GPU-based and capable of reporting over one quadrillion flops (a *petaflop*) under the standardised Linpack benchmark [DL11]. Some examples of the so-called petascale infrastructure are shown in Table 2.1, which includes the top five positions in the Top500 ranking of November 2015 [DMS+97].

System	Performance (Pflop/s)	Power (MW)	Location
Tianhe-2	33.86	17.81	China
Titan	17.59	8.21	USA
Sequoia	17.17	7.89	USA
K-Computer	10.51	12.66	Japan
Mira	8.59	3.95	USA

Table 2.1: Top five positions in the Top500 ranking of November of 2015.

Despite performance is a proper quantitative measure of an HPC system' s quality, researchers, developers and end-users are increasingly aware of other critical characteristics that must be considered in order to show the actual capabilities of the tested system for the efficient execution of 3D simulations and analytics workflows, while minimizing computing cost.

The Graph500 rank [MWBA10] includes shared-memory, distributed memory and cloud benchmarks for large scale graph-oriented algorithms. Its goal is to evaluate HPC system' s behaviour when approaching complex data-intensive applications, measured in traversed edges per second (*TEPS*). Current leading positions in the November of 2015 Graph500 ranking are shown in Table 2.2 [Top15].

System	Performance (TTEPS)	Location
K-Computer	38.62	Japan
Sequoia	23.75	USA
Mira	14.98	USA
JUQUEEN	5.84	Germany
Fermi	2.57	Italy

Table 2.2: Top five positions in the Graph500 ranking of November of 2015.

2.1.4 Future Goals: Green HPC, Exascale Infrastructures, and Big Data

Nowadays, sustainability and energy efficiency is key in the development and evaluation of HPC infrastructures. Following the Top500 philosophy, the Green500 list [FC07] is dedicated to rank supercomputers, but in terms of their efficiency, which is measured in performance-per-Watt.

Table 2.3 shows that current leading positions in the rank do not match any of the Top500 systems [Gre15], and their total power consumption is significantly less that the shown by the latter. This indicates that there is still a lot of research to be done in order to reduce the gap between performance and efficiency, especially considering that supercomputers will keep increasing their target performance to reach the exascale goal [SSSF13].

System	**Performance (Mflops/W)**	**Power (kW)**	**Location**
Shoubu -ExaScaler-	7031.6	50.32	RIKEN - Japan
TSUBAME-KFC/DL	5331.8	51.13	GSIC Center - Japan
ASUS ESC4000	5271.8	57.15	GSI Helmholtz Center - Germany
Sugon Cluster	4778.4	65.00	Institute of Modern Physics - China
XStream	4112.1	190.00	Stanford RCC - US

Table 2.3: Top five positions in the Green500 ranking of November of 2015.

Exascale systems will become the next generation of supercomputers, capable of performing with at least one exaflop. Scientific simulations will likely benefit from the upcoming exascale infrastructures [ABC+10], however many challenges must be overcome [BBC+08, GL09] including, processing speed [Cou13], data locality and power consumption; among them, energy efficiency seems to be the most limiting factor [Hem10].

Nowadays, cheaper and lower power alternatives are on research to overcome such difficulties. For instance, low-end processors are being considered to build large scale supercomputers. Besides, multiple efforts are currently under way in order to reduce energy consumption without reducing compute power, from scaling dynamically the number of compute cores [FL05], to deploy power-aware techniques in the I/O subsystem [LBIC13].

Big Data [MCB+11] is a term closely related to exascale systems, and one of the challenges that must be overcome. Big Data refers to the task of dealing with huge data sets, processing, analyzing, and storing vast amounts of information. Big Data challenge arises as a result of data explosion in society: web traffic, social networks, sensors, and pervasive or ubiquitous computing. Present information systems do not achieve nowadays the required capacity to deal with all data generated by current society. Besides, unpredictable events may lead to data explosions (see [GALM07]), so it is required an elastic dimensioning of compute and storage infrastructures in order to adapt system’ s capacity to service demand.

2.2 Cloud Computing

Cloud Computing appeared as a cheaper, elastic possibility to achieve the ideal situation of unlimited sustainable scalability. Cloud Computing is a popular paradigm that relies on resource sharing and virtualization to provide the end user with a transparent scalable system that can be expanded or reduced on-the-fly.

There were many definitions of ” Cloud Computing” . The NIST provided its own[MG09], which was considered the most relevant: *Cloud computing is a model for enabling ubiquitous, convenient, on-demand network access to a shared pool of configurable computing resources (...) that*

can be rapidly provisioned and released with minimal management effort or service provider interaction. The International Organisation for Standardisation (ISO) have adopted this definition [ISO14] and now is a standard. Nevertheless, other definitions are listed by [VRMCL08], which include the concepts of virtualization, web-based services, and user-friendly among others. Several efforts have been carried out in order to standardize terminology and concepts of Cloud Computing. [RCL09] proposes a taxonomy of Cloud Computing systems, and performs a survey of Cloud Computing service providers, and [YBDS08] defines an ontology of Cloud Computing.

The NIST states five essential characteristics of Cloud Computing which are listed below (shortened):

On-demand self-service A consumer can unilaterally provision computing capabilities, without requiring human interaction.

Broad network access These capabilities are available over the network, and accessed through standard mechanisms.

Rapid elasticity These capabilities can be elastically provisioned and released, to scale rapidly outward and inward commensurate with demand. To the consumer, the capabilities available for provisioning often appear to be unlimited.

Resource pooling The provider’ s computing resources are pooled to serve multiple consumers using a multi-tenant model, with different physical and virtual resources dynamically assigned and reassigned according to consumer demand. There is a sense of location independence in that the customer generally has no control or knowledge over the exact location of the provided resources but may be able to specify location at a higher level of abstraction.

Measured service Cloud systems automatically control and optimize resource use by leveraging a metering capability at some level of abstraction appropriate to the type of service.

Cloud providers operate at several levels of virtualization, which are known as service models. The NIST definition of Cloud Computing provides also a description of the three basic service models: Infrastructure as a Service, Platform as a Service, and Software as a Service. But as Cloud Computing services have become more popular, different authors have coined specific specific service models as a characterization of one of the three basic aforementioned services. For instance, [ZZZQ10] proposes three additional service models: Network as a Service (NaaS), Identity and Policy Management as a Service (IPMaaS), and Data as a Service (DaaS). The following subsections show a brief survey of the three basic service models and those derived from them.

2.2.1 Infrastructure as a Service

In this model, providers offer physical or virtual resources like instances of raw virtual machines, block storage, virtual networks and disk imaging. The consumer is able to deploy and run arbitrary software, which can include operating systems and applications. The consumer does not manage or control the underlying cloud infrastructure but has control over operating systems, storage, and deployed applications; and possibly limited control of selected networking components (e.g., hostfirewalls).

In [PO09], a taxonomy of this service model is proposed. IaaS clients can configure ***Virtual Dedicated Servers*** (VDS), also called instances in Amazon WS terminology. These VDS are virtual machines which can be customized by the user through deploying on top his/her own OS and software. Besides, in order to ease servers deployment, most of IaaS providers supply pre-configured generic VDS images. A number of images of a particular VDS can be deployed as separate independent machines. Each one of these images can be allocated in different availability zones: distinct locations (presumably distinct data centres) that are engineered to be decoupled from failures in other zones.

The hardware settings of these images are based on three kinds of resources: compute units, memory, and hard disk. A compute unit is an abstract term which defines the processing power of the machine. Theoretically, one compute unit is equivalent to one core, but the clock speed and the concrete core architecture is not always specified, and varies between different providers. The memory indicates the RAM size of the image, while the disk indicates the number and capacity of volatile disks (i.e. cleaned up after image termination).

Finally, most of IaaS providers offer additional services with regard to VDS administration and management. The following list describes the most regular:

Load balancing Refers to spreading a service workload between two or more VDS in order to avoid overloaded servers.

Resizing Adjustment of the amount of resources provisioned to an VDS based on the exhibited load. More compute unit, memory or disk can be added dynamically.

Checkpointing Refers to the capability of saving a snapshot of the running VDS (including all applications, data, conguration les, etc.) at any time instance.

The Cloud360 website [Clo14] provides a list of the top 20 IaaS providers. Amazon WS leads the list as the world’ s most important provider. Amazon EC2 sets the standard for spinning up and taking down cloud capacity. AT&T follows, offering Compute as a Service and Storage as a Service with SLA of 99.99 percent availability.

2.2.2 Platform as a Service

This model provides a full computing environment in which developers can create their own applications without having to concern themselves with hardware infrastructure. The capability provided to the consumer is to deploy onto the cloud infrastructure consumer-created or acquired applications, while the provider supplies programming frameworks, libraries, services or tools. This allows developers to have access to a wide range of licensed software ready to create or deploy their applications, without managing the underlying hardware. For instance, a provider may offer a database platform where the PaaS user can deploy his/her own relational model.

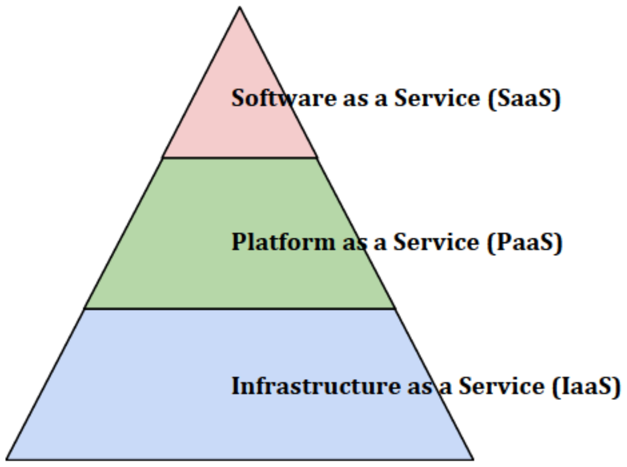

Software as a Service (SaaS)
Platform as a Service (PaaS)
Infrastructure as a Service (IaaS)

FIGURE 2.2: Services pyramid in Cloud Computing presented by [Mah11].

This model provides several advantages to its consumers. The main benefit is that developers do not have to be worried about the underlying infrastructure, including servers, storage space, and backing up their data. Besides, PaaS offers an holistic view of development environments, so developers do not have to acquire multiple software licenses necessary to build an application (programming framework, runtime, database server, etc.) [Law08]. Finally, PaaS inherits the Cloud Computing paradigm advantages, eliminating maintenance costs, and providing an elastic way to allocate/discard resources. Note that the consumer does not manage or control the underlying cloud infrastructure, but may be concerned about QoS, so PaaS providers allow users to allocate more computing resources to their hosted applications, in a similar way as it is done in IaaS services.

The Cloud360 website [Clo14] provides also a list of the top 20 PaaS providers. On the top of the list we find Amazon AWS again. Amazon AWS provides Elastic Beanstalk, in which developers can upload their applications and Beanstalk handles the deployment details, capacity provisioning, load balancing, auto-scaling and health monitoring. Another popular platform is AppScale [CBP$^+$10], which extends the Google App Engine cloud technology. AppScale gives developers the power to deploy and monitor their App Engine apps in an open-source environment while providing mechanisms to debug and profile applications as needed.

2.2.3 Software as a Service

This model provides the user with the capability to use applications running on a cloud infrastructure. Such applications are accessible from various client devices through either a thin client interface, such as a web browser (e.g., web-based email), or a program interface. It constitutes a higher level of abstraction in which users are provided with direct access to applications and databases without getting involved in the platform of infrastructure in which the software runs. Examples of SaaS are the wide variety of services provided by Google (GMail, Google Docs).

These three basic models are usually presented as a pyramid (see Figure 2.2) in which the highest levels of abstractions are supported by the lowest ones [Mah11]. Software products offered through SaaS are supported by virtual platforms offered through PaaS. Finally, those platforms can be hosted by virtual infrastructures provided as IaaS. The consumer of one service (such as PaaS) can provide the upper level of abstraction (i.e. SaaS) to other clients. At the and all actors are virtual instances executed on the cloud.

Other authors introduce slight variations on the model, adding or removing some components, but maintaining the same basic structure. For instance, the Figure 2.3 shows a schema proposed by [YBDS08], very similar to the aforementioned pyramid, in which cloud applications (SaaS) can be supported by software environments (PaaS). The infrastructure layer is divide in a more specific subsets: computational resources (i.e. virtual cores), storage (i.e. virtual hard disk drives or storage spaces) and communications (virtual networks). All items rely on the software kernel, which can be any cloud virtualization layer such as OpenStack. Finally, the physical hardware stands on the bottom of the schema.

2.2.4 The Upcoming Anything as a Service Model

The former models have been proved successful in current economies of scale and have been extended to higher levels of abstraction like Database as a Service [HIM02, CJP+11], Network as a Service [CMPW12] and Security as a Service [SDP13]. This is leading to a generic Anything as a Service (XaaS) vision. Simulations are not unaware of this trend, and there are current efforts to deploy simulation services on the cloud, like [AM13] and [Xia11]. With the explosion of cloud services and the Anything as a Service (XaaS) model, cloud service providers have also started to offer several HPC paradigms [APK+12]. Examples of this are MapReduce [Ama], MPI implementations [RBA11], and GPGPU processing [ECW10, SCSL12].

The so-called Simulation as a Service model and the native frameworks offered by Cloud providers seem promising for scientific simulations that are required to be scalable, but there is also a number of challenges that must be faced. The Magellan Final Report [YCD+11] exposes that scientific applications executed on the cloud suffer the overhead associated to the virtualization layer and the absence of high-bandwidth, low-latency interconnections in current virtual machines. Considering that nodes can be located in different data centres, communication-sensitive paradigms such as MPI would show decreased performance in such environments against traditional infrastructures.

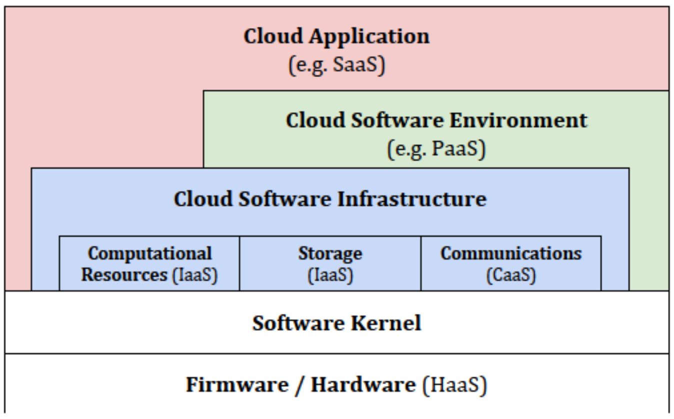

Cloud Application
(e.g. SaaS)
Cloud Software Environment
(e.g. PaaS)
Cloud Software Infrastructure
Computational Resources (IaaS)
Storage (IaaS)
Communications (CaaS)
Software Kernel
Firmware / Hardware (HaaS)

FIGURE 2.3: Cloud Computing services stack proposed by [YBDS08].

Several works have tackled the challenge of migrating scientific simulations to the cloud. A discussion about the use of clouds in science is conducted on [Lee10], where benefits and issues are analysed. [TLSS11] proposes SimSaaS (Simulation Software as a Service), a framework that combines a cloud multi-tenant architecture with simulation software, strongly focusing on data isolation and security. This framework is an evolution a service-oriented architecture proposed by the same author in [TFCP06].

2.2.5 Current Challenges in Cloud Computing

Cloud Computing is nowadays a widespread model used by enterprises all over the world. Nevertheless, this business model is still considered far from reaching maturity. Gartner's hype cycle of Cloud Computing [Smi12] still places most of the cloud key concepts far from the plateau of productivity. Besides, a survey carried out by Cloud Security Alliance [CSA12] finds that cloud market has not yet reached a level of maturity that will support major industry disruptions. Survey participants believe that platform and infrastructure service offerings are still in the infancy stage of maturity, while software service offerings are just emerging from infancy and are in the early stages of market growth.

There are still many challenges to be overcome in order to consider Cloud Computing as a completely mature technology. The following list provides a brief description of these challenges, obtained from several sources:

Security and privacy in clouds Data security and privacy in clouds is the main issue that concerns potential users of Cloud Computing [AFG$^+$10, DWC10]. Following the service models, cloud users are placing his/her data onto the provider's infrastructure, which represents a security issue due to intentional or non-intentional provider's malpractices. This security issue can be analysed from several perspectives:

1. Companies are reluctant to give its sensible data to third-party enterprises which could access and use, (or sell) this information to external agents. Otherwise, failures in providers security infrastructure may lead to involuntary data leaks. Recent NSA scandal has situated the focus on this particular aspect [Art13].
2. Companies are concerned about whether its services or data will have the required availability. Provider infrastructure failures have a direct impact on the client, and may lead to services interruption or data loss [Cla12].
3. Virtualization technologies used in Cloud Computing difficult the traceability and auditability of applications and data. Security records may expire when virtual machines are terminated. Besides, as long as many parties are involved on a cloud service delivery (cloud user, cloud provider, third-party vendors, etc.), it is difficult to provide consistent logging across all these parties.

Finally, the concept of "reputation fate-sharing" has arisen between companies which use cloud services [AFG$^+$10]. One costumer's bad behaviour can affect the reputation of others using the same cloud, since all customers are sharing the same computational resources (network addresses, physical machines, etc.).

Portability and interoperability One of the current issues in Cloud Computing is the absence of a common specification of Cloud services. An early stage of maturity in this industry leads to absence of standards and fierce competition in order to get dominance in markets. Practically every cloud provider offers a custom API to access its services, implementing different interfaces and behaviours. As a result, portability and interoperability between different cloud providers gets hard, since potential clients who want to interoperate with several providers have to implement several of these interfaces and behaviours. Besides, one of the main issues in cloud industry is the so-called "*vendor lock-in*", in which cloud clients get tied to its providers due to the high costs of re-implementing its applications adapting them to APIs of another providers.

There are several scenarios in which the use of multiple clouds is desirable: guarantee performance or availability, change of cloud vendors, or distribute a deployment across federated or hybrid clouds. Petcu et al. [Pet11, PMPC13] enumerates a list of requirements which have to be accomplished before performing cloud interoperability with an acceptable chance of success. Some of them are stated below:

1. At programming level, moving from one provider to another shouldn't imply a dramatic reimplementation. This can be reached through the existence of a common set of interfaces which would allow to manage simultaneously clouds from different providers. Besides, a common ontology of cloud computing is necessary in order to standardize components and behaviours, which may vary across different providers. With regard to this requirement, currently small cloud providers tend to implement the most popular APIs even if they are property of a competitor. For instance, OpenStack implements the Amazon AWS interface in order to attract Amazon clients. This may lead to a *de facto* standardization of APIs of the strongest providers.
2. At application level, the ability of spanning multiple cloud services should be performed in a transparent fashions. Examples of this could be moving data across different clouds or allocate computing resources on public clouds when a private cloud application hasn't enough available resources on its private cloud.
3. At monitoring level, SLA and performance monitoring should be delivered in an homogeneous and standardized fashion. This imply the creation of a set of benchmarks to evaluate performance factors, equivalent to all providers, as well as a common interface for supporting monitoring and management of load balanced applications. Besides, equivalent SLA metrics should be established between all providers in order to compare the quality of delivered services.
4. At deployment level, the ability to allocate resources from multiple cloud services should be managed with a single tool, in order to ease application deployment, configuration and management. Common platforms should be provided, in order to ensure that users can navigate between services/applications, enabling that a service hosted on one platform could automatically call another service hosted by other platform.
5. At authentication and security level, single sign-on for users accessing multiple clouds would be necessary, as well as integration of different security technologies, in order to provide an holistic vision of the security architecture, shared by all participants in the cloud service delivery (consumer, provider, third-party vendors, etc.).

Energy issues Energy efficiency is a major concern in current ICT, as well as one of the major challenges that must be overcome in order to achieve Exascale systems. Cloud Computing is not aware of this trend, so efforts are under way to increase energy efficiency in data centres, (i.e. decreasing power consumption while maintaining SLAs). As it is stated in [BGDG+10], energy-related costs amount to 42% of the Amazon data centre TCO, including both direct power consumption (19%) and the cooling infrastructure (23%).

Several techniques to improve energy efficiency in data centres have been already developed and deployed, and several others are under research. The following list describes briefly some of them:

1. Energy-efficient hardware. This approach is focused on developing hardware (CPUs, motherboards, disks) that consumes much less energy. Computer power can be saved by means of various well-known techniques, such as power down the CPU or switch off disks if there isn't any I/O activity.
2. Energy-aware scheduling in MP systems. These techniques schedule workload on a data centre trying to optimize power consumption across the servers. Tasks with different characteristics (compute bound, memory bound, I/O intensive) may have different footprint on server consumption. Moreover, virtualization may be used to consolidate several (virtual) servers in only one physical server.
3. Power minimization in clusters of servers. This technique is based on maintaining active a small set of active servers, while other servers are down to a low-power state. Due to the time required to turn up servers, it is necessary to foresee data centre utilization and keep a number of servers ready to face unexpected peak demands.

2.2.6 Trends in Cloud Migration and Adaptation Techniques

As already mentioned, scientific applications and their adaptability to new computing paradigms like the Cloud have been dragging increasing attention from the scientific community in the last few years.

The possibility to run simulations in the Cloud in terms of cost and performance was studied in [JDV+09], concluding that performance in the Abe HPC cluster and Amazon EC2 is similar –besides the virtualization overhead and high-speed connectivity loss in the cloud– and that clouds are a viable alternative for scientific applications. Hill [HH09] investigated the trade-off between the resulting performance and achieved scalability on the cloud versus commodity clusters; despite at the time of this work the Cloud could not properly compete against HPC clusters, its low maintenance and cost made it a viable option for small scale clusters with a minimum performance loss. Amazon [PBB15] proposes migrating HPC applications to its Cloud, but (surreptitiously) establishes restrictions to the size of the virtual cluster in those applications which are tightly coupled.

In this context, trends are naturally evolving to migrate applications to the Cloud by means of several techniques, and this includes scientific simulations as well. D'Angelo [D'A11] describes a Simulation as a Service schema in which parallel and distributed simulations could be executed transparently, which requires dealing with model partitioning, data distribution and synchronization. He concludes that the potential challenges concerning hardware, performance, usability and cost that could arise could be overcome and optimized with the proper simulation model partitioning.

In [SJV12], Srirama et al. study how some scientific algorithms could be adapted to the Cloud by means of the Hadoop MapReduce framework. They establish a classification of algorithms according to the structure of the MapReduce schema these would be transformed to and suggest that not all of them would be optimally adapted by their selected MapReduce implementation, yet they would suit other similar platforms such as Twister or Spark. They focus on the transformation of particular algorithms to MapReduce by redesigning the algorithms themselves.

Application adaptation middle-wares have also been developed to allow legacy code migration to the Cloud. For instance, in [YWH+11] a virtualization architecture is implemented by means of a Web interface and a Software as a Service market and development platform. This generalist approach is suitable to provide multi-tenancy in desktop applications, but might not suffice for the resource-intensive computations required by large-scale simulations.

Finally, in [SIJW13] there can be found interesting efforts to move desktop simulation applications to the Cloud via virtualized bundled images that run in a transparent multi-tenant fashion from the end user's point of view, while minimizing costs. However, the virtualization middleware might affect performance since it does not take into account any structural characteristics of the model, which could be exploited to minimize migration effects or drastically affect execution times or resource consumption.

Despite Cloud Computing has proven itself useful for a wide range of scientific applications, its utility for tightly-coupled HPC applications is still under research and development, mostly because of the added communication overhead and the heterogeneous underlying hardware [JRM+10]. Lately, several efforts have been made in the opposite direction: trying to adapt HPC resources and infrastructures in order to offer a Cloud-fashioned interface, bringing elasticity and pay-per-use model but avoiding the virtualization layer and maintaining the applications close to the real hardware. An example of this trend is the solution provided by Penguin Computing [Sch15], which offers a cloud service with bare-metal access, Infiniband interconnects, and support by HPC experts.

2.3 MapReduce

As seen in the previous section, one of the promising models that has been increasingly considered to adapt simulations to the Cloud is the MapReduce parallel computing framework, specially in cases in which data locality is key to improve performance by reducing data transmission overhead. The MapReduce paradigm [DG08] consists of two user-defined operations –*map* and *reduce*– and three additional phases that handle the original data, the intermediate results and the final output. Figure 2.4 shows the MapReduce dataflow and their stages, which behaves as follows:

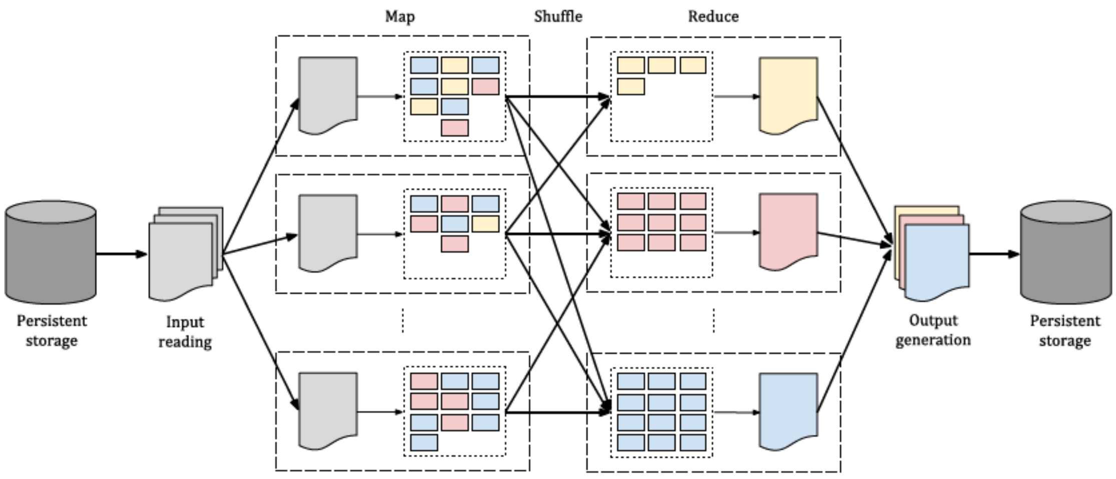


FIGURE 2.4: MapReduce dataflow.

Input reading The framework reads the input data from persistent storage and generates data chunks and assigns each of them a key, k_1, and a specific processor in the system.

Map Each input chunk is processed by a single independent map, thus spawning as many maps as k_1 values the previous phase had generated. The map's output is constituted by a set of intermediate pairs organized by a new key, k_2.

Shuffle The intermediate output is organized in lists of values for each k_2, which are assigned to a specific reducer.

Reduce As in the map function, each k_2 value list is manipulated by an autonomous reducer. The output is indexed by a new key, k_3, to allow the framework to produce the final output.

Output generation The reducer's output is collected and sorted by the framework, according to k_3, in order to write the final results to disk.

As a data-centric paradigm in which large amounts of information can be potentially processed, the *map* and *reduce* operations run independently and only rely upon the input data they are fed with. Thus, several instances can run simultaneously with no further interdependence. Moreover, data can be spread across as many nodes as needed to deal with scalability issues.

Given its popularity, there are several MapReduce implementations for distributed environments, with different capabilities and specifications. Some of the most popular are listed below:

Twister As previously mentioned, MapReduce performs poorly with iterative algorithms given the need of spilling intermediate data to disk between iterations. This system supports an efficient implementation of MapReduce for such applications by means of static data reusage among the tasks involved [ELZ$^+$10].

Peregrine This system eliminates the need of intermediate output writes. This feature, along with its implementation of MapReduceMerge [YDHP07], result in an overall improvement of MapReduce's capabilities. Moreover, it allows broadcasts of global-like variables and supports automatic task execution plan optimizations, so that the developer does not have to be tied to the classic MapReduce structure.

Hadoop MapReduce The most popular MapReduce implementation derived from the original Google's MapReduce and Google File System (GFS), providing an open-source alternative for both of them, is designed to be run on commodity hardware. Nowadays, Hadoop MapReduce is executed on top of the Hadoop Distributed File System (HDFS), the Hadoop Common platform and the Yet Another Resource Negotiator (YARN) resource manager, while sharing this environment with other related projects such as HBase (database system), Hive (data warehouse infrastructure) and Mahout (machine learning algorithms). It was designed to deal automatically with failures in one or several nodes of the cluster, thus resulting in a high-availability solution for data-processing infrastructures.

Spark This Hadoop-related project is focused on improving MapReduce's deficient performance regarding iterative jobs and interactive analytics [ZCF$^+$10]. Examples of these uses cases include parameter optimization on a static dataset, in which each iteration constitutes a job, and queries on large partitioned datasets, requiring a job per query. Spark's approach is based on a read-only Resilient Distributed Dataset that can be loaded into memory across many machines allowing multiple parallel operations on the same input data with no need for intermediate writes. Furthermore, Spark is not tied to the MapReduce framework and supports other programming models.

Elastic MapReduce Amazon's Elastic MapReduce (EMR) is a web service dedicated to process data on Hadoop MapReduce. It provides further advantages regarding multiple cluster manipulation, virtual cluster on-the-fly resizing, Simple Storage Service (S3) integration and HDFS support on local ephemeral storage.

Cloud MapReduce Similarly to EMR, this is another MapReduce implementation for the Cloud built on top of Cloud OS, a resource manager for the set of machines integrated to build the underlying cloud. Besides allowing incremental scalability and resizing, its most interesting feature is its decentralized and symmetric architecture in which all the nodes have the same responsibilities, even on heterogeneous environments [LO11].

2.3.1 Hadoop MapReduce

Apache Hadoop [Whi09] has been selected as main platform given its increasing popularity and community support. Its distributed file system is a great addition to the framework, since it allows automatic load balance and includes a distributed cache that supports auxiliary read-only file storage for tasks among all nodes. Besides the former technical features, Hadoop has been increasingly adopted into cloud environments along with other MapReduce frameworks, resulting in reduced costs given its parallelism exploitation capabilities [KPP09].

In addition, studies regarding the relationship between the Cloud and Hadoop MapReduce for scientific applications have established that performance and scalability results are similar between traditional clusters and virtualized infrastructures running this platform [GWQF10].

As a constantly changing technology, Hadoop evolves fast into more sophisticated and flexible versions, moving from the MapReduce-only infrastructure (versions 1.x) to the all-purpose YARN manager (versions 2.x). The following paragraphs give an overview of both platforms architectures and features, and describe their common underlying distributed file system, HDFS.

2.3.2 HDFS

HDFS was designed to suit Hadoop's requirements and needs. It supports the large data sets (from GB to TB of data) that Hadoop is meant to operate with, and is was built for batch read and write operations according to the MapReduce model.

In order to comply with Hadoop's fault tolerance goals, HDFS was designed for reliability and automatic recovery in case of error in one of the components of the cluster, thus providing block-level data replication and coherency mechanisms across the involved nodes.

Figure 2.5 gives an architectural overview of this file system. In it there is a *NameNode* that contains all the metadata of the system such as file-block mapping, block location among the nodes, paths and replication information. This information is requested by the client in order to perform read and write operations directly on the nodes themselves, once it has been provided with block locations. Since the *NameNode* constitutes a single point of failure in this system, it is replicated into a *Secondary NameNode* as backup; the latter would serve clients' metadata requests in case of failure.

