CONTROLLING THE PARALLEL EXECUTION OF WORKFLOWS RELYING ON A DISTRIBUTED DATABASE

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Dissertação de Mestrado apresentada ao Programa de Pós-graduação em Engenharia de Sistemas e Computação, COPPE, da Universidade Federal do Rio de Janeiro, como parte dos requisitos necessários à obtenção do título de Mestre em Engenharia de Sistemas e Computação.

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Rio de Janeiro

Julho de 2015

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DISSERTAÇÃO SUBMETIDA AO CORPO DOCENTE DO INSTITUTO ALBERTO LUIZ COIMBRA DE PÓS-GRADUAÇÃO E PESQUISA DE ENGENHARIA (COPPE) DA UNIVERSIDADE FEDERAL DO RIO DE JANEIRO COMO PARTE DOS REQUISITOS NECESSÁRIOS PARA A OBTENÇÃO DO GRAU DE MESTRE EM CIÊNCIAS EM ENGENHARIA DE SISTEMAS E COMPUTAÇÃO.

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RIO DE JANEIRO, RJ - BRASIL
JULHO DE 2015

Souza, Renan Francisco Santos

Controlling the Parallel Execution of Workflows Relying on a Distributed Database / Renan Francisco Santos Souza. – Rio de Janeiro: UFRJ/COPPE, 2015.

XI, 86 p.: il.; 29,7 cm.

Orientadora: Marta Lima de Queirós Mattoso

Dissertação (mestrado) – UFRJ/ COPPE/ Programa de Engenharia de Sistemas e Computação, 2015.

Referências Bibliográficas: p. 83-86.

1. Scientific Workflows. 2. Databases. 3. Distributed Data Management. I. Mattoso, Marta Lima de Queirós II. Universidade Federal do Rio de Janeiro, COPPE, Programa de Engenharia de Sistemas e Computação. III Título.

Agradecimentos

Primeiramente, agradeço a Deus, porque dele, por ele, e para ele são todas as coisas, inclusive minha vida e este trabalho.

Agradeço ao meu pai, ao Marcos, e, principalmente, à minha mãe. É notória sua vontade de me apoiar e de me ver crescendo. Agradeço pelos sacrifícios necessários para investir na minha educação. Tenho plena ciência de que sem sua ajuda, eu não teria conseguido chegar até aqui e, por isso, serei eternamente grato.

Agradeço à Gisele, minha namorada, por ter sido minha principal motivação por todos esses anos e por continuar dando um significado maior a todo meu esforço. Também agradeço a seus pais e irmão pelo apoio e compreensão durante as ausências.

Agradeço à minha professora orientadora Marta Mattoso, de quem eu tenho orgulho de ser aluno. Agradeço por ter me recebido tão bem em seu grupo de pesquisa, por ter me ensinado não só técnicas de bancos de dados, mas principalmente a ter uma visão crítica e analítica para trabalhos científicos, que vão muito além dos detalhes técnicos. Sua dedicação ao trabalho e seu esforço me inspiram.

Agradeço ao Vítor Sousa, colega, amigo e orientador. Incontáveis pedidos de ajuda atendidos, nas mais altas horas até de madrugada às vezes, foram essenciais para o desenvolvimento deste trabalho. Sua orientação bem próxima e, principalmente, seu incentivo foram determinantes para que eu prosseguisse adequadamente até o fim desta dissertação. Muito obrigado, como sempre!

Agradeço ao professor Alexandre Lima, de quem eu sou fã, pelas incansáveis trocas de e-mails, respondidos quase sempre imediatamente, e reuniões até sanar todas minhas dúvidas, que frequentemente eram muitas. Sua ajuda foi essencial para que eu compreendesse um problema difícil da minha dissertação, logo, para resolvê-lo também. Obrigado pela paciência e insistência para que meus trabalhos fiquem sempre melhores. Ah, também agradeço pelos cabelos brancos que ganhei depois de cursar suas disciplinas :).

Agradeço ao professor Daniel de Oliveira pela colaboração tão próxima e, principalmente, pela sua dedicação. Também agradeço à professora Kary Ocaña por sua bondade e palavras de incentivo. Agradeço à professora Maria Luiza Campos pelo carinho e orientação de sempre. Também agradeço aos professores Cláudio Amorim, Myriam Costa e Álvaro Coutinho pelas aulas de paralelismo. Agradeço à professora Lúcia Drummond por aceitar fazer parte da banca desta dissertação.

Agradeço a todos os amigos que me apoiam e incentivam, seja com discussões e ideias para meu trabalho, seja com singelas palavras de incentivo. Sua amizade é muito importante para mim.

Também agradeço à Mara Prata, Ana Paula Rabello, Solange Santos e Gutierrez da Costa, pela ajuda nas questões administrativas. Também agradeço à Sandra da Silva pelo carinho.

Agradeço à CAPES pela concessão da bolsa de mestrado.

Finalmente, agradeço à equipe do NACAD-COPPE/UFRJ e ao professor Patrick Valduriez (Grid5000) pela ajuda com os equipamentos usados nos experimentos e durante o desenvolvimento deste trabalho.

A todos, muito, muito obrigado!

Resumo da Dissertação apresentada à COPPE/UFRJ como parte dos requisitos necessários para a obtenção do grau de Mestre em Ciências (M.Sc.)

GERÊNCIA DA EXECUÇÃO PARALELA DE *WORKFLOWS* APOIADA POR UM BANCO DE DADOS DISTRIBUÍDO

Renan Francisco Santos Souza

Julho/2015

Orientadora: Marta Lima de Queirós Mattoso

Programa: Engenharia de Sistemas e Computação

Simulações computacionais de larga escala requerem processamento de alto desempenho, envolvem manipulação de muitos dados e são comumente modeladas como *workflows* científicos centrados em dados, gerenciados por um Sistema de Gerência de *Workflows* Científicos (SGWfC). Em uma execução paralela, um SGWfC escalona muitas tarefas para os recursos computacionais e Processamento de Muitas Tarefas (MTC, do inglês *Many Task Computing*) é o paradigma que contempla esse cenário. Para gerenciar os dados de execução necessários para a gerência do paralelismo em MTC, uma máquina de execução precisa de uma estrutura de dados escalável para acomodar tais tarefas. Além dos dados da execução, armazenar dados de proveniência e de domínio em tempo de execução permite várias vantagens, como monitoramento da execução, descoberta antecipada de resultados e execução interativa. Apesar de esses dados poderem ser gerenciados através de várias abordagens (*e.g*, arquivos de log, SGBD, ou abordagem híbrida), a utilização de um SGBD centralizado provê diversas capacidades analíticas, o que é bem valioso para os usuários finais. Entretanto, se por um lado o uso de um SGBD centralizado permite vantagens importantes, por outro, um ponto único de falha e de contenção é introduzido, o que prejudica o desempenho em ambientes de grande porte. Para tratar isso, propomos uma arquitetura que remove a responsabilidade de um nó central com o qual todos os outros nós precisam se comunicar para escalonamento das tarefas, o que gera um ponto de contenção; e transferimos tal responsabilidade para um SGBD distribuído. Dessa forma, mostramos que nossa solução frequentemente alcança eficiências de mais de 80% e ganhos de mais de 90% em relação à arquitetura baseada em um SGBD centralizado, em um cluster de 1000 cores. Mais importante, alcançamos esses resultados sem abdicar das vantagens de se usar um SGBD para gerenciar os dados de execução, proveniência e de domínio, conjuntamente, em tempo de execução.

Abstract of Dissertation presented to COPPE/UFRJ as a partial fulfillment of the requirements for the degree of Master of Science (M.Sc.)

CONTROLLING THE PARALLEL EXECUTION OF WORKFLOWS RELYING ON A DISTRIBUTED DATABASE

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July/2015

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Large-scale computer-based scientific simulations require high performance computing, involve big data manipulation, and are commonly modeled as data-centric scientific workflows managed by a Scientific Workflow Management System (SWfMS). In a parallel execution, a SWfMS schedules many tasks to the computing resources and Many Task Computing (MTC) is the paradigm that contemplates this scenario. In order to manage the execution data necessary for the parallel execution management and tasks' scheduling in MTC, an execution engine needs a scalable data structure to accommodate those many tasks. In addition to managing execution data, it has been shown that storing provenance and domain data at runtime enables powerful advantages, such as execution monitoring, discovery of anticipated results, and user steering. Although all these data may be managed using different approaches (*e.g.*, flat log files, DBMS, or a hybrid approach), using a centralized DBMS has shown to deliver enhanced analytical capabilities at runtime, which is very valuable for end-users. However, if on the one hand using a centralized DBMS enables important advantages, on the other hand, it introduces a single point of failure and of contention, which jeopardizes performance in a large scenario. To cope with this, in this work, we propose a novel SWfMS architecture that removes the responsibility of a central node to which all other nodes need to communicate for tasks' scheduling, which generates a point of contention; and transfer such responsibility to a distributed DBMS. By doing this, we show that our solution frequently attains an efficiency of over 80% and more than 90% of gains in relation to an architecture that relies on a centralized DBMS, in a 1,000 cores cluster. More importantly, we achieve all these results without abdicating the advantages of using a DBMS to manage execution, provenance, and domain data, jointly, at runtime.

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1 INTRODUCTION

Large-scale computer-based scientific simulations are typically complex and require parallelism on a High Performance Computing (HPC) environment, *e.g.*, cluster, grid or cloud. These simulations are usually composed of the chaining of different applications, in which data generated by an application are consumed by another, forming a complex *dataflow*. These applications may manipulate a large amount of non-trivial data, making their processing even more complex and time-consuming (*i.e.*, weeks or even months of continuous execution). For this reason, many scientific scenarios rely on the paradigm of *scientific workflows* which have their executions orchestrated by a *Scientific Workflow Management System* (SWfMS). SWfMSs provide the management of those scientific applications, the data that flows between each application, and the parallel execution on the HPC environment. A scientific workflow is composed of a set of *activities* – which are often seen as scientific applications that represent solid algorithms or computational methods – and a dataflow between each of them (Deelman *et al*., 2009). In Sections 2.1 and 2.2, we further explain these concepts.

In addition to the aforementioned aspects, during the long run of such simulations, each activity in the workflow is repeatedly and extensively invoked in order to explore a large solution space just varying the parameters or computational methods. For instance, optimization problems, computational fluid dynamics, comparative genomics, and uncertainty quantification problems are examples in which scientific applications need to compute a result for each combination of parameters or input data (as cited in Dias, 2013). If the execution of the linked scientific applications is managed by a SWfMS, it may handle each application invocation that consumes a given combination of parameters and produces result (output data) associated to that given combination. Additionally, we may say that an application or activity is completely executed for a given workflow execution if, and only if, all those invocations are completely finished. Moreover, each of these many invocations may be executed in parallel on the HPC environment. The paradigm that contemplates this scenario is called *Many Task Computing* (MTC), where each activity invocation is treated as a *task* (Raicu *et al*., 2008). Furthermore, Walker and Guiang (2007) call the specific type of parallelism that simultaneously executes each of those many tasks for a given combination of parameters as *parameter sweep* (as cited in Mattoso *et al*., 2010). In Section 2.3, these terms will be further elucidated.

In this work, we focus on independent tasks within the parallel execution of a single activity consuming multiple data. In other words, despite the inherent data dependency between activities in a complex dataflow, each task of a single activity is independent of other tasks from this same activity execution for other data. This type of problem, in which tasks *embarrassingly* run in parallel, is dominant in many scientific scenarios (Benoit *et al*., 2010; Oprescu and Kielmann, 2010). Further, we are especially concerned about how the SWfMS manages the execution of those independent tasks for each activity of a workflow on the HPC environment. For this reason, we use a classic term that is widely adopted by literature when referring to independent tasks scheduling on HPC: *Bag of Tasks* (BoT) (Carriero and Gelernter, 1990). In Section 2.4, we present different BoT variations, their scheduling policy, and also how they relate to our approach that relies on scientific workflows.

Furthermore, a SWfMS must not only manage tasks scheduling in workflow executions, but also needs to collect *provenance data* to support the life cycle of a large-scale computer-based scientific simulation (Mattoso *et al*., 2010). Provenance data contemplates both information about workflows specification and information about how the data generated during the workflow execution were derived, and that provenance may be even more important than the resulting data. Storing provenance data is essential to allow result reproducibility, sharing, and knowledge reuse in scientific communities (Davidson and Freire, 2008). In addition to data about workflow execution (needed to manage the parallel execution) and data provenance, a SWfMS needs to manage domain-specific data. Enriching provenance databases with domain data enables richer analyses (Oliveira *et al*., 2014). Thence, these three types of data are expected to be managed by a SWfMS: (i) execution control data, (ii) provenance data, and (iii) domain data. As a matter of simplicity, we are going to use the term *Provenance Database* to refer to these three types of data, jointly, from now on.

In short, (i) execution control data are related to information about scheduling tasks to computing resources, which computing resources are being used and how, and it is also possible to register data about the health of the system and hardware. (ii) Provenance data are related to how the data were derived, including computing methods or algorithms used in the process, data owner, workflow specification, simulation site, and other pieces of information. (iii) Domain data are mostly the main interest for the scientists and are specific for each problem, application or scientific domain and are closely related to both previous types of data. Further explanation will be given in Section 2.5

Managing all these data may not be trivial in large-scale scenarios and at least two issues are discussed. First, most SWfMSs manage their execution data using a centralized

data repository, which may generate bottlenecks, jeopardizing the performance of the system. Second, a trade-off between performance and analytical capabilities needs to be addressed. On the one hand, a system may use a distributed data control by storing multiple flat log files during execution, which is in general easier and faster to store, but harder to analyze, especially when there are many big log files. On the other hand, a system may store data in a structured database management system (DBMS) during execution, which amplifies the analytical capabilities, but it is in general more complex and slower to store than simply appending into log files. Further, the more data a SWfMS gathers and stores in a DBMS, the more analytical features it provides to the end-user, but also the more complex it becomes to manage. To tackle this, a system may attempt to combine performance and analytical capabilities by storing only one of the three types of data (*e.g.*, execution data) in a DBMS during execution, whereas provenance data are captured in log files and eventually stored in the DBMS usually in the end of the execution. In related work section (Section 2.9), we are going to mention SWfMSs that uses a distributed data control based on flat files and another one that stores execution data in a DBMS. Mostly, known SWfMSs do not store domain data in the DBMS. Hence, provenance data analyses at runtime are limited and, more importantly, joint analyses of the provenance database (*i.e.*, including execution and domain data) are not enabled in such systems.

However, it has been shown that storing all three types of data, jointly, in a provenance database during workflow execution delivers many powerful advantages. The advantages include discovery of anticipated results (Oliveira *et al.*, 2014), workflow execution monitoring associating to domain data generated throughout the dataflow (Souza *et al.*, 2015), and interactive execution, also known as user steering (Mattoso *et al.*, 2015). Moreover, in such integrated database, a data model may be used to structure fine-grained information enabling even greater analyses. For example, it is possible to register which specific task (from all those many tasks) is related to a specific domain datum and where this task is running among all the computing resources on the HPC environment – all this may be associated to the domain data in the dataflow. Additionally, if a SWfMS uses a data model that contemplates provenance data following a recognized standard, such as the PROV-DM proposed by the World Wide Web Consortium (Moreau and Missier, 2013), interoperability between existing SWfMSs that also collect provenance data may be facilitated.