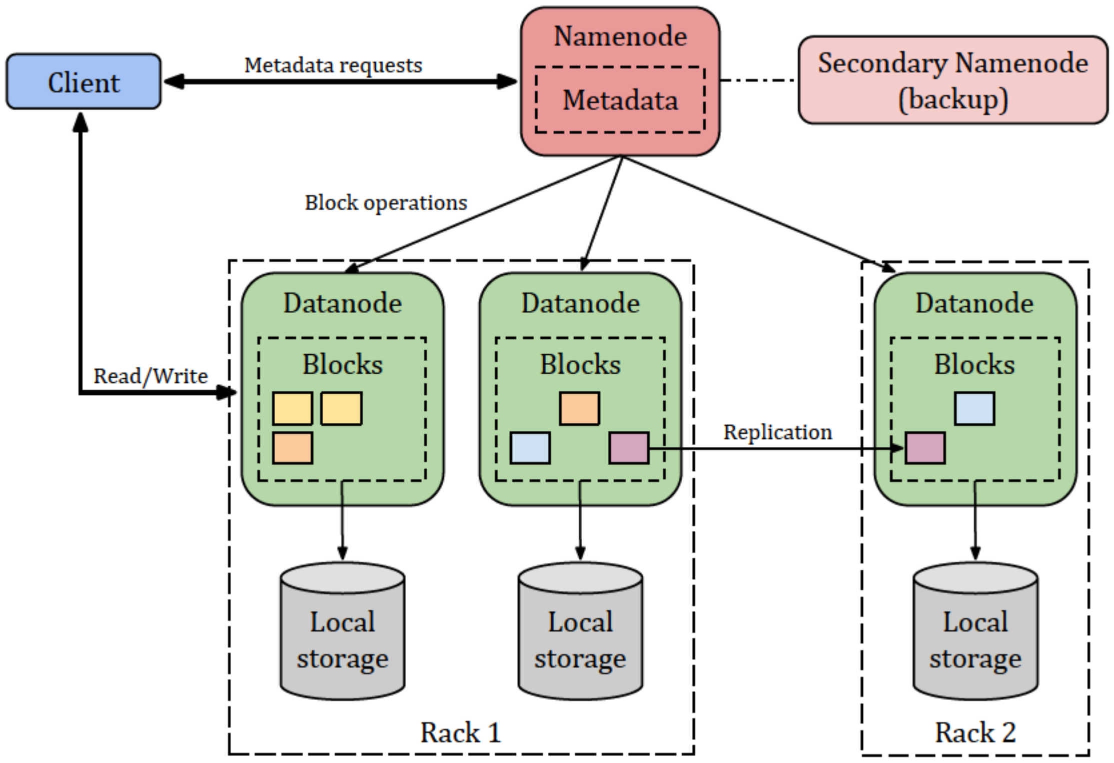


FIGURE 2.5: HDFS architecture.

A very interesting feature of the *NameNode* is its rack-awareness, for it is possible to configure the network's hierarchy to let it know which nodes are topologically closer to each other. This is crucial as data exchange between closer nodes is faster and replication is more effective if performed between two different racks, since the failure of a section of the network would not affect the system's availability.

In order to remain updated, the *NameNode* is in contact with the *DataNodes*, which constitute the actual storage nodes since blocks are stored in their local disks. This communication is performed by means of block operations that provide metadata to the *NameNode* and request operations such as replication to the *Datanode*. In case of replication, data copy is performed between *DataNodes* once it was authorized by the *NameNode*.

2.3.3 First Generation MapReduce Runtime (MRv1)

Hadoop 1.1.2 MapReduce's architecture –shown in shown in Figure 2.6– is based on a fixed number of slots that can be assigned to mappers and reducers equally. These are fully managed across the nodes by a unique *JobTracker*, which also coordinates mappers and reducers, provides progress information to the client which also assigns a *TaskTracker* per node to handle local operations and slot usage.

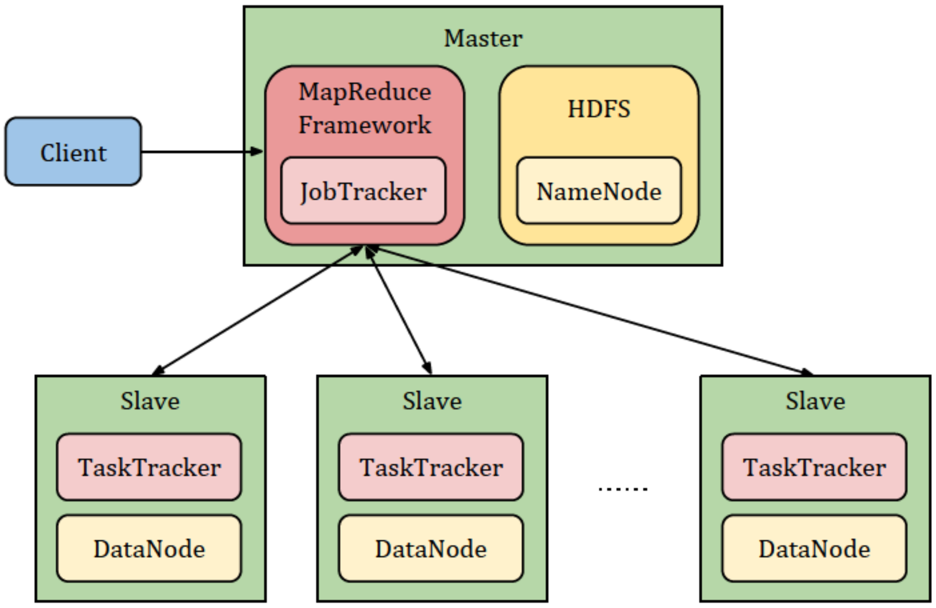


FIGURE 2.6: MapReduce 1.x architecture.

The *JobTracker* constitutes a single point of failure and may become a bottleneck in very large clusters [YKSM13]. It also lacks resource allocation flexibility, so it is starting to become obsolete and it is being increasingly replaced by Next Generation MapReduce.

2.3.4 Next Generation MapReduce (MRv2) and YARN

Next Generation MapReduce (MRv2) encapsulates cluster resource management capabilities into Yet Another Resource Negotiator (YARN), leaving MapReduce-specific functionalities and configuration in an independent module. This allows to avoid some scalability issues originated in the *JobTracker* by dividing its functionality, and results in a general-purpose platform for other programming paradigms and applications [The13].

Figure 2.7 shows MRv2's architecture and Hadoop's component communication with solid lines for resource managing, and dashed lines for MapReduce application control. The MapReduce functionalities handled by the previous *JobTracker* were moved to the new *ApplicationMaster*, while a *ResourceManager* is in charge of the cluster's resource management and a *HistoryServer* provides clients with information of completed jobs. *TaskTrackers* were replaced with *NodeManagers* that are responsible for the resources and container management on each node. Each container can hold a map or reduce task and can be configured regarding the available computational power, memory and input/output capabilities of the node, which yields an increased flexibility for task scheduling.

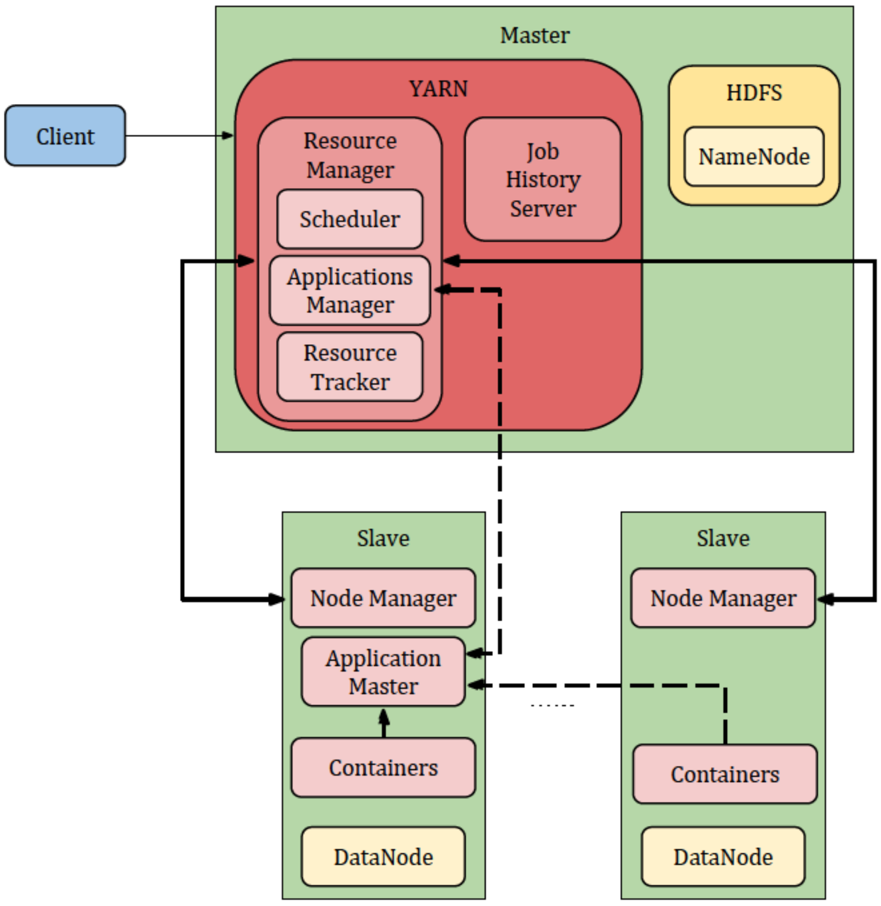


FIGURE 2.7: MapReduce 2.x architecture.

2.4 Cloud Computing and Scientific Applications

Scientific applications and their adaptability to new computing paradigms have been dragging increasing attention from the scientific community in the last few years. The applicability of the MapReduce scheme for scientific analysis has been notably studied, specially for data-intensive applications, resulting in an overall increased scalability for large data sets, even for tightly coupled applications [EPF08].

Hadoop MapReduce is nowadays widely used as base platform for new programming languages and architectures. Hadoop MapReduce is used in Pig Latin [ORS+08], an associative language used in Yahoo for taking advantage of both declarative languages and map-reduce programming style. This approach is strongly focused on processing data sets, and does not tackle the issue of scientific workflows. Apache Hive [TSJ+10] and Bigtable [CDG+08] are two storage systems developed on the top of Hadoop. Hive expresses data queries in an SQL-like declarative language which is compiled into map-reduce jobs. Bigtable uses a sparse, distributed, multi-dimensional sorted map to provide a fast method to access data, although de data structures exposed to the user are rows, columns, and tables.

Nevertheless, the most popular evolution of Hadoop MapReduce is Spark [ZCF+10]. Spark evolves the map-reduce programming style operating on resilient in-memory distributed data sets, thus improving performance in workflows (since the data does not have to be written to disk between tasks). Finally, an approach more related to scientific simulations is Twister [ELZ+10], a runtime specifically designed for iterative map-reduce works and, therefore, more suitable for repetitive computations over the same data.

The relationship between Apache Hadoop MapReduce and the cloud for scientific applications has also been tackled in [GWQF10], which establishes that performance and scalability results are similar between traditional clusters and virtualized infrastructures. In [SJV12], Srirama, Jakovits and Vainikko study how some scientific algorithms could be adapted to the cloud by means of the Hadoop MapReduce framework. They establish a classification of algorithms according to the structure of the MapReduce schema these would be transformed to. They suggest that not all of them would be optimally adapted by their selected MapReduce implementation, yet they would suit other similar platforms such as Twister or Spark. They focus on the transformation of particular algorithms to MapReduce by redesigning the algorithms themselves, and not by wrapping them into a cloudification framework as this thesis proposes. A similar approach is HAMA [SYK+10], a framework which provides matrix and graph computation primitives on the top of MapReduce. An advantage of this framework over traditional MPI approaches to matrix computations is the fault tolerance provided by the underlying Hadoop framework. Finally, an approach for using Hadoop MapReduce in scientific workflows is that explained in [XZSA13], whose authors propose a new architecture named SciFlow. This architecture consists on a new layer added on the top of Hadoop, enhancing the patterns exposed by the framework with new operations (join, merge, etc.). Scientific workflows are represented as a DAG composed of these operations.

More related with the proposed approach is the so-called *parameter sweep* [CLZB00], in which the same simulation kernel is executed multiple times with different input parameters, thus providing task independence. A related point of view is the many-task computing paradigm [RFZ08], in which a high number of loosely coupled tasks are executed over data sets for a short time. In this context, cloud computing has been proved as a good solution for scientists who need resources instantly and temporarily for fulfilling their computing needs [IOY^{+}11]. On the other hand, these evaluations show that better performance is needed for clouds to be useful for daily scientific computing. SciCumulus [dOOBM10] is proposed as a lightweight cloud middleware to explore many-task computing paradigm in scientific workflows. This middleware includes a desktop layer to bring the scientist the possibility of composing their own workflows, a distribution layer to schedule the flows in a distributed environment, and an execution layer to manage the parallel execution of the tasks. The preliminary results demonstrate the viability of the architecture.

2.5 Summary

In this chapter, the state of the art in HPC and Cloud Computing has been described. An overview of the current state, trends, and application suitability for both paradigms has been provided, pointing also the differences between them in terms of efficiency, elasticity, and adaptability. A survey of Hadoop MapReduce, a popular platform designed to process big amounts of data, that can be deployed on both HPC and Cloud infrastructures, has also been presented, as well as a thorough research on those simulators or engineering applications that are currently being migrated from HPC to Cloud, usually through MapReduce. These applications are very demanding in terms of computing power and efficiency, and therefore their migration must be studied carefully. In the next chapter the problem types that must be addressed in order to migrate a simulator from HPC to Cloud environments are studied.

Chapter 3

Problem Statement

There is a huge catalogue of simulation problems associated to scientific and engineering domains, but from the viewpoint of exploiting HPC and Cloud resources, it is meaningful to classify those problems according to its suitability for each particular infrastructures. HPC resources, in general terms, provide higher CPU power, on the basis of a similar number of computing resources such as CPUs, nodes, and disks. This is due to several reasons:

- HPC infrastructures do not use a virtualization layer (or at least, not as thick as its cloud counterparts) in order to detach the real hardware from the user point of view. And it is not only the added overhead of the virtualization layer, but also the possible collision of different users for the same hardware. In clouds, resources like processors or nodes are masked to the user, and several users can share (unwittingly) the same node, interfering each others in shared resources like cache memories, main buses, etc. Besides, the virtualization layer hampers those architecture-specific optimizations which cannot be translated dynamically at run time (e.g. SIMD instructions).
- HPC infrastructures are deployed using low-latency networks, specifically intended to decrease performance penalty in those problems which require a great amount of communications. Besides, all nodes in a cluster are held together arrayed in racks, the layout known by the network stack, so optimizations in communications can be performed. While clouds can perfectly deploy the same kind of networks, the virtualization layer, and the variable allocation of virtual machines prevent the application from knowing the underlying topology. Besides, cloud infrastructures can be spread across several data centres, which implies the possible allocation of virtual machines far from each other.
- HPC infrastructures deploy parallel file system in order to manage massive I/O. Such parallel file systems are hard to deploy in cloud infrastructures due to topology unawareness and software/hardware decoupling. The same principle can be applied to tuned computing libraries like [1]ScaLAPACK, which usually are optimized for the underlying hardware.

[1]`http://www.netlib.org/scalapack/`

On the contrary, Cloud Computing paradigm provides with more elastic infrastructures. The key feature of Cloud is that the user can size computing resources according to its particular needs. This is particularly useful on simulation, where workloads are strongly dependent on the size of the simulation, and the deadline the user wants to meet. Variable simulation sizes, or urgent necessities for obtaining immediately results may lead to big differences in the computing resources required.

Given the former, it is necessary to find how to make simulators suitable for both HPC and Cloud Computing, considering these big differences between both models. The fist step towards this direction is analysing and classifying problem types according to its suitability to these kinds of platforms.

3.1 Problem Types

On analysing a problem suitability for HPC or Cloud infrastructures, data and communications are the factors that have more relevance. There are two issues about data that should be analysed: data quantity and data structure. Data quantity is relevant because of the economic factor associated to Cloud Computing. Storing and processing information on the Cloud may suppose an expense proportional to the amount of data processed and stored. While the key advantage of Clouds is the elasticity of the infrastructure, the more resources you allocate, the more costs you have to pay. Therefore big amounts of data imply big expenses. Data structure is relevant because high latencies in clouds penalize applications which perform a lot of communication. Therefore a parallel application which has to swap much data between compute nodes in order to process the information (e.g. a parallel simulator performing a simulation), will behave poorly on clouds.

Due to the fact that economic aspects of Cloud Computing exploitation fall out of the scope of this thesis, the following analysis will be focused on data structure, classifying the problems according to the structure and dependences between its data.

3.1.1 Pleasingly Parallel Problems

Pleasingly parallel problems (also called embarrassingly parallel problems) are those kind of problems which are the easiest to implement in parallel. In pleasingly parallel problems the input data set can be decomposed and processed in several independent tasks, with no communication required between those tasks. Thus, the initial workload can be split among a number of compute nodes, and each node can process its part of the data independently. Because no communication is required between tasks, high network latencies have a minimal impact on performance (only at the initial stage of distributing the workload). Therefore this kind of problems are the best suitable for Cloud Computing, though they also perform well on HPC.

The following list contains several examples of pleasingly parallel problems:

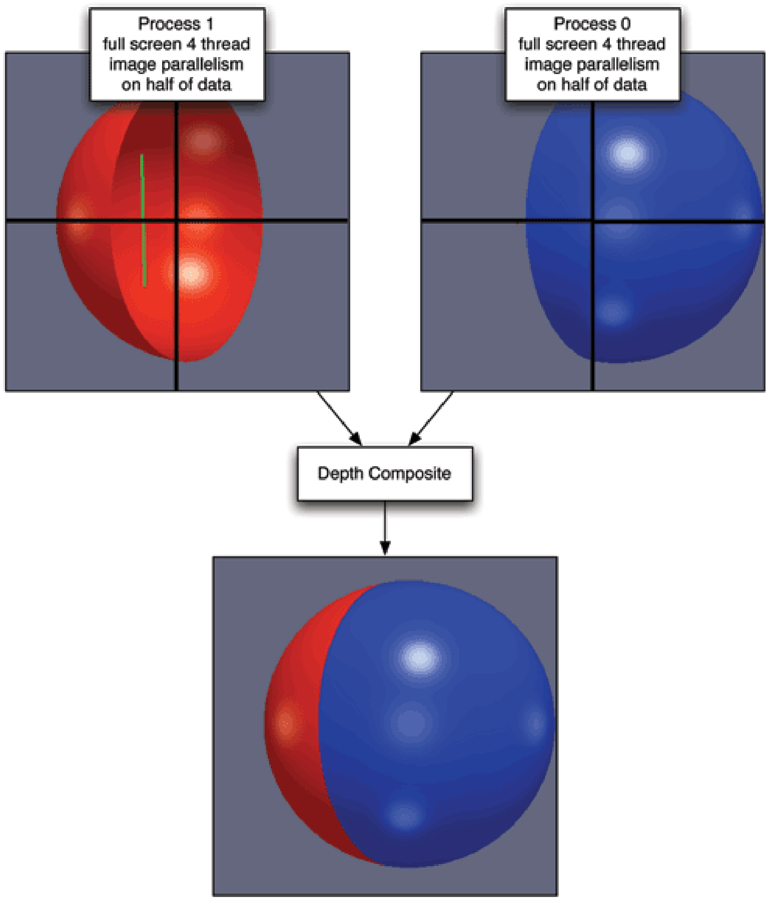


FIGURE 3.1: Parallel rendering in computer graphics as an example of a pleasingly parallel problem.[2]

- Distributed relational database queries. If a table is split among multiple nodes, each node can process its own part of the table without interacting with other nodes, apart from merging the results of all nodes on finalization.
- Fractals (*e.g.* Mandelbrot set). Each point of the set can be calculated independently, so the problem domain (i.e. a set of complex numbers) can be split among the compute nodes.
- Rendering of computer graphics. The same principle stated before applies to computer graphics, in which each pixel of the screen can be rendered independently. Finally all pixels are merged forming the final picture. Figure 3.1 illustrates an example of parallel rendering in computer graphics.
- Matrix multiplication. On multiplying matrices $A\dot{B} = C$. Each element c_{ij} of the resulting matrix can be calculated using only i row from A and j column from B, so the workload of calculating the resulting elements can be split across compute nodes, provided each node has access to the corresponding rows and columns from A and B.

[2]`http://www.kitware.com`

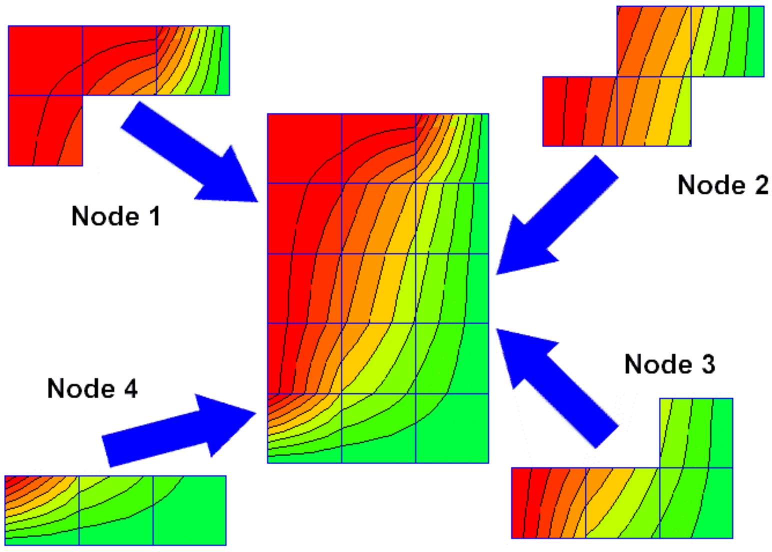


FIGURE 3.2: Parallel finite element simulation as an example of a loosely coupled problem.[3]

3.1.2 Loosely Coupled Problems

In this type of problems, the problem domain can be decomposed easily in several subdomains. but there is a (weak) dependence between those subdomains. They have to share information with their neighbours, or they influence its neighbours somehow. A certain amount of communication between compute nodes is required in order to solve the problem in parallel. While the boundaries of these communications are limited to a local scope, for instance adjacent CPUs in the virtual topology (otherwise we would be talking about tightly coupled problems), the impact of high latencies gets worse as the problem becomes bigger or it is required a higher degree of accuracy in the simulation.

All problems which involve partial differential equations, such as FEM or CFD, are loosely coupled problems. In such problems, the simulated structure/body/fluid is decomposed and simulated in several independent pieces, but the iterations between those decomposed pieces have to be calculated also in order to reflect a realistic behaviour (see Figure 3.2). Another loosely coupled problem is a (parallel) convolution, in which two functions are compared across the problem domain trying to find overlapped areas. One example of this would be a filter applied to an image. The image can be decomposed in several pieces, so the filter is applied in parallel to those pieces, but the boundaries between pieces have to be checked also, so a bordering region should be shared between neighbours.

3.1.3 Tightly Coupled Problems

These problems are the hardest to implement in parallel. In tightly coupled problems, every single entity (or most of the entities) of the problem domain has a certain amount of influence on the others. Therefore, there is a strong dependence, and each partition of the problem needs information of the others to solve the problem. A large amount of communications is required

[3] `http://ccpforge.cse.rl.ac.uk/gf/project/parfel`

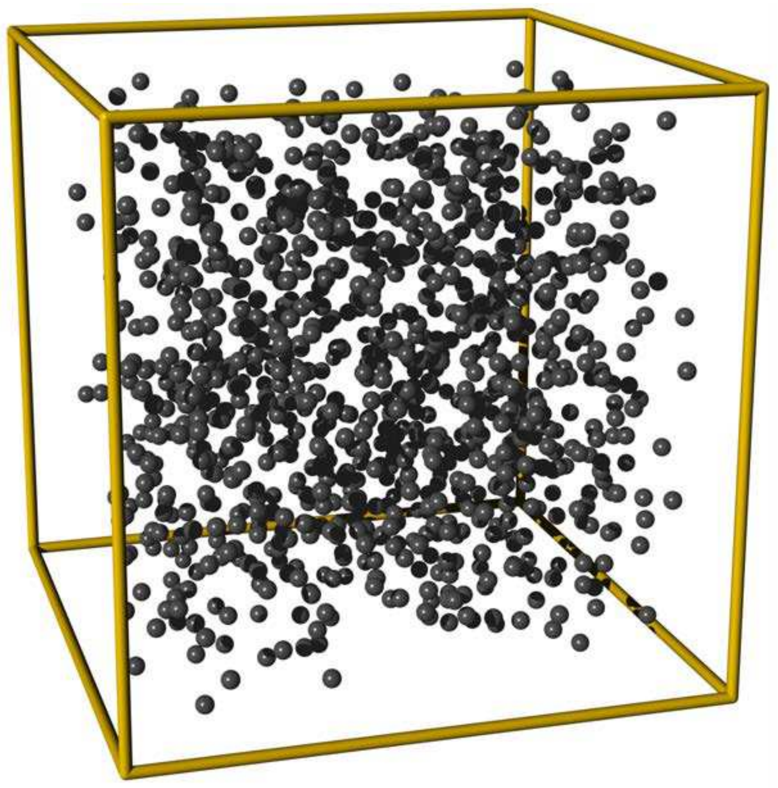


FIGURE 3.3: N-bodies problem as an example of a tightly coupled problem.[4]

to solve this problem in parallel, and this amount is increased exponentially as the problem size grows. Hence, communication latencies have a great impact on performance when solving this kind of problems.

A classic example of a tightly coupled problem is the N-bodies problem. In the N-bodies problem, the behaviour of a number of bodies have to be simulated, provided that each body interacts with the others (see Figure 3.3). Examples of interactions are gravitational (each body attracts and it is attracted by the others) or electromagnetic. Provided a domain decomposition based on bodies (each node calculates and updates a subset of the total bodies), since every different body influences all the others, some kind of information have to be exchanged between the nodes in an all-to-all fashion. Another example of a tightly coupled problem is the parallel implementation of Dijkstra's Algorithm, in which each node tries to find the shortest path independently, but on each interaction all results have to be merged in order to find what is the global shortest path.

3.1.4 Multivariate analysis: A Pleasingly Problem Particular Case

Simulators are widely used as tools not only for developing new designs or solutions, or improving existing ones, but also as part of optimization processes, with the aim of exploring a problem search space, trying to find the optimal components of a system. In other approaches, it is required to understand the behaviour of the system in response to variations of the input

[4]`http://parallel.massey.ac.nz/projects.html`

parameters. These approaches are called *multivariate analysis*, in which the value of one parameter is adjusted by sweeping the parameter values through a user defined range, checking for each value the behaviour of the system through simulation. *Multivariate analysis* usually implies performing not one but many simulations, using the same simulator but varying the input data.

In this context, the whole task of exploring the problem's search space obtaining the optimum (or optimums, if performing a multi-objective optimization) can be considered as a pleasingly parallel problem. Each single simulation is a sub-part of the a whole search problem. Apart from scoring and comparing the solutions once simulated (which can be considered as a kind of "merge" operation), there are no dependences between simulations, and therefore they can be executed independently. Note that this can be considered a pleasingly parallel problem regardless of whether the simulation problem itself is a pleasingly parallel problem, a loosely coupled problem, or a tightly coupled problem. In this case, there are two levels of parallelism:

- *Data-level parallelism*, based on the multiple independent simulations which can be performed concurrently, each one of them with a different input.
- *Task-level parallelism*, if each one of those simulations can be performed in parallel (either in a pleasingly parallel, loosely coupled, or tightly coupled fashion).

Examples of such kind of simulators can be found in [SGG+12] and [GGS+13]. These works introduce a simulator that designs and calculates railway portal frames. The structural calculations of an structure are performed using the direct stiffness method (DSM) which can be considered as task-level parallelism, but the tool also proposes different designs, looking for the best-suited structure that fills some requirements, thus performing multiple calculations of different structures, which can be considered as data-level parallelism.

3.1.5 Problem Types, Infrastructures and Platforms

Hadoop MapReduce have become in one of the most suited platforms for running applications on the Cloud. In Section 2.3 the main characteristics and architecture of MapReduce are detailed. As conclusions, it was stated that MapReduce uses data locality to improve performance, reducing data transmission overhead. This makes MapReduce an ideal platform on those environments where a huge amount of distributing processing is required, and communication latencies penalize the throughput according to amount of data transmitted through the network. MapReduce is also suitable for cluster environments on those operations which can be adapted to the map-reduce paradigm, yet it's lack of flexibility makes it a secondary option, with MPI performing the leading role.

As said in Section 2.1.2 MPI represents a standard *de facto* when developing HPC applications to be executed on HPC environments. MPI low-level optimizations and topology awareness makes MPI the best option on low-latency networks such as clusters or supercomputers. However, [5]MPI lacks of integrated fault-tolerance mechanisms for fault-tolerance and elasticity, as well as

[5]At least in the MPI specification document. Particular implementations may integrate non-standard mechanisms

the possibility of adapting the workload dynamically if the infrastructure changes. This makes MPI a non-optimal (yet possible) choice to execute applications on the Cloud. Even so, MPI gives the programmer much more flexibility with regard to network operations, thus parallel implementations of all problems can be developed using MPI.

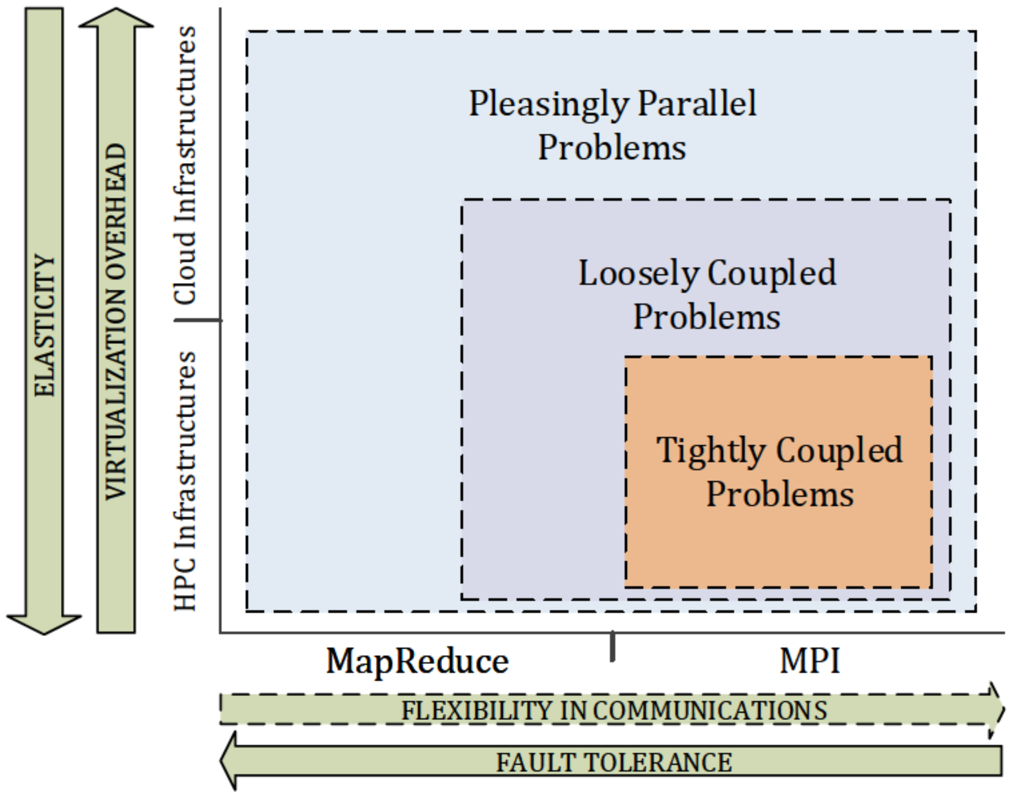


FIGURE 3.4: Platform and infrastructure suitability depending on the problem type.

All things considered, there is no best platform which could perform well in both HPC and Cloud environments. Figure 3.4 represents this trade-off on developing and deploying a parallel application. While MPI is more flexible than MapReduce, and can be used on either pleasingly parallel, loosely coupled, or tightly coupled problems, in Cloud environments MapReduce is more appropriate for pleasingly parallel problems.

3.2 Problem Statement: Applying Parallelism to Current Simulators

Current simulators make use of extensive computing resources. Nevertheless, a simulator may not be associated to just one of the problem types defined before, but several of them. Parallelism can be applied to different layers in the simulator, and depending on what layer is tackled, different levels of granularity, different data decomposition, and different communication patterns can result. Because these factors have direct impact on application performance (along with the infrastructure and platform type) they should be analysed carefully.