Nevertheless, the trade-off between such fine-grained analytical capabilities and performance remains an open issue. SciCumulus/C (SCC) is a SWfMS that stores fine-grained data in a provenance database, managed by a DBMS during workflow execution

(Silva *et al*., 2014). As we are going to explain in details in Chapter 3, SCC is based on Chiron (Ogasawara *et al*., 2011) and on SciCumulus (Oliveira *et al*., 2010), which introduced this approach of storing the three types of data in a provenance database managed by a centralized DBMS (*e.g*., PostgreSQL [1] or MySQL [2]). By doing this, SCC enables many important analytical capabilities, but its performance may be compromised in large-scale scenarios. Not only performance may be an issue, but also the utilization of a centralized DBMS may introduce other typical problems in HPC, such as single point of failure and contention. For this reason, the data gathering mechanism at runtime must be highly efficient and take these known HPC issues into account to attempt to provide both performance and analytical capabilities.

Therefore, the problem we want to tackle in this dissertation can be enunciated as follows. To the best of our knowledge, SCC is the only SWfMS that uses a DBMS to manage the entire provenance database at runtime, which enables powerful analytical capabilities, but it relies on a centralized DBMS. By relying on a centralized DBMS, a single point of failure is introduced – that is, if a node that hosts the DBMS fails, the workflow execution is interrupted. Furthermore, when compared with a distributed DBMS, a centralized DBMS has less ability to handle a very large number of requests per unit of time. To cope with this, SCC implements a centralized architecture in which there is a single node that is the only one able to access the database and is responsible for scheduling tasks to other nodes and for storing gathered data in the provenance database, as we are going to explain in details in Section 3.4 Nevertheless, such centralized architecture introduces a contention point in a single central node. This contention is more evident in a large scenario with multiple processing units requesting tasks to the node, which would also downgrade performance.

As a solution, decades of theoretical and practical development and optimizations on *Distributed Database Management Systems* (DDBMS) motivate their usage on a distributed system such as a parallel SWfMS. It is known that, compared with a centralized DBMS, a DDBMS can handle larger datasets, take more advantage of the HPC environment, and consider important issues in distributed executions, *e.g*., fault tolerance, load balancing, and distributed data consistency (Özsu and Valduriez, 2011). Thus, using a DDBMS may be a potential alternative for supporting an efficient structured data gathering mechanism at runtime. For this reason, in our solution, we propose a novel architecture for scheduling MTC tasks in a parallel workflow execution relying on a DDBMS to manage the entire provenance

[1] www.postgresql.org
[2] www.mysql.com

database. Our main goal is to provide a decentralized parallel execution management. To do so, we propose taking off the responsibility of a central node to receive requests from and send tasks to all other processing nodes. Instead, we want the distributed database system to serve as a decentralized data repository which all processing nodes are able to access. Furthermore, by using a DDBMS, we are able to enhance the data gathering mechanism at runtime; take more advantages of the HPC environment; and improve the system's performance, load balance, fault tolerance, and availability. More importantly, we do not abdicate all the advantages of using a DBMS to manage the provenance database at runtime.

We call the SWfMS that runs on top of such architecture as ***SciCumulus/C²*** *on a* ***D****istributed Database System* (**d-SCC**). We especially discuss important issues like synchronization, availability, load balancing, data partitioning, and task distribution among all available resources on the HPC environment.

Particularly, by developing d-SCC we can enumerate the following contributions. (i) We proposed a novel design of a distributed architecture for a parallel SWfMS that relies on a DDBMS, describing tasks scheduling, load balancing, fault tolerance, distributed data design (*i.e.*, fragmentation and allocation), and parallel data placement; (ii) We implement it based on a SWfMS that uses a centralized DBMS to manage the provenance database and discuss the main difficulties; (iii) We remove the single point of failure introduced by the centralized DBMS; (iv) We alleviate the contention introduced by the centralization on a single central node; (v) We take more advantages of the HPC environment by distributing the database on more computing resources; (vi) By using a DDBMS, we may handle larger datasets maintaining good efficiency; (vii) Since a DDBMS can handle a larger number of requests, we rely on it and make a lot of use of its synchronization mechanisms to keep our distributed provenance database consistent; (viii) Like SCC, d-SCC also manages the provenance database at runtime, maintaining all its inherited advantages previously mentioned.

The remainder of this dissertation is organized as follows. In Chapter 2, we present the background needed for this dissertation. In Chapter 3, we show SciCumulus/C (SCC), the SWfMS on which this work is based, explaining its architecture and workflow algebra. In Chapter 4, we introduce our novel distributed architecture that relies on a DDBMS. In Chapter 5, we present our parallel SWfMS solution called d-SCC, which runs on top of our proposed architecture. We especially discuss its implementation details and challenges faced during development. In Chapter 6, we show our experimental evaluation. Finally, we conclude this dissertation and foresee future work in Chapter 7.

2 BACKGROUND

In this chapter, we introduce the theoretical principles that give foundation for this dissertation. This dissertation is inserted in the context of supporting large-scale computer-based scientific experiments that require HPC (Section 2.1). These experiments are composed of the chaining of scientific applications with a dataflow in between. One acknowledged approach is to model these experiments as data-centric scientific workflows that are managed by a parallel SWfMS (Section 2.2). In addition, our previous works, on which this current dissertation is based, fit in the paradigm of MTC and, more specifically, Parameter Sweep parallelism (Section 2.3). We will explain that Parameter Sweep parallelism may be seen as a BoT application consisting of many tasks that consume and produce data; and we survey different implementations of BoT applications (Section 2.4). Furthermore, we argue that a SWfMS needs to store three types of data and that storing them in a provenance database enables powerful advantages (Section 2.5). We introduce principles of a DDBMS (Section 2.6), which, if used to manage the Provenance Database, more advantages could be taken from an HPC environment that can be built according to at least three different basic parallel architectures (Section 2.7). In Section 2.8, we explain the performance metrics we used to evaluate our parallel system. Finally, we conclude this section with related work in Section 2.9.

2.1 Large-scale Computer-Based Scientific Experiments and HPC

Mattoso *et al*. (2010) explain that traditional scientific experiments are usually classified as either *in vivo* or *in vitro*. However, in the last decades, scientists have used computer applications to simulate their experiments, which enabled two new classes of experiments: *in virtuo* and *in silico* (Travassos and Barros, 2003). Due to evolution of technology, a new challenge is being addressed in the computer science community, since these computer-based scientific simulations have been manipulating a huge amount of data which keeps increasing over the years. As a result, they demand continuous evolution of both hardware architecture and computational methods such as specialized programs or algorithms.

Additionally, large-scale computer-based simulations require massive parallel execution on *High Performance Computing* (HPC) environments. According to Raicu, an HPC environment is a collection of computers connected together by some networking fabric and is composed of multiple processors, a network interconnection, and operating systems.

They are aimed at improving performance and availability compared with a single computer (2009). As examples of HPC environment, we have clusters, grids, virtual machines (VM) on clouds, and supercomputers like IBM Blue Gene (IBM100, 2015). Moreover, we say that an HPC environment is homogeneous if the computing units (*e.g.*, individual computer or *nodes*, as usually called) that compose it are the same (Özsu and Valduriez, 2011).

2.2 Data-Centric Scientific Workflows, Dataflows, and SWfMS

One way to facilitate dealing with the complexity of a large-scale computer-based scientific experiment is by modeling it as a *scientific workflow* (Deelman *et al*., 2009). Scientific workflows extend the original concept of workflows. Traditional workflows, usually seen in business scenarios, systematically define the process of creation, storing, sharing, and reviewing information. Analogously, scientific workflows is a method of abstracting and systematizing the experimental process or part of it (as cited in Dias 2013). As previously mentioned, these computer-based experiments consist of one or many specialized scientific applications, which are represented by *activities* in the workflow. Moreover, a scientific workflow is usually formed by the chaining of activities; hence we say that there is data dependency between activities. That is, data produced by an application are consumed by another, forming a *dataflow* (as cited in Dias 2013). A scientific workflow with these characteristics are usually data-intensive and we claim that it is driven by data or, as Ogasawara *et al*. call, it is a *data-centric scientific workflow* (2011). Yet, Ogasawara *et al*. explain that such flow can be modeled as a Directed Acyclic Graph (DAG) on which vertices represent activities and edges represent the dataflow between them (2011).

Due to its complexity, there is a necessity of a system to manage the execution of a scientific workflow. Mattoso *et al*. argue that not only does the execution need to be managed, but also such a system needs to enable composition and analyses of a computer-based experiment (2010). Additionally, given the large-scale requirements, this system needs to implement special directives to deal with an HPC environment. A system with these characteristics is known as a *Scientific Workflow Management Syst*em (SWfMS) (Deelman *et al*., 2009). Examples of SWfMS are Pegasus (Lee et al., 2008), Swift/T (Wozniak et al., 2013), and SciCumulus (Oliveira *et al*., 2010).

2.3 Tasks, MTC and Parameter Sweep

In computer science, a concept called *divide and conquer* is widely used to solve a complex problem dividing it into smaller sub-problems. When all sub-problems are solved, that first complex problem is said to be solved (Cormen *et al*., 2009). Based on this concept, we define *task* as a smaller sub-problem of a greater complex problem. An application that runs tasks in parallel to solve a complex problem is known as a parallel application and they are broad and historically used in HPC (Raicu *et al*., 2008). Moreover, Raicu *et al*. (2008) qualify tasks as small or large (we also say light or heavy, short or long), uniprocessor or multiprocessor, compute-intensive or data-intensive, and dependent or independent of others. Yet, a set of tasks may be loosely or tightly coupled and homogeneous or heterogeneous.

In large-scale computer-based scientific experiments, a paradigm of parallel tasks takes part in: *Many Task Computing* (MTC). Raicu *et al*. (2008) define MTC as a paradigm to deal with a large number of tasks. Each task has the following characteristics. It takes relatively short time to run (seconds or minutes long), it is data intensive (*i.e*., it manipulates tens of MB of I/O), it may be either dependent or independent of other tasks, it may be scheduled on any of the many available computing resources on the HPC environment, and the execution of all tasks achieves a larger goal.

In this context, recall from the introduction (Chapter 1) that a typical scenario is that each application (or computational method or algorithm) is repeatedly and extensively invoked in order to explore a large solution space just varying the parameters or computational methods. As examples, there are optimization problems, computational fluid dynamics, comparative genomics, and uncertainty quantification (as cited in Dias 2013). Each invocation consumes a given combination of parameters (input data) and produces result (output data). A parallel system may manage all these invocations in parallel. This type of parallelism is called *Parameter Sweep* (Walker and Guiang, 2007) and it fits in the MTC paradigm where each invocation is treated as a task. For this reason, from now on, we are going to use the term task to refer to an application invocation. Merging this context with the context of data-centric scientific workflows, we claim that an activity is composed of many tasks and an activity is completely executed for a given workflow execution if, and only if, all those tasks are completely finished.

2.4 Bag of Tasks

As previously stated, the MTC paradigm contemplates both dependent and independent tasks. However, for a given single application, each application invocation that sweeps a combination of parameters and produces output data is treated as independent of each other. That is, in Parameter Sweep parallelism, there is neither data nor communication exchange between different invocations of a single application. In other words, using the considerations enunciated in Section 2.3, we say that all tasks for a given single activity of the workflow are independent of each other. This is a very typical scenario in a broad variety of scientific applications (Benoit *et al*., 2010; Oprescu and Kielmann, 2010). The specific type of parallel application that is especially concerned about scheduling many independent tasks on the available resources of the HPC environment is called *Bag of Tasks* (BoT) parallelism. In this dissertation, we propose a distributed architecture for BoT parallelism that relies on a DDBMS. We especially discuss its tasks scheduling mechanism and other related issues, such as load balancing. For this reason, we revisit BoT applications in order to study its singularities and apply them on the tasks scheduler that composes the core of our proposed architecture on top of which our SWfMS that manages data-centric workflows will run.

The concept of a bag of tasks may be implemented within different approaches. Most of them differ in distinguishing the owner or manager of the bag of tasks that need to be executed to solve the determined problem. In each of these approaches, task distribution design and scheduling over slaves are also different. In this section, we present these implementations and their specificities.

Although these implementations have many differences, a common issue that is in question over all approaches is load balancing. Since tasks' cost may be heterogeneous (*i.e*., some tasks are heavier than others) and slaves' efficiency may be heterogeneous (*i.e*., some slaves execute tasks faster than others), load imbalance may occur. For this reason, *load balancing* is discussed in all approaches presented in this section.

In order to cope with this load imbalance problem, *work stealing* is one of the techniques that frequently appear in most approaches. The idea is simple. If a fast slave executes the entire load that was under its responsibility, it will become idle. Then, the fast slave may choose a slower busy slave as victim so the fast slave can steal tasks from. There are different strategies to implement work stealing and to choose victim nodes (Mendes *et al*., 2006), but this is out of the scope of this current work. However, how work stealing would

work may differ in each approach and the general idea of the strategy will be briefly discussed in following sections.

In addition to load imbalance, communication overhead is also an important issue that is commonly addressed in BoT implementations. Since tasks may need to be transmitted over the network, this might become a bottleneck depending on the implementation and on the problem. Ergo, we discuss communication overhead in each of the presented approaches.

Regarding nomenclature, even though tasks in a BoT are independent hence may be executed in an arbitrary order (Silva *et al*., 2003), many authors frequently use the term *work queue* (WQ) when referring to the data structure that holds the bag of tasks (Cario and Banicescu, 2003; Silva *et al*., 2003; Senger *et al*., 2006; Anglano *et al*., 2006; da Silva and Senger, 2010). However, we highlight that tasks do not need to be executed in a first-in-first-out policy.

Having all this considered, in next sections we show three known implementations of bag of tasks. How tasks are distributed and scheduled within each of these approaches is discussed. Their advantages and disadvantages regarding load balance and communication overhead are discussed as well. This survey on existing BoT designs is important because we propose a novel BoT design in Section 4.1, which inspired us to propose our architecture for a parallel workflow engine that relies on a distributed database management system.

2.4.1 Centralized Work Queue

Centralized Work Queue (CWQ) is the simplest design of a bag of tasks (Silva *et al*., 2003). In a master-slave fashion, the centralized master owns and manages the entire bag of tasks. It is the masters' responsibility to schedule tasks over all slaves. Scheduling is also simple. As soon as a slave becomes available (*i.e*., it is ready to execute tasks), it requests the master for work. The master listens to the slave's request and sends one or a chunk[3] of runnable tasks, which are marked as "in execution". Then, after the slave having received those sent tasks, it becomes busy while executing its load until completion. When a slave finishes and becomes available again, it both sends a feedback with execution results to the master, who marks the

[3] Determining an efficient chunk size, commonly referred to *K*, to provide load balance may be a complex problem depending on the application characteristics (Cariño and Banicescu, 2007). We also note that due to the provenance database, we could use it as a knowledge database to predict future tasks cost, which would lead to more accurate choice of *K* hence better load balancing.

tasks as “completed” accordingly, and requests more work. The procedure is repeated until all tasks from the queue are completed. Figure 1 shows a diagram of this design.

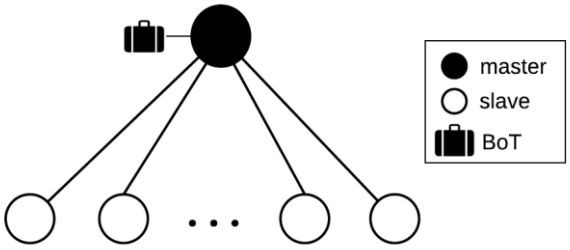


Figure 1 – Centralized Work Queue design

In spite of the advantage of being easier to understand and to implement, this model has some disadvantages in a scenario with a large number of slaves. The main disadvantage is communication overhead due to centralization on master which may lead to a bottleneck if a large number of slaves is present. The scheduling work is totally concentrated in the single centralized point. In addition, tasks need to be sent multiple times between master and slaves, which may drive to network congestion. Hence, loss of performance may happen.

Regarding work stealing for load balancing, it is not common in classic CWQ implementations since tasks are only transmitted between the master and slaves. When a fast slave finishes its work load, asks the master for more work, and the master replies that the bag of tasks is empty, this fast slave becomes idle until the end of the application execution even if there are other slower busy slaves. This is more evident if a larger chunk of tasks is transmitted at once, instead of only one task. For this reason, load imbalance may occur in a heterogeneous scenario within this approach.

Furthermore, another disadvantage is that it introduces a single point of failure. That is, if the single centralized master fails while there are still runnable tasks in the bag, the whole parallel application stops since other idle slaves will not be able to get them. In addition, it is shown that the simplest CWQ implementation is the one that performs worst compared to other WQ models (Silva *et al*., 2003), which will be presented next.

Therefore, the CWQ design would only be a good option in a more sophisticated implementation that considers enhanced strategies for load balancing and communication overhead. However, these are not common in most CWQ classic implementations.

2.4.2 Work Queue with Replication

Silva *et al*. (2003) propose Work Queue with Replication (WQR), which basically adds task replication to the classic CWQ design. There is a master processor that is only responsible for coordinating scheduling, as shown in Figure 2.

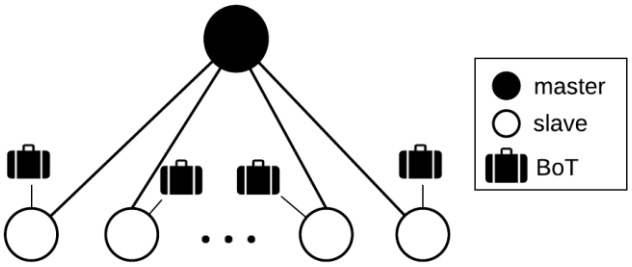


Figure 2 – Work Queue with Replication design

In the beginning, scheduling is like simple CWQ. Slaves request tasks to the master, which assigns ready tasks to the requesting slaves. However, WQR takes better advantage of data locality than other WQ strategies with no replication. Since each slave owns a replica of the bag of tasks, the master just sends a short message so the slave can start executing a task, instead of sending the task itself (Silva *et al*., 2003). A message containing a task is usually larger than simple scheduling messages, which can be implemented using a convention of simple constants (*e.g*., an integer to signify the message "give me some work" or "execute such task"). In addition, whereas in a simple CWQ implementation slaves that finish their work become idle during the rest of the application execution, in WQR the master requests idle slaves to execute tasks that are still ready to run. This improves load balancing (Silva *et al*., 2003). Then, when a replica finishes, the master coordinates the abortion of all other replicas.

It is important to mention that this architecture implies a similar scheduling behavior to work stealing. A valuable difference, though, is that there is no task transmission in WQR because the tasks that will be stolen are replicated. Since only short messages inherent to the scheduling algorithm are needed, there is an important reduction in data transmission in the network.

More advantages of WQR are related to performance and availability. Replicating tasks increases the probability of running one of the replicas on a faster machine, which reduces overall execution time (Anglano *et al*., 2006). For this reason, the number of replicas also affects performance. That is, the greater the number of replicas, the greater this

probability is, which may imply in better performance, as shown in (Paranhos *et al*., 2003). Compared to a simple implementation of CWQ, WQR is shown to perform significantly better. In some cases, it performs better than other techniques that require *a priori* information about the tasks and the system, which may be unfeasible in complex scenarios. In addition to the performance advantage, WQR enables enhanced failure recovery strategies to provide high availability. However, like in simple CWQ, the master scheduler still remains a single point of failure (Silva *et al*., 2003).

Despite the advantages, the utilization of replication in WQR introduces a concern related to problem size. Performance evaluations are provided, but the greatest number of tasks evaluated is 5,000 and no scalability or speedup tests are presented (Silva *et al*., 2003). Especially, full replication of the work queue (even two replicas only), as proposed by Silva *et al*. (2003), may not be viable if the bag of tasks is very large.

To tackle this issue, Cariño and Banicescu describe a work queue with *partial* replication (2007). Instead of replicating the entire work queue on each slave node in the cluster, a smaller part of the queue is given to each slave. Scheduling initially occurs in a similar fashion to the full replicated WQR until one of the slaves consumes its whole share of the queue and becomes idle. Then, the idle slave requests the master for more work. The master selects a busy slave to be the victim. Then, the master calculates whether or not it is advantageous to move tasks from one slave to another. If it is, the master asks the idle slave to steal tasks from the victim slave. In this case, not only are scheduling messages transmitted, but tasks themselves are also sent from a slave to another. Therefore, although partial replication may involve tasks transmission, it is an alternative to the WQR proposed by Silva *et al*. (2003) to deal with a really large bag of tasks.

2.4.3 Hierarchical Work Queue

Both designs previously presented require a centralized master node to coordinate all slaves in the cluster. This may lead to congestion at the master in a scenario with a large number of slaves. To deal with this, we present a hierarchical architecture with many masters. The Hierarchical Work Queue (HWQ) design presented in this section is based on the 2-level hierarchical platform described by Senger *et al*. (2006) and Silva and Senger (2011). The architecture consists of one *supervisor*, which is responsible for scheduling tasks among M *masters*. Then, each master m_i is responsible for scheduling tasks among S_i *slave* processors in one cluster c_i. Finally, each slave is only responsible for performing computation, *i.e*.,

executing the tasks. Figure 3 illustrates this architecture. Each master has its own BoT that is populated by the supervisor's BoT.

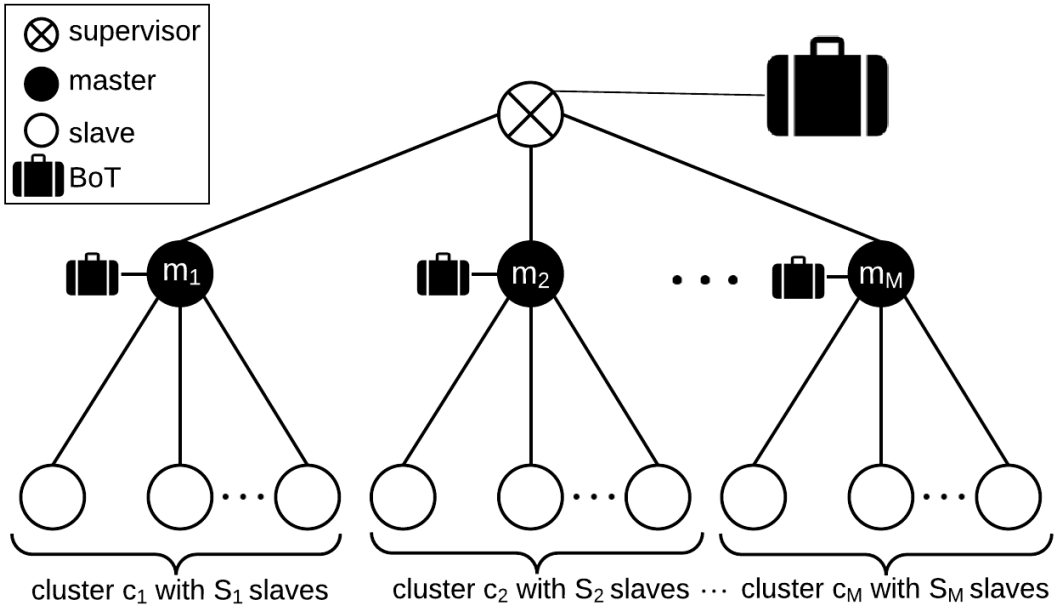


Figure 3 – Hierarchical Work Queue design

HWQ characteristics leads to less communication overhead in a centralized node compared to a simple CWQ. Since there are multiple masters, scheduling overhead is not fully concentrated in a single point (*i.e.*, the single master in a CWQ model). Although this facilitates communication load balancing, if there are too many masters, there will be a bottleneck at the supervisor. As a consequence, this will eventually lead to load imbalance and loss of performance as well.

For this reason, one sensitive issue in this hierarchical model is to find M and S_i for each cluster c_i so the architecture can be dynamically set up. Regarding M, one the one hand, if M is too small compared to the total of slaves, masters will suffer communication bottleneck; on the other hand, if M is too large, more contention will happen at the supervisor. Regarding S_i, a simple solution is to even up the number of slaves, S, for each master (*i.e.*, $S_i = S$, for $i = 1..M$). In other words, all masters in the system are responsible for a same number, S, *of* slaves.

To cope with this, Senger *et al*. (2006) propose a strategy for hierarchical scheduling which includes finding static M and S_i. Their proposed strategy relies on estimating S_{eff}, the maximum number of slaves a master can efficiently control. Since they assume a homogeneous and dedicated hardware, all masters have the same S_{eff}. Under "some

assumptions" (Senger *et al*., 2006), this number is estimated utilizing the sum of the mean response time of the executions of the tasks and the mean time required to transmit input and output files from one machine to another, since this is common in the scenario they aimed their solution at. However, considering our motivating problem as described in previous sections, tasks do not necessarily share or transmit any data or file, limiting the utilization of this estimate on our problem.

Although communication bottleneck is less likely to occur in a single point due to masters' decentralization, there is an added up layer of bureaucracy between slaves and tasks which is inherent in a hierarchical model. That means that a task executed in a slave was originally owned by the supervisor, who is two levels upon the hierarchy. There will be more data transmission in the network caused by task transmission in two levels. Thus, this is a disadvantage in the hierarchical design.

Moreover, in typical HWQ implementations there are no clear strategies to provide computation load balancing (Senger *et al*., 2006; Silva and Senger, 2011). For example, if a fast slave finishes much earlier than all others, it is not considered whether the slave should remain idle until the end of the execution or should steal work from others. Ergo, to provide computation load balance, it is necessary to investigate improvements in the original HWQ.

Finally, regarding availability, it is noted that HWQ also contains a single point of failure, the supervisor node, just like CWQ and WQR. Therefore, it is important to deal with this and propose a more sophisticated model if one wants to eliminate a single point of failure.

2.5 Provenance Database: storing the three types of data

Up to this point, we were mostly essentially worried about parallel execution and tasks scheduling. However, in addition to execution data required by a distributed system, a parallel SWfMS is expected to also manage other two types of data: provenance and domain data. In this section, we explain each of the three types of data in further details and how we deal with them in our work.

First, the underlying parallel engine needs a scalable data structure that accommodates the bag of tasks and is capable of storing execution status of each single task in order to manage the workflow parallel execution. Information such as which tasks should be scheduled to which processors, number of tasks, which input data a task should consume, etc. is necessary to be maintained by a SWfMS. We call this type of data as *execution control data*.

Second, in addition to maintaining execution data, a SWfMS needs to collect *provenance data* in order to support a large-scale computer-based scientific simulation (Davidson and Freire, 2008; Mattoso *et al*., 2010). Provenance data may be defined as the information that helps to determine the history of produced data, starting with their origins (Simmhan *et al*., 2005). In other words, it is simply "the information about the process used to derive the data" (Mattoso *et al*., 2010). Moreover, Goble *et al*. summarize that provenance data serve for (2003): providing data quality; tracking each process utilized to derive the data; keeping data authorship information; and providing powerful means for analytical queries for data discovery and interpretation (as cited in Oliveira, 2012). Additionally, according to Davidson and Freire, provenance data may be even more important than the resulting data and may be further categorized as *prospective provenance* – information about workflows specification – and *retrospective provenance* – information about how the data generated during the workflow execution were derived (2008).

Third, *domain data* are of extreme interest for scientists and are specific for each application domain. They are closely related to execution data because the SWfMS needs to be aware of which domain data will be consumed by a task. They are also closely related to provenance data because since each task may generate output domain data, the SWfMS needs to keep track of how such domain data was generated. In a Bioinformatics application, an example could be the number of alignments of a phylogenetic tree; in a Seismic application, an example could be the speed of seismic waves; and in an Astronomy application, an example could be the coordinates (x,y) of a specific point of an image of the sky.

All those data may be hard to manage and Dias (2013) claims that many approaches to store them have been proposed (Altintas *et al*., 2006; Bowers *et al*., 2008; Gadelha *et al*., 2012; Moreau and Missier, 2013). We argued that storing all those data, especially in fine granularity, in a structured database enable powerful data analytical capabilities. For instance, it enables execution monitoring associating to domain data generated throughout the dataflow (Souza *et al*, 2015), discovery of anticipated results (Oliveira *et al*, 2014), and interactive execution, also known as user steering (Mattoso *et al*., 2013). In this dissertation, we call such database, which jointly contemplates the three types of data, as *Provenance Database*.

In addition to facilitating such analyses within a single experiment or scientific research group, a widely accepted standard model for data enables possible future data interchange, interoperability, and ease of communication among scientists from different communities. For these reasons, the World Wide Web Consortium, acknowledged for defining standards and recommendations on the web, recommends the Provenance Data

Model (PROV-DM) (Moreau and Missier, 2013). Moreover, for structuring provenance data for workflows, we need a provenance data model for workflows. This is called PROV-Wf (Figure 4), which is an extension of PROV-DM (Costa *et al*., 2013). PROV-Wf is the data model for our Provenance Database. Further explanation on PROV-Wf, as well as on most of the attributes within each entity and a real practical example of its utilization, can be found in (Costa *et al*., 2013).