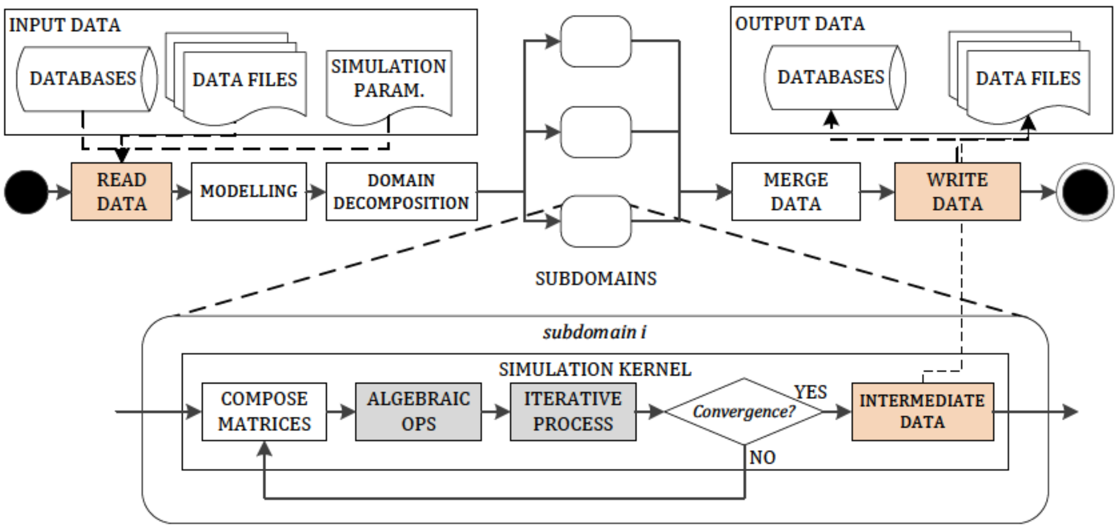


FIGURE 3.5: Generic architecture of a modern simulator and its elements.

3.2.1 Generic Architecture of a Modern Simulator

Prior to study the different ways of parallelizing modern simulators, and the advantages brought by such ways, it is required to identify a generic architecture of modern simulators, with the aim of defining shared characteristics and common elements. Although there is a huge variety of high-performance simulators, from different domains, operating different mathematical models, and with different characteristics, this proposal of generic architecture contains the most common elements, present in almost all simulators. By this way, any measure can be applied to as many simulators as possible, provided that such measure is based on this common architecture.

The proposed architecture is shown on Figure 3.5. This figure represents common components present in most simulators. As the figure is described in the forthcoming paragraphs, some concepts are going to be proposed as key components or features of that generic architecture. Later, these concepts will be applied to the analysis of modern simulators from a parallel point of view. Note that these definitions may differ from the widespread meaning, known by everybody. They will be used in the context of this thesis. The more general terms will be defined first of all:

- *Simulation.* A simulation is defined as the process of, starting from an input data set, producing an output data set by translating the input data into a simulation model, and operating such model. The whole process is represented in the Figure 3.5 between the start point (black circle) and end point (black circle with white edge).
- *Simulation model.* The structures and data used to represent the simulated domain, and the mathematical model and operations that process such data in order to produce the output. Ontologies are widely used to represent particular domains as structured data in order to be simulated.
- *Input data.* The data that contains a particular scenario or case study to be simulated. Usually on permanent storage such as databases or data files.

- *Output data.* The results obtained from the simulation. They must be stored in permanent storage such as databases or data files.
- *Multivariate analysis.* The concept of performing multiple simulations, varying on each one the input data set in order to obtain different results according to the variation. Optimization processes or ANOVAs are examples of multivariate analyses. A multivariate analysis constitutes several of the processes depicted in Figure 3.5.

Secondly, more specific concepts are defined, restricted to the scope of this generic architecture:

- *Modelling module.* The module that receives the input data and translates such data into the representation determined by the simulation model (matrices, graphs, etc.).
- *Domain decomposition.* The process of splitting the domain representation into smaller parts. These parts may have a degree of dependence between them, depending on the particular domain and simulation model. The more dependence, the more communication will be required between subdomains to perform the simulation. Domain decomposition is not strictly an essential element of common simulators, but should be present in those simulators intended to perform on parallel high-end infrastructures.
- *Subdomain.* A division of the original domain that can be operated by the simulation model independently (to a certain extent) from the others. Although, it may be necessary to merge some data in order to complete the simulation.
- *Simulation kernel.* A set of mathematical operations that constitutes the mathematical solver of the simulation model. Matrix operations and iterative processes (e.g. Newton-Raphson or the conjugate gradient method) usually compose the simulation kernel of most operations. [LKC$^+$10] enumerates a list of popular simulation kernels along with its characteristics in terms of resource usage, and opportunities for parallelization.
- *Intermediate data.* Many simulators generate intermediate data during the execution of the simulation kernels on each of the subdomain partitions. These data may be too large to be kept in memory and usually is sent to permanent storage on the last phase of the simulation kernel. Later, these data may be merged in a final phase of the simulation, in order to extract the definitive results.

Finally, some concepts that are present in a representative set of simulators but have not been included in the architecture are listed, as well as the reasons for such decision:

- *Data workflows.* Some simulators are composed of several consecutive phases, in which the output data of the previous phase is the input data of the next one. On each one of these phases different operations are applied to the data, forming a bound graph. These workflows are not represented on the proposed architecture, though they can be seen as several different simulation kernels applied in sequence, thus applying the same techniques taken to one simulation kernel.

- *Iterative processes.* In the same way, some processes require to apply the same kernel several times to the same set of data. On each one of these phases the same operations is applied to the data resulting from the previous iteration. In a similar way, they can be seen as the same simulation kernel applied in sequence.

3.2.2 Parallelization Layers

Once a generic architecture has been defined, the different ways of applying parallelization are analyzed. As said before, parallelization can be applied to different layers in the simulator. Figure 3.6 displays these layers. They are analysed from the top to the bottom. First of all, current simulators may not be limited to performing one single simulation. Instead, they can perform multiple simulations, as part of an optimization problem, or a parameter sweep engine. On a first stage, different scenarios are generated starting from an initial test case, through sweeping the parameters or just modifying the inputs by some way. Then, all simulations are executed, and the results are evaluated through the metrics associated to the optimization problem. In this top level a pleasingly parallel problem can be found, because the simulator has to execute multiple simulations, each simulation totally independent from the others.

Secondly, each one of the aforementioned simulations can be performed in parallel following classic approaches of domain decomposition. A particular simulation domain can be decomposed

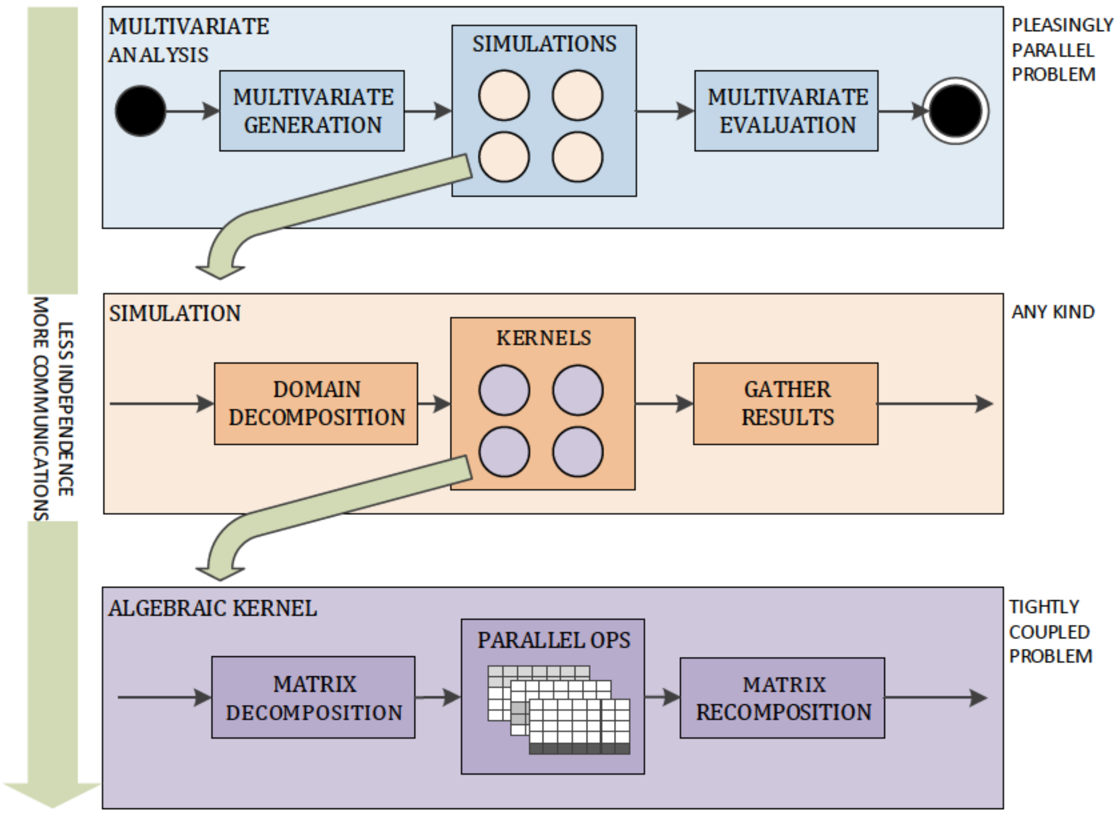


FIGURE 3.6: Parallelization layers on current simulators, from the top level (pleasingly parallel) to the bottom level (tightly coupled).

in several subdomains, simulating each subdomain separately and finally recomposing the domain again. Therefore another opportunity for paralelization can be found at this middle level, yet this time it is possible that the resulting problem will not be a pleasingly parallel problem. The kind of problem depends strongly on the particular domain characteristics. On FEM or CFD problems, domain can be split with few dependences (only boundary conditions), thus resulting in a loosely coupled problems. On other domains, pleasingly parallel or tightly coupled problems may appear.

Finally, each one of the domain decomposition described before are usually translated to partial differential equations or linear equation systems, and simulated through algebraic operations, involving huge matrices (dense or sparse) that have to be added, multiplied or inverted. On operating these huge matrices, lies another level of parallelism. Algebraic operations can be operated in parallel, yet there is a strong dependence between the matrix elements, thus leading to a tightly coupled problem. Parallel algebraic operations are usually conducted on clusters and supercomputers, making use of specialized libraries such as BLAS and ScaLAPACK, optimized for the underlying hardware.

These three levels can coexist in the same simulator. On making the decision of migrating a simulator to a HPC cluster or a Cloud, these three levels should be considered, taking into account the suitability of a particular infrastructure to certain problem types, as described in Figure 3.4.

3.2.3 Computational Complexity

On analysing the complexity and computational workload of current simulators, all three levels have to be considered also. On multivariate and optimization problems, the number of simulations to be conducted is related to the number of dimensions of the problem to be explored, and the cardinality of each one of these dimensions. We denominate dimension of the problem to one particular variable that can be changed in order to generate different scenarios, and expecting different behaviours according the this variable's value. Optimization problems may be conducted on several dimensions, trying to optimize a function of several variables (the basics of Multi-Objective Optimization). Assuming a basic search based on brute force (without heuristics or advanced algorithms) the number of simulations to be conducted is the set of combinations of all different values from all dimensions considered. Let P a particular problem that can be explored on four dimensions. $P = \{A \mid B \mid C \mid D\}$, where $A = \{a_1, a_2, ..., a_m\}$ is the set of possible values of the dimension A, $B = \{b_1, b_2, ..., b_n\}$ is the set of possible values of the dimension B, $C = \{c_1, c_2, ..., c_p\}$ is the set of possible values of the dimension C, and $D = \{d_1, d_2, ..., d_q\}$ is the set of possible values of the dimension D. The number of possible simulations to be conducted S, is

$$S = \|A\| \cdot \|B\| \cdot \|C\| \cdot \|D\| = m \cdot n \cdot p \cdot q \tag{3.1}$$

As Figure 3.7 shows, this may lead to an exponential outburst of possible simulations to be executed. The figure represents an outburst due to three variables of 3, 3, and 2 dimensions

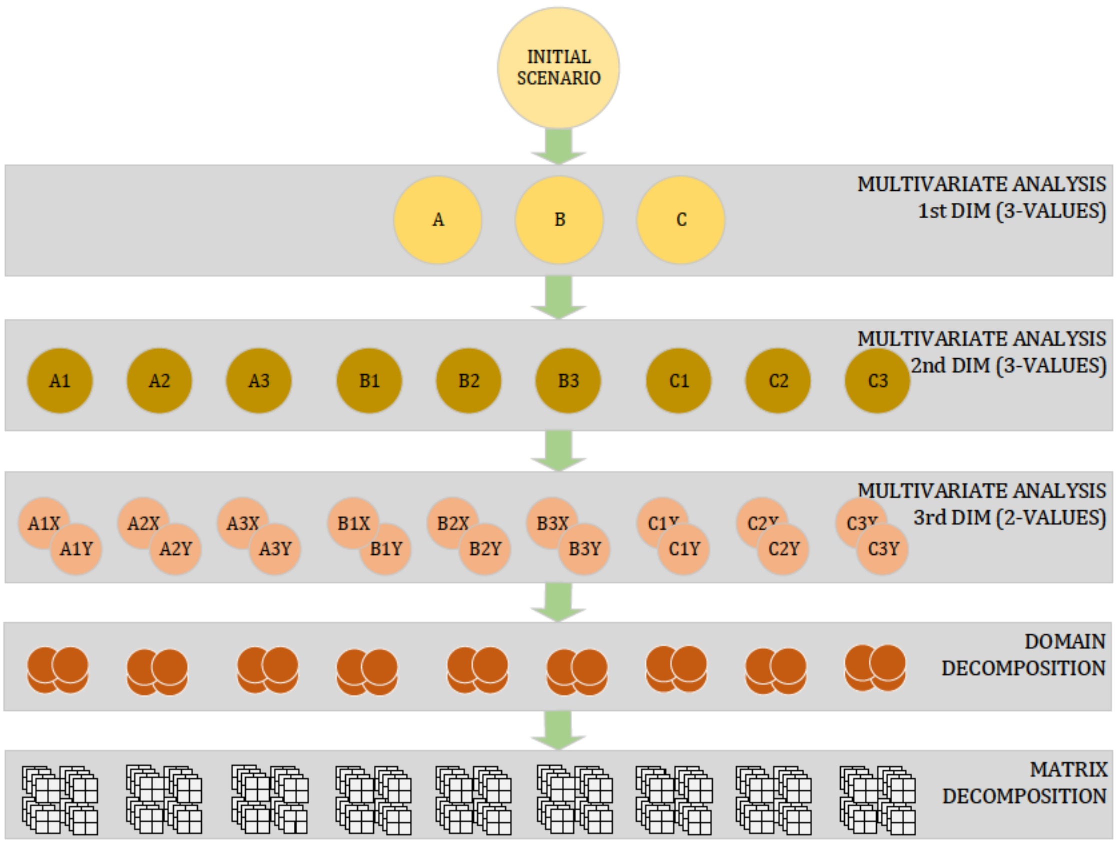


FIGURE 3.7: Workload outburst in multivariate analysis. Each dimension adds a level of complexity.

respectively. Note that, as it is shown in the figure, each one of these simulations can be also decomposed using domain or algebraic decomposition. Two more factors have to be taken into account within an unique simulation:

- The domain size D_s, provided by the number of times the simulation kernel has to be applied during the simulation. The domain size sets the maximum number of subdomains that can be obtained through domain decomposition.
- The problem size P_s, provided by the size of the data that has to be processed by the simulation kernel. In kernels that operate with matrices like LU factorization, Jacobi method, or Conjugate gradient method, the size of the (most significant) matrix establishes the problem size.

Note that, while in some applications both sizes may be related, in others may be not. In applications like FEM or CFD, the more partitions of the simulated domain are created, the smaller the size of the matrices needed to simulate each partition will be. In other kinds of applications, this relationship may not be present.

The Table 3.1 resumes the different characteristics of each parallelization layer, in terms of computational resources like processing power or memory. For each layer, the table indicates the maximum number of partitions in which each problem may be decomposed applying parallelization at that layer, the memory needed to process each partition using the sizes defined before,

Level	**Type**	N_{max} **partitions**	**Mem. partition**	**Serial part**	**Comms**
Multivariate analysis	Pleasingly parallel	$m \cdot n \cdot p \cdot q$	$D_s \cdot P_s$	Simulation	$\emptyset$
Simulation	Pleasingly parallel	$m \cdot n \cdot p \cdot q \cdot D_s$	P_s	Simulation kernel	$\approx \emptyset$
Simulation	Loosely coupled	$m \cdot n \cdot p \cdot q \cdot D_s$	P_s	Simulation kernel	K
Simulation	Tightly coupled	$m \cdot n \cdot p \cdot q \cdot D_s$	P_s	Simulation kernel	$\mathcal{O}(D_s)$
Matrix operations	Tightly coupled	$m \cdot n \cdot p \cdot q \cdot D_s \cdot \mathcal{O}(P_s)$	K	None	$\mathcal{O}(P_s)$

Table 3.1: Characteristics of different parallelization layers in terms of computational resources.

the part of the problem that must be treated sequentially (because parallelism is being applied at a different level), and a function of the amount of communications between partitions demanded by that layer. Note that this table does not include communications required to spawn the processes or distribute the partitions across a theoretic cluster. Only communications between layers due to data dependences are reflected:

- At the top level, applying parallelization on the multivariate analysis brings the advantage of absence of communication between partitions, because there is no dependence between simulations. On the counterparts, the maximum number of partitions is the number of simulations performed, each simulation must be performed sequentially, and memory must be available to store the whole simulation.
- At the middle levels, parallelization can be applied on each simulation by decomposing the simulation domain. The maximum number of partitions can be up to the number of decompositions allowed by the domain multiplied by the number of simulations. The memory must be large enough to hold the problem size (allocate all matrices necessary to solve one partition), but shorter than the previous case. On the counterpart, the simulation kernel must be processed sequentially, and the amount of communications are dependant on the problem type. On the worst case, a tightly coupled problem may require communications between all domain partitions.
- At the lowest level, parallelization can be applied on the simulation kernel, performing the matrix operations concurrently. This allows the largest degree of granularity, and the smallest amount of memory per partition. On the contrary, parallel matrix operations require usually a high degree of communications.

All things considered, current simulators may lead to unexpected demand of resources, with different ways of performing the parallelization, and each one of them suitable for different platforms and infrastructures.

3.3 Case Study: RPCS

In collaboration with [6]ADIF, the Spanish railway company, the Computer Architecture Group at University Carlos III of Madrid developed during the last years a railway electric power consumption simulator (RPCS) with the aim of evaluating and verifying different scenarios: developing new routes, increasing train traffic across the tracks, or testing failure situations where services have to be operated on degraded mode. This simulator is introduced as part of the contributions of this thesis.

The initial specification and requirements of the simulator specified that the software should be used on desktop PCs and laptops (for usability and productivity reasons). Therefore, a shared-memory simulator based on threads was developed. Nevertheless, the potential of the tool goes beyond simulating those cases that can be allocated on a laptop, being capable of simulating larger and larger cases, provided there are sufficient computing resources available. Hence, it is meaningful to migrate the simulator to parallel infrastructures such as HPC clusters or Clouds. To illustrate the proposed parallel architecture of current simulators, the RPCS was analysed with the aim of identifying on the simulator all layers exposed on Figure 3.6, determining the problem types, and finally exploring the possibilities of implementing that simulator focusing on HPC and Cloud infrastructures.

The tool is suitable for this analysis due to several facts. First of all, the tool requires a high amount of computing power, performing multiple matrix operations for each simulated instant (and a typical train traffic scenario has to be simulated during the whole day), so it is worthwhile improving the application scalability in order to reduce simulation times. Secondly, the application is bound to local resources, as previously mentioned, so it is a perfect test case for exploring parallel implementations on different platforms and infrastructures. Thirdly, it is a real tool currently used by ADIF, the Spanish railway company, to evaluate and verify different scenarios, so it portraits a general sort of engineering simulators commonly used which would be desirable to move to the cloud.

3.3.1 Application Description

The aim of this simulator is, provided a number of trains circulating across the lines, to calculate if the amount of power supplied by the electrical substations is enough or not. Starting from a description of the railway infrastructure (i.e. tracks, catenaries deployed over the tracks, electric substations placed along the tracks, as well as additional elements like feeders and switches, the simulator reads the position of the trains and their instantaneous power demand. Then, the electric circuit formed by the trains and the infrastructure is composed and solved using modified nodal analysis (MNA). The MNA general formulation is:

$$\begin{bmatrix} A_1 Y_1 A_1^T & A_2 \\ M_2 A_2^T & N_2 \end{bmatrix} \cdot \begin{bmatrix} u^n \\ i_2^r \end{bmatrix} = \begin{bmatrix} -As \cdot is \\ ws2 \end{bmatrix} \tag{3.2}$$

[6]http://www.adif.es

In this problem, branches are considered resistors, and there are only independent voltage sources, so the previous equation can be simplified as:

$$\begin{bmatrix} G & B \\ C & 0 \end{bmatrix} \cdot \begin{bmatrix} u^n \\ i^r \end{bmatrix} = \begin{bmatrix} i \\ e \end{bmatrix} \tag{3.3}$$

where G, B, and C are matrices of known values obtained from the circuit elements (connection, conductances, etc.), u^n and i^r are the unknown voltages and and currents, and finally i and e contain the sum of the currents through the passive elements, and the values of the independent voltage sources respectively. More details about MNA can be found on [JMHJ].

Useful mean voltages, voltage drops, and temperatures of the wires are examples of results provided by the tool. The structure of the selected application is a shared-memory application that has a preparation phase in which all the required input data is read and fragmented to be executed in a predefined number of threads. Two classes of input files are handled:

- A shared infrastructure specification file containing the initial and final time of the simulation, besides a wide range of domain-specific simulation parameters such as station and railway specifications and power supply definition.
- A set of train movement data files, structured in a time-based manner, in which each line contains the values of speed and distance profiles for a particular train at a specific instant regarding the infrastructure constraints, with a one second interval.

Once all data has been read, the simulator executes the simulation kernel for each instant to be simulated. This simulator kernel translates the infrastructure and train positions on the current instant into an electric circuit, and solves that circuit using an iterative algorithm (see Section 3.3.2). Electric results are calculated by the kernel on every instant, and will be merged in the main thread to constitute the final output files.

The simulator outputs electric data indicative of the state of the circuit, and all its components. This includes voltages and currents in all trains, voltages and currents in the converter-rectifier groups, and currents in all branches. Additional data is post-processed calculating useful mean voltages on trains and zones of the circuit.

3.3.2 Algorithm

Simulator internals consist on composing the electric circuit on each instant, and solving that circuit using modified nodal analysis. Algorithm 1 summarizes the process. Let $T = \{t_1, t_2, ...t_i\}$ be the set of instants to be simulated, let $C = \{C_1, C_2, ...C_i\}$, where $C_i = \{c_i^1, c_i^2, ...c_i^n\}$ is the set of trains at instant t_i, including they position and power. Let R be the infrastructure that covers all rail tracks, centenaries, feeders and electrical substations. Let $V = \{V_1, V_2, ...V_i\}$, where $V_i = \{v_i^1, v_i^2, ...v_i^n\}$ are the voltages of each train that must be calculated at t_i instant, and $I\{I_1, I_2, ...I_i\}$, where $I_i = \{i_i^1, i_i^2, ...i_i^n\}$ are the currents of each train that must be calculated at t_i instant. The algorithm performs the steps detailed as follows:

1. Given infrastructure data, and train positions at current instant, the matrices representing the electric circuit are composed following the MNA technique (see lines 3 to 11 in Algorithm 1).
2. The main matrix is inverted using LU decomposition (see line 12).
3. Given train consumption at present instant, the aim is to obtain the corresponding values of current and voltage (both unknown). An iterative process is conducted, performing the following substeps:
   (a) A value for train voltage is proposed (e.g. the system nominal voltage U_{nom}) (see line 13).
   (b) The current is obtained as the quotient of power (provided as input data) between the voltage proposed (see lines 16 and 17).
   (c) The circuit is solved using that tentative values. New voltages are obtained. These new values are compared against the previous ones (see lines 18 and 19).
   (d) If the error is less than certain percentage over the nominal voltage (e.g. 0.5 %), the algorithm converges, so current and voltage values for each train have been found, and the algorithm ends. If not, another iteration is conducted, proposing as voltages those values calculated in this iteration (see line 20).
4. Finally, results are written to the disk.

The application is multi-threaded, so simulation workload is split among the available cores in the computer. Each thread simulates a different subset of the total simulated time. This split is performed as follows: let $tini$ and $tfin$ the initial and final simulated times defined in the input files, and let $th_0, th_1, ...th_{n-1}$ the n threads of the application, the thread th_j simulates all $t_i \in [tini_j, tend_j)$ following the equations:

$$\begin{aligned} tini_j &= (j \cdot (tend - tini)/n) + tini \\ tfin_j &= ((j+1) \cdot (tend - tini)/n) + tini \end{aligned} \tag{3.4}$$

3.3.3 RPCS Problem Stack

As it is mentioned in Section 3.2.2, a simulator may not be associated to just one of the problem types defined in Section 3.1, but several of them. This is the case of the RPCS, where several opportunities for applying parallelization arise at different levels. These levels are depicted in Figure 3.6 from the bottom to the top:

1. *Matrix decomposition.* The RPCS algorithm operates huge matrices, performing an inversion (currently through an LU decomposition) and multiplications (in order to solve the equations) for each simulated instant. These operations can be decomposed following classic approaches to parallel algebraic operations, splitting the matrices among available cores

Algorithm 1 SimulateScenario

```
Input: $T, C, R$
Output: $V, I$
1: $ElectricBranches \leftarrow Translate(R)$
2: for all $(t_i \in T)$ do
3:     $ElectricBranches_i \leftarrow AllocateTrains(ElectricBranches, C_i)$
4:     $NodeMatrix_i \leftarrow CreateNodeMatrix(ElectricBranches_i)$
5:     $BranchMatrix_i \leftarrow CreateBranchMatrix(ElectricBranches_i)$
6:     $A_i \leftarrow CreateA(BranchMatrix_i)$
7:     $M_i \leftarrow CreateM(BranchMatrix_i)$
8:     $N_i \leftarrow CreateN(BranchMatrix_i)$
9:     $Ws_i \leftarrow CreateWs(BranchMatrix_i)$
10:    $A_i^t \leftarrow Transpose(A_i)$
11:    $NodalMatrix_i \leftarrow CreateNodal(A_i, M_i, A_i^t, N_i)$
12:    $NodalMatrix_i^{-1} \leftarrow Invert(NodalMatrix_i)$
13:    $V_i^j \leftarrow U_{nom} \forall j$
14:    $error \leftarrow U_{nom}$
15:    while $error > 0.005 \cdot U_{nom}$ do
16:        $P_i^j \leftarrow GetMaxPowerAvailable() \forall j$
17:        $I_i^j \leftarrow GetCurrent(P_i^j, V_i^j) \forall j$
18:        $Vr_i \leftarrow Solve(NodalMatrix_i^{-1}, I_i)$
19:        $error \leftarrow CheckError(V_i, Vr_i)$
20:        $V_i = Update(Vr_i)$
21:    end while
22:    $WriteResults(V_i, I_i)$
23:    $i = i + 1$
24: end for
```

and performing row and column operations in parallel. Therefore, there is an opportunity for parallelizing such operations using libraries such as ScaLAPACK.

2. *Domain decomposition.* RPCS simulations consist of a period of simulated time during which each instant must be represented as an electric circuit and solved. Because the train positions and consumptions of the trains are known all along the simulated time, there is no dependence between one instant and the following, so all instants are independent from the others. There is an opportunity for parallelizing the simulation through splitting that workload among available cores, each one of them simulating a different set of instants.

3. *Multivariate analysis.* Currently, RPCS does not implement any kind of multivariate analysis. If any kind of analysis requiring more than one simulation is desired, the tasks of varying the inputs, performing several simulations, and comparing the results, are left to the user. Nevertheless, there is a huge potential in the tool, and multiple features could be developed, should a proper multivariate engine (scenario generator, evaluation, optimization metrics, etc.) be implemented. Some of them are listed below:

    - Optimization of the energy consumed by the trains, search for the best electrical substation placements, or sizing the converter-rectifier groups to the optimal capacity. In order to do this, multiple simulations can be performed varying the position of the electrical substations or the number of active groups, comparing the average power consumed.

- Optimization of traffic across the lines, allocating the maximum number of trains allowed by the energy provisioning infrastructures. In order to do this, multiple simulations can be performed varying the number of trains, checking the absence of voltage drops on each train.
- Optimization of the mesh, configuring the best railway connections in order to maximize passengers or goods lifted, etc. In order to do this, multiple simulations can be performed varying the placement of the stations or yards, checking the timetables and paths of the trains.
- Fault tolerance analysis, through simulating downtimes in converter-rectifier groups, power losses, etc. In order to do this, multiple simulations can be performed disconnecting each time one electrical substation (or one group) and checking that the trains can keep on travelling.

Besides, several of these features can be combined in a multi-objective optimization pattern, leading to an outburst of the number of simulations to be performed. While the first point would result in a tightly coupled problem, due to the high degree of coupling on matrix operations, the last two would result in pleasingly parallel problems, due to the high independence between simulation subdomains or different simulations.

3.3.4 RPCS Analysis

As said before, the application is compute and memory-bound, because its memory usage pattern leads to a lack of scalability if the user wants to simulate bigger and bigger problems. There are two independent factors that have influence on application memory usage, and should be analyzed independently:

- Circuit size. The number of simulated elements on the same instant (e.g. trains, tracks, catenaries, etc.) is proportional to the size of the circuit to be calculated (problem size). Actually, for each new element, a minimum of two nodes and one branch are added to the circuit (the twice as much for certain elements such as trains). Following the MNA technique, this means two more rows and one more column in the problem matrix.
- Number of simulated instants. The circuit must be solved for each instant of the simulation. As said before, a typical train traffic scenario has to be simulated during the whole day, leading to 86400 instants with the duration of one second. While this workload can be split across the node cores using threads, for each thread solving an instant the matrices must be allocated in memory. This increases the memory usage linearly to the number of threads. There is a trade-off between execution time and memory usage. The more threads we add to shorten the simulation time, the more memory we consume.

The application is also very demanding in terms of processing power, since it deals with several matrix operations per simulated instant: LU decomposition, inversion, multiplication, etc. which traditionally require a great amount of floating point operations. But unlike the memory, this limitation can be addressed either by adding more cores to a compute node, or extending the execution time of the simulation.

In order to illustrate this analysis, a study of the application memory consumption given different problem and simulation sizes was conducted. Four test cases were considered with variations on the circuit size, simulation's initial and final time and, consequently, input data volume, execution time, and memory consumption. A description of these simulations is provided in Table 3.2. Cases I and II should not yield any significant load, yet simulation III is expected to reflect the system's behaviour under average problems. The biggest experiment, case IV, should reveal the platforms' actual limitations as simulations become larger. All test cases are based on the same real case, a particular railway line at Madrid surroundings, with increasingly levels of detail and simulation periods. This line has been used before in other works [CPGC$^+$03] because it is a good example in size and complexity of a real railway project.

In addition to the four test cases previously described, a fifth test case is considered. We selected as benchmark a standard railway scenario described in the proposed draft of the European normative *prEN-50641*[7]. [CEN15]. This proposal of normative, drawn by the CENELEC committee [8], establishes the requirements for the validation of simulation tools used for the design of traction power supply systems. Therefore, it is meaningful to apply such normative when conducting a research based on that kind of application. Key parameters of all test cases are also indicated in Table 3.2.

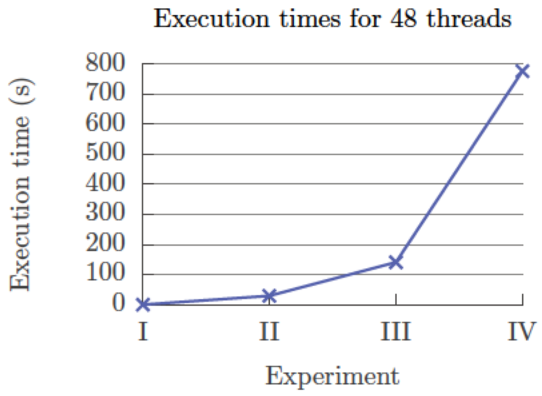
Experiment	**Trains**	**Tracks**	**Electric subs.**	**Avg. circuit branches**	**Simulated time**	**Input size (MB)**
I	3	3	2	77	$\approx$ 1 hour	1.7
II	207	8	7	179	$\approx$ 1 day	170
III	1449	8	7	525	$\approx$ 1 week	1228.8
IV	6417	8	7	755	$\approx$ 1 month	5324.8
CENELEC	6	2	3	564	1 h 20 min.	4.2

Table 3.2: Test cases definition

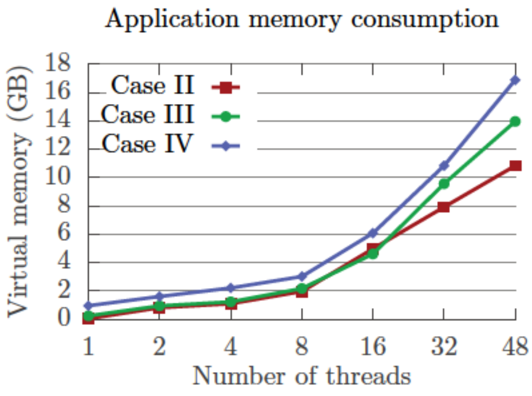
Figure 3.8b displays the execution times using 48 threads, whereas Figure 3.8b displays the memory consumption of the application the number of concurrent threads is increased. Measurements have been taken by means of the Linux *proc*. OS policies about memory pages assignment introduce a slight randomness, so each measurement has been repeated 10 times. As it can be seen in the figure, this application does not scale well for large test cases in terms of memory usage in a standalone environment (tests were conducted on a single node with 48 cores and 110 GB of RAM).The most determining factor is the number of simultaneous threads, which increases the memory consumption linearly. As said before, each thread operates a different matrix which can reach a size of thousands of elements. On the other hand, using more threads is the best option to shorten the simulation time.