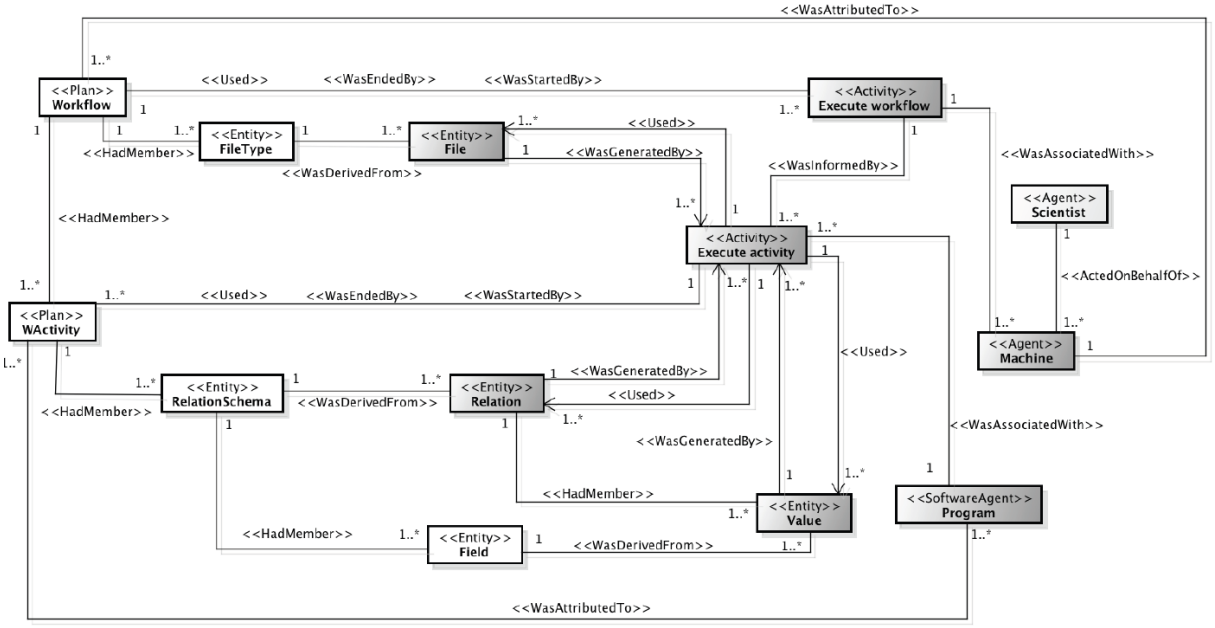


Figure 4 – The PROV-Wf data model (Costa *et al*., 2013)

2.6 Principles of Distributed Databases

As briefly argued in introduction, although gathering provenance data in a fine level and storing in a common centralized DBMS during execution enables rich advantages, it might introduce contention points that would jeopardize execution time. Thus, the provenance gathering mechanism must be highly efficient to accommodate both those advantages and good performance. Moreover, decades of theoretical and practical development and optimizations on Distributed Database Management Systems (DDBMS) motivate their usage on a distributed system such as a parallel SWfMS. Additionally, many important concepts in HPC problems are discussed in the same context of a DDBMS, *e.g*., fault tolerance and synchronization. Since our proposed architecture relies on a DDBMS, in this section, we review some principles that are important for this dissertation. Most of the concepts briefly reviewed in this section are further explained in details by Özsu and Valduriez (2011).

2.6.1 Data Fragmentation and Replication

Data fragmentation is related to the division of a database table into disjoint smaller tables (or fragments) (Özsu and Valduriez, 2011). The objective is to make distributed transactions more efficient when they access different fragments in parallel (Lima, 2004). There are three types of fragmentation: Horizontal, Vertical, and Hybrid (Özsu and Valduriez, 2011). In the scope of this dissertation, we only explore Horizontal Fragmentation.

In *Horizontal Fragmentation*, a table is cut into fragments each of which having a shorter number of rows (or smaller cardinality) but having the exact same schema. The fragmentation happens following rules based on values of determined attribute on the table. For example, suppose we have a table for storing data about employees of a multinational company. One of the attributes of this table defines the country where each employee belongs to. One possible horizontal fragmentation for this table is fragmenting it into smaller tables where each table contains all employees of only one country. Horizontal Fragmentation has many advantages such as speeding up parallel transactions that manipulate data from different fragments and decreasing complexity of transactions that do not manipulate data from all fragments.

Furthermore, to increase availability, reliability and query performance, all or some fragments may be *replicated* (Özsu and Valduriez, 2011). Each fragment replica needs to be allocated to the nodes that host the distributed database. There are *total* and *partial replications*. Total replication means that each node owns a replica of the entire distributed database while partial replication means that only some fragments are replicated. Total replication is recognized for achieving the best availability requirements and flexibility for query executions. However, in very large databases, total replication may not be possible if the entire database size exceeds a host's storage capacities (Lima, 2004). We highlight that regarding availability, replication is highly important because if a node fails, a different (living) node may host a replica that the failed node was hosting. Thus, the application is still available even if a node fails.

2.6.2 OLTP, OLAP, Transaction Management, and Distributed Concurrency Control

In data management, there are two important classes that differ on how data is processed: On-Line Transaction Processing (OLTP) and On-Line Analytical Processing (OLAP). OLAP applications, *e.g.*, trend analysis or forecasting, need to analyze historical and summarized

data and they utilize complex queries that may scan very large tables. OLAP applications are also read-intensive and updates occur less frequently, usually in specific times. In contrast, OLTP applications are high-throughput and transaction-oriented. Extensive data control and availability are necessary, as well as high multiuser throughput and fast response times. Moreover, queries tend to be simpler, manipulating a smaller amount of data, they are also short, but they are many. Queries execution performance is usually greatly increased if indices are used. Additionally, updates tend to occur more frequently in OLTP applications than in OLAP ones (Özsu and Valduriez, 2011). Although an OLAP database would be desirable since data analyses are very important in our scenario, the tasks distribution mechanism with provenance gathering alludes to an OLTP access pattern. For this reason, since in this dissertation we mainly focus on tasks distribution and parallel execution, we also focus on typical characteristics in OLTP parallel applications. We note, however, that our solution does not abdicate of analytical capabilities, even though it is not focused.

Because data updates are frequent in OLTP applications, transaction management becomes crucial to keep the database consistent. For example, when two clients try to update a same piece of data, the DBMS needs to manage synchronization to guarantee consistency. A *transaction* is a basic unit of consistent and reliable computing in database systems. If the database is in a consistent state and then a transaction is executed, the database must remain consistent in the end of the execution. A DBMS that employs *strong consistency* transaction management guarantees that all transactions are *atomic*, *consistent*, *isolated*, and *durable* (ACID). In addition to managing synchronization of multiple client requests, strong consistency is important for *transaction* and *crash recovery*. Furthermore, in distributed databases, ensuring data consistency is more complex, since if a piece of data is modified in a node, all nodes need to "see" this modification so the entire distributed database can be consistent. If the DDBMS employs strong consistency distributed transaction management mechanisms, it needs to guarantee that all transactions are ACID even being distributed. For this, the DDBMS implements sophisticated distributed algorithms for distributed concurrency control to ensure consistency and reliability (Özsu and Valduriez, 2011).

Years of significant research in both centralized DBMSs and DDBMSs regarding transaction management and distributed concurrency control endorse a distributed architecture for Many Task Computing parallelism that relies on a distributed database management system. We highlight that the topics mentioned in this section are extremely relevant for an application with intense data updates. If a database use is read-only, such complexities do not occur and these sophisticated mechanisms are not required (Özsu and Valduriez, 2011).

2.6.3 Parallel Data Placement

In DDBMSs, *parallel data placement* is similar to data fragmentation (Section 2.6.1). Nonetheless, one difference is that, in data placement, an important concern is about minimizing the distance between the processing and the data for maximizing performance. *Full data partitioning* is data placement solution that yields good performance. In this solutions, each table is horizontally fragmented across all the DDBMS nodes; however, it is highlighted that full partitioning is not adequate for small tables (Özsu and Valduriez, 2011). There are three strategies for data partitioning: (i) round-robin – it is the simplest and ensures uniform data distribution, although direct access to individual rows based on an attribute requires accessing the entire table; (ii) hash – a hash function is applied to some attribute based on which the partitioning will happen. This strategy allows efficient exact-match queries (*i.e.*, queries with `where attribute = 'value'`); and (iii) range – rows are distributed based on value intervals (ranges) of some attribute. This is a good alternative for both exact-match and range queries (Özsu and Valduriez, 2011).

2.7 Parallel Hardware Architectures

A parallel system (*e.g.*, a parallel SWfMS or a DDBMS) needs to be aware of the parallel hardware architecture on which the system will run in order to take more advantages of it. There are three basic parallel hardware architectures that determine how the main hardware pieces (processor, memory, and disk) are organized and interconnected in an HPC environment: *shared-memory* (SM), *shared-disk* (SD), and *shared-nothing* (SN) (Özsu and Valduriez, 2011). We highlight that although architectures may determine the hardware organization within each single machine in an HPC environment, we only consider how nodes (machines) are interconnected rather than how each of the pieces within each machine are interconnected.

In SM architecture, all nodes can access any memory module or disk unit through a fast interconnect network. In SD, all nodes can access a shared disk unit through the interconnection network, but each processor has its own memory module (distributed memory). In SN, each node has its own memory and disk space.

Regarding differences that are relevant for this work, comparing with SN and SD, systems that run on SM generally provides better performance and developing tem are usually simpler. However, SM is not as extensible as SD and SN. Indeed, adding or removing nodes

in SN architecture is simpler than in SD and SM because the architecture is more loosely coupled. SN has lower costs, high extensibility, and availability. However, data management is more complex and data redistribution is needed when nodes are added or removed. Moreover, in SD, since data may be exchanged across all nodes through the disk, it is easier to support ACID transactions and distributed concurrency controls. Thus, for OLTP applications, SD is preferred. Conversely, since OLAP applications are usually larger and mostly read-only, SN is preferred (Özsu and Valduriez, 2011).

In extremely large-scale computer-based scientific experiment scenarios, an HPC environment may consist of hundreds of processors or even more. These are the ones called supercomputers. Most of the Top 500 supercomputers in the world are built on top of SD (TOP 500, 2015). We note that, in a SD, there are multiple disks (*i.e.*, they are distributed), but they are all interconnected through a very fast network interconnect (*e.g.*, Infiniband) so data in all disks can be kept synchronized; otherwise, bottlenecks may happen. Network-Attached Storage (NAS) and Storage-Area Network (SAN) are technologies for implementing SD architectures. SAN is acknowledged for providing high data throughput and for scaling up to large number of nodes (Özsu and Valduriez, 2011). Thus, SAN is preferred when performance is a requirement.

2.8 Performance Metrics

To evaluate the performance of a parallel system, there are some known basic metrics that are commonly used. In this work, we utilize at least three metrics in our performance evaluation: speedup, efficiency, and scalability.

Speedup measures performance gain achieved by parallelizing a program compared with a sequential version of such program. Sahni and Thanvantri explain that although the basic idea to calculate the speedup of a parallel system is given by the ratio between sequential execution time and parallel execution time, the definition of sequential and parallel times may vary depending on what and how the system is being measured, which results in many different definitions of speedup (1995). In this work, we use two definitions of speedup: real speedup and an adapted version of relative speedup (Sahni and Thanvantri, 1995). The real speedup $Speedup$ to solve a problem I using the program Q running on P processors is given by

$$Speedup = \frac{time\ to\ solve\ I\ using\ the\ best\ sequential\ program\ using\ 1\ processor}{time\ to\ solve\ I\ using\ program\ Q\ using\ P\ processors} \quad (1)$$

1

The time to solve using the best sequential program is also known as *theoretical time*. This time may hide overheads and assumes a perfect case scenario, which may be utopic in most situations, causing performance gains to be hidden. For this reason, instead of using this theoretical time to calculate the real speedup, using a relative speedup seems fairer. The relative speedup $RelativeSpeedup$ is given by (Sahni and Thanvantri, 1995):

$$RelativeSpeedup = \frac{time\ to\ solve\ I\ using\ program\ Q\ using\ 1\ processor}{time\ to\ solve\ I\ using\ program\ Q\ using\ P\ processors} \quad (2)$$

However, in large-scale simulations, running the program Q on only one processor may not be possible because it is not rare to have an executing taking days or weeks to run on a single processor. Taking all this time to run may not be viable, because it means more costs (especially if the HPC environment is a cloud-based service), more energy consumption, and more time spent on queues on clusters that are shared with many users. For this reason, we adapt the (2 and define the $RelativeSpeedup*$ as:

$$RelativeSpeedup^{*} = \frac{time\ to\ solve\ I\ using\ program\ Q\ using\ B\ processors}{time\ to\ solve\ I\ using\ program\ Q\ using\ P\ processors} \quad (3)$$

where $B \leq P$ and B is the smallest number of processors the program Q could run for the evaluation. We use both $RealSpeedup$ and $RelativeSpeedup^{*}$ in our experimental evaluation in Chapter 6.

In addition to speedup, efficiency is another popular metric used to evaluate parallel systems. It measures the fraction of time for which a processor was efficiently employed (Sahni and Thanvantri, 1995). The efficiency of the system is calculated by dividing the speedup by the number P of processors used to run. Since we used two different definitions for speedup, we also use two different definitions for the efficiency. The real efficiency $Efficiency$ is calculated based on the real speedup (1):

$$Efficiency = \frac{Speedup}{P} \quad (4)$$

Analogously, the relative efficiency $RelativeEfficiency$ can be calculated based on the relative speedup as in Equation (2).

Finally, to measure how the system behaves when we vary the problem size and the number of processors, we use the $scalability$ metric. The ideal scalability is that the execution time remains constant when we multiply the problem size by a factor of F and multiply the number of processors by F.

2.9 Related Work

In previous sections, we argued that to support large-scale computer-based simulations, a SWfMS needs to manage three types of data: execution data, provenance data, and domain data, and we have defined the term provenance database to signify a data repository that contains all of them, jointly. In introduction, we explained that some SWfMSs use a distributed data control based on flat files and some of them use a centralized DBMS at runtime to store one of the three types of data. We also argued that managing a provenance database at runtime enables powerful advantages (Section 2.5). In this section, we are going to mention existing parallel SWFMs in respect to their data management capabilities.

To the best of our knowledge, only Swift/T (Wozniak *et al*., 2013) and Pegasus (Deelman *et al*., 2007) are acknowledged for running on large HPC environments. Swift/T is a highly scalable parallel SWfMS that uses a distributed data management based on flat files and stores provenance data in the end of the workflow execution. Thus, although it is good for performance, its data analytical capabilities, including execution monitoring at runtime and user steering, are limited. Pegasus stores execution data using a centralized DBMS and stores provenance data in flat files, which are loaded into the database in the end of execution. Since it uses a centralized DBMS, it suffers from a contention point. Moreover, since it does not store the other two types of data at runtime, its analytical capabilities and interactive execution are also limited.

For this reason, since SCC is the only existing SWfMS that manages a provenance database (composed of the three types of data – Section 2.5) at runtime using a DBMS, it is the only SWfMS that must be concerned about efficient mechanisms for capturing these data at runtime to enable the mentioned advantages and to keep good efficiency. We highlight that although SCC is directly related to this work, we do not mention it in this section. Instead, we dedicate the next chapter for it (Chapter 3). Several previous works from our research group have already surveyed with more details other existing SWfMS that enable provenance data analyses (mostly in the end of workflow execution). Some of these works are reported by Ogasawara (2011), Oliveira (2012), Dias (2013), and Silva (2014).

3 SCICUMULUS/C²

SciCumulus/C (SCC) (Silva *et al*., 2014) is a parallel Scientific Workflow Management System (SWfMS) developed by the High Performance Computing and Databases research group[4] at COPPE/Federal University of Rio de Janeiro and at Fluminense Federal University. It is based on a collection of works from many researchers, undergraduate students, and masters' and PhD's theses. Essentially, SCC was developed to benefit from the results of two main initiatives: SciCumulus (Oliveira *et al*., 2010) and Chiron (Ogasawara *et al*., 2011; Ogasawara *et al*., 2013). Chiron is a parallel workflow execution engine that takes advantage of clusters and grids. SciCumulus utilizes the main characteristics and algorithms of Chiron and adds special techniques to take advantages of cloud properties, such as elasticity, at runtime (Oliveira, 2012). SCC aims at integrating Chiron and SciCumulus in order to propose a more flexible parallel SWfMS that takes advantages of a wider variety of HPC environments (Silva *et al*., 2014). To the best of our knowledge, they are the only current parallel SWfMS that stores the three types of data jointly on the same Provenance Database (Section 2.5). We use most of the core concepts introduced in Chiron, we keep the special algorithms that take advantage of cloud environments introduced in SciCumulus, and use the most recent version of SCC, which integrates them all, to serve as a basis for our work. For this reason, the most important concepts of these systems that are for particular interest for this dissertation are explained in this chapter.

3.1 SciWfA: a workflow algebra for scientific workflows

SCC manages a scientific workflow and the data that flows between each activity that composes a workflow. We argue that scientific workflows in large-scale computer-based experiments are data intensive, require HPC (as seen in Sections 2.1 and 2.2, and should not miss relevant optimization opportunities, especially in parallel executions (Ogasawara *et al*., 2011). To cope with this, Ogasawara *et al*. (2011) propose an algebraic approach that facilitates complex dataflow definition, parallel data management of the data that flows between activities, and enables optimizations of scientific workflow executions at runtime. The *Scientific Workflow Algebra* (SciWfA) is an extension of the well-established relational algebra, which is the basis for query processing and optimizations in relational database systems (Özsu and Valduriez, 2011).

[4] hpcdb.wordpress.com

In SciWfA (Ogasawara *et al*., 2011), each activity $Y_k \in \{Y\}$ is associated to an algebraic operator ϕ. Where $\{Y\}$ is a set containing all activities in a determined workflow and $\phi \in \{SplitMap, Map, Reduce, Filter, SRQuery, MRQuery\}$. Moreover, Y_k consumes a set (or relation, as it is traditionally called in relational algebra) R_i of input tuples and produces a set R_o of output tuples. The operator ϕ may also need an additional operand o. Hence, we may state that

$$R_o \leftarrow \phi(Y_k, o, R_i) \quad (5)$$

Additionally, the algebraic operator ϕ is defined depending on the ratio between the number of tuples consumed and produced for a determined activity invocation, as we can see in Table 1.

Operator	Type of Operated Activity	Additional Operands	Ratio between consumed and produced tuples
Map	Application	Relation	1:1
SplitMap	Application	File Reference or Relation	1:m
Reduce	Application	Set of aggregating attributes or Relation	n:1
Filter	Application	Relation	1:(0-1)
SRQuery	Relational Algebra Expression	Relation	n:m
MRQuery	Relational Algebra Expression	Set of Relations	n:m

Table 1 – SciWfA operations (adapted from Ogasawara *et al*., 2011)

The ratio between consumed and produced tuples is calculated based on the cardinality (*i.e*., number of tuples) of the consumed input set and produced output set. This means that in a workflow execution, a same application is invoked multiple times each of which consuming a tuple (or set of tuples) and generating a tuple (or set of tuples) (recall from Section 2.3). However, these applications that are invoked and managed by SCC are usually made by third party companies or institutions that are not necessarily aware of SciWfA. As a consequence, each invocation may not produce the necessary output tuples, which are very important for the provenance gathering mechanism and to serve as input for the next linked activity. For this reason, the SciWfA relies on the definition of an important concept called *activation*.

3.2 Activation and Dataflow strategies

According to Özsu and Valduriez (2011), an activation is "the smallest unit of sequential processing that cannot be further partitioned", *i.e*., cannot be further parallelized. In Chiron,

the core of SCC, an activation can be simplified as an activity invocation. Further, Ogasawara *et al*. (2011) explain that it is a "self-contained object that holds all information needed to execute a workflow activity at any core" on the HPC environment. That is, it contains which application to invoke, which data to consume and what the schema of the data that will be produced is.

Moreover, due to the reasons mentioned in Section 3.1, the concept of activation in SCC is more than an activity invocation. It is necessary to define sub-concepts inside of it. These are *instrumentation*, *invocation*, and *extraction* that altogether form an activation (Ogasawara *et al*., 2011). Before the workflow execution, users define the data schema of the input and output relations of all activities in the workflow. In instrumentation, input tuples are extracted and the application invocation is prepared according to the defined input schema. An invocation launches an application on a processor in the HPC environment, consuming the input tuples defined in instrumentation and produces output tuples. Finally, in extraction, produced output tuples are collected. Provenance data are gathered since the beginning until conclusion of an activation. Typical gathered provenance data aids the scientists to answer, in a high level of details, questions like: Is an activation still running? Has any error occurred? If yes, which errors? How long did an activation take to completely execute? More importantly, since different values for domain-specific parameters (*e.g*., speed of wave – seismic – or point of the sky – astronomy) may impact of application performance or even may introduce application errors, all those provenance data can be associated to domain-specific input and output data. This enables rich analyses at runtime and execution monitoring (Oliveira *et al*., 2014; Souza *et al*., 2015). The formal definition of an activation and its composing parts can be found in (Ogasawara *et al*., 2011).

Regarding dataflow strategies, there are two in SCC: *First Tuple First* (FTF) and *First Activity First* (FAF) (Ogasawara *et al*., 2011). To explain this, we use a simple workflow example: two activities A_1 and A_2, being A_2 dependent on A_1. In FTF, an A_2 activation only waits until its necessary input tuples are produced by an A_1 activation. This is a typical pipeline dataflow. In contrast, in FAF, A_2 only begins to execute when all A_1 activations are completely executed. In other words, A_2 remains blocked until A_1 finishes. We only used the FAF strategy in our experiments as in almost all experiments executed in SCC (Chapter 6).

3.3 Centralized DBMS

SCC relies on a centralized DBMS to manage its Provenance Database. Although this brings powerful advantages as mentioned in Section 2.5, this also leads to some drawbacks. We highlight five disadvantages, especially comparing with the utilization of a DDBMS.

First, a centralized DBMS introduces a single point of failure in the parallel system. That means that if the node that hosts the DBMS fails, the entire system fails. Second, if compared with a DDBMS, it cannot handle a large dataset as efficiently as a DBMMS. Third, it does not have special algorithms or techniques to take advantages of parallel execution on multiple nodes in an HPC environment. Forth, a centralized DBMS is not as scalable as a DDBMS. Finally, a DDBMS can handle a higher number of requests from clients than a centralized DBMS. However, it is important to notice that despite the drawbacks, a centralized DBMS uses less computing resources than a DDBMS, since only one node is necessary whereas in a DDBMS, generally, the greater the data size, access rate, or availability requirements, the more nodes are required to keep latency low and the system available.

3.4 Architecture and Scheduling

SCC's architecture is organized in a distributed fashion consisting of multiple nodes, which we especially call SciCumulus Nodes (SCN). The core of SCC is instantiated on each SCN, where the scientific workflow is effectively executed. The architecture is managed following a master-slave policy. The master node manages the distribution of activations among all SCN. Moreover, the master node is also an SCN node, which means that it also runs activations, but it will not need to send MPI messages to get tasks, since tasks are just one hop away from the database, and not two, like the other SCNs that are not masters. In addition to managing activations distribution among all SCN, the master node is also responsible for storing data in the Provenance Database. All slaves are connected to the master via a network interconnect and all SCN access a shared disk. We note that there may be bottlenecks at the master node due to a centralized management at a single site and due to the fact that the master node is the only SCN enabled to access the provenance database. Furthermore, a database server is utilized to host the DBMS that manages the Provenance Database. This architecture is illustrated in Figure 5.

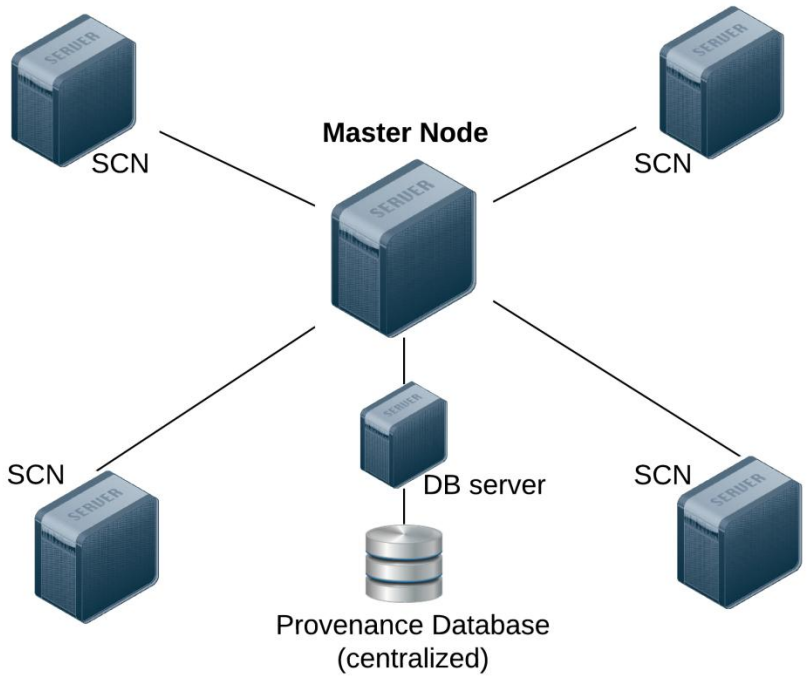


Figure 5 – SCC architecture

Regarding activations scheduling, SCC implements a CWQ BoT architecture and tasks scheduling (recall from Section 2.4.1). Basically, master node is the only one that can access the BoT (which is managed by a DBMS) to retrieve tasks and distribute them among slaves. More specifically, it works as follows. The master node waits for requests from slaves. A slave requests work and waits until the master sends an activation. Then, the master accesses the database to retrieve the next activation that is ready to be executed. Following, the master sends a massage containing the activation to the requesting node. The requesting node receives the activation, executes it, and sends the master a feedback message containing provenance data about the execution. Finally, the master receives the sent data, stores them in the database, and waits for new requests. The execution finishes when all activations from all activities are completely executed and provenance data of each individual execution is stored. SCC is implemented in Java and utilizes MPJ[5] (MPI for Java) for message passing among all nodes in the cluster and Java built-in threads[6] for concurrent programming in the shared-memory architecture within each node.

Concerning software architecture, SCC is organized in four modules (Silva *et al*., 2014). (i) SciCumulus Starter (*SCStarter*) – which facilitates workflow execution submission on HPC environments. Common actions include automatic preparation of all machines that

[5] http://mpj-express.org
[6] http://docs.oracle.com/javase/tutorial/essential/concurrency/procthread.html

will be used during execution (*e.g.*, VM instantiation in a cloud environment), conceptual workflow insertion into the database, and instantiation of the workflow execution engine on each machine; (ii) SciCumulus Setup (*SCSetup*) – which is used to insert, update or delete conceptual workflows into or from the provenance database; (iii) SciCumulus Core (*SCCore*) – which is the main module. It concretizes the conceptual workflow. It contains the main SCC logic, including runtime optimizations based on the SciWfA (Ogasawara *et al.*, 2011), fault tolerance (Costa *et al.*, 2012), intra-node parallelism taking advantage of shared-memory architecture within each machine, adaptive execution (Oliveira *et al.*, 2010), and so on. This is the module that is effectively instantiated on each `SCN`; and finally (iv) SciCumulus Query Processor (S*CQP*) – which aids users to submit SQL queries to the provenance database. Although users can connect to the DBMS via other means (such as the ones provided by the DBMS itself), this module simplifies the database connection so analytical queries can be conveniently submitted to the provenance database by users. Queries results are returned to users' standard output, which can be redirected to semi-structured files (*e.g.*, CSV) and consumed by services that plot graphs to facilitate data visualization. These are the main features, functionalities, and characteristics of the parallel WFMS we base this dissertation on.

4 BAG OF TASKS ARCHITECTURES SUPPORTED BY A DISTRIBUTED DATABASE SYSTEM

In this chapter, we propose our main theoretical contribution. We propose two conceptual distributed architectures for a BoT that relies on a Distributed Database Management System (DDBMS). We define these architectures' tasks scheduling, load balancing, fault tolerance, and other issues. In Section 4.1, we propose a novel design of a BoT application. It is a high level tasks distribution design and scheduling in a BoT application and does not depend on a DBMS. However, it serves as inspiration and basis for our architectures that rely on a DDBMS. In Section 4.2, we briefly introduce and explain the two architectures. In Section 4.3, we discuss common characteristics between them. In Section 4.4, we define the first architecture and, in Section 4.5, the second.

4.1 Work Queue with Replication on multiple Masters

Before introducing our architectures proposal, we first propose a novel task distribution design and scheduling of a BoT application. Although this does not depend on a DBMS, we will show that it serves as an inspiration and basis for our actual architectures proposal.

We begin this proposal by enumerating advantages and disadvantages of two designs studied in Section 2.4: Work Queue with Replication (Section 2.4.2) and Hierarchical Work Queue (Section 2.4.3).

WQR advantages
i. It May achieve higher performance than the simple CWQ (Silva *et al*., 2003); ii. Comparing with CWQ and HWQ, it has better use of data locality (Paranhos *et al*., 2003; Anglano *et al*., 2006). In WQR, the necessary data is likely to be locally stored, which does not occur in CWQ and HWQ; iii. Higher availability than simple CWQ and HWQ because of the replicas; iv. No task transmission between master and slaves; v. Ability to accommodate large problems when partial replication is used.
WQR disadvantages
i. Communication bottleneck may occur due to centralization at the master node; ii. If partial replication is used, choosing the victim node for work stealing needs to be carefully evaluated because it may lead to communication overhead; iii. If partial replication is used, there may exist tasks transmission (work stealing) among slaves; iv. Single point of failure at the central node.
HWQ advantages

i. Multiple masters lead to less congestion at a centralized node; ii. If M and S are *wisely* chosen, congestion at the central node is avoided; iii. HWQ may accommodate larger problems (Silva and Senger, 2011).
HWQ disadvantages
i. HWQ model does not take as much advantage of data locality as WQR; ii. HWQ has single points of failure; iii. There is task transmission in both levels of the hierarchy. That is, between supervisor and masters and between masters and slaves. iv. There is an added layer of bureaucracy between the slaves and the main owner of the BoT. That is, compared with a one-level hierarchy (*e.g.*, CWQ), more communication is needed so a slave can reach a task; v. To the best of our knowledge, there is not an optimal general method to find M and S, even statically. As a result, the choice remains empirical; vi. Computation load balancing is not clearly specified; vii. Single point of failure at the central node.