[7]This normative has been accepted and is now on *public comment* phase, but has not been approved yet. See `https://standardsdevelopment.bsigroup.com/Home/Page/StageCodes`

[8]See `http://www.cenelec.eu/`



(A) Original application execution times.



(B) Simulation kernel memory consumption.

Generic concept	RPCS concept
Multivariate analysis	Find fault tolerance on substation crash. Optimization of the mesh. Optimization of the traffic. ...
Simulation	A number of trains circulating for a period of time.
Modelling	Translate railway elements into a MNA electric circuit.
Input data	Infrastructure definition and train positions and consumptions
Output data	Train voltages and currents Converter-rectifier group voltages and currents. Current across feeders. Energy consumed ...
Domain size	Period of simulated time.
Domain decomposition	Divide the period in independent instants of simulated time.
Subdomain	Each simulated instant.
Simulation kernel	For each instant, conduct a MNA and an iterative process.
Problem size	Matrix sizes of the MNA analysis

TABLE 3.3: Generic architectural concepts identified in RPCS and its domain characteristics.

Finally, as summary of the RPCS analysis, Table 3.3 describes the concepts defined in Section 3.2 identified in the RPCS, with the particular RPCS domain characteristics reflected.

3.4 Summary

This Chapter has described the problem statement by characterizing the different problem types that can be faced when working with simulators. This characterization is based on the ease of splitting the problem in order to perform the computation in parallel. The way the problem is decomposed has a direct impact on data and communication patterns, and should be studied carefully according to the target infrastructure and platform. It is also stated that several problem types can coexist in the same simulator, insofar as several parallelizations can be applied to different layers of that simulator.

As contribution, the chapter also has described the RPCS, a railway power consumption simulator developed by UC3M in collaboration with ADIF, the Spanish railway company. With the aim of serving as case study, this simulator is analysed from the point of view described before, pointing the different layers where opportunities for applying parallelization lie. In subsequent chapters, parallelization on such layers will be applied, targeting different infrastructures and platforms, and analysing the results obtained.

Chapter 4

High Performance Computing Approaches to Problem Decomposition

The previous chapter has described the different problem types that must be faced when working with simulators. This characterization is based on how easy the problem domain can be split, provided that it has a direct impact on data and communication patterns. The previous chapter has also shown two kinds of infrastructures (HPC and Cloud), and two kinds of solutions (MPI and MapReduce) very related to the execution of extensive parallel simulations.

This chapter explores different HPC-based approaches to problem decomposition. Starting from the generic architecture proposed in the previous chapter (see Figure 3.5), two different approaches using message-passing techniques are described. The first one tackles the medium layer of those described in Figure 3.6, applying parallelism through domain decomposition. This approach will be described in Section 4.1. The second one tackles the lowest layer (see Figure 3.6 again) applying parallelism to the algebraic operations that usually represent the main computing workload of the simulation kernels. This approach will be described in Section 4.2.

In order to evaluate the feasibility of both approaches, the RPCS (described in Section 3.3) will be used as case study, so both will be implemented within the application, and evaluated separately using MPI, which is the *de-facto* standard in HPC. Implementation details will be described in Section 4.3. The evaluations will be conducted under HPC and Cloud infrastructures, in order to analyze the performance with regard to the underlying infrastructure which is running the simulation. These results will show the suitability and limitations of the aforementioned approaches according to the infrastructure used.

4.1 Domain Decomposition Approaches in HPC

The first HPC approaches to be explored are based on domain decomposition. This approach starts from the generic simulator architecture described in Section 3.2.1, and the possible parallelization layers and their complexity exposed in sections 3.2.2 and 3.2.3. In domain decomposition, the whole simulation domain is scattered across the compute nodes, and each compute node executes the simulation kernel once per received partition. Resulting from the kernel executions, partial results are obtained on each node. Finally, these partial results are merged in order to obtain the final simulation result.

The key aspect in this approach is the degree of coupling in the simulation domain. If such domain can be decomposed easily in partitions, and processing each partition does not require to swap data with another one, the communications required to conduct the simulation will be reduced to the minimum. On the contrary, a tightly coupled domain may require exchanges of data between all partitions, leading to an explosive amount of communications as the number of nodes is increased.

Besides, this approach implies that the whole simulation kernel is going to be executed sequentially, and each partition will be stored in the memory of the node. CPU intensive simulation kernels may take too long to be solved, and memory intensive kernels may require more memory than that available in the compute node. The advantages of this approach lie in the best case: a pleasingly parallel problem and a not so demanding kernels. In this case this approach is the easiest to implement, and the fastest (in terms of execution times) due to absence of communication delays.

Two generic algorithms for domain decomposition are described: using a coordinator process and using collective I/O. We assume familiarization with MPI-like programming model (same program, multiple processes), and communications (point-to-point and collective operations).

4.1.1 Domain Decomposition Using a Coordinator Process

Algorithm 2 illustrates the code of a simulator implementing domain decomposition, and using a coordinator process. In this code, a coordinator process (usually rank 0 in MPI applications) is accountable for the initial and final stages of reading the simulation data and writing the results. The coordinator process reads from the storage both the global data I_{glob} (used all through the simulation) and the domain data I_{dom} (which can be decomposed). The global data is then broadcasted, and the domain data is scattered to all other processes. Each process receives a subset I_p which contains one or more partitions I_i so that they are able to execute the simulation kernel over their own subset of data.

After (or during) the executing of the simulation kernel, exchanges of data between domain partitions may occur. A pleasingly parallel problem may not require any exchange, but some simulations may require communication between a constant, reduced set of related processes (like the ghost region, the boundaries between mesh partitions, or any other kind of neighbourhood), and some others may require that each process broadcasts its partial results. This has been

Algorithm 2 Message-passing approach to domain decomposition using a coordinator process.

```
Input: {$Path\text{-}I_{glob}, Path\text{-}I_{dom}$}
Output: $O$

if coordinator then                          ▷ Coordinator reads data and splits the simulation domain.
    $I_{glob} \leftarrow Read(Path\text{-}I_{glob})$
    $I_{dom} \leftarrow Read(Path\text{-}I_{dom})$
    $Broadcast_{snd}(I_{glob})$
    $Scatter_{snd}(I_{dom})$
else
    $I_{glob} \leftarrow Broadcast_{rcv}()$
    $I_p \leftarrow Scatter_{rcv}()$
end if

for all ($I_i \in I_p$) do        ▷ Every process executes the simulation kernel on its own partition.
    $O_i \leftarrow SimulationKernel(I_{glob}, I_i)$
    SolveCoupling($O_i$)
    $O_p \leftarrow O_p + O_i$
end for

if coordinator then                          ▷ Coordinator gathers all output and writes the results.
    $O \leftarrow Gather_{rcv}()$
    $Write(O)$
else
    $Gather_{snd}(O_p)$
end if

function SolveCoupling($O_i$)                ▷ Depends on domain coupling, it can be:
    if Pleasingly parallel then do-nothing
    end if                                   ▷ Communications not required
    if Loosely coupled then send-to-k-processes
    end if                                   ▷ K exchanges per process
    if Tightly coupled then all-gather
    end if                                   ▷ All processes exchange data
end function
```

represented in the algorithm with the *SolveCoupling* function. Finally, after the execution of the kernels, the coordinator process is accountable for gathering the partial results of each process O_p and merging the final output O.

This algorithm is easy to implement, provided it does not require the use of advanced I/O, data layouts, and parallel file systems. Nevertheless, it does not scale up as the simulated domain increases in size. This is due to the asymmetry in the role of the coordinator process, which has to maintain in memory the whole domain data, between reading it from storage and scattering it to the other processes. Most exascale simulation problems tackle domain sizes that do not allow one single node to maintain the whole domain in memory. In order to cope with this issue, collective I/O has to be used.

Algorithm 3 Message-passing approach to domain decomposition using collective I/O.

```
Input: {$Path\text{-}I_{glob}, Path\text{-}I_{dom}$}
Output: $O$
 1:
 2: $I_{view} \leftarrow TypeCommit(Layout\text{-}I_{dom})$
 3: $O_{view} \leftarrow TypeCommit(Layout\text{-}O)$
 4:
 5: $I_{glob} \leftarrow Read(Path\text{-}I_{glob})$
 6: $I_p \leftarrow MPI\text{-}IO\text{-}Read(Path\text{-}I_{dom}, rank, I_{view})$
 7:
 8: for all ($I_i \in I_p$) do      ▷ Every process executes the simulation kernel on its own partition.
 9:     $O_i \leftarrow SimulationKernel(I_{glob}, I_i)$
10:     SolveCoupling($O_i$)
11:     $O_p \leftarrow O_p + O_i$
12: end for
13:
14: $MPI\text{-}IO\text{-}Write(O_p, rank, O_{view})$
15:
16: function SolveCoupling($O_i$)      ▷ Depends on domain coupling, it can be:
17:     if Pleasingly parallel then do-nothing
18:     end if                          ▷ Communications not required
19:     if Loosely coupled then send-to-k-processes
20:     end if                          ▷ K exchanges per process
21:     if Tightly coupled then all-gather
22:     end if                          ▷ All processes exchange data
23: end function
```

4.1.2 Domain Decomposition Using Collective I/O

Algorithm 3 illustrates the code of a simulator implementing domain decomposition, and using collective I/O. In this case, there is no coordinator role, so all processes perform a collective read operation. The data layout in the storage system should be arranged properly, in order to ease the data reading and distribution performed by the processes collectively. This is done in MPI by committing a representative type so that all processes can share a global view of the data. The *MPI-IO-Read* shown in the algorithm (as simplification of the available I/O functions that can be found in the MPI standard), is able to read and scatter the data to all processes all at once. The same principle can be applied to the *MPI-IO-Write* function, which is able to make all processes write the data to the storage neatly. Note that, while MPI-IO is referred as the most common example of collective I/O, this description can be applied to any other kind of I/O performed parallel and collectively by all ranks, even if these ranks are using the POSIX inteface, HDF5, or any other kind of I/O.

This approach is more complicated (in terms of development complexity) than the previous one. It requires the use of advanced I/O and parallel file systems. Besides, the data layout must be arranged properly. But due to the characteristics of exascale problems, this fashion is usually required, because when the domain size goes bigger and bigger, it becomes harder to fit in any node which could act as coordinator. Finally, note that while this approach avoids the necessity of maintaining the whole domain in physical memory, several issues remain as in the previous algorithm: the degree of coupling, the serial execution of the kernel, and the need of fitting that kernel in the physical memory.

4.1.3 Communication and Resource Modelling

In order to give an insight into the workings of both implementations, a basic modelling of the communication and memory usage pattern is proposed. The aim of this basic model is, provided a simulation domain, to give a rough estimate of the suitability of both implementations in order to take a first decision. Table 4.1 summarizes the meaning of the symbols used in this section.

Table 4.1: Symbol table for the proposed communication and memory model

Symbol	**Meaning**
α	Network latency
β	Network bandwidth
m	Message size (generic)
T_{msg}	Time required to perform a generic point-to-point communication
T_{Scat}	Time required to perform a collective *Scatter* operation
T_{Gath}	Time required to perform a collective *Gather* operation
T_{Brd}	Time required to perform a collective *Broadcast* operation
$T_{AllGath}$	Time required to perform a collective *AllGather* operation
p	Number of compute processes
d	Number of I/O servers
I_{glob}	The (input) global data
m_{glb}	The size of I_{glob} data
I_{dom}	The (input) domain data
m_{dom}	The size of I_{dom} data
I_p	Fraction of the domain data handled by each process
O	Output data
m_O	The size of O data
T_{ker}	Time to execute the simulation kernel
T_{Cp}	Time to exchange data after executing the simulation kernel
T_{Alg2}	Time to perform the whole algorithm (w/ coordinator proc.)
T_{Alg3}	Time to perform the whole algorithm (w/ collective I/O)
M_{Alg2}	Memory per proc. required by the whole algorithm (w/ coordinator proc.)
M_{Alg3}	Memory per proc. required by the whole algorithm (w/ collective I/O)

The basis of this model is the algorithms and formulas proposed by Thakur and Gropp in [TG02], based on the Hockney model [Hoc94]. This work focuses on switched networks, which represent a very simple kind of cluster. Besides, it is unaware of optimizations based on particular technologies or platforms, so the model can be taken as the worst-case scenario. Given the wide variety of infrastructures performing HPC nowadays, the model tries to be as generalist as possible.

The time taken to send a message between any two nodes is independent of the distance, and can be modelled using the Equation 4.1:

$$T_{msg}(m) = \alpha + m\beta \tag{4.1}$$

where α is the latency per message, m is the message size, and β is the transfer time per byte. Once this basic transaction has been defined, collective operations can be modelled on the top of point-to-point communications, in terms of latency, message size, and bandwidth.

The *Scatter* and *Gather* operations can be modelled using a minimum spanning tree algorithm (MST), in which each process receives the data from its parent, retains its own slice, and relays the rest to its children. Let p the number of processes, the Equation 4.2 shows the time required to perform either *Scatter* or *Gather* operation:

$$T_{Scat}(m) = T_{Gath}(m) = \lceil \lg p \rceil \alpha + \frac{(p-1)}{p} m\beta \tag{4.2}$$

MST algorithm can be used also to implement the *Broadcast* operation, making the difference to the previous operation that each process relays the whole set of data, instead of relaying only a fragment. The Equation 4.3 reflects the time required to complete the operation:

$$T_{Brd}(m) = \lceil \lg p \rceil (\alpha + m\beta) \tag{4.3}$$

The *AllGather* operation can be implemented using a recursive-doubling algorithm. The Equation 4.4 reflects the time required to perform this operation:

$$T_{AllGath}(m) = \lg p\alpha + \frac{(p-1)}{p} m\beta \tag{4.4}$$

After modelling the collective communications, the time required to complete the whole Algorithm 2 can be estimated. Let:

- I_{glob} be the global data.
- I_{dom} be the domain data.
- I_p be the fraction of the domain data handled by each process (according to Equation 4.5). Each process is assumed to share the same amount of data.

$$|I_p| = \frac{|I_{dom}|}{p} \tag{4.5}$$

- O be the output data.
- T_{ker} be the time required to execute the simulation kernel, which is assumed constant regardless the input data simulated.

The Equation 4.6 represents the total execution time of the Algorithm 2 without considering the times related to the storage devices:

$$T_{Alg2} = T_{Brd}(I_{glob}) + T_{Scat}(I_{dom}) + (|I_p| \cdot T_{ker}) + ((|I_p| - 1) \cdot T_{Cp}(O)) + T_{Gath}(O) \tag{4.6}$$

T_{Cp} represents the data exchange after executing the kernel, depending on each domain's degree of coupling. Equation 4.7 represents this time as a no-op in a pleasingly parallel problem, a constant, small number of communications between nodes (e.g. neighbourhood communication) for loosely coupled problems, and an *AllGather* operation in tightly coupled problems where all nodes have to broadcast their results.

$$T_{Cp}(m) = \begin{cases} \varnothing & \text{for} \quad PP \\ K \cdot T_{ms}(m) : K \ll p & \text{for} \quad LC \\ T_{AllGath}(m) & \text{for} \quad TC \end{cases} \tag{4.7}$$

Note that this exchange is performed $(|I_p| - 1)$ times. Due to the fact that the algorithm executes a *Gather* operation as final stage, it is redundant to perform the final data collection twice.

Substituting in Equation 4.6 all terms related to collective communications, the total time can be expressed as a function of the data sizes, the number of processes, and the network latency and bandwidth, obtaining Equation 4.8. Let:

- m_{glb} be the size of I_{glob} data.
- m_{dom} be the size of I_{dom} data.
- m_O be the size of O data.

$$\begin{aligned} T_{Alg2} = &\lceil \lg p \rceil (\alpha + m_{glb}\beta) \\ &+ \lceil \lg p \rceil \alpha + \frac{(p-1)}{p} m_{dom}\beta \\ &+ \frac{|I_{dom}|}{p} T_{ker} \\ &+ (\frac{|I_{dom}|}{p} - 1) \cdot (\lg p\alpha + \frac{(p-1)}{p} m_O\beta) \\ &+ \lceil \lg p \rceil \alpha + \frac{(p-1)}{p} m_O\beta \end{aligned} \tag{4.8}$$

Finally, grouping terms α, m_{glb}, m_{dom}, and m_O, Equation 4.9 is obtained:

$$\begin{aligned} T_{Alg2} = &(3\lceil \lg p \rceil + \frac{|I_{dom}| \cdot \lg p}{p} - \lg p)\alpha \\ &+ \lceil \lg p \rceil m_{glb}\beta \\ &+ \frac{(p-1)}{p} m_{dom}\beta \\ &+ \frac{|I_{dom}|}{p} T_{ker} \\ &+ (((\frac{|I_{dom}|}{p} - 1) \cdot \frac{(p-1)}{p}) + \frac{(p-1)}{p}) m_O\beta \end{aligned} \tag{4.9}$$

Analysing the limits of T_{Alg2} as p approaches to 1 (pure sequential) and to $|I_{dom}|$ (the maximum degree of parallelism), we obtain:

$$\lim_{p \to 1} T_{Alg2} = |I_{dom}| \cdot T_{ker} \tag{4.10}$$

$$\lim_{p \to |I_{dom}|} T_{Alg2} = 3\lceil \lg p \rceil \alpha + (\lceil \lg p \rceil m_{glb} + \frac{(p-1)}{p} m_{dom} + \frac{(p-1)}{p} m_O)\beta + T_{ker} \tag{4.11}$$

This allows to establish when it is worthwhile decomposing the problem across a number of processes, provided the characteristics of the problem (m_{glb}, m_{dom}, etc..) and the network (α, β) are known.

The maximum memory usage of the algorithm in a single process can be expressed as the maximum between the domain data (loaded in memory by the coordinator prior to performing the *Scatter* operation) and the memory usage required by the kernel at any node (i.e. the size of the problem):

$$M_{Alg2} = I_{glob} + \max(I_{dom}, I_p + SimulationKernel + O_p) \tag{4.12}$$

The total execution time of the Algorithm 3 can also be expressed in the same terms, modelling its communications and the execution time of the simulation kernel. Nevertheless, in this algorithm the I/O phases are performed collectively by all processes, and therefore is more difficult to predict the behaviour of the application in such phases. The Equation 4.13 represents the total execution time of the algorithm using IO_{read} and IO_{write} as the times required to execute the I/O read and write phases respectively:

$$T_{Alg3} = T_{Brd}(I_{glob}) + IO_{read} + (|I_p| \cdot T_{ker}) + ((|I_p| - 1) \cdot T_{Cp}(O)) + IO_{write} \tag{4.13}$$

Collective I/O involves different participants that may influence the global behaviour of the system: the parallel file system, the number of I/O servers, the I/O network, and the storage devices. In order to keep the strategy of providing a simple approach, this model focuses on the number of I/O servers, assuming a switched network similar to that assumed between compute nodes. Other elements are not considered, and the algorithms implemented within MPI-IO are considered to be the same as those previously described in common collective communications (e.g. MST when an IO server is gathering the data). Let d the number of I/O servers, Equation 4.14 represents the times required to perform the collective I/O, without considering the storage devices:

$$\begin{aligned} IO_{read} &= \frac{\lceil \lg p \rceil}{\lceil \lg d \rceil} \alpha + \frac{(p)}{d} m_{dom} \beta \\ IO_{write} &= \frac{\lceil \lg p \rceil}{\lceil \lg d \rceil} \alpha + \frac{(p)}{d} m_O \beta \end{aligned} \tag{4.14}$$

With this approach, if there is only one I/O server (the worst case), IO_{read} and IO_{write} operations become *Scatter* and *Gather* respectively (see equations 4.6 to 4.9), sending the data from the server to the compute nodes, or receiving the data from the compute nodes to the server. The best case is achieved when there is a one to one ratio between I/O servers and compute nodes. In that case, IO_{read} and IO_{write} operations become single point to point communication: each compute node exchanging data with its I/O pair.

$$\begin{aligned} T_{Alg3} &= \lceil \lg p \rceil (\alpha + m_{glb}\beta) \\ &+ \frac{\lceil \lg p \rceil}{\lceil \lg d \rceil}\alpha + \frac{(p)}{d} m_{dom}\beta \\ &+ \frac{|I_{dom}|}{p} T_{ker} \\ &+ (\frac{|I_{dom}|}{p} - 1) \cdot (\lg p\alpha + \frac{(p-1)}{p} m_O\beta) \\ &+ \frac{\lceil \lg p \rceil}{\lceil \lg d \rceil}\alpha + \frac{p}{d} m_O\beta \end{aligned} \tag{4.15}$$

Finally, grouping terms α, m_{glb}, m_{dom}, and m_O, Equation 4.16 is obtained:

$$\begin{aligned} T_{Alg3} &= (\lceil \lg p \rceil + 2\frac{\lceil \lg p \rceil}{\lceil \lg d \rceil} + (\frac{|I_{dom}|}{p} - 1) \lg p)\alpha \\ &+ \lceil \lg p \rceil m_{glb}\beta \\ &+ \frac{(p)}{d} m_{dom}\beta \\ &+ \frac{|I_{dom}|}{p} T_{ker} \\ &+ (((\frac{|I_{dom}|}{p} - 1) \cdot \frac{(p-1)}{p}) + \frac{p}{d}) m_O\beta \end{aligned} \tag{4.16}$$

In this algorithm, the maximum memory usage per single process can be expressed as the size of its corresponding share of domain data, plus the global data and the memory consumption brought by the simulation kernel (i.e. the size of the problem):

$$M_{Alg3} = I_{glob} + I_p + SimulationKernel + O_p \tag{4.17}$$

4.2 Matrix Decomposition Approaches in HPC

Once the domain decomposition has been explored, the next approaches to be analysed are the matrix decompositions. In matrix decomposition, the algebraic operations that represent the simulation kernel are performed in parallel across all cluster nodes (e.g. multiplication, transposition, inversion, etc.) and the fragments of the matrices used by the simulation are scattered (or read in parallel) across the cluster. Usually a simulation requires several executions of the simulation kernel, In such cases each one of these executions will be performed in parallel across the whole cluster, but sequentially regarding the simulation life cycle, because each execution makes use of all available resources.

Far from the previous approach where the degree of coupling was dependant on the particular domain, matrix operations are always tightly coupled, requiring a high number of communications to be performed. This supposes a serious handicap in medium or low speed networks with high latencies, and that is the main reason for putting a lot of effort in optimizing high-performance networks, topologies, and those related topics. The main advantage of this approach is that due to the fact that the whole simulation kernel is decomposed, it is possible to lower the amount of memory required by the compute nodes to execute the kernel. By sharing each node a piece of the matrix (or matrices), no matter how big the problem size is, we can just add more and more nodes to tackle it.

4.2.1 Matrix Decomposition Using Master-Slaves

Algorithm 4 illustrates the code of a simulator implementing matrix decomposition. This code uses a master-slaves scheme, where a leading process drives the simulation stages (see *Master* function), and dispatches the operations, whereas the slave processes (see *Slave* function) take the bulk of the simulation sharing the workload associated to the matrix operations. The leading process may also share its own part of the workload, so as to make all processes use the same resources.

This scheme is useful when the simulation requires additional logic apart from the simulation kernel, having to choose, for instance, between different kernels, or different operations within the same kernel, depending on some data. In order to do so, the coordinator, which is driving the simulation, and therefore knows what is the forthcoming operation, broadcasts a corresponding code as well as any additional arguments of such operation (see *SimulationKernel* function), making all slaves proceed in coordination. The slaves follow the pattern of a finite-state machine (FSM), waiting for a code, and then executing the corresponding operation, until the simulation finishes.

As in the previous algorithms, I/O can be performed through the coordinator process or collectively. Regarding this, the same advantages and shortcomings described in the previous section remain, being the collective I/O the most suitable code as the domain and/or problem sizes become large. Algorithm 4 illustrates the coordinator process case, but a collective I/O approach could be implemented easily by adding to the slaves another *DistributedMatrixOP* operation, which could read (or write) the matrix data collectively, and remaining the master as the driver of the simulation.

4.2.2 Communication and Resource Modelling Example: LU Inversion

Whereas in Section 4.1.3 a basic model has been given, in order to estimate roughly the communication burden of the algorithms described in sections 4.1.1 and 4.1.2, it is not possible to proceed in the same way with the matrix decomposition approach. The fact is that there is a

Algorithm 4 Message-passing approach to matrix decomposition using master-slave scheme.

```
Input: $\{Path\text{-}I_{glob}, Path\text{-}I_{dom}\}$
Output: $O$

if $coordinator$ then                                   ▷ Master process drives the simulation.
    $Master(Path\text{-}I_{glob}, Path\text{-}I_{dom})$
else
    $Slave()$
end if

function $Master(Path\text{-}I_{glob}, Path\text{-}I_{dom})$
    $I_{glob} \leftarrow Read(Path\text{-}I_{glob})$                  ▷ I/O through coordinator process.
    $I_{dom} \leftarrow Read(Path\text{-}I_{dom})$
    for all $(I_i \in I_{dom})$ do
        $O_i \leftarrow SimulationKernel(I_{glob}, I_i)$
        $O \leftarrow O + O_i$
    end for
    $Write(O)$
end function

function $SimulationKernel(I_{glob}, I_i)$
    ...                                ▷ Master distributes matrix op. codes across the slaves.
    $Broadcast_{snd}(OP_1)$
    $DistributedMatrixOP_1(Matrix)$
    ...
    $Scatter_{snd}(OP_2)$
    $DistributedMatrixOP_2(Matrix)$
    ...
    $Broadcast_{snd}(OP_{end})$
end function

function $Slave$                                    ▷ Slaves execute matrix operations.
    while $!end$ do
        $OP \leftarrow Broadcast_{rcv}()$
        if $OP = OP_1$ then $DistributedMatrixOP_1()$
        end if
        if $OP = OP_2$ then $DistributedMatrixOP_2()$
        end if
        ...
        if $OP = OP_{end}$ then $end \leftarrow true$
        end if
    end while
end function
```

huge amount of different simulation kernels and algebraic operations, each one of them performing a different communication pattern. A very brief list of some of these kernels can be found in [Jam12].

Nevertheless, it is possible to develop the same model with one example of matrix operation, and then extend the conclusions to those operations that are more complex than the illustrated one. The operation to be analysed is matrix inversion based on the LU factorization. Let a system of linear equations in matrix form:

$$Ax = b \tag{4.18}$$

The square matrix $A \in \mathbb{R}^{n\times n}$ is invertible if there exists a matrix $A^{-1} \in \mathbb{R}^{n\times n}$ such that:

$$A^{-1}A = AA^{-1} = I \tag{4.19}$$

If we have computed the LU decomposition: $A = LU$ then we can replace A in the system. This leads to two linear systems:

$$Ly = b \tag{4.20a}$$

$$Ux = y \tag{4.20b}$$

Solving both systems brings the solution b easily. Note that we are not analysing the LU factorization, but the matrix inversion once the matrix has been factorized. The Listing 4.1 shows a simplified code of the LU inversion that does not perform partial pivoting, using MPI:

```
// Solve L*Y = I
for (int k = 0; k < cols; k++){
  MPI_Barrier( MPI_COMM_WORLD );

  //Send k row to all
  if(k >= startingrow[slaverank] && k < finalrow[slaverank]){
    for(int p = slaverank + 1; p < slavesize; p++){
      MPI_Send( &ret[k * cols], cols , MPI_DOUBLE, p, 1980, MPI_COMM_WORLD);
    }
  }
  else if(k < startingrow[slaverank]){
    //Receive
    MPI_Recv( &ret[k * cols], cols, MPI_DOUBLE, MPI_ANY_SOURCE, 1980, MPI_COMM_WORLD,
     MPI_STATUS_IGNORE);
  }

  //Update lower rows using k
  for (int i = max(k + 1, startingrow[slaverank]); i < finalrow[slaverank]; i++){
    for (int j = 0; j < cols; j++){
      ret[i * cols + j] = ret[i * cols + j] - (ret[k * cols + j] * lu[i * cols + k]);
    }
  }
}

// Solve U*X = Y;
for (int k = cols - 1; k >= 0; k--){
  MPI_Barrier( MPI_COMM_WORLD );
  if(k >= startingrow[slaverank] && k < finalrow[slaverank]){
    //Update k row using diagonal
    for (int j = 0; j < cols; j++){
        ret[k * cols + j] /= lu[k * cols + k];
    }

    for(int p = slaverank - 1; p >= 0; p--){
      //Send k row to all
      MPI_Send( &ret[k * cols], cols , MPI_DOUBLE, p, 1975, MPI_COMM_WORLD);
    }
  }
  else if(k >= finalrow[slaverank]){
    //Receive
    MPI_Recv( &ret[k * cols], cols, MPI_DOUBLE, MPI_ANY_SOURCE, 1975, MPI_COMM_WORLD,
     MPI_STATUS_IGNORE);
  }

  //Update upper rows using k
  for (int i = startingrow[slaverank]; i < min(k, finalrow[slaverank]); i++){
    for (int j = 0; j < cols; j++){
      ret[i * cols + j] = ret[i * cols + j] - (ret[k * cols + j] * lu[i * cols + k]);
    }
  }
}
```

Listing 4.1: MPI implementation of a matrix inversion using LU decomposition w/o partial pivoting

The main matrix is scattered (or read collectively) across the processes by rows. Then, there are two main loops in the code that iterate across the rows of the matrix. Up to down in the first one, and down to up in the second. For each iteration, the process accountable for the current (k) row broadcasts it to the processes holding the inferior (in the first loop) or superior (in the second loop) rows. Then, all processes update their part of the matrix using the received row. The following enumeration summarizes the estimation of the communications:

1. For simplicity, it is assumed that the matrix (of size $n \times n$) has been evenly distributed across a number of p processes. Therefore each process shares $\frac{n}{p}$ rows, each one of size n.

2. Each process $p_i \in p$ has to send its $\frac{n}{p}$ rows to the lower (or upper) ranks. Let $r_i \in [0, p-1]$ the rank of the process p_i, and let t_i the times the process p_i sends a message:

$$\forall p_i \in p, t_i = \frac{n}{p}(p - r_i + 1) \tag{4.21}$$

3. Therefore, the total number of messages for each loop t_{tot} will be:

$$t_{tot} = \sum_i \frac{n}{p}(p - r_i + 1) = \frac{n}{p}\sum_i (p - r_i + 1) \tag{4.22}$$

4. Considering both loops, Equation 4.1 which defines the time required to send a message, and the fact that all messages are equal in size $m = n$, the total communication time required to perform the LU inversion is:

$$T_{LU^{-1}} = 2 \cdot t_{tot} \cdot T_{msg} = \frac{2n}{p}\sum_i (p - r_i + 1)(\alpha + n\beta) \tag{4.23}$$

5. Finally, applying the divergent series:

$$\sum_{k=1}^{n} k = \frac{n(n+1)}{2} \tag{4.24}$$

6. The $T_{LU^{-1}}$ can be approached as follows:

$$T_{LU^{-1}} = n(p+1)(\alpha + n\beta) \tag{4.25}$$

Therefore the communication time $T_{LU^{-1}}$ is quadratic to the matrix dimension d and linear to the number of processes p, but due to the fact that, as the matrices go bigger, more nodes have to be used (in order to decrease the execution times), both magnitudes can be considered directly proportional: $p \propto n$. So we can consider that the communication time $T_{LU^{-1}}$ is cubic to matrix dimension d or cubic to the number of processes p if a proportionality constant $n = kp$ is established.