Table 2 – A summary of the advantages and disadvantages of both WQR and HWQ.

Given these facts, we can combine characteristics of replication and hierarchy to propose the *Work Queue with Replication on multiple Masters* (WQRM). In WQRM (Figure 6), there are M masters and σ slaves in the cluster. The number σ of slaves in the whole cluster is given by the sum of all slaves in all clusters c_i. That is:

$$\sigma = \sum_{i=1}^{M} S_i \tag{2}$$

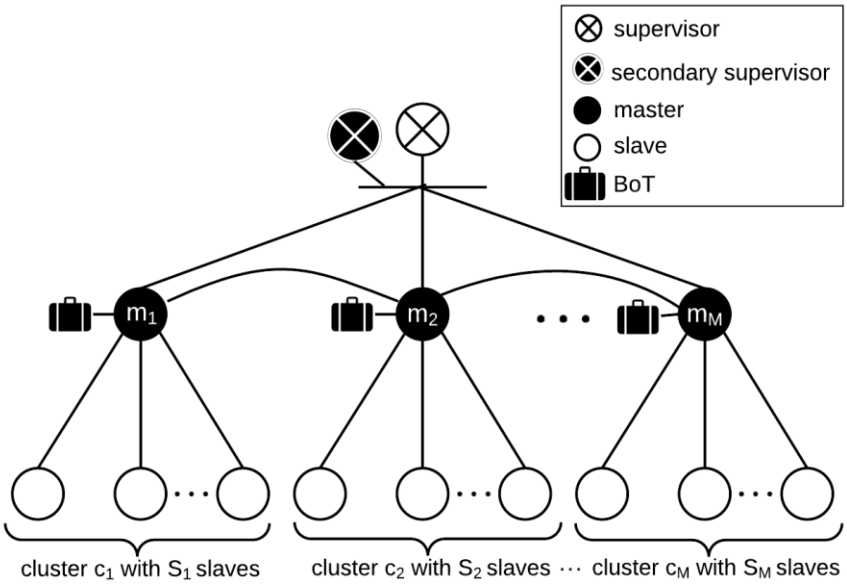


Figure 6 – Work Queue with Replication on Masters design.

Like in WQR, the supervisor does not own the bag of tasks. Instead, the BoT is replicated in all masters. This increases availability because if a master fails, another master may own the failing portion of the BoT and the supervisor coordinates the failure recovery. Identically to WQR, between master nodes and the supervisor there are only scheduling messages, *i.e.*, no task transmission. Each cluster c_i works exactly like the CWQ, that is, there is task transmission between a master and slaves. Just like in WQR with partial replication, when one master node ends its portion of the work queue and becomes idle, the supervisor helps calculating whether or not it is advantageous to ask the idle master to steal tasks from a victim busy master.

Regarding availability, failure recovery strategies may be applied in the slave nodes by taking advantage of replication (Anglano *et al.*, 2006). In addition, to provide higher availability, the secondary supervisor's role is just to eliminate a single point of failure. That is, if the main supervisor fails, the secondary supervisor takes its place.

Regarding advantages and disadvantages in WQRM:

a) From WQR, in respect to the advantages, WQRM inherits most of them. Only the advantage (iv) is not fully given because even though there is no task transmission between supervisor and masters, there is between masters and slaves. In respect to the disadvantages, all of them are inherited. However, since there are many masters, contention in a single centralized point is less likely to occur, like in the hierarchical model.

b) From HWQ, the only inherited characteristic is having multiple masters, which is its greatest advantage. For his reason, in respect to the advantages, WQRM inherits all of them. In respect to the disadvantages, (i) still remains because WQRM only takes advantage of data locality between masters and the supervisor (just like slaves and master in WQR). This is useful for work stealing among masters, but not useful for scheduling tasks among slaves. Moreover, disadvantage (v) is still an open problem. All other disadvantages are canceled because of replication, addition of a second supervisor, and work stealing among masters.

By proposing WQRM, we want to add an extra option to the existing BoT designs (Section 2.4) so that we can choose among them which we will use as inspiration and basis for our architecture that relies on a DDBMS, which will be responsible to hold the BoT. It is important to avoid communication bottleneck due to centralization, which motivates us to choose a design with multiple masters (managers of the BoT). Especially, a design based on replications has many advantages that we are very interested in. For this reason, we decide to

choose WQRM, which combines advantages of replication and hierarchy (specifically, multiple masters). Therefore, among the four tasks distribution designs previously presented (CWQ, HWQ, WQR, and WQRM), we choose WQRM so our architecture supported by a database system will be based on. In next section, we discuss two architecture alternatives and explain which one we choose to implement our solution.

4.2 Brief introduction to Architectures I and II

Most BoT implementations found in literature do not utilize a database system (Silva *et al*., 2003; Anglano *et al*., 2006; Silva and Senger, 2011). For this reason, we need to highlight three important motivations for using a DBMS, a distributed DBMS in special, in a BoT problem.

The primary motivation for using a DBMS in our architecture (in a SWfMS context) is that in a workflow execution, lots of data are continuously managed in a fine grained level as data are processed all over the dataflow. Thus, by using a DBMS, it is possible to query complex experiments' execution logs, perform advanced data analyses, as well as enable humans to interact with the remaining tasks to be executed through updates on the database, everything during runtime, as we have argued in Section 2.5. We do not want to abdicate these powerful advantages.

The secondary, but also very important, motivation for using a database system is that most DBMSs implement very efficient mechanisms that are essential in a HPC scenario. For example, any DBMS implements efficient concurrency control mechanisms. Especially, most relational DBMS (including the centralized ones) implement well-known algorithms and strategies to guarantee atomicity, consistency, isolation, and durability in transactions. Moreover, distributed database systems enable robust parallel access and storage of data, usually in larger sizes than regular centralized DBMS. Further, sharding, *i.e*., partitioning the database into multiple nodes is also well-studied and implemented in many distributed DBMSs. Besides, failure recovery is also an important functionality in a DDBMS. Furthermore, efficient utilization of cache memory is also a common feature in DBMSs, including centralized ones (Özsu and Valduriez, 2011). Additionally, a DBMS (either centralized or distributed) may be implemented to run completely in-memory instead of performing I/O operations to disk, which would enhance performance. Therefore, having a DBMS – which already implement most of these mechanisms usually very efficiently – to take care of all these complex issues, will alleviate the effort on developing such complex

controls in a given parallel application. In this way, the developers would focus on specific concerns that are related to specific uses of the application, instead of having to worry about implementing tasks scheduling and dealing with complex concurrency issues. In our case, we want to focus on controlling the parallel execution of workflows and store important data in the provenance database.

The tertiary motivation specifically relies on a *distributed* database system. In addition to the above arguments regarding the utilization of a distributed database system, there is still the fact that, by using one, we can take more advantage of the parallel hardware architecture, which is common in HPC environments. Furthermore, a centralized database system will likely suffer from congestion in a scenario with many processing nodes. For these reasons, a distributed database system is more convenient in an HPC scenario.

In next sections, we describe two architectures, based on WQRM design, supported by a distributed database system: **Architecture I**, which uses WQRM by making an analogy between masters and data nodes; and **Architecture II**, which has many similarities with Architecture I, but has different number of partitions and data nodes.

4.3 Common Characteristics

Similarities and differences between Architectures I and II are in respect to the work queue. In common, the work queue is managed by a distributed database system and it is fully partitioned, that is, horizontally fragmented across all nodes in the cluster of database nodes. This significantly increases parallelism (Özsu and Valduriez, 2011). Moreover, regarding availability, both architectures share the same characteristics inherited from WQRM design. Yet, if a node hosting a work queue partition fails, there is still at least an extra replica that may be utilized.

Although inspired by WQRM and many analogies will be made to explain both architectures, WQRM and the architectures are not exactly one-to-one analogous. The architectures do not explicitly have multiple master nodes functioning as schedulers. We may, rather, establish the DDBMS (as a whole) as a great “centralized” scheduler, which implies a similar behavior to CWQ.

Nonetheless, instead of having slaves requesting tasks to a master through regular message passing, like in common CWQ implementations, we have slaves sending structured queries to a distributed database system. Instead of having a master to receive the slave

request, get the next ready task and send it to the slave, we have the DDBMS to play the very same role.

In spite of the fact that the message passing primitives (*e.g.* *send* and *receive*) are basically the same in either implementations (common CWQ implementation or DBMS supported implementation); and that data transfer happens in a similar way, the main advantage is that we rely the scheduling on a third party system. That is, we apply the idea of outsourcing. More importantly, this third party system we rely on is known to be specialized in concurrency control mechanisms (Özsu and Valduriez, 2011). Furthermore, all benefits we pointed out in our secondary motivation in the beginning of this section are applicable. Thus, we count on a trusted and highly specialized third party system to alleviate our work so we can spend more efforts on the actual application.

Despite noting a CWQ behavior resemblance, we emphasize that a DDBMS is utilized instead of a single central node, as it is in CWQ. In other words, there is not a centralized single master at all. A DDBMS is composed of many data nodes which diminishes the centralization problem that causes congestion in CWQ. We use the term *data node* (*dn*) to signify a node that hosts the process that manages partitions of the database. A data node also contains data of the DDBMS. In other words, a data node owns and manages part of the bag of tasks. This also resembles the fact that multiple master nodes hold BoTs in the WQRM design.

It is important to highlight that since we are relying on a database solution, a new role takes place in the scenario: the database server, which we shorten as `dbs`. Database servers just listen to connections and applications commonly connect to the database through connection drivers (*e.g.*, JDBC or ODBC[7]). Even though the `dbs` are usually just responsible for listening to connections, they may play an important role regarding communication load balance. Some distributed DBMSs implement mechanisms to improve communication load balance so contention at the database may be avoided, which is very valuable for us. However, the presence of a new role introduces a new problem that we need to deal with because of the database utilization. There is a need to determine a good number of `dbs` in the cluster, which may also be empirical. We denote this number by q.

Furthermore, an initial connection distribution is needed. That is, each slave needs to know in advance which `dbs` it will connect to. A supervisor node needs to take care of this. Plus, it is important to even up communication load across the q `dbs`. Otherwise, there may be

7 http://en.wikipedia.org/wiki/Java_Database_Connectivity and http://en.wikipedia.org/wiki/Open_Database_Connectivity

a `dbs` with a heavy load of slaves connecting to it while there are others lightly loaded. This communication load balance may be easily achieved by making use of a circular distribution policy, as we show in the algorithm proposed in Section 4.4.4. Next, we describe both architectures in details.

4.4 Architecture I: Analogy between masters and data nodes

Just like there are *M* masters in WQRM, there are *M* data nodes in Architecture I (Figure 7). In next sections we will explain the scheduling process, which consists of slaves querying the data nodes in order to retrieve tasks (analogous to slaves asking masters for work).

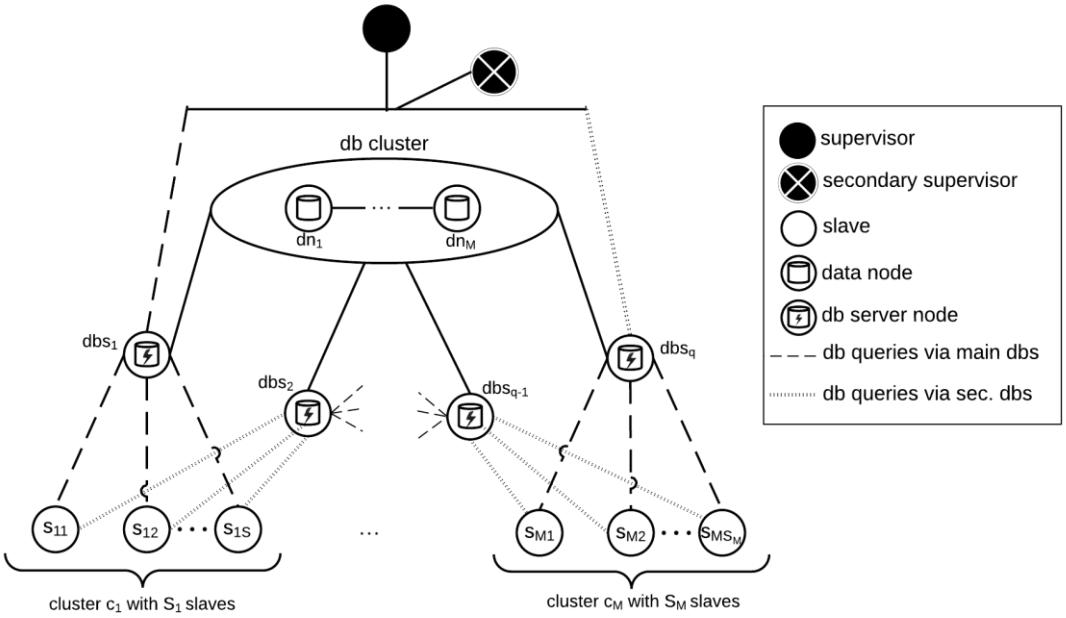


Figure 7 – Architecture I: Master nodes are data nodes

Furthermore, to increase availability in the system, each slave S_{ij} may connect and query the database cluster via two different `dbs` nodes: the main `dbs` node connection, represented by dashed lines in Figure 7 and the secondary `dbs` node connection, represented by dotted lines. If one `dbs` fails, all slaves that were connected to it just need to connect to their secondary `dbs`.

4.4.1 Parallel data placement

Regarding parallel data placement in the database system (recall from Section 2.6.3), the whole work queue is horizontally fragmented into *M* (number of data nodes in the cluster)

partitions. Each partition ρ_i is responsibility of and physically stored in dn_i and replicated elsewhere. Each partition ρ_i initially contains $T = ceiling(T_{total}/M)$ tasks, where T_{total} is the total number of tasks in the BoT. To place T tasks in each partition, a hash function on the data node *id* may be applied.

4.4.2 Task distribution and scheduling

This is how initial task distribution happens in this architecture. Initially, given that there are M data nodes, the supervisor is responsible for assigning each task to a data node in a circular fashion. This is done inserting tasks in the work queue relation in the database assigning the data node *id* to the task and the hash function mentioned previously (Section 4.4.2) will take care of placing the task in the right data node. Similarly, the supervisor also assigns a data node to each slave node so that each slave will know which data node will be queried.

It is worth noting that only in close-to-homogeneous problems (that is, all tasks cost approximately the same), the static initial distribution will provide near to optimal load balance. In heterogeneous problems, though, this initial distribution needs to be dynamically "corrected" during runtime. However, even in homogeneous problems, load imbalance may still occur in very long running executions. Thus, work stealing and more sophisticated load balancing may still be needed.