4.3 Application to RPCS

To illustrate and evaluate how the HPC approaches shown in the previous sections perform on different infrastructures, both of them were implemented within the RPCS simulator described in Chapter 3. Parallelism to the RPCS can be applied at different layers, either performing a domain decomposition, or applying parallelism to the simulation kernel that performs the MNA. So Section 4.3.1 will describe the domain decomposition approach implemented within the RPCS, and Section 4.3.2 will describe the matrix decomposition implementation within the RPCS. Both implementations do not overlap, and are maintained as separate subversions of the application.

4.3.1 Domain Decomposition in RPCS

The RPCS simulates the electric behaviour of a railway infrastructure during a period of time in which the trains are circulating across the lines. This period is defined by the user, and may be from several minutes in the smallest simulations, to several weeks or even one month if the user wants to analyse the behaviour of the system in a long-term plan. The simulation is conducted analysing the behaviour of the electric circuit in each one of the seconds that compose this period. The positions and consumptions of the trains are know for each one of such seconds, and taken as input data of the simulations, so there are no dependences between the simulations of different seconds even if they belong to the same period.

As it is described in Table 3.3, the simulated time period can be considered as the simulation domain, and the MNA performed in each one of the simulated seconds is the simulation kernel. Therefore, the whole simulation period will be decomposed in several subintervals with lower magnitude, and each one of this subintervals will be simulated by a different worker. For instance, if the whole simulation period is from the 06:00:00 hours to the 22:00:00 hours and the number of workers is 4:

- The 1st worker will handle from 06:00:00 hours to 09:59:59 hours.
- The 2nd worker will handle from 10:00:00 hours to 13:59:59 hours.
- The 3rd worker will handle from 14:00:00 hours to 17:59:59 hours.
- The 4th worker will handle from 18:00:00 hours to 22:00:00 hours.

In order to avoid the asymmetric role of a coordinator process, the algorithm to be implemented will be based on collective I/O (see Algorithm 3). Implementation details are listed below:

- The infrastructure file, which defines the invariant elements of the circuit common to all simulated instants (tracks, catenaries, power stations, etc.), is considered as the global data.
- The train data files, which contain the positions and consumptions of each train along the simulated period, are considered as the domain data. The domain distribution will be based on MPI ranks: the process with the first rank will handle the first subinterval, and son on.
- All I/O will be handled by POSIX system calls, and MPI-IO will not be used. This is because most of the input data is based on text, so the structured layout usually used in MPI-IO does not fit properly when reading lines of variable length. Besides, test-based input and output is a requirement of the original application, in order to ease the post-processing and analysis of the results. On reading data, this does not suppose a problem, because common file systems can handle parallel readings easily. Besides, parallel file systems implement also the POSIX interface in order to give support to basic operations. On the contrary, writing data in parallel to the same file supposes a risk of losing coherence, due to interleaved or disordered writings. In order to cope with this issue, each worker will write data to its own file, and all files created by workers will be merged in a final stage.

- Apart from the final merger of the files created by workers, there are no dependences between domain partitions, so no data must be exchanged between workers every time the simulation kernel is executed.

4.3.2 Matrix Decomposition in RPCS

In order to apply matrix decomposition to the RPCS, it is necessary to analyze first what are matrix operations that are performed within the kernel. Two different sources are used to get this information: the application technical report which contains the description of the mathematical and electrical principles implemented, and an application profile, obtained using *gconf* utility, which identifies the top execution time functions. The list is displayed in Table 4.2.

Table 4.2: Execution profile of RPCS from gprof utility: top execution time functions list

Each sample counts as 0.01 seconds						
% time	cumulative seconds	self seconds	calls	self s/call	total s/call	name
66.84	1086.57	1086.57	16752	0.00	0.00	ArrayOperator::Inv(...)
22.85	1458.02	371.45	16752	0.00	0.00	LUMatrix::Factorize()
9.70	1615.74	157.72	47658	0.00	0.00	ArrayOperator::MultiplyMatrix(...)
0.28	1620.36	4.62	25521	0.00	0.00	ArrayOperator::MultiplyMatrix(...)
...						

These analyses identify four major matrix operations which are conducted during the execution of the kernel. They are listed below, ordered proportionally according to their relative execution times respect to the whole kernel:

- Matrix inversion, provided that the matrix has been factorized before (performed by the *ArrayOperator::Inv()* function).
- LU factorization with partial pivoting (PA-LU) (performed by the *LUMatrix::Factorize()* function).
- Matrix multiplication (performed by the *ArrayOperator::MultiplyMatrix()* function).

Matrix factorization and inversion take the most of the simulation kernel's execution time, so applying parallelism to that functions is the most urgent task. LU decomposition with partial pivoting complicates the implementation and significantly affects potential performance [Hea11]. Nevertheless, partial pivoting is required to ensure existence and numerical stability of the factorization. In order to optimize as much as possible these two operations, a specialized algebraic library such as ScaLAPACK (as well as its dependences LAPACK and BLAS) is integrated with the RPCS. ScaLAPACK [BCC$^+$97] implements a a block cyclic data distribution for dense matrices and block-partitioned algorithms that minimize the frequency of data movement between different levels of the memory hierarchy (including off-processor memory of other processors). The following routines will be invoked from the RPCS:

- PDGEADD: this routine performs the sum operation between two distributed matrices, but it can be used also to distribute a local matrix in the memory of one node among the rest of the nodes using the block cyclic data distribution, required to perform the further operations. It can be used also to gather back the resulting matrix to one node.
- PDGETRF: this routine computes the LU factorization of a general m-by-n distributed matrix. The function uses partial pivoting, with row interchanges. The matrix is expected to be distributed using the block cyclic data distribution among the cluster nodes, and remains distributed once factorized. L and U factors are stored together in the same buffers. Unit diagonal elements of L are not stored. The pivoting information is stored in an additional distributed array.
- PDGETRI: this routine computes the inverse of a general distributed matrix using the LU factorization. This method inverts U and then computes the inverse of A by solving the system. On entry, the routine receives local pieces of the L and U and the pivoting information computed by PDGETRF.
- Auxiliary functions: some auxiliary functions are also used by RPCS to make use of the previous routines. The two-dimensional rectangular process grid arrangement recommended by ScaLAPACK is configured using *blacs_gridinit* and *blacs_gridinfo*, and destroyed using *blacs_gridexit*.

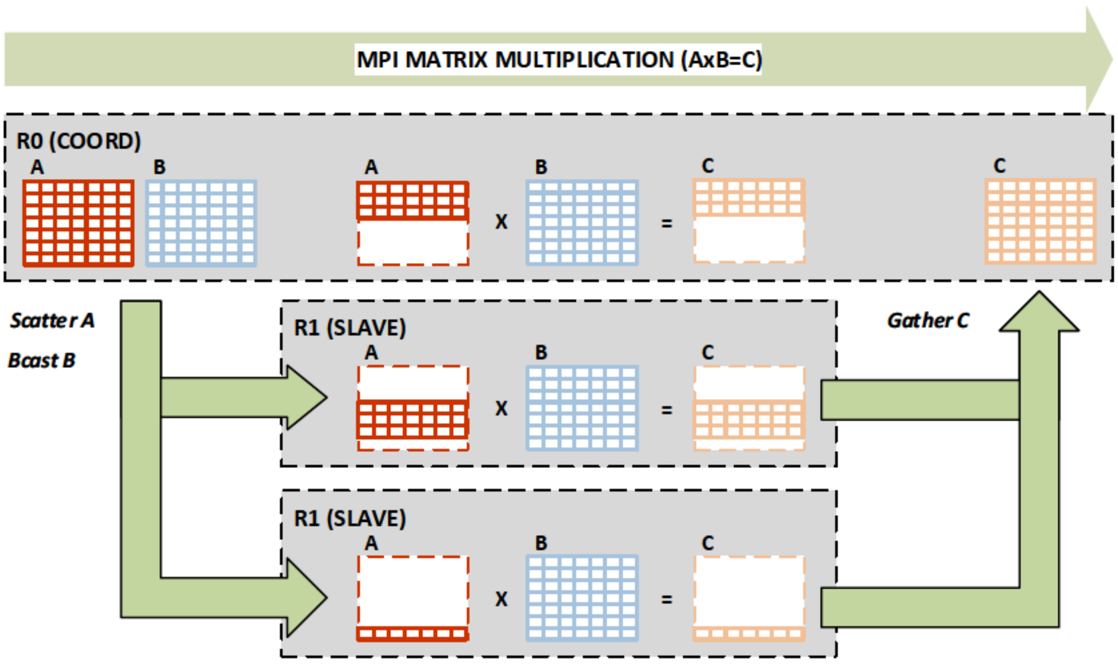


FIGURE 4.1: Matrix multiplication implemented within the RPCS simulation kernel.

Matrix multiplication ($AB = C$) comes in third place with less than a 10% of the execution time. Due to this low percentage, a custom algorithm has been implemented using a coordinator process that scatters the A matrix, distributing the rows of the matrix between the slaves, and broadcasts the matrix B. Then every process performs the multiplication calculating its own part of the C matrix, which is finally gathered back by the coordinator process. Figure 4.1 represents a scheme of the whole process.

4.4 Evaluation

In order to assess the behaviour of the two approaches described in this chapter, an evaluation is conducted using the two versions of the RPCS described in the previous section: with domain decomposition and with matrix decomposition. This evaluation is conducted under two kinds of infrastructures, an HPC cluster and a Cloud of virtual instances deployed in Amazon EC2. The aim is to identify the trends of both approaches as the low level optimizations characteristic of HPC systems disappear in favour of the Cloud characteristics and limitations. Table 4.3 summarizes the characteristics of the nodes that compose these two kinds of infrastructures.

Table 4.3: Node features for the HPC cluster and the Cloud used in the evaluation

	HPC cluster node	**Amazon EC2 Cloud node**
Processor	Intel® Xeon® E5405 2.00GHz	Intel® Xeon® E5-2680 (v2) 2.80GHz
Physical mem.	8.0 GB DDR2	7.5 GB DDR3
Network	InfiniBand DDR	Unspecified (moderate performance)[1]
Topology	Flat	Unknown
Compiler	ICC 15.0.1	GCC 4.8.1
Libraries (DD)	Netlib LAPACK	Netlib LAPACK
Libraries (MD)	Intel® MKL 11.3	Netlib ScaLAPACK OpenBLAS
File System	GlusterFS	NFSv4
Op. mode (DD)	Process per core (MPI)	Process per core (MPI)
Op. mode (MD)	Process per node (MPI + OpenMP)	Process per node (MPI + pthreads)

The HPC cluster features the common characteristics of HPC infrastructures. It deploys a high-bandwidth low-latency interconnect network, in a well-known static topology. RPCS implementations have been compiled using the Intel® ICC compiler, in order to take advantage of that optimizations available for the particular processor model and architecture installed in the cluster nodes. Besides, the Intel® Math Kernel Library (MKL) has been used as implementation of ScaLAPACK, LAPACK, and BLAS routines.

On the contrary, the Cloud allocated in Amazon EC2 features the characteristics of Cloud environments, with little or no optimizations based on the particular hardware architecture. The *c3.xlarge* has been selected as the instance type most similar to the cluster nodes in terms of processing power and physical memory. While Amazon describes in the documentation that the processor model supporting the *c3.xlarge* instance type is an E5-2680 Ivy Bridge, it has been decided to not take advantage of this information when compiling the application, provided that other instance types, and therefore other processor models (or even other processor brands), may be selected according to the particular requirements of the user at forthcoming executions. Following the same philosophy, the compiler used has been GCC, and the ScaLAPACK, LAPACK, and BLAS implementations used have not been those provided by Intel®. Instead, the Netlib implementation of ScaLAPACK and LAPACK, and the GotoBLAS2[GVDG08] implementation of BLAS have been used, because they target a wider catalog of architectures than the MKL

[1]Measurements through *iperf* commands suggest a 1Gbps network

Table 4.4: Test cases definition for the HPC-based approaches.

Experiment	**Simulated time**	**Input size (MB)**	**Version tested**
I	$\approx$ 1 hour	1.7	Matrix dec. only
II	$\approx$ 1 day	170	Domain dec. and Matrix dec.
III	$\approx$ 1 week	1228.8	Domain dec. and Matrix dec.
IV	$\approx$ 1 month	5324.8	Domain dec. only

[Edd10]. Finally, Amazon EC2 does not provide information about the network that supports the virtual machines, apart from an ambiguous ”Moderate” referred to the quality of the network connection. Nevertheless, measurements through *iperf* tool between allocated instances suggest that the network bandwidth is approximately 1Gbps.

The test cases simulated during this evaluation are summarised in Table 4.4. These tests are the same that were used in Chapter 3 to conduct a resource analysis of the original RPCS application (also the same that will be used in Chapter 5). Each one of these experiments (numbered as I, II, III, and IV) suppose an increment in both domain size (period of time to be simulated) and problem size (size of the electric circuit) with regard to the previous one. They will be tested using both approaches implemented (domain decomposition and matrix decomposition), in both infrastructures (the HPC cluster and the Cloud), and with a variable number of nodes in infrastructure (for 2, 4, 6, 8, and 10 nodes).

Due to the large amount of experiments that are going to be simulated, the simulation step has been increased to from 1 to 120 seconds. Therefore, only one of each 120 instants of the simulation interval will be simulated. Besides, due to the fact that the domain size of the *Experiment I* is very small, it will not be tested using the domain decomposition approach. Similarly, due to the fact that the domain size of the *Experiment IV* is very large, it will not be tested using the matrix decomposition approach.

4.4.1 Domain Decomposition Evaluation

The domain decomposition approach was the first to be evaluated. Figure 4.2 shows the RPCS execution times, when simulating the Experiments II, III, and IV, as the number of nodes in both the HPC cluster and the Amazon Cloud is increased. The figure shows times corresponding to the initial input phase in which all the global and domain data is loaded (a, c, and e), and the times corresponding to the actual simulation (b, d, and f). The following conclusions can be extracted from the results shown:

- Regarding the compute phase, the application expresses a good degree of scalability up to 10 nodes (40 MPI processes) regardless of the infrastructure used. Compute times descend linearly as more nodes are added for all infrastructure size tested. The absence of communication inside the simulation kernel, as well as the fact that the whole simulation

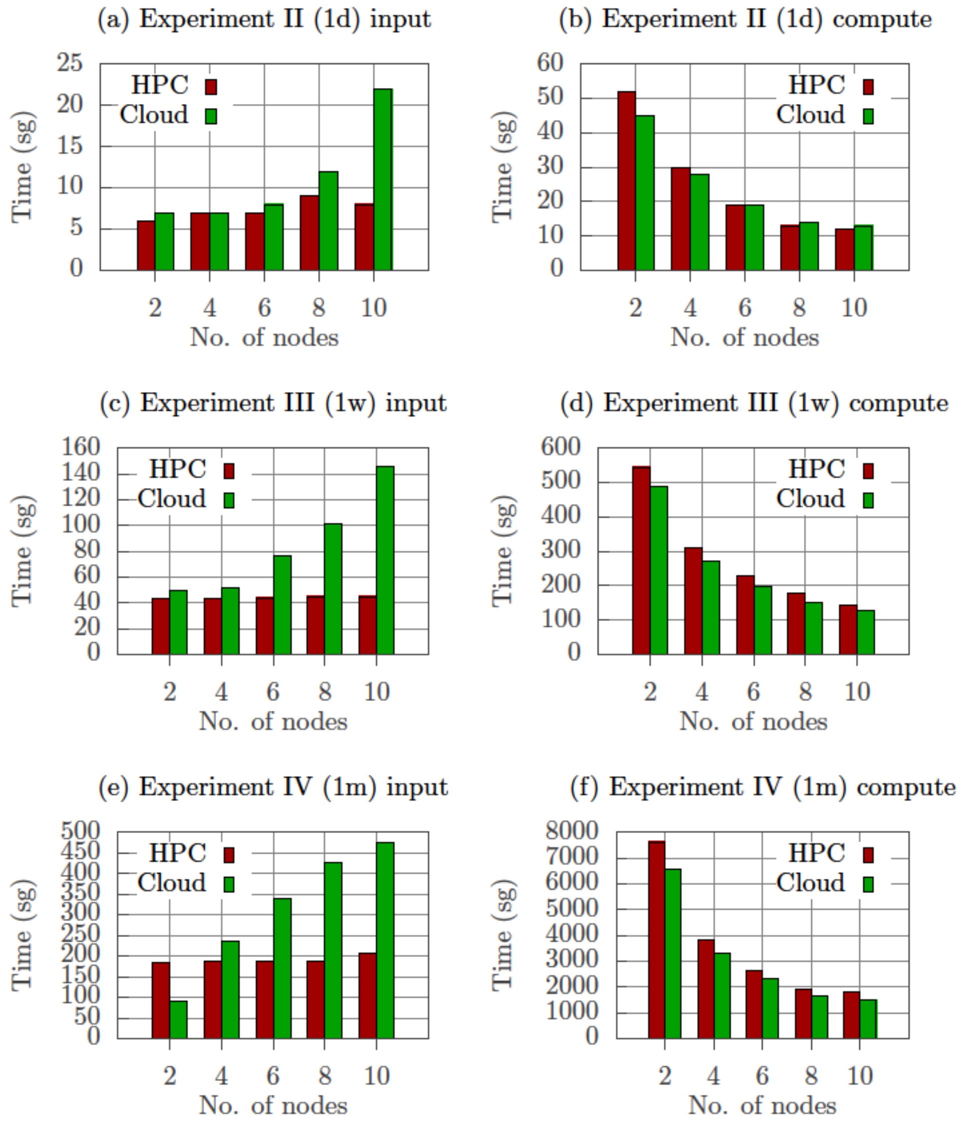


FIGURE 4.2: Execution times for the domain decomposition approach in the HPC cluster and the Amazon Cloud.

kernel fits in the memory of the node (actually it fits in the memory-per-cpu slice) favours the scalability of the solution.

- For this application, and using domain decomposition, this Cloud infrastructure allocated in Amazon seems to outperform the computing power of the HPC cluster used in these evaluations, obtaining lower compute times in the majority of the tests. While the application executed in the HPC cluster has been optimized compiling with the Intel® ICC compiler for that particular processor model, the CPU of the nodes in the Cloud infrastructure is superior enough (more up-to-date processor model, 2.80GHz vs. 2.00GHz clock speed, larger cache sizes, etc.) to overcome the absence of optimizations and the virtualization overhead for the CPU. In this type of problem, the absence of communications due to the use of domain decomposition downplays the role of the network in favour of the CPU characteristics.

- Regarding the input phase, the GlusterFS in the HPC cluster shows overall better results than the NFSv4 in the Amazon Cloud for the Experiments II and III. Actually, the input phase times in the cluster remains constant for these experiments, indicating that the volume of the input data is not big enough to overcome the bandwidth of the file system. The same is not happening in the Cloud, where the input phase times are increased as more nodes read the data from the NFS server.

4.4.2 Matrix Decomposition Evaluation

After evaluating the domain decomposition approach, we proceeded to evaluate the matrix decomposition implementation. Figure 4.3 shows the RPCS execution times, when simulating the Experiments I, II, and III, as the number of nodes is increased in both the HPC cluster and the Amazon Cloud. The figure shows times corresponding only to the actual simulation, discarding the initial and final phases. The following conclusions can be extracted from the results:

- For all experiments tested, and for both architectures, the application's execution times are increased as more nodes are added to the infrastructure. This demonstrates how sensible is the application to the communication overhead, as expected using matrix decomposition (see Equation 4.25), but also denotes that the size of the operated matrices is not big enough to make the parallel execution worthwhile. The number of operations performed in parallel does not compensate the latencies suffered when communicating through the network, even if using a high-performance low-latency network. Nevertheless, the main advantage of this approach is the distribution of the memory workload among all the cluster, in that cases where the simulation kernel does not fit in the memory of a single node.
- As expected, the HPC cluster achieves better overall performance, since outperforms the Amazon Cloud in every direct comparison. Besides, the HPC cluster shows better scalability, since the growth in the execution times is far less steep than in the Amazon Cloud. Even through the HPC cluster is somewhat outdated compared to the underlying Amazon infrastructure (see Table 4.3 for comparison), the superior quality of the network has a great impact on these tightly coupled algorithms.

4.5 Summary

In this chapter we have explored HPC approaches to problem decomposition, starting from the generic architecture proposed in Chapter 3. Two different approaches using message-passing techniques are described: domain decomposition and matrix decomposition. Domain decomposition relies on splitting the simulation domain in multiple subdomains and executing in parallel the simulation kernel on each subdomain, while matrix decomposition applies parallelization in the matrix operations that compose the simulation kernel.

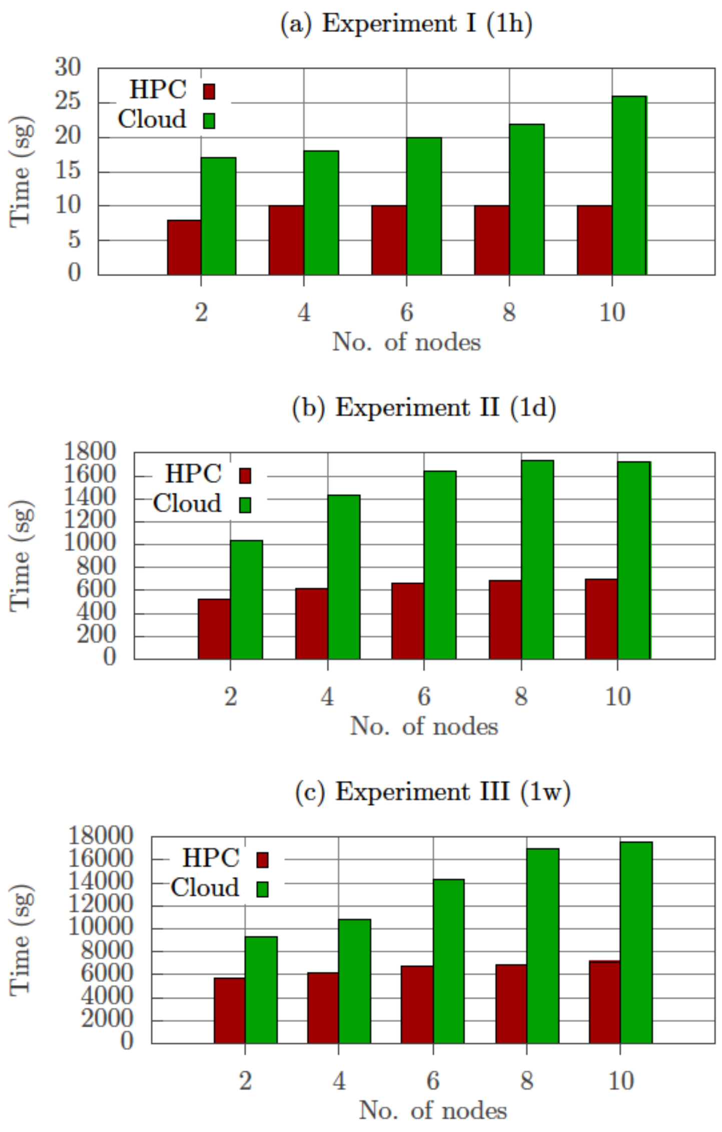


FIGURE 4.3: Execution times for the matrix decomposition approach in the HPC cluster and the Amazon Cloud.

A basic model of the communication burden is proposed for both the domain decomposition approach and a representative example of matrix decomposition approach: a LU inversion. Performance in the first approach depends heavily on that degree of coupling inherent in the simulation domain, while the second one is a tightly coupled operation requiring a high degree of communication. Nevertheless matrix decomposition is the only valid model if the memory required by the simulation kernel exceeds the memory available in the compute node.

The evaluation was conducted on both HPC and Cloud infrastructures, implementing both approaches on the RPCS. The results show that the matrix approach is much more sensitive to network latencies, thus making it not recommended for Cloud environments. The domain decomposition is therefore the best choice if the simulation kernel fits in memory.

The tendencies show how the application behaves, provided there are a tightly coupled simulation kernel and a pleasingly parallel simulation domain. Should the simulation kernel be executed sequentially, the most relevant feature in the infrastructure is the CPU (even if platform specific optimizations are not available). On the contrary, should the simulation kernel be executed in parallel, the network has the deepest impact on the execution times. In terms of workload sharing, the bigger the simulation domain is, the easier is to distribute the workload evenly among the cluster through domain decomposition. On the contrary, if the computing requirements of the simulation kernel are high enough, it can be meaningful to perform the matrix computations in parallel, even through these operations are tightly coupled.

Finally, there are several shortages common to both approaches. First of all, MPI (at least at the standard level) does not bring any fault tolerance to the applications. Secondly, MPI neither provides elasticity mechanisms to adapt the application to changes in the infrastructure, so Cloud elasticity can not be exploited. All things considered, we turn towards domain decomposition using data centric approaches based on the MapReduce framework, which can bring these desired features.

Chapter 5

A Methodology to Migrate Simulations to Cloud Computing

In the previous chapter, the traditional approaches to parallelizing modern simulators have been explored. Message-passing techniques were used over cluster resources, applying the parallelization at different levels of the simulator proposed as case study. Once traditional approaches have been explored, this thesis turn towards Cloud technologies.

In this chapter, a generic methodology to transform modern simulators into a cloud-suitable data-centric scheme via the MapReduce framework is proposed. The aim of this thesis proposal is to exploit Cloud advantages in modern simulators, such as virtual unlimited scalability of hardware resources, platform independence, and flexibility according to instantaneous user needs (through adapting computing resources). The focus is on Map-Reduce because this platform, as well as the data-centric scheme that proposes, is suitable for Cloud Computing, but also can perform efficiently on clusters and supercomputers.

5.1 Methodology Description

The MapReduce paradigm consists of two user-defined operations: *map* and *reduce*. The former takes the input and produces a set of intermediate $(key, value)$ pairs that will be organized by key by the framework, so that every reducer gets a set of values that correspond to a particular key [DG08].

As a data-centric paradigm, in which large amounts of information can be potentially processed, these operations run independently and only rely upon the input data they are fed with. Thus, several instances can run simultaneously with no further interdependence. Moreover, data can be spread across as many nodes as needed to deal with scalability issues.

Simulations, however, are usually resource-intensive in terms of CPU or memory usage, so their scalability is limited to hardware restrictions, even in large clusters. The goal is to exploit the data-centric paradigm to achieve a virtually infinite scalability. This would permit the execution of large numeric simulations independently of the underlying hardware resources, with minimal effects to the original simulation code. From this point of view, numeric simulations would become more sustainable, allowing us to spread simulation scenarios of different sizes in a more flexible way, using heterogeneous hardware, and taking advantage of shared inter-domain infrastructures.

To achieve this, this proposal takes advantage of MapReduce's lack of task interdependence and data-centric design. This will allow to disseminate the simulation's original input to distribute its load among the available nodes, which will yield the scalability we aim for. The steps involved in the proposed methodology are described in the following sections.

5.1.1 Methodology Terms and Definitions

The first step is defining several key concepts in which the methodology is going to be based on. Let S be the whole simulation process, which receives an input data set I, applies a function $f_{sim}(x)$ over that input, and produces an output data set O.

$$S \equiv f_{sim}(I) = O \tag{5.1}$$

The output data O can be organized in multiple files, each one containing different results from the simulation:

$$O \equiv \{O_0, O_1, ..., O_m\} \tag{5.2}$$

The input data I can be classified in two different types:

- *Global data I_{glob}*. This kind of data does not vary with regard to the problem domain, maintaining all values constant all along the simulation. In this category may fall those parameters which are used to configure the simulation globally, read once, applied many times.
- *Domain data I_x*. This kind of problems represents the particular scenario to be simulated. It can be decomposed in different subsets with regard to the problem domain, representing different dimensions of the problem: a collection of registers that can be processed independently, different sub-areas of a continuous domain, or different instants in a time independent simulation.

Therefore, $I = \{I_{glob}, I_0, I_1, I_2, ..., I_k\}$ where there are k subdivisions of the domain input data. Assuming that the problem can be solved in a parallel manner, the function $f_{sim}(x)$ is formulated as a reduction, f_{red}, of multiple sub-pieces of the input data, after being processed by some function $f_{ker}(x)$, which implements the main logic of the simulation, but applied only to a part of the problem domain.

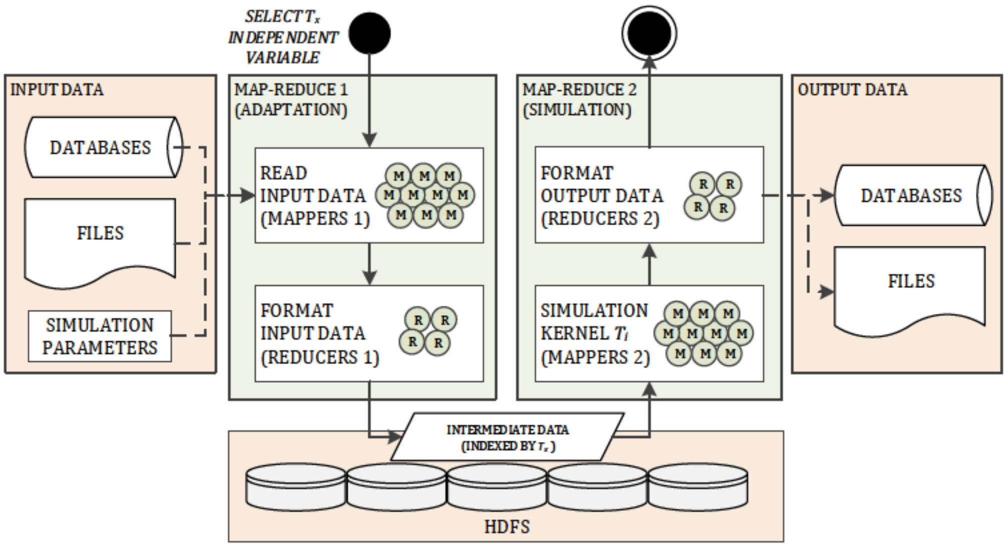

SELECT T_x INDEPENDENT VARIABLE
INPUT DATA
DATABASES
FILES
SIMULATION PARAMETERS
MAP-REDUCE 1 (ADAPTATION)
READ INPUT DATA (MAPPERS 1)
FORMAT INPUT DATA (REDUCERS 1)
MAP-REDUCE 2 (SIMULATION)
FORMAT OUTPUT DATA (REDUCERS 2)
SIMULATION KERNEL T_i (MAPPERS 2)
OUTPUT DATA
DATABASES
FILES
INTERMEDIATE DATA (INDEXED BY T_x)
HDFS

FIGURE 5.1: Methodology overview.

$$s(I) = f_{red}(f_{ker}(I_{glob}, I_0), f_{ker}(I_{inv}, I_1), f_{ker}(I_{inv}, I_2), ..., f_{ker}(I_{inv}, I_k))) \tag{5.3}$$

Form the previous equations, the following definitions are provided:

- *Adaptation.* The process of rearranging the input data set I into multiple independent subsets of global and domain data $\{I_{glob}, I_0, I_1, I_2, ..., I_k\}$
- *Simulation Phase.* The process of simulating and reducing all the independent subsets that compose the simulation domain (i.e. performing $s(I)$).
- *Simulation Kernel.* The function $f_{ker}(x)$ that implements the main logic of the simulation. If it can be applied to only a part of the problem domain, it outputs only a chunk of the total simulation data.
- *Reduction.* The function $f_{red}(x)$ that recomposes the output corresponding to the original global simulated domain from the data outputted by the different simulation kernels executed.

In order to apply the proposed methodology, the aforementioned entities should be identified in the context of a particular problem domain. Finally, on simulations based on workflows, composed of several tasks, or the same task performing iteratively, the entities described can be applied to each one of the individual tasks, applying the methodology separately for each one of them.

5.1.2 Application Analysis

The purpose is to divide the application into smaller simulations that can run with the same simulation kernel, but on a fragment of the full partitioned data set, so that the executions can be performed in parallel and the hardware requirements for each can be lowered.

Hence, the original simulation domain must be analysed in order to find an independent variable –T_x in Figure 5.1– that can act as index for the partitioned input data and the following procedures. This independent variable would be present either in the input data or the simulation parameters and it could represent, for example, independent time-domain steps, spatial divisions or a range of simulation parameters.

At the moment, the analysis and selection of such variable is done by direct examination of the original application. As this process is critical, and it is intimately related with the application's structure, procedures and input, it should be performed by an expert in the simulator to be cloudified. Future work could simplify this stage by mean of automatic analysis and variable proposal, yet an expert would still be needed to assess the correctness of the suggestion.

5.1.3 Cloudification Process Design

Once verified that the application is suitable for the process, it can be transformed by matching the input data and independent variables with the elements in Figure 5.1. This results in the two MapReduce jobs described below:

- **Adaptation stage:** reads the input files in the *map* phase and indexes all the necessary parameters by T_x for every execution as intermediate output. The original data must be partitioned so that subsequent simulations can run autonomously with all the necessary data centralized in a unique $(T_x, parameters)$ entry.
- **Simulation stage:** runs the simulation kernel for each value of the independent variable along with the necessary data that was mapped to them in the previous stage, plus the required simulation parameters that are shared by every partition. Since simulations might generate several output files, mappers would organize the output by means of file identifier numbers as keys, so as reducers could be able to gather all the output and provide final results as the original application.

The two algorithms for the adaptation stage are described in Algorithm 5 and Algorithm 6. Algorithm 5 describes the *map* phase. During this phase, the input files of the simulation are processed line by line, in order to extract and arrange all data according to the independent variable T_x. The task is performed as follows:

1. The input data of the simulation is stored in an HDFS cluster. Chunks of these data are spread across all nodes and mappers are dispatched to each node in order to process that chunks.
2. For each chunk, the contents are processed line by line, arranging all lines according to key-value pairs.
3. If the line contains global data, a specific terminal indicating global contents is assigned as key, and the value is assigned to the whole line of data.

Algorithm 5 Adaptation phase mapper

```
Input: $I$
Output: $KV1 = \{(k_0, v_0), (k_1, v_1), ..., (k_n, v_n)\}$
 1:
 2: for all ($chunk \in I.files$) do
 3:     MAP($chunk$)
 4: end for
 5:
 6: function MAP($chunk$)
 7:     for all ($line \in chunk$) do                ▷ Process input files line by line
 8:         if ISGLOBAL($line$) then                  ▷ If line contains global data
 9:             $key \leftarrow GLOB$
10:             $value \leftarrow line$
11:         else                                      ▷ If line contains domain data
12:             $T_x \leftarrow$ FINDTX($line$)             ▷ Find $T_x$ within the line
13:             $key \leftarrow T_x$
14:             $value \leftarrow line$
15:         end if
16:         EMIT($key, value$)    ▷ Adds pair to KV1, $T_x$ value as key, the line as value
17:     end for
18: end function
```

4. If the line contains domain-specific data, the mapper looks for the value of the independent variable T_x. Once found, this value acts as key, and the value is again the whole line of data.

5. All key-value pairs are emitted to the *reduce* phase.

During the *reduce* phase (described in Algorithm 6) the reducers can group all lines associated to each value of T_x, thus arranging the input data in an $\{I_{glob}, I_0, I_1, I_2, ..., I_k\}$ layout, where I_{glob} contains the global data which does not vary with regard to the problem domain, and I_i contains all data belonging to the ith subdomain partition. The task is performed as follows:

Algorithm 6 Adaptation phase reducer

```
Input: $KV1 = \{(k_0, v_0), (k_1, v_1), ..., (k_n, v_n)\}$
Output: $I_{glob}, I_0, I_1, I_2, I_3, ...I_k$
 1:
 2: for all ($(k_i, v_i) \in KV1$) do
 3:     REDUCE($(k_i, v_i)$)
 4: end for
 5:
 6: function REDUCE($(key, value)$)
 7:     $I_i \leftarrow$ DATASETOF($key$)     ▷ Find sub-domain partition associated to $T_x$
 8:     $I_i \leftarrow I_i + value$        ▷ Group all data associated to $T_x$ in the same set
 9: end function
```

1. Each key-value pair emitted by the previous phase is processed by the reducers of this phase.

2. For each member of the keys set, a dataset is created in order to group all values corresponding to that key.

3. Values are aggregated as the key-value pairs are being processed. The datasets represent groups of data associated to simulation subdomains.

4. Once all keys have been processed, the datasets are stored in the HDFS.

Once the adaptation stage ends, the simulation stage takes as input the datasets. The simulation stage is described in Algorithm 7 and Algorithm 8. Algorithm 7 describes the *map* phase. Starting from the data layout obtained from the previous stage, the mappers execute the simulation kernel, using as input each one of the subdomain partitions. The *map* task is performed as follows:

Algorithm 7 Simulation phase mapper

```
Input: $I_{glob}, I_0, I_1, I_2, I_3, ...I_k$
Output: $KV2 = \{(k_0, v_0), (k_1, v_1), ..., (k_p, v_p)\}$

for all $I_i \in I_0, .., I_k$ do
    MAP($I_{inv}, I_i$)            ▷ Execute simulation kernel on sub-domain partition
end for

function MAP($I_{inv}, I_x$)
    $O^x = O^x_0, O^x_1, ..., O^x_m \leftarrow$ SIMULATIONKERNEL($I_{inv}, I_x$)
    for all $O^x_i \in O^x$ do            ▷ For each chunk outputted by the kernel
        $key \leftarrow i$
        $value \leftarrow O^x_i$
        EMIT($key, value$)        ▷ Adds pair to KV2, file ID as key, chunk contents as value
    end for
end function
```

1. First of all, the global dataset is spread across all mappers, because it contains data associated to the whole simulation, so it is needed in all simulation kernels. In order to do this, the HDFS cache is used. This cache allows to make a small amount of data available to all nodes in an efficient way. Global data are usually orders of magnitude smaller than domain data.

2. Datasets containing all simulation subdomains, obtained from the previous stage, are read by the nodes in the HDFS cluster.

3. The mappers in the nodes execute the simulation kernel on each subdomain. As result, the simulation is conducted in (concurrent) steps according to the partitions produced in the previous stage.

4. Each mapper obtains a collection of chunks, fragments of the output files which contain only the results associated to the simulated partition. The number of chunks depends on each particular simulation domain characteristics.

5. Finally, mappers emit each chunk using as key an identifier of the final files of the simulation (e.g if the simulation kernel produces five files, the keys will be $k = \{0, 1, 2, 3, 4\}$).

The *reduce* task (described in Algorithm 8) is accountable for merging each chunk gathering the results from all mappers. The task is performed as follows:

Algorithm 8 Simulation phase reducer

```
Input: $KV2 = \{(k_0, v_0), (k_1, v_1), ..., (k_p, v_p)\}$
Output: $O = \{O_0, O_1, ...O_m\}$

for all $((k_i, v_i) \in KV2)$ do
    REDUCE($(k_i, v_i)$)
end for

function REDUCE($(key, value)$)
    $O_i \leftarrow$ DATASETOF($key$)          ▷ Find output file associated to that ID
    $O_i \leftarrow O_i + value$          ▷ Gathers all chunks which corresponds to each output file
end function
```

1. Each key-value pair emitted by the previous phase is processed by the reducers of this phase.
2. Each key represents a final file of the simulation. Data from all simulation kernels are aggregated and grouped following the same arrangement used in original simulation.

By this way, the resulting files can be composed as if the simulation domain were never split across the cluster.

5.1.4 Virtual Cluster Planning

The former stages would most likely require different amounts of CPU and memory resources depending on the application to be cloudified. In this section, a heuristic to detect the slaves' instance requirements to maximise resource utilisation is provided. First of all, the concept of an *entry* is defined. An entry is a piece of data processed by the mappers on any of the methodology stages. There will be different entries for the adaptation and simulation phases:

- For the adaptation phase, an entry is one of the registers by which the input files are arranged. Mappers in adaptation phase process these registers indexing them according to the independent variable T_x.
- For the simulation phase, an entry is one of the $I_i = (T_x, parameters)$ pair. This is the autonomous piece of data which is going to be simulated by the mappers of the simulation phase.

Next, the following assumptions are considered:

- All the slaves must be equal in terms of memory and number of cores.
- The execution time required to process an entry, $t_e \in \mathbb{R}^+$, is previously known by the user, and homogeneous for all the entries. For the adaptation phase, this is the time required to parse an index the parameters according to the independent variable. For the simulation phase, this is the time required to execute the simulation kernel over a single autonomous piece of the input data.

- The amount of memory required to process an entry, $m_e \in \mathbb{R}^+$, is known and homogeneous for all the entries. For the adaptation phase, this is the memory needed to perform the grouping of input parameters according to the independent variable. For the simulation phase, this is the memory needed to allocate and simulate one single simulation kernel and merge the results.
- The number of entries, $n_e \in \mathbb{N}$, is known.

Of course, t_e and m_e may vary, depending on the problem domain. In that case the expert should either estimate an accurate value, or consider inserting probabilistic distributions in formulae. In the first approach, let assume t_e and m_e constant along all entries, in order to simplify the heuristic. Given these parameters and assumptions, *the objective is to minimise the total execution time of the cloudified application*, $T \in \mathbb{R}^+$. The minimisation problem is defined as follows:

$$\min_{n_I, c_I} T = \frac{t_e n_e}{n_I c_I} + \alpha \tag{5.4}$$

Where $c_I \in \mathbb{N}$ represents the number of cores per instance, $n_I \in \mathbb{N}$ is the number of instances in the targeted cluster, and $\alpha \in \mathbb{R}^+$ is a parameter that represents the compute overhead factor of the underlying platform (spawning the tasks, etc.), which is considered constant.

The following constraint is applied:

$$m_e c_I + \beta \leq m_I \tag{5.5}$$

Where $m_I \in \mathbb{R}^+$ represents the amount of memory per instance and β represents the memory overhead added by the platform on each instance. Equation 5.5 indicates that the aggregated memory required by the entries that can be concurrently processed by each node must not exceed the total memory of it.

Once n_I, c_I and m_I are found, one can select the instances that have greater or equal resources for both metrics, simultaneously.

This minimisation problem can be modified by letting T be a fixed value, in order to find suitable instances to meet a specific deadline. This deadline-oriented planning can be very beneficial to minimise costs in pay-as-you-go infrastructures, as deadlines can be multiples of the time slices covered by successive charges. For instance, Amazon charges the user for slices of one hour (even if the user only allocates VMs for 15 minutes). Therefore, this heuristic can be used for:

a) Providing a VM configuration and calculate the expected execution time using that configuration.

b) Choosing the best VM configuration in order to meet a given deadline.

TABLE 5.1: Examples of virtual cluster planning using different instance types, $\alpha = 30\text{s}$ and $\beta = 1\text{GB}$.

Objective	**Problem domain**			**Instance type**			**Ex. time**
	n_e	m_e	t_e	c_I	m_I	n_I	T
Calculate T	10^5	1GB	1s	8	17GB	30	**447s**
Size cluster	10^5	1GB	1s	2	8GB	**15**	3600s
Calculate T	10^5	1GB	1s	1	4GB	15	**6697s**

Examples of the former formulation are shown on Table 5.1, using different instance types. Let E be the set of $n_e = 10^5$ entries the user wants to process, each one requiring $m_e = 1\text{GB}$ of memory and $t_e = 1\text{s}$ for its execution. The first and third rows illustrate contain examples of calculations of the execution time T provided that the user wants to use 30 instances of 8 cores and 17GB each (first row), or 15 instances of 1 core and 4GB each (third row). The second row illustrates the opposite procedure. Assuming the user wants to process E within one hour, using instances with $c_I = 2$ and $m_I = 17\text{GB}$, the execution time, T, becomes a deadline of 3600s. Solving the resulting equation, the number of instances necessary to process all entries within one hour is 15. Let assume in all examples $\alpha = 30\text{s}$ and $\beta = 1\text{GB}$. Note that memory optimised machines are meant to favour the memory-bound tasks with a high ratio memory-to-CPU, whereas compute-bound tasks would benefit from compute optimised instances, as a large number of cores would allow the execution of more mappers simultaneously.

5.2 Application to RPCS

To illustrate how this methodology works on a real-world use case, we applied it to the RPCS simulator. This applications is widely described in Chapter 3, as well as the different ways of applying parallelization at its different layers. Also, as has been explained, the application is memory-bound, so it is a perfect test case for the methodology. There are multiple advantages that Cloud Computing could bring to the application. In Section 3.3.4, the analysis of resource usage performed to the application shows how the workload is strongly dependant on the particular scenario to be simulated. Different scenarios may have different computational requirements, so Cloud flexibility to size infrastructures could suppose a big feature to end users. Besides, the original application is based on multi-threading, so it cannot be deployed on more than one node.

5.2.1 RPCS Application Analysis

The key to adapt such algorithm to a cloud environment resides in its input files, for they hold an indexed structure that stores in each line an $(instant, parameters)$ pair. As said before, each simulated instant (t_i in Equation 3.4 at Section 3.3.2) is independent from the others, because for each instant the circuit has to be composed, solved, and the results obtained, so the whole simulation period can be divided (e.g. from 06:00:00 to 22:00:00) in multiple smaller simulations, each one of length 1 second. Therefore, the temporal key can be considered as the independent variable required for the theoretical model. But in order to do that, first the input data have to be adapted, rearranging that data from the initial set to multiple smaller subsets, each one containing those information necessary to simulate one single instant.

5.2.2 RPCS Cloudification Process Design

Following the cloudification schema, the application was transformed into two independent MapReduce jobs executed sequentially. In the first job, which matches the first MapReduce in Figure 5.1, the movement input files, I, are divided into input splits by the framework according to its configuration. Each split is then assigned to a mapper, which reads each line and emits $(key, value)$ pairs where the key is the instant, t_i, and the value is the corresponding dddset of parameters for such instant. The intention behind this is to provide reducers with a list of movement parameters per instant $I_n, \ldots, I_m$ –each element representing the movement of one of the trains involved in the overall system for a particular t_i– to concatenate and write to the output files, so that the simulation kernel can be executed once per instant with all the required data.

As described in Figure 5.1, the output of the previous job is used as input to the mapper tasks by parsing each line. Then, the resulting data –which corresponds to the instant being processed– is passed to the electric algorithm itself along with the scenario information obtained from the infrastructure file that is also read by the mapper. The mappers' output is compound by an output file identifier F_j as key and the actual content as value.

Reducers simply act as mergers gathering and concatenating mappers' output organized by file identifier and instant as a secondary key injected in the value content. This arranges the algorithm's output so that the full simulation results are shown as in the original application, in which each output file contains the results for the whole temporal interval of the simulation.

5.2.3 Implementation and platform configuration

The previous design could be implemented in any of the available MapReduce frameworks. Among them, Apache Hadoop platform [Whi09] is selected given its increasing popularity and community support. Its distributed file system is a great addition to the framework, since it allows automatic load balance. Moreover, it includes a distributed cache that supports auxiliary read-only file storage for tasks among all nodes, which suits neatly the shared infrastructure parameter file's needs.

Besides the former technical features, Hadoop has been increasingly adopted into cloud environments along with other MapReduce frameworks, resulting in reduced costs given its parallelism exploitation capabilities [KPP09].

This design was implemented via Hadoop Pipes API, since the original code was written in C++ and we wanted to maximize code re-usage. Despite Pipes does not allow to take full advantage of Hadoop's potential given its limited functionality, it provided all the necessary tools to execute

Table 5.2: Job-specific configurations on MRv1

Parameter	**Job 1**	**Job 2**
Maximum no. of map slots (GB)	16	6
Number of reducers	2	4
JVM memory (GB)	4	8

the framework, including *map* and *reduce* interfaces, basic data type support and Distributed Cache access on job submission.

The framework was configured assuming no robustness or availability is needed nor desired in this application. Therefore, Hadoop's Distributed File System (HDFS) replication was disabled in order to make HDFS interactions less time-consuming. The parameters shown in Table 5.2 permitted to achieve a significant balance between memory consumption –especially in the second job– and the required time to finish the job in the worst case tackled. Besides the former, reducers were forced to wait for at least the 85% of the mappers to finish before start processing their output. This was considered to minimize the shuffle overload and maximize the available resources at the map phase, which is especially relevant in the second job.

Given the eager algorithm in terms of memory that constitute the kernel of the RPCS, the container configuration shown in Table 5.3 aimed to provide enough memory for the second job in the worst case tackled. With similar purposes, the configuration for node resource dedication that can be seen in Table 5.4 is set. Moreover, the slow-start configuration is maintained in both phases and the HDFS parameters mentioned previously.

Table 5.3: Job-specific configurations on MRv2

Parameter	**Single-node cluster**		**Virtual cluster on EC2**	
	Job 1	Job 2	Job 1	Job 2
Container memory (GB)	1.5	7	1	6
Number of reducers	2	13	5	10

Table 5.4: Platform configuration parameters for MRv2

Parameter	**Single-node cluster**	**Virtual cluster on EC2**
Node memory (GB)	92	16
Virtual cores	16	4
Minimum allocation (GB)	1	0.5
Virtual memory ratio	4	8

Table 5.5: Execution environments.

Configuration	**Platform**	**Underlying infrastructure**
1	Multi-thread	Cluster node
2	Hadoop 1.1.2 (MRv1)	Cluster node
3	Hadoop 2.2.0 (MRv2)	Cluster node
4	Hadoop 2.2.0 (MRv2)	EC2

5.3 Evaluation

In order to asses the methodology applicability and the performance its execution time on both a cluster and the cloud is compared. The following sections describe the utilized resources and a discussion on the obtained outcome.

5.3.1 Execution Environments and Scenarios

Table 5.5 summarizes the infrastructures and software platforms on which the evaluations were conducted. In a first place, there were tested the original multi-thread application's memory consumption and performance on a cluster node consisting of a 48 Xeon E7 cores and 110GB of RAM (Configuration 1). This node was also used to test the resulting cloudfied application to avoid variations that may arise from heterogeneous configuration, resource differences, or network latency in case of the MapReduce application [JDV+09]. This isolation favours the multi-thread application, which is especially designed to perform in standalone environments. However, it allows to focus on the actual limiting factors that may affect scalability in large test cases like I/O, memory consumption and CPU usage. Both Hadoop versions –MRv1 and MRv2– were installed and configured on the single-node cluster to benchmark their performance against the original application (Configurations 2 and 3, respectively).

MRv2 was chosen to be deployed on EC2 given its improved resource management options and better overall performance (Configuration 4). The cloud infrastructure consisted of a general purpose *m1.medium* node as dedicated master and several memory optimized *m2.xlarge* machines as slaves; Table 5.6 shows the main aspects of the selected instances. The number of slaves was selected to match roughly the resources present in Configuration 1, so that the comparison is fair for both infrastructures, leading to a total of 24 slaves to match the 48 cores present in Configuration 1. Additionally, further evaluations have been conducted on EC2 using a variable number of slaves, in order to check if scalability issues arise as the number of nodes increases.

Table 5.6: EC2 instances description.

Type	**Role**	**Virtual CPUs**	**Memory (GB)**	**Local storage (GB)**
m1.medium	master	1	3.75	410
m2.xlarge	slave	2	17.1	420

Table 5.7: Test cases definition for the original vs. cloudified application

Experiment	**Avg elements per instant**	**Simulated time (hours)**	**Input size (MB)**
I	77	1	1.7
II	179	33	170
III	525	177	1228.8
IV	755	224	5324.8

The test cases simulated during this evaluation are summarised in Table 5.7. These tests are the same that were used in Chapter 3 to conduct a resource analysis of the original RPCS application, as well as those used in Chapter 4. Now, they are meant to indicate the performance of the cloudified adaptation versus the original application under an increasing amount of input data and simulation time. Each one of these experiments (numbered as I, II, III, and IV) suppose an increment in both domain size (period of time to be simulated) and problem size (size of the electric circuit) with regard to the previous one.

5.3.2 Results Discussion

As was already discussed in Chapter 3, the original multi-thread application's memory usage suggests a lack of scalability in a shared memory environment. The evaluation will now analyse whether the cloudified simulation behaves as expected in relation to performance and scalability by examining its execution times on several execution environments, which are shown in Figs. from 5.2 to 5.5. These figures show the time measurements obtained on the configurations in Table 5.5, in which the EC2 cluster is constituted by five slaves –graphs (a), (b) and (c)–. The EC2 values also served as baseline for the scalability study shown in (d). Additionally, Table 5.8 includes the execution times, as the values for the extreme cases make the first experiment hard to compare with the others visually.

(a) Cloudification phase

The execution times of the cloudification phase are shown in Figure 5.2. Several conclusions can be extracted from these results. First, the cloudification performs better on EC2 than on he same MapReduce version in the local cluster for the three largest experiments (at least a 55% faster, in the worst case, up to a 74%). This is because input files reside locally on the EC2 virtual cluster, thanks to the HDFS filesystem that spreads the chunks of the files across all nodes. However, the node cluster rely on Lustre to store the input files externally, so data must be sent to the cluster node to be processed. The smallest experiment, however, runs a 57% slower, mainly due to the execution time being too short to make up for the platform's launching and synchronisation overhead; this issue can be observed in all of the remaining stages.

(b) Kernel execution

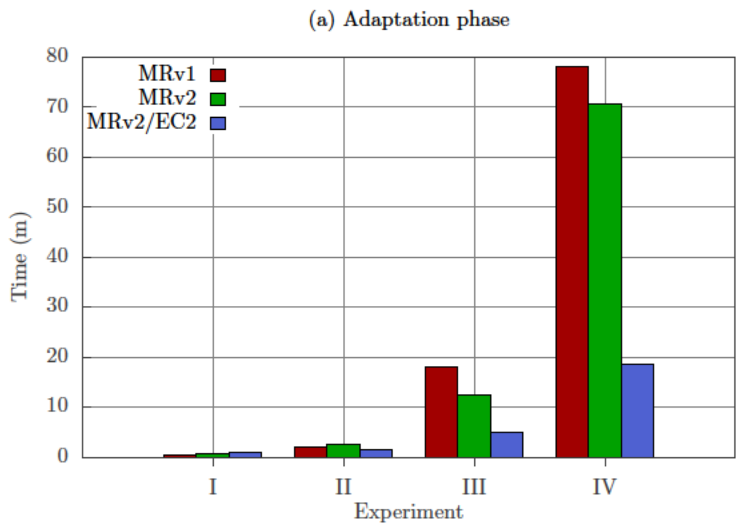


FIGURE 5.2: Evaluation results: adaptation phase times of the four test cases using different execution environments.

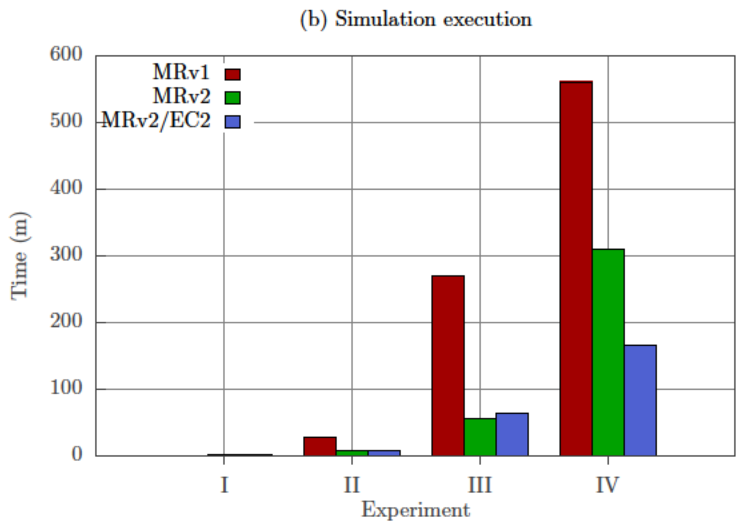


FIGURE 5.3: Evaluation results: kernel execution times of the four test cases using different execution environments.

The simulation execution stage is shown in Figure 5.3. It is the most determinant phase in the whole process, ranging from the 46% of the whole execution time, in case I on EC2, to a 91%, in case III in the same environment. Since the virtual cluster was selected to match the number of cores of the physical environment, we can claim that the application deployed in the Cloud shows outstanding performance against the other configurations for the largest experiment (47% faster in the worst case against MRv2 on the local node). Experiments I, II and III, however, have similar execution times in EC2 and the physical node running MRv2, yet this sustains the scalability of the application, as no signingicant performance loss (14% tops) is perceived in average sized experiments after cloudification.

(c) Aggregated time

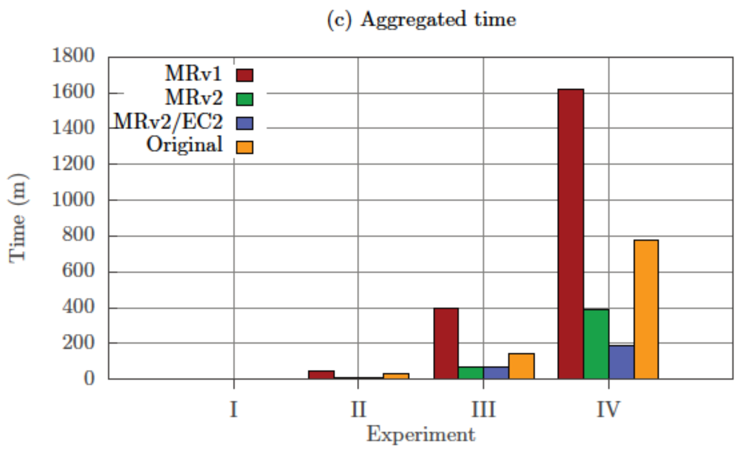


FIGURE 5.4: Evaluation results: aggregated times of the four test cases using different execution environments.

In Figure 5.4 it is observed that the overall execution time for the application including both MapReduce jobs and input data upload. The latter has to be considered given that replication and balance must be achieved by the platform to distribute load evenly. The graph indicates that the performance obtained with MapReduce on Yarn in both the single-node cluster and the elastic cloud is remarkably better than the original multi-thread application –68% and 85% less total simulation time for the largest experiment, respectively–. The shared memory simulator's results might be caused by the bottleneck constituted by the physical memory and the disk. The latter is particularly critical, as all threads write their results to disk while they perform their computations in the original simulator.

As said before, the smallest experiment is an interesting exception, with execution times ten times greater than the original application in all the platforms. This reflects how the MapReduce framework's overhead significantly affects the time taken to complete such a small simulation compared to the original application benchmark.

(d) Scalability study

Finally, in Figure 5.5 it is observed the speed-up obtained on EC2 running YARN when the number of slaves is increased. The speed-up shown in the figure is related to the execution times commented in the previous paragraphs, which were obtained in a five-slave cluster. Nevertheless, it has been normalized using one slave as reference, in order to understand better how the speed-up evolves as we add more nodes to the virtual cluster. As the figure indicates, increasing the number of slaves decreases the total simulation time. However, the performance does not scale up linearly with the number of nodes: while with 16 nodes the speed-up is 16.55, with 64 nodes it is only 37.99. The reason behind this result is that the problem size becomes small for the cluster size as more nodes are added. Hence, less data is assigned to each slave and some resources become underutilised. Moreover, as it is mentioned in the previous paragraph, in very small experiments the measured execution time is mostly spent in the platform's task preparation and scheduling, and not in the actual simulation. This results in degraded performance due to platform overhead.

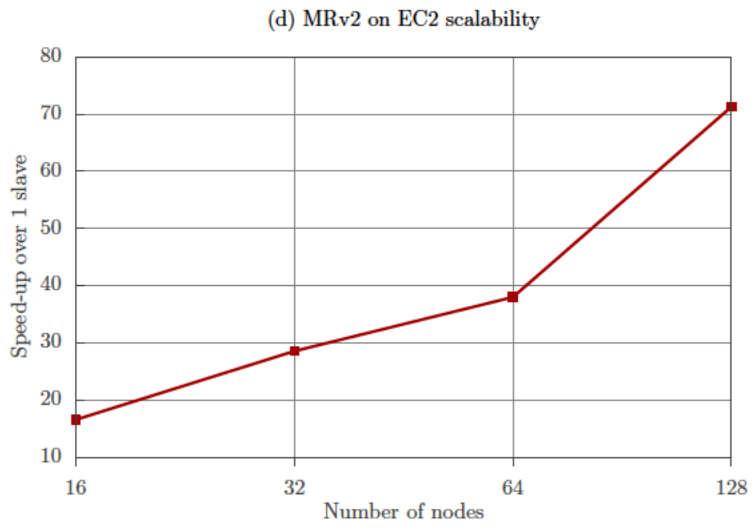


FIGURE 5.5: Evaluation results: scalability study of the largest case on EC2 using 1 slave as baseline.

Therefore, it is necessary to increase the problem size as well as the number of slave nodes in order to achieve linear scalability.

TABLE 5.8: Execution times per stage in minutes. Configurations and experiments defined in tables 5.5 and 5.7.

Configuration	Experiment	Copy to HDFS	Adaptation	Simulation	Aggregated
MRv1	I	2.17	0.43	0.53	3.13
	II	17	2	28	47
	III	110	18	270	398
	IV	977	78	561	1616
MRv2	I	0.05	0.63	0.88	1.57
	II	0.18	2.62	8.23	11.03
	III	1.43	12.43	55.5	69.37
	IV	5.68	70.52	310.27	386.47
MRv2/EC2	I	0.12	1	0.95	2.07
	II	0.4	1.45	7.15	9
	III	1.28	4.87	63.7	69.85
	IV	5.53	18.63	165.57	189.73
Original	I	-	-	-	0.095
	II	-	-	-	29.47
	III	-	-	-	140.9
	IV	-	-	-	777

5.4 Summary

As the cloud is increasingly shown as a viable alternative to traditional computing paradigms for high-performance applications and resource-intensive simulations, this chapter proposes a general methodology to transform simulations into a highly scalable MapReduce application that re-uses the same simulation kernel while distributing the simulation load across as many nodes are desired in a virtual cluster running on the cloud.

The procedure requires an application analysis phase in which at least one independent variable must be found, since this element will act as index for the cloudification phase. The cloud adaptation stage transforms the original input into a set of partitions indexed by the the previous variable by means of a MapReduce job; these partitions are fed to a second MapReduce job that executes the simulation kernel independently for each, merging the final results as well.

This methodology performs a paradigm shift from resource-bound applications to a data-centric model; such cloudification mechanism provides effective cloud migration of simulation kernels with minimal impact on the original code and achieves great scalability since limiting factors are scattered. The promising results obtained in the particular use case studied, in terms of performance and scalability, support the model's viability. Moreover, we think that this cloudification methodology may improve its results on parameter sweep problems, due to its pleasingly parallel pattern and the benefit from data locality on such kind of problems. The results of the methodology on multivariate analysis through parameter sweep will be studied in the next chapter.

Chapter 6

Multivariate Analysis of Simulation Problems

In the previous chapter, a methodology to transform simulations into a highly scalable MapReduce application has been proposed. Up to this point, the methodology focuses on splitting a single simulation into multiple tasks that use the same simulation kernel, distributing the simulation load across as many nodes are desired. Nevertheless, modern workflows that make use of simulation tools usually perform not one but many simulations, in the context of MOO problems, parameter sweep applications, or rapid prototyping.

This chapter focuses on extending the proposed methodology to include multivariate analysis simulations, as a particular case of pleasingly parallel problem. The kinds of applications that benefit the most of this paradigm are the ones with many loosely coupled tasks, including those simulations based on parameter sweep. Most simulators that fulfil the proposed enhancement rely on several parameters to configure a specific experiment. All of these variables can be changed independently, yielding an exponential number of possible experiments. This complexity is further problematic if one decides to combine more than one variable at a time in a multidimensional experiment analysis. Therefore, it is meaningful to consider multivariate analysis within the methodology, thus providing a mechanism to execute concurrently a large number of simulations in the same infrastructure.

6.1 Multivariate Analysis on Current Simulators

As computer systems have been evolved, the role of simulators have turned, from merely imitators of the real world, to expert systems with the ability of taking decisions and complement the user knowledge with metrics in order to achieve the best solutions. The main goal of a modern simulator is not reduced to perform the simulation and output the results to the user. It has to generate candidate solutions (experimental designs, prototypes, or models), evaluate if they are acceptable or not, and provide a degree of fitness.

This procedure is composed of several tasks: first, a candidate solution must be selected, either being provided by the user, or being generated by the simulator itself. Then, the simulation is performed and the results are analysed. The candidate solution is scored, and a decision to accept it or reject it is taken. This procedure is repeated across all areas in which simulators are used on. A simulator must not be restricted to evaluate solutions provided by the user, but also it should find acceptable solutions by itself, with a high degree of fitness, and in a reasonable amount of time.

6.1.1 Proposal of Simulation Enhancement

To achieve these targets an enhanced simulation structure is presented, which allows increasing the output of simulators by covering more capabilities than the main procedure described before. This enhancement is focused on four main issues which we proceed to describe.