After all initial task distribution and data placement, the actual scheduling begins and it works similarly to what we described for the CWQ (recall from Section 2.4.1). A *slave* sends a query to retrieve tasks from its partition which is physically stored in dn_i and replicated elsewhere. The DDBMS is responsible for an efficient concurrent management from the multiple requests and then it delivers the right tasks to the requesting slave. The requesting slave becomes busy while executing its tasks. When a slave finishes its work load, it stores the results in the provenance database. Then, it becomes idle and ready to retrieve more tasks from the database. This is done until all tasks in the bag of tasks are completed.

4.4.3 Load balancing

Load balancing happens analogously as specified in WQRM. When all tasks in a data node are completed, a slave notifies the supervisor of the situation. Then, the supervisor calculates whether or not work stealing is advantageous. If it is, a victim data node must be selected. If we use the heuristic of choosing the most loaded data node, we just need to query the database

to easily get this information. Finally, after selecting the victim, say dn_j, the supervisor needs to move data from the partition ρ_j to partition ρ_i.

4.4.4 Algorithm for distributing dbs to achieve better communication load balance

In our architectures, slaves access the distributed database via connection to the dbs nodes. In other words, the dbs are the only nodes that the slaves are aware of to get access to data in the distributed database. A common scenario is when the number of slaves is much greater than dbs nodes and communication load imbalance may occur. If, for example, there are 20 slaves and only 2 dbs nodes, (say dbs_1 and dbs_2) there would be communication load imbalance if 19 slaves connect to dbs_1 e only one slave connects to dbs_2. For this reason, we need extra functionalities to improve communication load balance. To tackle this, we also propose our own algorithm for distributing dbs nodes to all slaves in a balanced way. In our previous example, one balanced way to distribute dbs nodes would be 10 slaves connecting to the DDBMS via dbs_1 and the other 10 connecting via dbs2. Moreover, we also need to assign a secondary dbs_2 for each slave to increase availability in case the primary dbs fails. In other words, each slave has a primary dbs through which it connects to the DDBMS and a secondary dbs that is used if the primary dbs fails.

The algorithm is divided into three parts. In part (i), if a physical machine is both slave and database server, then, this slave machine connects to the distributed database through the database server that is hosted on this machine. In other words, if a machine is both slave and dbs, it assigns itself as the dbs. In part (ii), each slave assigns a dbs to it in a circular fashion. Each dbs can serve at most W/q, where W is the number of remaining slaves to be assigned and q is the number of dbs nodes. In part (iii), each of the W remaining slaves is assigned to a dbs, also in a circular fashion. This algorithm is formalized as shown in Figure 8. In addition to this algorithm, we discuss in Section 5.3 that in our implementation, we may also make use of features provided by the DDBMS to improve communication load balance.

Algorithm 1: Distributing database servers to slaves

Input:
L_{dbs}: List of database server machines
L_w: List of slave machines
Output:
-

```
1.    function distributeDatabaseServers(Ldbs, Lw)
2.       int circular ← 0
3.       int i ← 0
4.       int quotient ←0
5.       int primDBindex ← 0
6.       int secDBindex ← 0
7.
8.       // Part (i)
9.       for each machine in Ldbs do
10.         if exists machine in Lw then
11.            machine.mainDBS ← machine
12.            circular ← circular + 1
13.            remove(machine, Lw)
14.         end if
15.      end do
16.
17.      quotient ← |Lw| div |Ldbs|
18.
19.      // Part (ii)
20.      while i < |Lw| do
21.         primDBindex ← circular mod |Ldbs|
22.         Lw[i].mainDBS ← Ldbs[primDBindex]
23.         if |Ldbs| >= 2 then
24.            secDBindex ← abs ( ( |Ldbs| − 1 − circular ) mod |Ldbs| )
25.            Lw[i].secondaryDBS ← Ldbs[secDBindex]
26.         end if
27.         i ← i + 1
28.         if quotient = 0 then
29.            circular ← circular + 1
30.            exit while
31.         end if
32.         if i mod quotient = 0 then
33.            circular ← circular + 1
34.         end if
35.      end do
36.
37.      // Part (iii)
38.      while i < |Lcn| do
39.         primDBindex ← circular mod |Ldbs|
40.         Lw[i].mainDBS ← Ldbs[primDBindex]
41.         if |Ldbs| >= 2 then
42.            secDBindex ← abs ( ( |Ldbs| − 1 − circular ) mod |Ldbs| )
43.            Lw[i].secondaryDBS ← Ldbs[secDBindex]
44.         end if
45.         i ← i + 1
46.         circular ← circular + 1
47.      end do
48.   end function
```

Figure 8 - Algorithm for dbs distribution to slaves

4.4.5 Advantages and disadvantages

Advantages of using Architecture I are: (i) Assuming that M is *wisely* chosen (recall from Section 4.1) as well as q is good enough, there will be less congestion at the database and parallel query execution may be well explored; (ii) due to utilization of secondary nodes (for master node and for db server nodes) and due to reasons inherited by basing on WQRM, this architecture is able to provide high availability; and (iii) this architecture provides great flexibility for adding slaves, even dynamically during runtime. Everything a slave needs to do to join the executing team is to connect to the DBMS through any `dbs`. Despite being likely unnecessary, a more sophisticated strategy to choose the least loaded `dbs` may be accommodated to preserve communication load balancing. Then, after connecting, the recently joined slave can start executing by following the scheduling policy described previously. Removing slaves is similar to the slave failure recovery process as discussed in the beginning of this section.

The disadvantages of Architecture I are related to scalability problems, which are likely to occur in a scenario with a large M because it will be harder for the DBMS to manage a large number of data nodes. A large number of data nodes means that data will be spread throughout many actual machines. Many distributed DBMSs do not scale data nodes up to a really big number, say hundreds of nodes. In addition, the more partitions, the more it will be taken advantage of parallel executions. However, requiring that each partition needs to be physically stored in each data node implies that many data nodes will be needed in order to achieve greater parallelism. This, as mentioned, may also lead to a scalability problem. Since we want our architecture to be adaptable to a large environment, this is a critical limitation.

4.5 Architecture II: Different number of partitions and data nodes

Architecture II (Figure 9) functions mostly like Architecture I. The main difference is that in Architecture II, we do not force each partition ρ_i to be physically stored in dn_i. This implies that the number of partitions does not need to be equal to the number of data nodes. Rather, the cluster of database nodes is composed of d data nodes and the work queue is partitioned into M partitions.

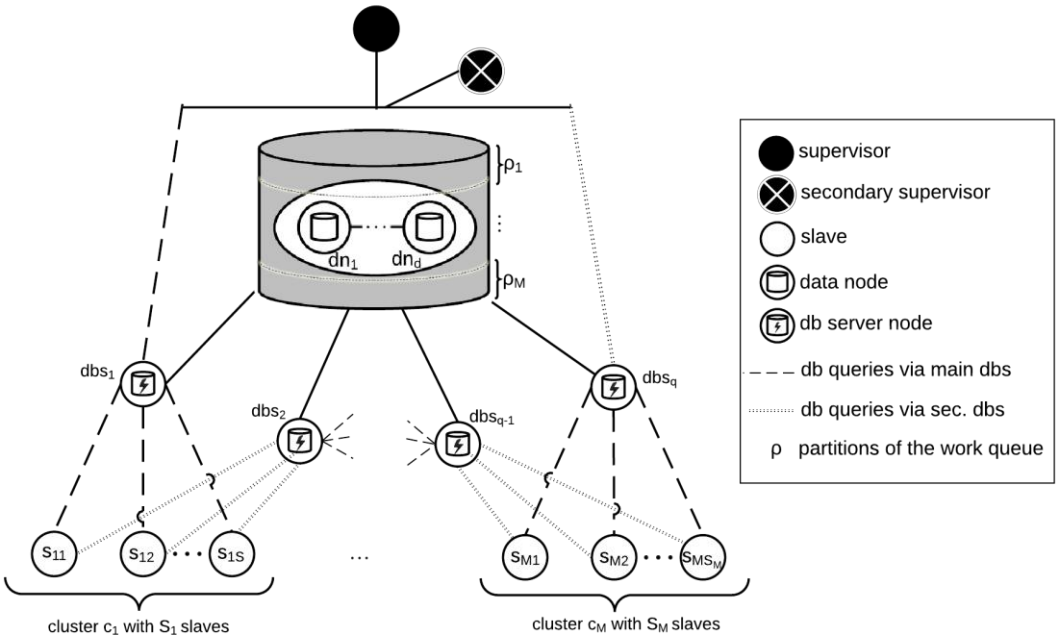


Figure 9 – Architecture II: Analogy between masters and partitions of the work queue

This introduces much more flexibility than in Architecture I, since we may have a greater number of partitions than of physical data nodes. As said previously, more partitions lead to better parallelism. Multiple data nodes are more costly than multiple partitions.

Although more flexibility and generality are given to Architecture II, it introduces one new problem: choosing d. Table 3 summarizes which parameters need to be adjusted in order to achieve good performance.

Parameter	Meaning
d	Number of data nodes in the database cluster
q	Number of `dbs` nodes
M	Number of partitions of the work queue
S	Number of slaves that connect to a dbs node. If q is known, this may be simplified as $S = \sigma / q$. Recall from Section 4.1 that σ is the total number of slaves on the HPC environment.

Table 3 – Parameters that need to be adjusted

In spite of seeming very complex to define all these parameters, a simplification of the problem is presented in Section 5.5.

4.5.1 Parallel data placement

Regarding parallel data placement in the database, the work queue is *fully partitioned* (Özsu and Valduriez, 2011) into M horizontal fragments, or partitions, across all data nodes. Each partition ρ_i initially contains $T = ceiling(T_{total}/M)$ tasks, where T_{total} is the total number of tasks in the BoT. To place T tasks in each partition, a hash function on the partition id may be applied, as in Architecture I.

It is important to highlight that M may be very large in a large-scale scenario. Although it is harder to manage by the DDBMS, this will significantly improve parallelism. Especially, this may cause so much improvement in parallelism that congestion at the DBMS might be highly alleviated. However, it needs to be carefully evaluated (*e.g.*, testing speedup and scalability) to investigate if no overhead will occur.

4.5.2 Task distribution and scheduling

Initial task distribution happens in an analogous way to Architecture I. Initially, given that the work queue is partitioned into M partitions, the supervisor is responsible for assigning each task to partition in a circular fashion. This is done inserting tasks in the work queue relation in the database assigning a partition id to the task and the hash function mentioned above will take care of placing the task in the right partition. Similarly, the supervisor also assigns a partition *id* to each slave node so that each slave will know which partition will be queried.

Load balancing also works similarly to Architecture I. The algorithm proposed for improving communication load balance (Section 4.4.4) is also applied in Architecture II.

4.5.3 Advantages and disadvantages

Finally, the advantages of using Architecture II are the same of Architecture I. In addition, Architecture II is more flexible since it does not require a large number of data nodes (*e.g.* hundreds) to achieve enhanced parallelism. Moreover, Architecture II does not require that the number of data nodes to be equal to the number of slave nodes, removing the main disadvantage of Architecture I. However, Architecture II introduces more complexity since a new parameter needs to be adjusted. This is explored in our experimental evaluation (Chapter 6).

In this section, we proposed two architectures supported by a distributed database system. We described their main ideas, how they would work and discussed the benefits and losses of using each of them. We chose to use Architecture II to implement because it has all advantages of Architecture I and is more flexible. In the next section, we describe how we implemented Architecture II.

5 SCICUMULUS/C² ON A DISTRIBUTED DATABASE SYSTEM

In this chapter, we explain details of the implementation of SciCumulus/C on a Distributed Database System (d-SCC). In Section 5.1, we explain how we chose the DDBMS technology we used. In Section 5.2, we present MySQL Cluster. In Section 5.3, we present the architecture of d-SCC, which is the Architecture II, presented in the previous section, fitting MySQL Cluster's architecture. In Section 5.4, we show an extra module we developed to manage DDBMS issues. In Section 5.5, we describe parallel data placement and fragmentation in our solution. In Section 5.6, we explain how we implemented tasks scheduling and why we removed MPI for this. Finally, In Section 5.7, we discuss fault tolerance and load balancing.

5.1 Technology choice

In order to accommodate either Architecture I or II, presented in the previous section, we need a DDBMS technology. For this reason, we list necessary and desirable requirements.

First, the necessary requirements are: (i) It needs to provide efficient parallel and distributed strategies (parallel query optimization and distributed concurrency control mechanisms); (ii) It needs to be highly scalable – both (i) and (ii) are required because of the distributed DBMS features that Architecture II relies on; and (iii) It has to be optimized for OLTP queries – because multiple short and simple queries based on indexes are very frequently performed in order to retrieve next runnable tasks and to update their status and execution time when they finish.

Second, the desired requirements are: (i) It would be better if it were free licensed – because we do not want to close our solution to a very specific DBMS technology; (ii) SQL/relational model – SQL queries on a relational database with good indexes are known to be efficient for quick and simple lookups, which are very frequent because of the scheduling we described in Chapter 4, hence SQL queries would be desirable; (iii) it should implement strong consistency – because besides retrieving tasks, slaves need to store back results of their executions in the database. Thus, many updates occur at runtime and taking advantage of strong consistency provided by the DBMS is desirable to facilitate our work; and (iv) it should be able to be executed in shared disk architecture – because our motivating problem is mainly focused on complex scientific applications, which are usually executed in very large clusters operating on shared disk architecture Section 2.7)

Given these facts, we build up the following table.

Technology	Relational/SQL	Architecture	License	Main Disadvantage
NuoDB	NewSQL	SN	Very limited free version	License
VoltDB	NewSQL	SN	Proprietary	License
MemSQL	NewSQL	SN	Free trial	License
SparkSQL	SQL	SN	Proprietary	Little support for OLTP
MySQL Cluster	SQL	SN	Open	No support for SD
Oracle TimesTen	SQL	Both	Proprietary	License
Oracle Coherence	KeyValue	Both	Proprietary	License and NoSQL
MongoDB	Document	SN	Open	NoSQL
Impala	SQL-like	SN	Open	SN and OLAP optimized
HBase	Column	SN	Open	SN and little support for OLTP
Presto	SQL-like	SN	Open	SN and little support for OLTP
MonetDB	Column	SN	Open	SN and OLAP optimized

Table 4 – DBMS technologies comparison

In Table 4, we mainly compare the technologies according to our needs previously listed. All of them are said to be scalable and work on a distributed environment, with distribution features. We first eliminate all options that provide little support for OLTP or are mainly optimized for OLAP (online analytical processing), since we are mainly interested in fast transactions rather than heavy analyses during execution. Proprietary technologies are highly discouraged because of the reasons we stated; hence we cross out all DBMS technology with a proprietary disadvantage. This leaves us to choose between MySQL Cluster and MongoDB.