- *Layer 1: computing elasticity.* First of all, modern simulators should be capable of taking advantage of modern Cloud architectures, which can allocate computing resources upon user request. Productivity issues in industry require to shorten the deadlines when evaluating new designs. Besides, the design process may require evaluating a lot of candidate solutions. We state that an efficient simulator should be adaptable to the underlying hardware, so as to let the user to control the simulation times, allocating more computing resources to shorten the deadlines, or giving up time if the computing resources are low.
- *Layer 2: automatic generation and evaluation.* In the second place, automatic generation and simulation of solutions falls outside the scope of most simulators. Therefore, the user must feed the simulator providing new possible solutions, which leads to productivity losses. Moreover, the capacity of finding good (maybe optimal) solutions is tied to the user and her own ability to explore the problems search space. We state that an efficient simulator should evaluate and simulate a set of solutions with a minimal user involvement. To achieve that: a) the user should provide the simulation parameters as a set of possible values (e.g. [minimum, maximum, increment]), and the simulator uses them to generate candidate solutions; b) the simulator should be able to generate new solutions starting from an initial database (e.g. an inventory or catalogue).
- *Layer 3: include stakeholders.* Thirdly, there are many stakeholders taking part in the design process which usually fall out of the scope of the simulation models. These parts can influence, or even determine, the final acceptance of the candidate solutions [NHC13]. For instance, the set of possible solutions when looking for a valid design of a railway portal frame, can be limited by the availability of constructive pieces in the company's inventory, and once found, a portal frame that stands could not be in compliance with legal normative in certain countries. All issues that have to be considered throughout the design process, but fall out the scope of the simulation model, should be also taken into account when simulators generate and evaluate candidate solutions. This category includes provider specifications, client requirements, technical security, legal normative and even budget limitations. Different ways of including such restrictions in the simulation model

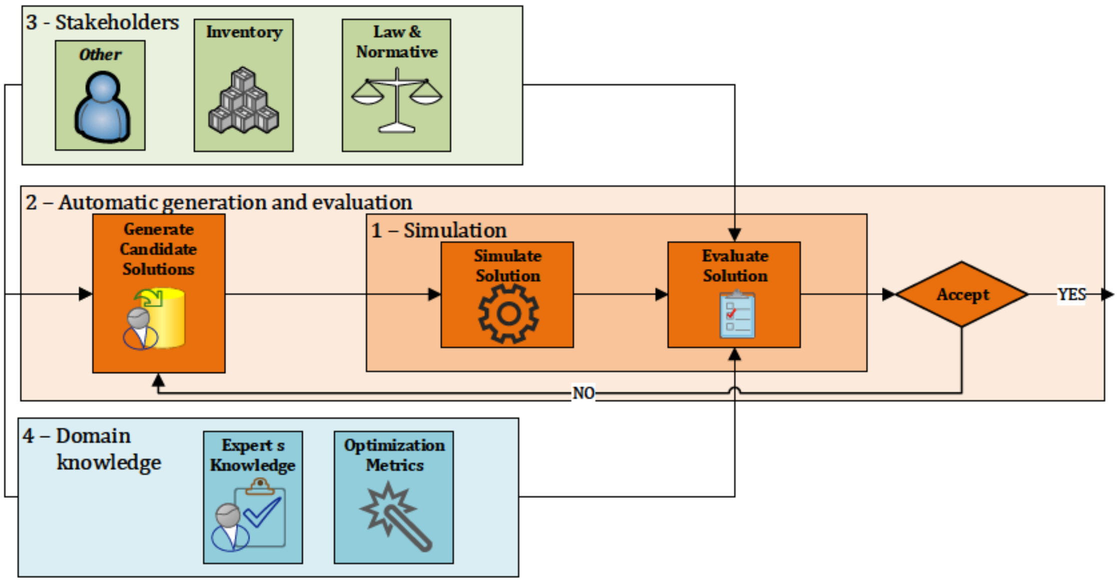


FIGURE 6.1: Enhanced structure of a simulator presented by the authors

are, a) restrictions to generate candidate solutions, so that the simulator only generates candidate solutions that fulfill with these initial restrictions; b) restrictions to evaluate a candidate solution, so that the simulator evaluates these restrictions as well as any other conditioned by the simulation model.

- *Layer 4: include expert's knowledge.* Finally, expert's domain knowledge is a fundamental part in the engineering design process [Ade03]. Expert's knowledge defines heuristics that allow speeding up the search process and achieving the best solutions in the problem's search space. Therefore it should be included as a part of the simulation, particularly in those simulators that include automatic generation of candidate solutions (described as the second issue). In a similar way to other participants in the design process, expert's knowledge can be included when generating candidate solutions in the form of decision rules. Those rules guide the search process to generate better candidate solutions. They can also be included to evaluate a candidate solution in the form of optimization metrics, which can be used to score the solution and compare it with others, thus choosing the best one.

In [GGGCC14], a general structure which includes all these components is introduced, as well as a proposal to translate this structure into a cloud-based design. Therefore we use this architecture as a starting point. This approach is showed in Figure 6.1. This figure is layered following the four issues previously mentioned. The core procedure of simulating and evaluating candidate solutions compounds layer 1. Issue 2 is covered by the layer 2, which contains the task of generate automatically new solutions to be evaluated. This task could be fed from other elements in layers 3 and 4 (e.g. requirements related to an inventory of constructive pieces, or expert's domain knowledge, applied to generate better candidate solutions). Layer 3 is composed by those stakeholders that are not included in the simulation procedure (layer 1), but have impact on the solution, thus adding restrictions. Those restrictions can be applied either when generating or when evaluating a candidate solution. Examples of such restrictions are availability of constructive pieces in company's inventory when proposing a design, or compliance with legal normative when evaluating the proposed design. Finally, layer 4 represents the expert's domain knowledge that allows to obtain better solutions. Decision rules used to generate better candidate solutions, or optimization metrics used to choose the best one, are included in this layer. This approach improves the efficiency of the simulators by giving them the ability of searching for the best solutions in the problem space. Obtained solutions will be fully-integrated with the different actors of the design process, that have been included as a part of the structure proposed.

There are multiple examples of this trend in simulation techniques. In computational fluid dynamics, an aerodynamic design of a new vehicle can be tested in order to analyze its efficiency. In overhead contact line designs, structural behavior [NHAR13] of poles and portal frames are evaluated, checking their feasibility [SGG+12]. In nuclear physics, different designs of BWR reactors can be simulated to analyze different aspects such as efficiency, integrity, etc. In the field of energy provisioning, a proposal of electric installation locations may be simulated checking whether energy is available to all planned consumers [ASS13].

6.1.2 Cloud-Based Approach to Multivariate Analysis

The proposed structure allows to increase the output of the simulators, generating and evaluating multiple solutions, and taking into account different parts of the design process. Nevertheless, this theoretic approach have to be implemented and tested in order to make its advantages effective. In Chapter 3 we stated that multivariate analysis can be described as a pleasingly parallel problem, in which each simulation can be performed concurrently. We stated also that Cloud platforms were the best-suited in order to deploy pleasingly parallel problems. Therefore, we propose an approach to implement this structure in the Cloud.

- Regarding to issue 1, the system should have a flexible computing power which could adapt to the computational complexity of the simulated domain. Complex simulations may require more computing power to evaluate solutions, whereas simple simulations can lead to untapped resources. The user should be capable of set the trade-off between time and resources as desired, customizing the computational capacity of the infrastructure.
- Regarding to issue 2, the system should have a software engine which generates the specific domain solutions. Starting from the domain description and simulation parameters, this component should create a model of the solution, which will be simulated by a simulation engine. Also, this component should be able to vary the simulation parameters (or the simulation scenario) in order to generate different solutions and to explore the solutions space.
- Regarding to issues 3 and 4, the system should have a database which contains all restrictions from stakeholders taking part in the design process, and all the optimization metrics and heuristics that can influence the final acceptance of the solutions. Those factors must be formalized and stored as decision rules.

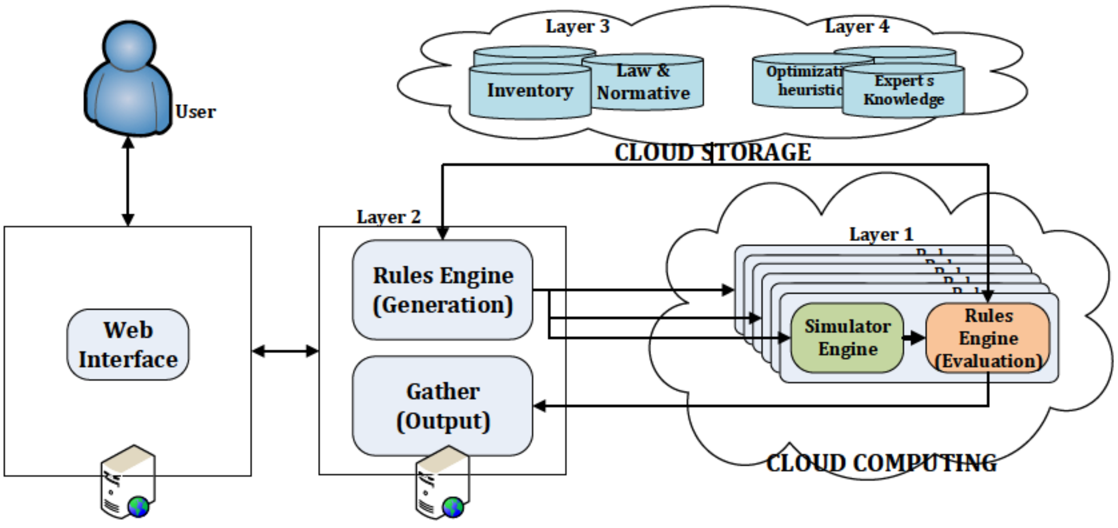


FIGURE 6.2: Cloud-based approach to simulation enhancement

In order to overcome these issues, we describe a proposal to map the structure provided to a Cloud-based design. This design is based on ontologies and decision rules. The user defines an ontology to represent the simulated domain, and decision rules to implement domain specific knowledge (restrictions, optimization metrics). This allows to keep the design aware of specific domain data. The user can define the simulation model as well as the rules in which are based both evaluation and optimization functions. Two rule engines have been included in the design in order to apply the rules described above in the generation and evaluation phases. The generation engine asks for restrictions (that limits the number of new solutions), and for heuristics (that help to choose the following one to be evaluated). On evaluation, the simulation engine asks for restrictions and optimization metrics to be used to score the solution. We rely on cloud computing paradigm to bring the flexible computing capacity required to address the issue 1. This paradigm allows to demand computational resources (i.e. computing power) in a transparent manner. If the user requires more computing power to perform more (or more precise) simulations, she can request to the cloud those resources. Cloud service providers (e.g Amazon or Google) or public/private clouds within the reach of the user (e.g enterprise private cloud) are part of the solution. Decision rules can be implemented as a database, which can be allocated in cloud infrastructure or not.

The Figure 6.2 illustrates the evolution of the structure proposed in this chapter. We map the layers of the Figure 6.1 to the software components in Figure 6.2. The core procedure to simulate and to evaluate a candidate solution is formed by the simulation and evaluation engines. Simulation engine reads the solution description (e.g. a mathematical model) and performs the simulation (e.g. solving the linear equation system). The evaluation engine decides whether it is acceptable or not, and scores the solution. This core procedure is supported by the cloud infrastructure, and can be scaled horizontally (adding more instances) allowing the user to perform more simulations if necessary. The task of generating automatically new solutions is mapped to the generation engine, which can create new scenarios or changing simulation parameters. Layers 3 and 4, which contains specific restrictions (e.g. legislation, normative, or restrictions from the providers), and experts knowledge (such as optimization metrics), are composed of decision rules databases. Generation and evaluation engines perform queries to these databases when applying decision rules. Finally, the user interacts with the simulator through a standard interface (e.g. web interface).

6.2 Methodology Enhancement for Multivariate Analysis

Since the methodology we described in Chapter 5 aims to provide task independence between concurrent simulation partitions, we can perform a multivariate analysis by spawning several simulations in a many-task manner. Many-task computing (MTC) is a new computing paradigm that mixes high throughput computing (HTC) and high performance computing (HPC). Its main goal is to make an efficient use of a large number of computing resources over short periods of time to execute many computational tasks [RFZ08]. The main difference with HTC is that the throughput is measured as tasks over very short periods of time –such as FLOPS, tasks/s, etc.– instead of jobs per month, for instance.

Scientific simulations such as DNA database analysis, data processing in the Large Hadron Collider (LHC) and climate modelling constitute examples of applications that make use of many-tasks to analyse their huge amount of data. These applications rely on large quantities of data, therefore data locality seems critical for large scale MTC. In fact, [RFZ08] states that data-aware scheduling minimises data movement across nodes and benefits performance. Given this context, it seems natural to enhance out data-centric methodology with a many-task deployment to support multidimensional analysis, while enforcing efficient resource utilisation and balance.

In the Section 6.1.1, the advantages of developing simulators with an increased set of capabilities have been exposed: not only simulating and evaluating scenarios provided by the user, but also generating a new set of scenarios by its own, thus exploring the solution search space. A simulator should also implement the evaluation function necessary to score the simulated scenario, off-loading this task from the user. Combining these two properties, a third one arises, since with a little additional development the simulator should be capable of conducting a guided search for optimal solutions across the problem's domain space.

Given this context, it seems natural to enhance out data-centric methodology with a many-task deployment to support multivariate analysis, while enforcing efficient resource utilisation and balance. The following sections describe, implement and evaluate a multivariate analysis tool, implemented as a many-task deployment based on our cloudification methodology.

6.2.1 Multivariate Terms and Definitions

First of all, it is important to note that not one, but many simulations have to be performed, so the Equation 5.1 evolves to Equation 6.1, that represents the concept of many simulations S^i, each one with its corresponding input data set I^i, and output data set O^i:

$$S^i \equiv f_{sim}(I^i) = O^i \tag{6.1}$$

Then, in order to include the multivariate analysis in the methodology, the following concepts have to be added to those defined in Section 5.1.1:

- *Generation engine.* The function $G \equiv f_{gen}$ that, starting from an initial scenario I, generates derivative scenarios as variations of the initial one, performing modifications to the input data set. This modifications can be performed through different ways: user-driven, parameter sweep, evolutionary algorithms, etc.

$$G \equiv f_{gen}(I, i) = I^i \tag{6.2}$$

- *Evaluation engine.* The function $E \equiv f_{ev}$ that process the output results from a simulation, and gives a score for that scenario indicating its suitability, optimality, or any other quality indicator θ related to the simulation domain.

$$E \equiv f_{ev}(O^i) = \theta^i \tag{6.3}$$

  The aim is to find the scenario I^k that maximizes the score obtained from that evaluation function, after evaluating the whole set of considered scenarios:

$$I^k \mid \theta^k = \max_{\forall x} \theta^x \tag{6.4}$$

  The evaluation engine can be expressed as the union of two different sets of evaluating conditions that influence the validity and optimality of the solution in different ways: restrictions rules f_{res}, and optimization metrics f_{opt}.

$$f_{ev}(O^i) = f_{res}(O^i) \cdot f_{opt}(O^i) \tag{6.5}$$

- *Restriction rules.* The restriction rules f_{res} are those evaluating conditions whose fulfilment is mandatory in order to consider a solution valid to the problem domain. These rules do not consider the optimality of the solution, only if it meets the minimum requirements. As result, the image of f_{res} is binary: 1 if fulfilled, 0 if not. Due to the fact that every and each of the restrictions rules must be satisfied in order to consider the solution valid, f_{res} is expressed as the product of each one of the functions f^i_{res} which corresponds to each evaluation rule.

$$f_{res}(O^i) = f^1_{res}(O^i) \cdot f^2_{res}(O^i) \cdot f^3_{res}(O^i) \cdot \ldots \cdot f^n_{res}(O^i) \tag{6.6}$$

$$f^i_{res} : O^i \to 0, 1 \tag{6.7}$$

- *Optimization metrics.* The evaluation rules f_{opt} are those evaluating conditions that indicate a degree of quality associated to the problem domain, so provided the set of valid solutions, they can be used to tell apart the good solutions from the bad ones. In order to score the optimality of a solution, the output of these functions is a real number, and the objective is to find the maximum (or minimum) value associated to the best solution across the simulated ones. If some optimization metrics have more impact than others in the problem domain, each metric f^i_{opt} can be weighted using a coefficient ω^i which helps to determine the influence on the metric i within the whole set of optimization metrics.

$$f_{opt}(O^i) = f^1_{opt}(O^i) \cdot \omega^1 + f^2_{opt}(O^i) \cdot \omega^2 + f^3_{opt}(O^i) \cdot \omega^3 + ... + f^n_{opt}(O^i) \cdot \omega^n \tag{6.8}$$

$$f^i_{opt} : O^i \to \mathbb{R} \tag{6.9}$$

$$\omega^i \in \mathbb{R} \tag{6.10}$$

- *Search engine.* The search engine defines the global strategy for exploring the problem space. While the generation engine is accountable for providing new scenarios, and the evaluation engine gives a score to that scenarios after the simulations, the search engine establishes how many simulations will be generated, what will be the seed for the generation, how many simulations will be performed simultaneously, how the evaluation results will influence the search, etc. A BFS, an A*, or evolutionary algorithms are examples of search engines that make use of the generation and evaluation engines to proceed with the exploration of the problem space.
- *Population.* This concept is strongly related to the search engine, but it is defined apart due to its relevance in terms of performance and efficiency. The population establishes how many simulations can be performed in the same lot, i.e. the maximum number of scenarios whose absence of dependences between them allows to conduct their simulations simultaneously. This means that the score of a particular scenario does not influence the possibility of conducting the simulation of any other of the same lot. The meaning is the same as the population concept of genetic algorithms, where a set of individuals are created, simulated, and evaluated all together, but applied also to other search algorithms where it is possible to conduct several steps simultaneously.

In order to establish a multivariate analysis problem, the generation engine G and the evaluation engine E should be defined, including all restriction rules, optimization metrics, and weights that constitute E. Besides, the global search engine should be determined by deciding what is the best strategy to explore the problem space. The population can be determined together with the search engine, but it may also be influenced by how much resources are available in the infrastructure.

6.2.2 Cloudification Process with Multivariate Enhancement

In order to enhance our methodology implementing the many-task programming paradigm, we added some elements to the methodology structure proposed in Figure 5.1. This enhancement is represented in Figure 6.3. The idea behind the figure is to wrap the adaptation and simulation

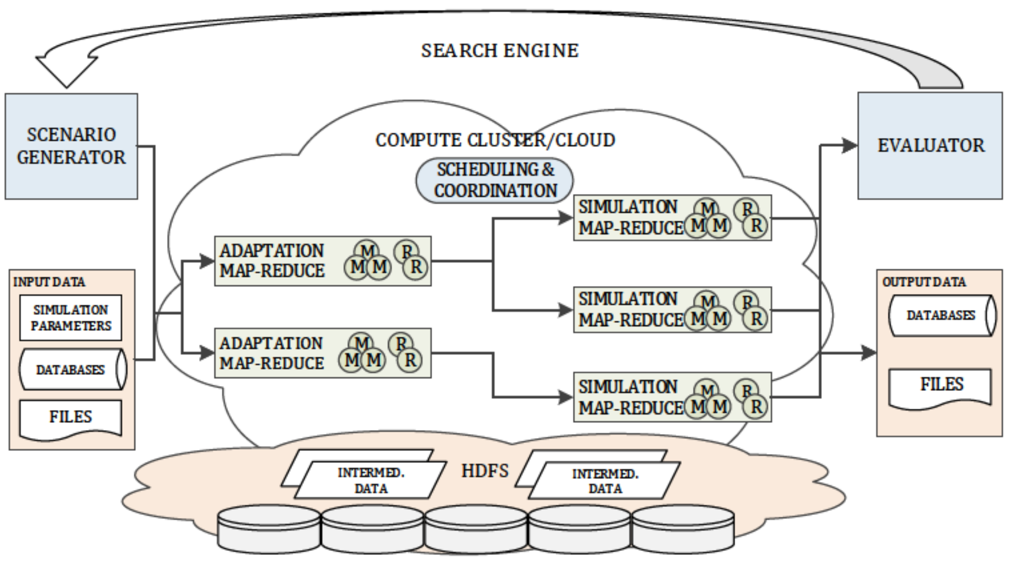


FIGURE 6.3: Methodology enhancement including many-task deployment and optimum search for multivariate analysis.

phases described in Section 5.1.3 with an scenario generator, an evaluator and a search engine that performs an iterative loop.

There are two major goals to be accomplished. The first is to increase the number of scenarios simulated concurrently to support multivariate analysis, instead of simulating just one case like in the aforementioned evaluation. By dispatching several concurrent simulations we follow a many-task paradigm and take further advantage of the Hadoop cluster resources.

The second goal is to provide further functionality for the end user by permitting the exploration of the solution space generated by introducing variations of the initial scenario, and simulating each of them. Through the proposed approach we can iteratively evolve the initial scenario in order to find better solutions according to an user-defined evaluation function and a search engine.

The elements included in the deployment's architecture are the following:

- *Adaptation and simulation stages.* These phases correspond to the ones belonging to the methodology described in Section 5.1.3, with a few considerations. First, we could make use of different adaptation procedures, each tailored for a subset of the generated experiments datasets. However, the simulation kernel would remain the same for every experiment, allowing to execute the same simulator while varying several parameters at the same time. Second, note that every task is independent among experiments. This means we can execute the adaptation stage of one experiment at the same time we run the simulation stage of a different one. Therefore, we can interleave many heterogeneous tasks as in MTC paradigms.

  This approach allows us to perform a better usage of the cluster resources, since a double-grained workload is distributed across the nodes. First, we run multiple simulation kernels (maps) which correspond to the same simulation scenario (i.e. the same map-reduce task).

Second, we run multiple map-reduce jobs, since we are simulating several scenarios concurrently. Note that, since multiple map-reduce jobs can be on execution at the same time, the task scheduling has a potential impact on performance across the global workload.

- *Scenario generator and evaluator.* We propose that an efficient simulator should evaluate and simulate a set of solutions with a minimal user involvement. New generation simulators should be capable of proposing and evaluating new designs based on a range of possible parameters. Besides, generating new scenarios to be evaluated allows us to deploy the many-task paradigm in an easy way, with minimal user involvement. The proposed methodology aims these objectives through two new components: a scenario generator and an evaluator. We define scenarios as independent simulations, each one of them with a different input data set (though parts, or even almost of the data can be similar), that have to be evaluated separately. Varying the input data leads to a different scenario (e.g. a different infrastructure to be evaluated, or different environmental conditions the current infrastructure have to be checked with).

  The scenario generator and the evaluator wrap the simulation model (i.e. the adaptation and simulation phases) generating different solutions to be evaluated. The scenario generator creates new scenarios through variations in the input data, thus allowing experimentation with different simulation parameters, components or domain restrictions. Those scenarios are provided to the map-reduce cluster, which performs the simulation as described in the Section 5.1.3. The evaluator analyses the output from that simulations and scores the generated solutions, stating whether they are acceptable or providing a measure of their quality.

- *Search engine.* In order to conduct the search across the problem space, it is necessary a component which implements a strategy defining the number and timing the scenarios are created and evaluated. This strategy can take the form of BFS, DFS, genetic algorithms, etc. and decides how many scenarios compound the population, how to guide the successive evolutions, how is the global progress of the search, when to stop searching, etc.

- *Scheduling and coordination* Due to the fact that multiple simulations are going to be executed in the cluster, it is necessary an management component which could act as resource manager. Some platforms do have a resource manager which can schedule the tasks efficiently (e.g. YARN on Hadoop MR), but others may lack of an adequate manager, so it should be implemented externally. This is accountable for deciding how many simulations will compound the batch of tasks be dispatched to the map-reduce cluster. The number of tasks executed concurrently in the cluster (population) is a crucial parameter in terms of performance and efficiency. An excessive number of tasks may lead to the saturation of the cluster resources, whereas an insufficient number of tasks may lead to resource underutilization.

Generating and evaluating multiple scenarios automatically allows a simulator to try different solutions, thus providing a faster way of exploring the solution space. Rather than obtaining a single solution, this method obtains a set of feasible solutions from which the user can select the best one. Moreover, advanced search algorithms may be implemented. For instance, the generator. the evaluator, and the search engine could implement a guided search using heuristics in order to find an optimal solution.

Algorithm 9 Multivariate engine: generation, simulation, and evaluation of multiple solutions

```
Input: $I^0, n, scheduler$
Output: $Bests$
1: $i \leftarrow 0$                                          ▷ Initialize variables
2: $j \leftarrow 0$
3: $Bests \leftarrow \emptyset$
4: while $!stopCondition$ do                                 ▷ Until the users decides to stop searching
5:     $i \leftarrow j$
6:     for $(i < j + n)$ do                                  ▷ Generate child solutions from the initial scenario
7:         $I^i \leftarrow$ GENERATE$(I^0, i)$
8:         $i \leftarrow i + 1$
9:     end for
10:
11:    $i \leftarrow j$                                      ▷ Dispatch adaptation phases (Map-Reduce tasks)
12:    for $(i < j + n)$ do
13:        WAIT$(scheduler.Allows)$
14:        $\{I^i_{glob}, I^i_0, I^i_1, I^i_2, I^i_3, ...I^i_k\} \leftarrow$ DISPATCH$(AdaptationPhase,\ I^i)$
15:        $i \leftarrow i + 1$
16:    end for
17:
18:    WAIT$(scheduler.AllFinished)$
19:
20:    $i \leftarrow j$                                      ▷ Dispatch simulation phases (Map-Reduce tasks)
21:    for $(i < j + n)$ do
22:        WAIT$(scheduler.Allows)$
23:        $O^i \leftarrow$ DISPATCH$(SimulationPhase,\ \{I^i_{glob}, I^i_0, I^i_1, I^i_2, I^i_3, ...I^i_k\})$
24:        $i \leftarrow i + 1$
25:    end for
26:
27:    WAIT$(scheduler.AllFinished)$
28:
29:    $i \leftarrow j$
30:    for $(i < j + n)$ do                                  ▷ Evaluate and score results
31:        $\theta^i \leftarrow$ EVALUATE$(O^i)$
32:        $i \leftarrow i + 1$
33:    end for
34:
35:    $Bests \leftarrow Bests \cup I^k \mid \theta^k = \max_{j \le i \le j+n} \theta^i$     ▷ Get the best solutions from those evaluated
36:    $j \leftarrow i$
37: end while
```

Algorithm 9 illustrates the pseudocode of a very basic search engine using the proposed methodology. The algorithm starts from three input parameters: an initial test case I used as base for generating new scenarios, and a population number n, used to establish how many simulations will compound the batch of tasks, and an scheduler object, either implemented by the user or provided by the platform, which acts as cluster resource manager.

While the stop condition is not reached (either established by the user or implemented through a decision rule), the algorithm generates child solutions from the initial scenario using the generation engine. An ordinal is provided in order to evolve the generations as more scenarios are created. Then, adaptation phases are dispatched in order to adapt those scenarios, following the same algorithms proposed in Chapter 5. Nevertheless, this stage can be optimized, reducing replication in those scenarios which share part of the input data. Thus, the number of generation stages can be lower than the number of simulations.

After the adaptation, the simulation tasks are dispatched to the cluster, performing concurrently among the cluster. This leads to an optimal use of cluster resources, where multiple map-reduce tasks are scheduled and executed so their phases can be interleaved. As the simulation tasks are finishing, the results can be evaluated using the evaluation engine. The aim is to find the bests solutions of those evaluated. In this case, the best of each bunch executed concurrently is added to the set of best solutions.

The scheduler acts as semaphore deciding whether or not there are available resources on the cluster. It has a direct impact on the cluster performance, being a trade-off between workload overhead (if we have too many simulations running) and waste of resources (if we have too few), so it should be implemented carefully.

There are different alternatives to the workflow shown in Algorithm 9. The best solutions can act as base cases for the next iterations, following a pattern commonly displayed on evolutionary algorithms. Besides, optimal solutions can be separated from the set of valid ones, in order to implement elitism or any other technique.

6.3 Case study: RPCS

The cloudified application selected to perform the multidimensional analysis was the railway electric power consumption simulator presented in Chapter 3. We have implemented an enhancement to the RPCS basic structure, turning towards a MOO problem. In this MOO problem, not one, but many simulations will be executed. Each one of these simulations constitutes a variation of the input data –either the infrastructure or the trains–, and the results are evaluated according to a set of optimisation metrics in order to find the optimum initial configuration, with regard to a specific optimisation criteria. The way we vary the input data defines the problem's search space, which constitutes the set of solutions obtained from the simulations, and the optimisation metrics and functions define the goal we pursue in our search.

The problem search space to be studied will be the placement of the electrical substations along the tracks –i.e. the connection milemarker of the substation to the track–. By modifying the substations' locations, we vary the electric circuit, thus we obtain different measures of instantaneous and mean voltages, as well as consumed potency. Therefore, substation placement has a direct impact on the power supply quality and energy savings.

In this particular case, we focus on the trade-off between energy saving and quality of energy provisioning. The quality of the power supply refers to the concept of maintaining the system as near to the nominal voltage, $U_{nom} = 3000V$, as possible. As trains circulate along the tracks demanding power, voltage oscillations may arise all across the electric circuit, leading to voltage drops or over-voltages. Note that trains do not always consume the same amount of power, and even more, they can return power to the circuit due to regenerative braking technologies.

TABLE 6.1: Variations of electrical substations placement on MOO optimization

Electrical substation	E1	E2	E3
Milemarkers(km) (initial, final, Δ)	(0, 20, 1)	(20, 40, 1)	(40, 50, 1)

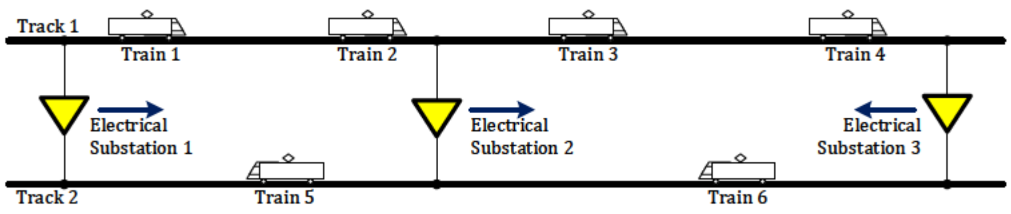


FIGURE 6.4: Schema of the main railway elements in the CENELEC test case. Parallel connections between catenaries or tracks are not shown.

These situations should be avoided, maintaining a constant flow of electric power to the trains. While voltage drops can be avoided by adding more electric substations on the tracks, this may lead to over-voltages due to excessive power. Besides, the more substations to be placed, the more expensive the deployment is, and the more aggregated energy is consumed by the electric substations. This leads to conflicting objectives, thus to a MOO problem: the goal of maintaining a constant power flow, in favour of providing more energy, against the target benefit of saving energy.

We aim to find the corresponding Pareto frontier of the MOO problem, thus giving the user the set of optimal solutions and letting him or her chose the preferred option. We propose a set of restriction rules that must be fulfilled by the design in order to be considered as acceptable, and set of optimisation metrics in order to score those accepted solutions. Both sets are obtained analysing the European regulations [AEN04], [CEN12], and [CEN15]. A formalisation of the resulting MOO problem is described next.

6.3.1 Problem Formalisation: Generation and Search Engines

We selected as benchmark the CENELEC standard railway scenario described in Section 3.3.4, whose data and key parameters are indicated in Table 3.2. As said before, this proposal of normative establishes the requirements for the validation of simulation tools used for the design of traction power supply systems. Therefore, it is meaningful to apply such normative in this case study. A general overview of the elements of the experiment are shown in Figure 6.4.

The search space was generated by conducting the simulation with a different positioning of several substations. Let E_k the position of the substation k, and let $I = \{..., E_1, E_2, E_3, ...\}$ the definition of the test case, which includes (among others) E_1, E_2, E_3 as the positions of the three substations. Let the initial and final points of the interval in which they can be placed –$E_{k_{ini}}$ and $E_{k_{fin}}$, respectively–, along with the distance between each planned position for the generation of the experiment set, Δ_k. Let also P_k be the amount of possible positions for the the substation k:

$$P_k = \frac{E_{k_{fin}} - E_{k_{ini}}}{\Delta_k} \tag{6.11}$$

The generation engine should vary the positions of the substations progressively, and according to their corresponding intervals as more derivative scenarios are created, so the function is defined as follows.

$$G \equiv f_{gen}(I,i,k) = \begin{cases} E_k = E_{k_{ini}} + i \mod P_k, & \text{if } k = 1 \\ E_k = E_{k_{ini}} + \frac{i}{\frac{E_{k-1_{fin}} - E_{k-1_{ini}}}{\Delta_{k-1}}} \mod P_k, & \text{if } k = 2 \\ E_k = E_{k_{ini}} + \frac{i}{\left(\frac{E_{k-1_{fin}} - E_{k-1_{ini}}}{\Delta_{k-1}} \cdot \frac{E_{k-2_{fin}} - E_{k-2_{ini}}}{\Delta_{k-2}}\right)} \mod P_k, & \text{if } k = 3 \end{cases} \tag{6.12}$$

where i, is the number of the i-th generated scenario, and k is the number of the k-th substation which is going to be placed.

As each substation can be assigned to any of the points within the former interval, and all of the substations have to be combined with the others to generate the experiment set, we would get as many different experiments as indicated by Equation 6.13, where M is the number of substations to be manipulated. The equation indicates that, the finer the grain of the planned experiments, the more simulations have to be executed in order to generate the solution space.

$$n = \prod_{k=1}^{M} P_k \tag{6.13}$$

For this evaluation, we generated a set of 4 000 solutions using the variations of the positions indicated in Table 6.1, displacing each substation from one kilometre to the next, without overlapping their ranges. From this set, we sampled for this evaluation only 1 000 random experiments as population, aiming to increase this number for future works. Note that, since each experiment is composed of 4 800 simulation steps –one per simulated instant, corresponding to $1h$ and $20m$ of simulated time–, it would be required to solve 4 800 equation systems per experiment. The search engine implements a basic BFS algorithm, in which we first evaluate all variations of the first substation, then we combine all these variations with variations of the second substation, and so on. Algorithm 10 illustrates the basic code for the generation of cases.

Algorithm 10 BFS multivariate engine implemented on the top the RPCS

```
1: $i \leftarrow 0$
2: for $(i < 4000)$ do
3:     $I^i \leftarrow \text{GENERATE}(I^0, i, 1)$
4:     $I^i \leftarrow \text{GENERATE}(I^i, i, 2)$
5:     $I^i \leftarrow \text{GENERATE}(I^i, i, 3)$
6:     $i \leftarrow i + 4$
7: end for
```

6.3.2 Problem Formalisation: Evaluation Engine

As previously described, there are two objectives that guide the optimisation process:

- Improving the quality of the power supply.
- Reducing the amount of power consumed by the groups.

We define from these goals the following criteria:

- Maximise the mean useful voltage per train, f^1_{opt}.
- Minimise total amount of energy consumed by the groups, f^2_{opt}.

The mean useful voltage, described in European normative *UNE-EN-50388* [CEN12], is defined as the mean of all voltages at the pantograph of each train in the geographic zone, along all simulation steps. This measure indicates the quality of the power supply. The lower the mean useful voltage is, the less energy is transferred from the supply stations to the trains, on average.

For the formalisation of this problem, let T be the set of trains in the whole system, and G be the set of groups in the network. The first objective is defined in Equation 6.14, where U^t_{mu} is the mean useful voltage per train, and U_{max_1} constitutes the maximum permanent voltage.

$$\mathbf{max} \quad f^1_{opt} = \frac{U^t_{mu} - 2800}{U_{max_1} - 2800} \quad \forall t \in T \tag{6.14}$$

The second objective is formulated in Equation 6.15, where E^i_g is the energy consumed per group, in kW/h.

$$\mathbf{min} \quad f^2_{opt} = \sum_{i=1}^{G} E^i_g \quad i \neq g, \forall g \in G \tag{6.15}$$

As said before, the aim to find the corresponding Pareto frontier of the MOO problem, so no combination of both metrics will be performed, and no weights ω^1 and ω^2 will be used to modify such metrics. The problem is subject to the following constraints:

- According to the normative [CEN12], the mean useful voltage per train, U^t_{mu}, must never be lower than $2800V$, and it shall not surpass the maximum permanent voltage, U_{max_1}.

$$f^1_{res} \equiv 2800 \leq U^t_{mu} \leq U_{max_1} \tag{6.16}$$

- No sharp voltage drops or over-voltages shall exist on normal (non failure) operating conditions [AEN04]. Therefore, instantaneous voltages should be in the range of non-permanent conditions on every instant of the simulation. This derives Equation 6.17a and Equation 6.17b.

$$f^2_{res} \equiv U_{min_1} \leq U_t \leq U_{max_2} \quad \forall t \in T \tag{6.17a}$$

$$f^3_{res} \equiv U_{min_1} \leq U_g \leq U_{max_2} \quad \forall g \in G \tag{6.17b}$$

- The mean voltages on trains and the simulated zone, shall be within the limits of permanent operating conditions, even if voltages fall beyond that limits for a moment during the simulation [AEN04, CEN12]. This yields Equation 6.18a and Equation 6.18b.

$$f^4_{res} \equiv U_{min_1} \leq U^t_{mu} \leq U_{max_1} \quad \forall t \in T \tag{6.18a}$$

$$f^5_{res} \equiv U_{min_1} \leq U_{muz} \leq U_{max_1} \tag{6.18b}$$

6.3.3 Multivariate Analysis Evaluation: Results and Performance

A first evaluation was conducted aiming to solve the whole MOO problem, thus executing the population of 1 000 random experiments. The selected platform to deploy the evaluation of the multidimensional analysis was MRv2 on Amazon EC2. MRv2 outperformed MRv1 in the evaluation performed in Chapter 5, getting better results than its counterpart in all evaluations. Amazon EC2 was selected in order to take advantage of the cloud's possibility to allocate resources (slave nodes in this case) on demand. The selected cloud infrastructure consisted of a general purpose *m2.4xlarge* node as dedicated master and one hundred *m2.xlarge* machines as slaves. Table 6.2 shows the main aspects of the selected instances.

The results we obtained were parsed and evaluated according to the metrics defined in Section 6.3.2. The Pareto-optimal frontier for the former data is shown in Figure 6.5, along with the other solutions that resulted from the subsequent simulations. The solutions that belong to the Pareto-optimal frontier highlighted in Figure 6.5 are the ones that meet the optimisation criteria developed in Section 6.3.2, yet the preferred solution still has to be chosen by the end user. The final selection could balance the supply quality (O_1) and the wasted energy (O_2), or be directed towards emphasising one of the optimisation objectives. Table 6.3 gives the substation configuration for the limit solutions in the Pareto-optimal frontier, the positions are indicated with respect to the beginning of the rail track.

Table 6.2: EC2 instances description.

Type	Role	Virtual CPUs	Memory (GB)	Local storage (GB)
m2.4xlarge	master	8	68.4	2 x 840
m2.xlarge	slave	2	17.1	420

After solving the whole MOO problem, we performed a second battery of evaluations in order to illustrate the many-task deployment capabilities of our methodology. In the evaluation performed in Chapter 5, we only executed one of the test cases at a time. This was conducted to study the behaviour of the workload distribution in a cloud and cluster. In this evaluation, many experiments will be spawned in the same Hadoop cluster following the MTC paradigm, in order to check the resource usage when multiple tasks make use of the same infrastructure. While the

TABLE 6.3: Optimal configurations for each optimisation criteria for the CENELEC experiment set.

	E1 milespoint (km)	E2 milespoint (km)	E3 milespoint (km)
Best configuration for O_1	16	25	40
Best configuration for O_2	4	23	46

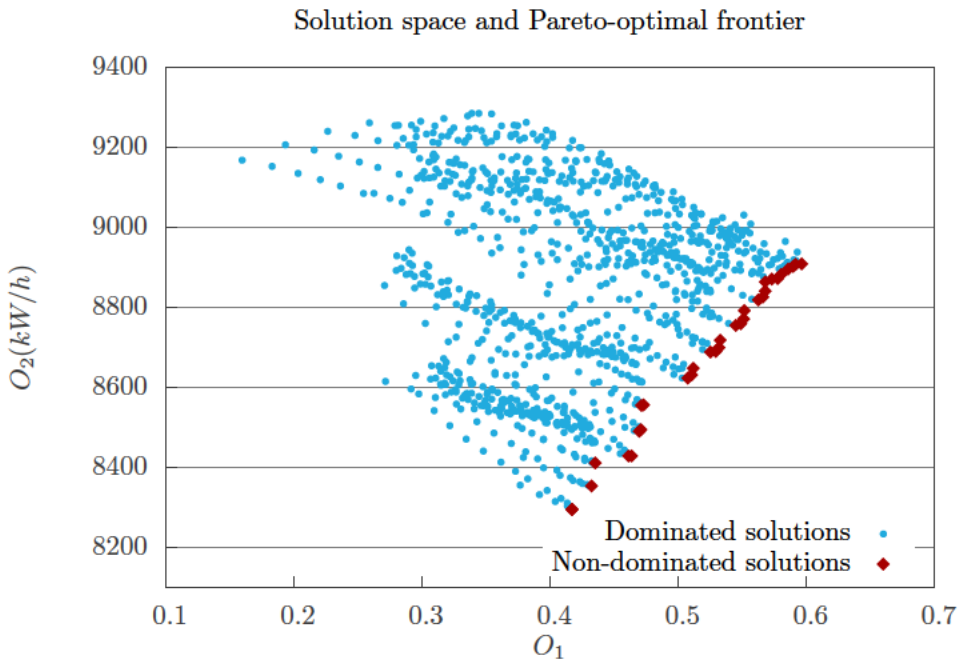


FIGURE 6.5: Resulting solution space and Pareto-optimal frontier for the CENELEC experiment set.

the evaluation performed in Chapter 5 focused on the speed-up and computing time required to perform a single test case, this evaluation is centred in the number of test cases simulated simultaneously and the obtained scalability and throughput.

Using the same type of instances as those used for solving the MOO problem (see Table 6.2), the virtual cluster consisted of a general purpose *m4.xlarge* node as dedicated master and memory optimized *m2.xlarge* machines as slaves. The battery of tests has been conducted using four virtual clusters of 1, 4, 16, and 64 slaves respectively. In each virtual cluster we simulate 1, 4, 16, and 64 experiments.

As shown by Figure 6.6, our evaluations indicate that the enhanced system scales linearly with the number of experiments for every cluster size tested. This suggests that the proposed methodology is suitable for multidimensional analysis via MTC, as we can run several interleaved heterogeneous tasks making an efficient use of the infrastructure's resources. Furthermore, we can see that linearity is not loss in any case, so the end user can run the many-task job successfully with either a few nodes or a larger infrastructure. This permits to tailor the underlying infrastructure to reduce of economical costs or provide higher performance.

In Figure 6.7 we show the resulting speed-up of the enhanced deployment, taking as base a single-node execution with increasing number of nodes and experiments. In Figure 6.8 we include the

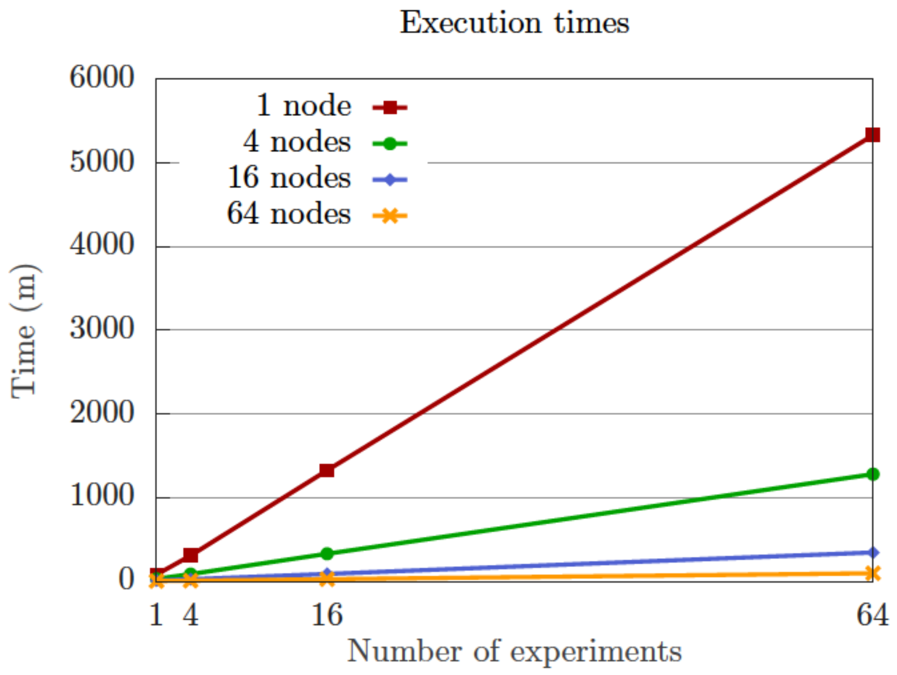


FIGURE 6.6: Execution times for the enhanced methodology with increasing number of nodes and experiments.

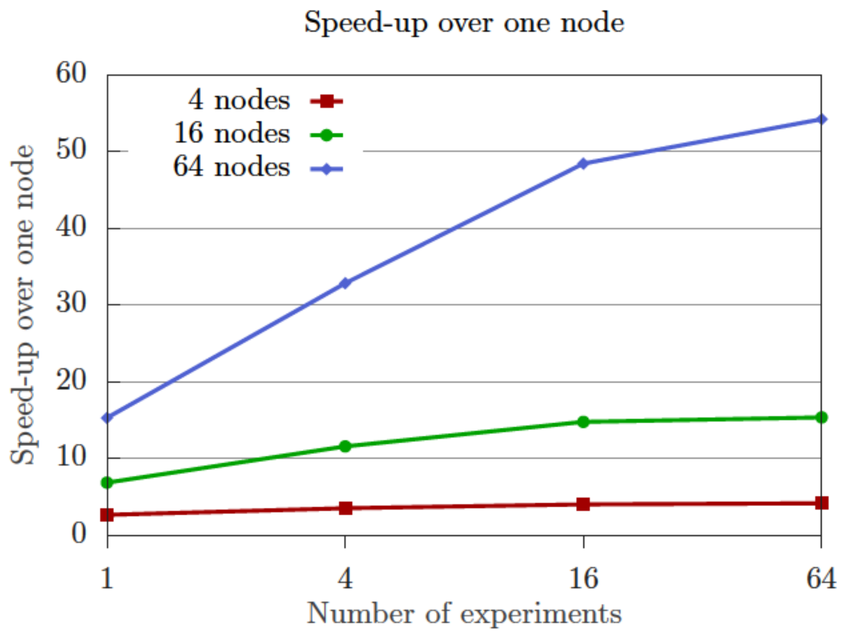


FIGURE 6.7: Speed-up for the enhanced methodology, over one node.

efficiency over one node, e, which corresponds to the normalised speed-up with relation to the number of slaves. Equation 6.19 shows the formulation of this concept, similar to the one found in [GWC$^+$11], where t is the total execution time on n nodes, and t_0 is the total execution time in one node. This is an interesting measure of the system's performance and resource utilisation as the number of experiments and nodes varies.

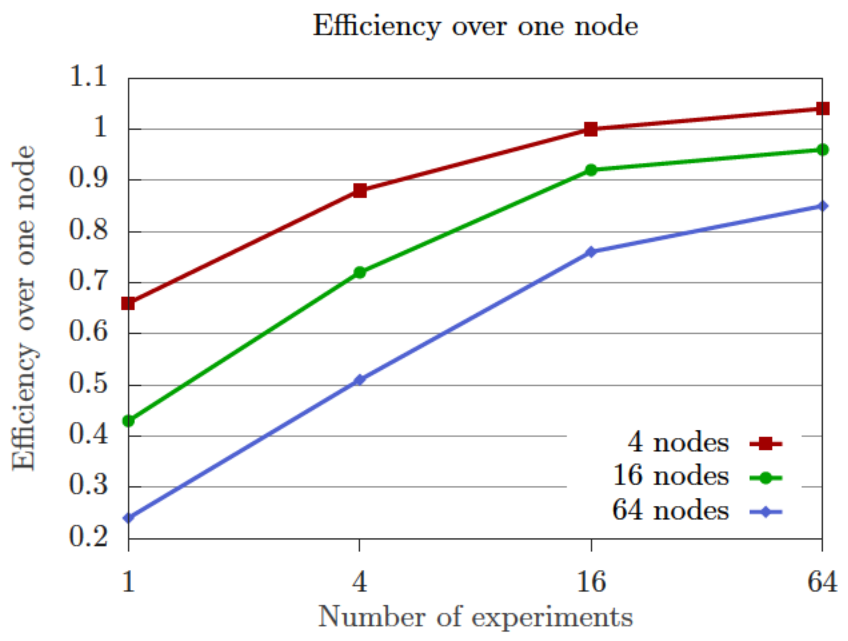


FIGURE 6.8: Efficiency of the enhanced methodology with increasing number of experiments.

$$e = \frac{t_0}{nt} \tag{6.19}$$

The worst result corresponds to 64 nodes and one experiment because of the significant impact of the Hadoop platform's overhead in the overall execution time. Noticeably, with four nodes and 64 experiments we obtain superlinear speed-up due to the efficient utilisation of the cluster resources. As seen in Figure 6.8, when more nodes are added, the system becomes underused and the platform's overhead becomes noticeable, thus losing efficiency. The same situation occurs if we run less experiments in the same environment. Therefore, the overall system's efficiency is tightly related to the ratio between the number of nodes and experiments. It is also remarkable that the system increases its efficiency as more experiments are executed, and that it is not needed to rely on a large cluster to execute them if efficiency is more relevant than total execution time.

6.4 Summary

In this chapter we have proposed a enhanced simulation structure in order to bring to current simulators multidimensional analysis, which allows increasing the output by covering more capabilities than the main procedure. This structure allows not only to evaluate solutions provided by the user, but also it find acceptable solutions by itself, with a high degree of fitness, and in a reasonable amount of time. In order to do so, different stakeholders of the design process have to be taken into account, as well as expert's domain knowledge and optimization metrics.

We describe a proposal to map the structure provided to a Cloud-based design. This design is based on ontologies and decision rules. The user defines an ontology to represent the simulated domain, and decision rules to implement domain specific knowledge (restrictions, optimization metrics). This allows to keep the design aware of specific domain data. The user can define the simulation model as well as the rules in which are based both evaluation and optimization functions. The Cloud infrastructure bring us the possibility of scale up or down the computing resources according to the particular needs of the simulation.

Since the methodology we described in Chapter 5 aims to provide task independence between concurrent simulation partitions, we can perform a multidimensional analysis by spawning several simulations in a many-task manner. Given this context, it seems natural to enhance out data-centric methodology with a many-task deployment to support multidimensional analysis, while enforcing efficient resource utilisation and balance. Our evaluations indicate that the enhanced system scales linearly with the number of experiments for every cluster size tested. This suggests that the proposed methodology is suitable for multidimensional analysis via MTC, as we can run several interleaved heterogeneous tasks making an efficient use of the infrastructure's resources. Furthermore, we can see that linearity is not loss in any case, so the end user can run the many-task job successfully with either a few nodes or a larger infrastructure. This permits to tailor the underlying infrastructure to reduce of economical costs or provide higher performance.

Chapter 7

Conclusions

In this thesis, we have analysed the suitability of performing simulations in clouds by performing a paradigm shift, from classic parallel approaches to data-centric models, more adequate to be executed on Cloud Computing infrastructures. We aimed to maintain the scalability achieved in traditional HPC infrastructures while we take advantage of Cloud features. We have fulfilled the objectives presented in Section 1.3:

O1 *To explore the simulator's characteristics that make them suitable or unsuitable to be deployed on HPC or Cloud infrastructures.* In Chapter 3, we characterize the different problem types that can be faced when working with simulators. This characterization is based on the ease of splitting the problem in order to perform the computation in parallel. The way we decompose the problem has a direct impact on data and communication patterns, and should be studied carefully according to the target infrastructure and platform. We also stated that several problem types can coexist in the same simulator, insofar as several parallelizations can be applied to different layers of that simulator.

O2 *To propose a methodology to adapt scientific simulations following a cloud-suitable data-centric scheme, while maintaining classic approaches to domain decomposition for those problems which cannot be split gracefully.* In Chapter 5, we propose a general methodology to transform simulations into a highly scalable MapReduce application that re-uses the same simulation kernel while distributing the simulation load across as many nodes are desired in a virtual cluster running on the cloud. The results show how the cloudfied simulator outperforms the original multi-threaded application in Cloud infrastructures of computing power similar to a single-node environment. Besides, we break the barrier between shared-memory environments and distributed memory environments, thus allowing us to increase the number of nodes as we demand more computing power. Nevertheless, the speed-up of the cloudified application is not as good as it would be desirable as this number of nodes is increased but the problem size remains constant. In that case, the problem size becomes small for the cluster size and less data is assigned to each slave. This results in degraded performance due to platform overhead.

O3 *To transform a memory-bound simulator into the proposed scheme, integrating the original application with both the MapReduce framework and MPI libraries.* In Chapter 3, the RPCS is introduced, as an example of memory-bound simulator. With the aim of serving as case study, this simulator is analysed from the point of view described before, pointing the different layers where opportunities for applying parallelization lie. In Chapter 4, the RPCS is parallelized following classic HPC approaches based on MPI, thus proposing and solving a tightly coupled problem. In Chapter 5, we apply the proposed methodology to the RPCS, and explore the performance of changing to a data-centric approach based on MapReduce.

O4 *To demonstrate the feasibility of the resulting architecture comparing the behaviour and efficiency of adapted vs. original applications in both HPC and Cloud environments.* Measurements and evaluations are conducted both in Chapter 4 and Chapter 5. In Chapter 4 we measure the performance of HPC approaches based on MPI, on both cluster and Cloud environments. In Chapter 5, we measure the performance of the cloudified application based on MapReduce, on both cluster and Cloud environments. The results show in that Chapter 4 how the domain decomposition is the best approach in order to avoid communications, and the shortages of these MPI-based approaches in terms of fault tolerance and stability. In Chapter 5, the promising results we got in the particular use case studied, in terms of performance and scalability support, our initial model's viability.

O5 *To enhance the proposed methodology in order to include multivariate analysis simulations, as a particular case that can benefit from a cloud-suitable data-centric scheme.* In Chapter 6, we have proposed a enhanced simulation structure in order to bring to current simulators multidimensional analysis, which allows increasing the output by covering more capabilities than the main procedure. Since the methodology we described in Chapter 5 aims to provide task independence between concurrent simulation partitions, we can perform a multidimensional analysis by spawning several simulations in a many-task manner. Our evaluations indicate that the enhanced system scales linearly with the number of experiments for every cluster size tested. This suggests that the proposed methodology is suitable for multidimensional analysis via MTC, as we can run several interleaved heterogeneous tasks making an efficient use of the infrastructure's resources.

Nowadays, HPC and Cloud Computing are two communities separated one from the other, and they diverge in their research lines and objectives proposed. HPC community focus on breaking the exascale barrier by developing more and more powerful infrastructures, and taking the maximum performance of such systems in all dimensions (processing, networking, energy efficiency, etc.). On the contrary, Cloud Computing model is more focused on enterprises and business world, bringing the users (no matter what type of user) the possibility of sizing computing computing power according to instantaneous needs, at the expense of some performance loss. This thesis explores the opportunities of establishing some common areas between both communities, studying when and how HPC applications (such as simulators) can be deployed on Clouds, and what are the advantages that Cloud Computing can bring to HPC community.

7.1 Contributions

This thesis makes the following contributions:

C1 *Classification of simulation problems according to its suitability to HPC and cloud infrastructures and the different ways of parallelizing such problems.* First, we define what are the key advantages on cluster on Cloud infrastructures, analyzing the performance in such systems in terms of processing power, network, file systems, storage, etc. Then, we define three types of problems according to the structure and dependences between its data: pleasingly parallel, loosely coupled, and tightly coupled problems. We state that a simulation may expose several of these problems, depending on the level you apply parallelization. Finally, we analyze what is the most suited type of infrastructure for each kind of problem.

C2 *Proposition of different mechanisms to split simulation domains in smaller sub-domains, with different degrees of data coupling, thus indicating the suitability of the simulator to different infrastructures, identifying architectural bottlenecks, and those aspects which limit the scalability of the application.* We explore domain decomposition and matrix decomposition as mechanisms to parallelize simulations in cluster environments using MPI. We propose domain decomposition as mechanism to parallelize simulations in Cloud environments, using MapReduce and the proposed Methodology. Finally, we propose using MapReduce and the proposed Methodology in order to perform multivariate analysis on Cloud environments.

C3 *Definition of a software framework suitable for both cloud and HPC systems, that makes use of data-centric schemes such as MapReduce.* We propose a software framework based on MapReduce as a part of the methodology proposed. The framework consists of two MapReduce tasks. The adaptation task rearranges the input data set into multiple independent subsets of global and domain data. The simulation task runs the simulation kernel for each multiple independent subset that was mapped to them in the previous stage, plus the required simulation parameters that are shared by every partition, so as reducers are able to gather all the output and provide final results as the original application. Finally, we enhance this software framework in order to conduct multidimensional analysis simulations, dispatching several concurrent simulations following a many-task paradigm, and taking further advantage of the Hadoop cluster resources.

C4 *Implementation of the mechanisms and frameworks proposed in a simulator, and performance study when different computing resources (e.g. HPC and cloud) are used.* We implement MPI version of the studied simulator, performing both domain and matrix decomposition. We also migrate the simulator to Cloud using the methodology described, obtaining promising results. Finally, we also implement multivariate analysis within the simulator using the methodology described, obtaining linear scalability with the number of experiments for every cluster size tested.

7.2 Future Work

The work described in this thesis could be further extended and improved in many different aspects. This section presents the future work derived from this thesis.

The first task to accomplish is to update the methodology, adapting it to novel frameworks like Spark. Apache Hadoop is nowadays considered an obsolete platform, with performance issues that have been solved in the last generation of data-centric frameworks. In particular, we are considering other implementations to migrate to, such as Spark, that provide further functionality and support for complex algorithms. Spark can help to improve the chained workflows like the adaptation and simulation phases which constitute the basis of the methodology. Therefore, we expect an improved performance if we adapt the algorithms and repeat the evaluations using Spark.

Another research line is to explore approaches to execute tightly coupled problems in Clouds by means of hierarchical decomposition. The thesis results have shown how sensible is the matrix decomposition approach to the network latencies, even more if the size of the operated matrices is not big enough to make the distributed parallel execution worthwhile. Therefore, domain and matrix decomposition could be implemented simultaneously at different levels, for instance, using domain decomposition to distribute workload across all nodes of the Cloud, and using matrix decomposition to distribute workload across the CPU cores within the node, or using small subsets of the Cloud nodes for matrix decomposition if the cores within the node are not enough.

Future works are strongly focused on extending the current methodology to a generalized framework which would allow to cloudify any scientific application, and conduct its execution in both both HPC and Cloud infrastructures. This framework should make use of local cluster resources if available, and allocate resources on cloud if the local resources are not enough. In order to do so, domain and matrix decompositions should be mixed in order to avoid the impact of the latencies between local and remote resources.

Finally, we aim to develop an interface for applications to make use of this framework. This interface will represent the different types of problems and problem decompositions described in this thesis, so as to develop applications in terms of domain, sub-domains, decompositions, simulation kernels, etc. In this way, functional programming models like MapReduce could be used, and more complicated communication patters like those present in the simulation kernels could be hidden to the programmer.

7.3 Thesis Results

The main contributions of this thesis have been published in international conferences and journals. We enumerate the publications classified into journals, conferences, and workshops. Additionally, we indicate the research stays, grants, and projects related to the results of this thesis.

- **Journals**

1. C. Gomez, R. Saa, A. Garcia, F. Garcia-Carballeira, and J. Carretero, "A model to obtain optimal designs of railway overhead knuckle junctions using simulation", *Simulation Modelling Practice and Theory*, vol. 26, pp. 16–31, August 2012. Impact Factor: 0.969. Q2
2. R. Saa, A. Garcia, C. Gomez, J. Carretero, and F. Garcia-Carballeira, "An ontology-driven decision support system for high-performance and cost-optimized design of complex railway portal frames", *Expert Systems with Applications*, vol. 39(10), pp. 8784–8792, August 2012. Impact Factor: 2.203. Q1
3. A. Garcia, C. Gomez, R. Saa, F. Garcia-Carballeira, and J. Carretero, "Optimizing the process of designing and calculating railway catenary support infrastructure using a high-productivity computational tool", *Transportation Research Part C: Emerging Technologies*, vol. 28, pp. 1–14, March 2013. Impact factor: 1.957. Q1
4. S. Caino-Lores, A. Garcia, F. Garcia-Carballeira, and J. Carretero, "A cloudification methodology for multidimensional analysis: Implementation and application to a railway power simulator", *Simulation Modelling Practice and Theory*, vol. 55, pp. 46–62, June 2015. Impact factor: 1050. Q2

- **Conferences**

1. R. Saa, A. Garcia, C. Gomez, F. Garcia-Carballeira, and J. Carretero, "A high-productivity computational tool to model and calculate railway catenary support structures", in *The 2012 International Conference of Computer Science and Engineering*, London, United Kingdom, July 2012. Best Student Paper Award.
2. A. Garcia, C. Gomez, F. Garcia-Carballeira, and J. Carretero, "Enhancing the structure of railway infrastructure simulators", in *International Conference on Engineering and Applied Sciences Optimization (OPT-i)*, Kos, Greece, June 2014.
3. J. Carretero, C. Gomez, A. Garcia, and F. Garcia-Carballeira, "A holistic approach to railway engineering design using a simulation framework", in *The 4th International Conference on Simulation and Modeling Methodologies, Technologies and Applications (SIMULTECH 2014)*, Vienna, Austria, August 2014.
4. A. Garcia, S. Caino-Lores, F. Garcia-Carballeira, and J. Carretero, "A multi-objective simulator for optimal power dimensioning on electric railways using cloud computing", in *The 5th International Conference on Simulation and Modeling Methodologies, Technologies and Applications (SIMULTECH 2015)*, Kolmar, France, July 2015.

- **Workshops**

1. S. Caino-Lores, A. Garcia, F. Garcia-Carballeira, and J. Carretero, "A cloudification methodology for numerical simulations", in *Euro-Par 2014: Parallel Processing Workshop*, Porto, Portugal, August 2014.
2. S. Caino-Lores, A. Garcia, F. Garcia-Carballeira, and J. Carretero, "Breaking data dependences in numerical simulations using Map-Reduce", in *XXV Jornadas de Paralelismo*, Valladolid, Spain, September 2014.

- **Research stays**

  West University of Timisoara, under the supervision of Prof. Dana Petcu, from November 2014 to February 2015.

- **Grants**

  - Convocatoria PIF UC3M 01-11112 de Personal Investigador en Formación, PhD fully granted (4 years), 2011, Universidad Carlos III de Madrid
  - Programa propio de investigación. Ayudas a la movilidad de investigadores en formación predoctoral, 1050 €, 2014, Universidad Carlos III de Madrid.

- **Bachelor thesis**

  - S. Caino-Lores. Adaptation, deployment and evaluation of a railway simulator in cloud environments. *Supervisor: Alberto Garcia.* B.Sc in Computer Science. University Carlos III of Madrid. June, 2014. itSMF award to the best bachelor thesis.

- **Projects**

  - Administrador de Infraestructuras Ferroviarias (ADIF), Estudio y realización de programas de cálculo de pórticos rígidos de catenaria (CALPOR) y de sistema de simulación de montaje de agujas aéreas de línea aérea de contacto (SIA), JM/RS 3.6/4100-.0685-9/00100
  - Administrador de Infraestructuras Ferroviarias (ADIF), Proyecto para la Investigación sobre la aplicación de las TIC a la innovación de las diferentes infraestructuras correspondientes a las instalaciones de electrificación y suministro de energa (SIRTE), JM/RS 3.9/1500.0009/0-00000
  - Spanish Ministry of Education, TIN2010-16497, Scalable Input/Output techniques for high-performance distributed and parallel computing environments
  - Spanish Ministry of Economics and Competitiveness, TIN2013-41350-P, Técnicas de gestión escalable de datos para high-end computing systems
  - European Union, COST Action IC1305, ”Network for Sustainable Ultrascale Computing Platforms” (NESUS)
  - European Union, COST Action IC0805, ”Open European Network for High Performance Computing on Complex Environments”
  - Spanish Ministry of Economics and Competitiveness, TIN2011-15734-E, Red de Computación de Altas Prestaciones sobre Arquitecturas Paralelas Heterogéneas (CAPAP-H)

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