MongoDB is a NoSQL database, document-oriented. In addition to the desired requirement (ii) previously mentioned, the SWfMS we are basing our implementation on utilizes a data model that is essentially relational: PROV-Wf (Costa *et al.*, 2013), as presented in Section 2.5. Because of this, there are many relational queries that are executed

at runtime needed by the execution engine, which is totally based on the provenance database. These queries generally involve both reads and writes, and joins among different relations. NoSQL DBMS are not as concerned about ACID transactions as relational databases are, which commonly implement strong consistent models. We need to keep all those writes consistent, and these kinds of relational queries, involving joins, are better performed by relational DBMS. Finally, one other important aspect is regarding development. Since SCC already relies on a relational DBMS and the entire execution is driven by SQL queries, using a different query language would require much more effort. By using a different DBMS, but still a relational one, we could save lots of effort by just adjusting small differences in specificities of the SQL dialect of this different relational DBMS.

MySQL Cluster is a relational DBMS, OLTP optimized, efficient for fast lookups, provides efficient concurrency control mechanisms, and claims to provide high availability[8] (Oracle, 2015a). Just like most conventional DBMS, it is also possible to execute OLAP queries on MySQL Cluster. Additionally, its fault tolerance mechanisms make it a good choice for removing a single point of failure introduced by using a centralized DBMS. Besides, it is an in-memory database cluster and it tends to be faster than regular on-disk DBMS. However, MySQL Cluster has a limitation for our needs. It does not support shared disk architecture[9]**.** Anyhow, especially because of our limited choices, we gave it a try.

5.2 MySQL Cluster

MySQL Cluster requires three types of database nodes (or roles, as we call): `ndbd`, `mysqld` and `ndb_mgmd`, which is a necessary manager node for MySQL cluster's architecture. The documentation recommends that each of these roles is placed on different physical machines for higher availability purposes (Oracle 2015a). In Figure 10, it is shown MySQL Cluster architecture and how its main components (*i.e.*, the roles) communicate to each other. The main role is the `ndbd` which is responsible for distributing queries, transaction management, and data management. That is, most of the database processing is responsibility of the `ndbd` role. `Mysqld` role basically works as a port through which clients or APIs may connect using connection drivers (*e.g.*, JDBC or ODBC) and issue SQL queries. `Ndb_mgmd` manages the

[8] www.mysql.com/products/cluster
[9] http://dev.mysql.com/doc/refman/5.1/en/mysql-cluster-overview.html

other roles, manage backups, and stores necessary configuration metadata.

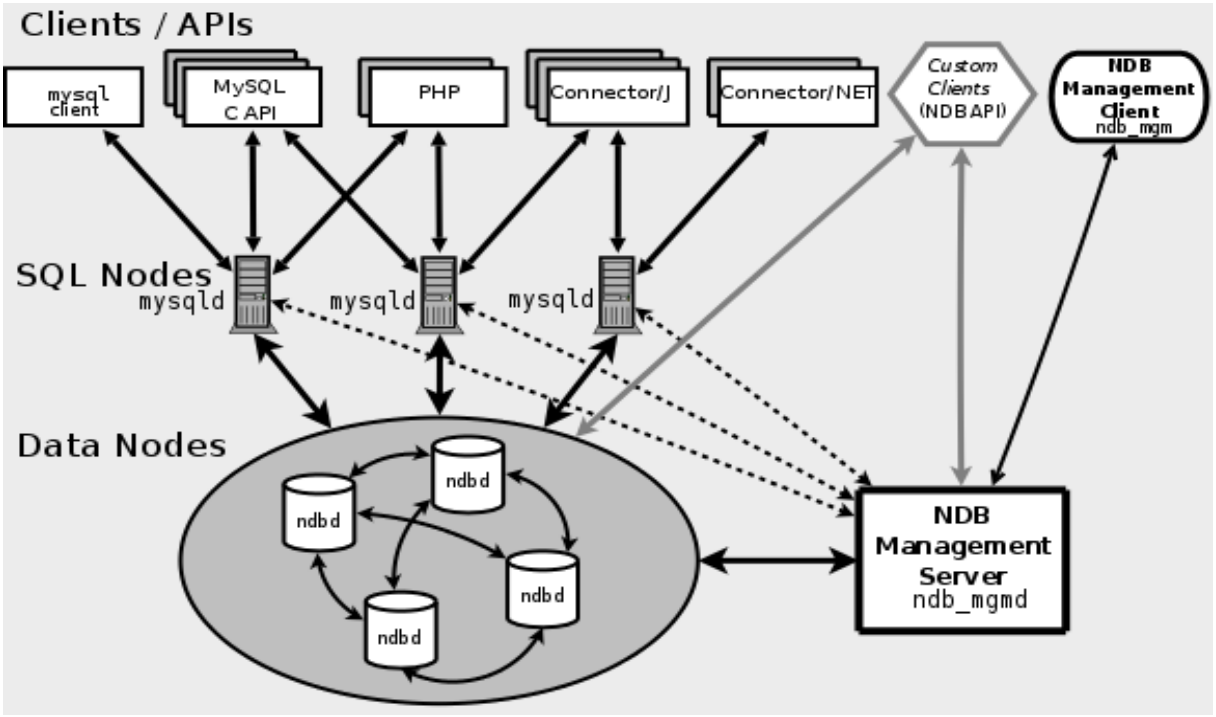


Figure 10 – MySQL Cluster architecture[10]

Database tables in MySQL Cluster need to run using NDB engine so they can be distributed and replicated over all data nodes' memory. As far as we know, full replication is utilized. Even though MySQL Cluster is an in-memory database cluster, it continuously executes check points on disk for failure recovery, even though this feature may be turned off by the user, making it completely diskless. If this feature is turned on, however, even if all database processes are finished or even if the entire cluster shuts down (assuming that the disk will not be damaged), the database will be safely stored on disk. Moreover, we usually save a backup of the database in the end of the workflow execution, enabling *a posteriori* analyses in addition to runtime analyses.

5.3 d-SCC Architecture

To accommodate our Architecture II in MySQL Cluster architecture, we have the data node (`dn`) role and the database server (`dbs`) role in Architecture II analogous to `ndbd` and `mysqld` nodes, respectively. Moreover, MySQL Cluster architecture requires an extra database node, the database manager node (`ndb_mgmd`). We note that a `ndb_mgmd` node in MySQL Cluster architecture is not to be confused with a supervisor node in Architecture II, because the

[10] Figure extracted from http://dev.mysql.com/doc/refman/5.1/en/mysql-cluster-overview.html

supervisor node is responsible for tasks distribution and other functions related to the management of the actual workflow execution; the `ndb_mgmd`, on the other hand, is a requirement for the MySQL Cluster architecture and is responsible for functions related to the management of the distributed database. Furthermore, we highlight that `ndb_mgmd` is not a requirement for our Architecture II. That is, if a different DDBMS is utilized in the future to implement Architecture II, this role does not need to exist. Thus, these are the three roles that compose the distributed database in our current implementation of d-SCC, which relies on MySQL Cluster: `dn`, `dbs`, and `ndb_mgmd`.

In addition to the databases roles, we also have SciCumulus Core Nodes (`SCN`). In a distributed execution, a *SCCore* module is instantiated on each machine that will play SCN role, *i.e.*, that will run the actual execution (recall from Section 3.4). `SCN`s are analogous to slave nodes in Architecture II. Moreover, one `SCN` is chosen to work as the supervisor node. Thus, using the notation introduced in Section 4.1, in an execution, there will be σ `SCN`s in the cluster and one of them will act both as a supervisor and as a slave in our current implementation of d-SCC. The characteristic of having a node to function both as a slave and as a supervisor is inherited from SCC architecture, as explained in Section 3.4. The architecture is illustrated in Figure 11.

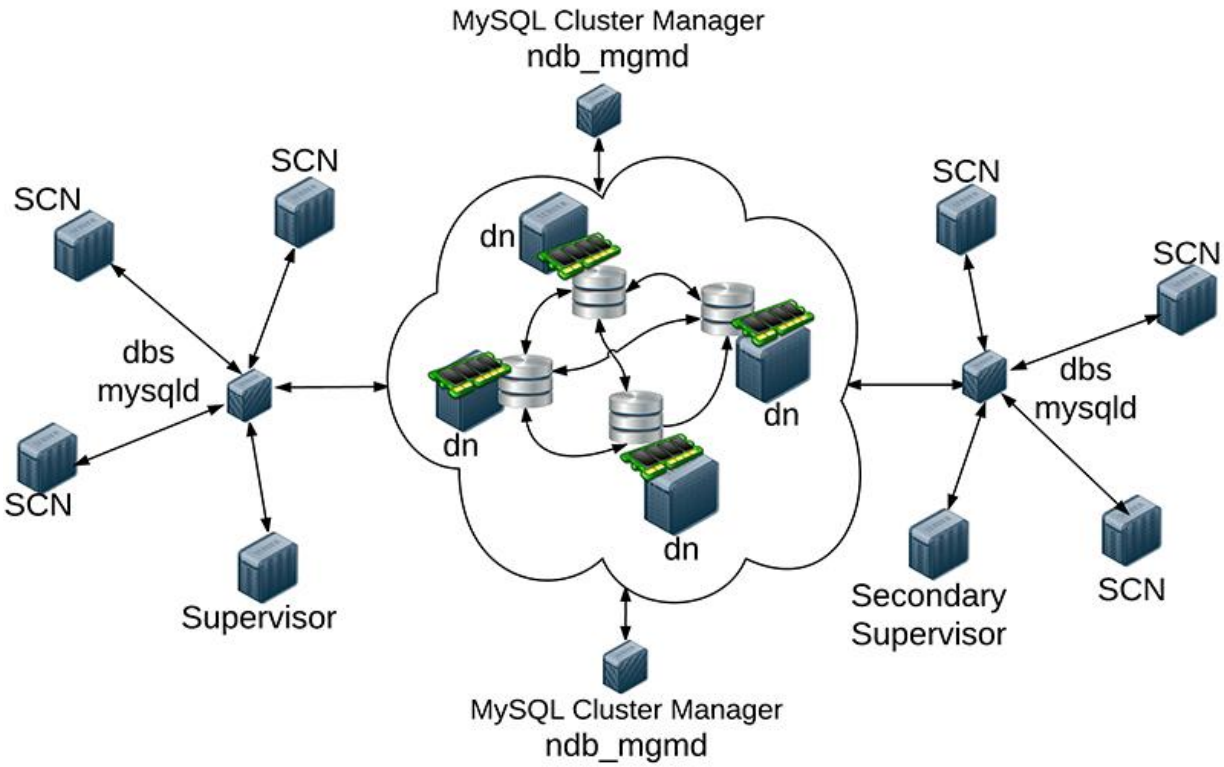


Figure 11 – Current d-SCC architecture: Architecture II accommodating MySQL Cluster roles

Furthermore, in d-SCC, the BoT is completely placed in a distributed table and we make use of MySQL Cluster features to improve communication load balancing[11], in addition to the algorithm presented in Section 4.4.4. We give more details on how we distribute it across all data nodes in Section 5.5

5.4 SciCumulus Database Manager module

As introduced in Section 3.4, SCC software architecture is built upon four modules: *SCStarter*, *SCSetup*, *SCCore*, and *SCQP*. To conveniently manage the distributed database in our solution, we developed an extra module: *SciCumulus Database Manager* (*SCDBM*). In this section, we explain in details our added *SCDBM* module and modifications we needed to adapt.

5.4.1 Pre-installation Configuration

In d-SCC, just like its predecessors, a list of machines on the HPC environment that will be used in the workflow execution needs to be provided. The list is historically saved on a file called `machines.conf` (Figure 12). These machines will compose the architecture and each of them will play one or more roles (`SCN`, `dn`, `dbs`, `ndb_mgmd`) defined in Section 5.3.

```
# Number of processes
10
# Protocol switch limit
131072
# Entry in the form of hostname@port@rank
node1@20919@0
node2@20919@1
node3@20919@2
node4@20919@3
node5@20919@4
node6@20919@5
node7@20919@6
node8@20919@7
node9@20919@8
node10@20919@9
```

Figure 12 – `machines.conf` file example containing 10 machines

[11] http://dev.mysql.com/doc/refman/5.1/en/mysql-cluster-basics.html

Configuring which role each machine will play may impact on performance, as we explain and show in our experimental evaluation in Chapter 6. For this reason, in d-SCC, one important configuration file, which we call `installation.properties`, is needed so users can vary the architecture according to their needs. For example, a tradeoff between performance and available resources needs to be analyzed, since the best performance may demand a lot of computing resources. In `installation.properties`, users define values for the parameters described in Table 3 from Section 4.5.1. More specifically, users need to define three parameters: d (= number of `dn`), q (= number of `dbs`), and the number of management nodes (`ndb_mgmd`).

After defining these three values, next step is to define which roles the machines may accumulate. That is, to save resources, one may want each machine to play more than one role. We divide this role accumulation concept into two types of accumulation: `SCN` and database nodes.

For `SCN` accumulation, users define which database roles (*i.e.*, `dn`, `dbs`, and `ndb_mgmd`) a *SCCore* instance will play together with. For example, suppose we have 10 machines available and we want all of them to play `SCN` role (*i.e.*, to actually execute the workflow). However, we need at least 3 roles for the database (`dn`, `dbs`, and `ndb_mgmd`). In this scenario (10 `SCN`, 1 `dn`, 1 `dbs`, and 1 `ndb_mgmd`), we need to indicate that we want machines that will play `SCN` role will also play `dn`, `dbs`, and `ndb_mgmd`. This means that three machines will play two roles concurrently. On the one hand, this saves resources and more *SCCore* instances can run hence more parallel execution; on the other hand, in three machines at least two processes will compete for resources (especially memory and processor), which may interfere in performance, as we discuss in our experimental evaluation (Chapter 6). Obviously, users are able to indicate that each *SCCore* instance will run dedicatedly, *i.e.*, machines that play `SCN` role are not going to play database role.

For database nodes accumulation, users may want to indicate that a machine that plays one of the database roles (`dn`, `dbs`, and `ndb_mgmd`) may accumulate more database roles. In our exemplary scenario (10 `SCN`, 1 `dn`, 1 `dbs`, and 1 `ndb_mgmd`), we may want `dbs` and `ndb_mgmd` roles to be played by the same machine, consequently the `dn` role will be played dedicatedly by a different machine. We may combine both accumulation types to indicate which of the four roles will be dedicated or will be concurrently played within a machine. This brings flexibility to build the architecture according to the users' interest. We vary the

architecture configuration and measure performance impact using these concepts in our experimental evaluation in Chapter 6.

Currently, it is only possible to define the parameters d (= number of `dn`), q (= number of `dbs`), the number of management nodes (`ndb_mgmd`), and which roles will be accumulated or dedicated. Although it may easily be changed, it is not possible to define the parameter σ for the number of `SCNs`. Instead, this number is derived from all previous definitions. For example, if, in a scenario of 10 available machines, we define 1 `dn`, 1 `dbs`, and 1 `ndb_mgmd` and we define that all database roles and all `SCN` will be dedicated, 3 machines will play one database role each. Consequently, there will be 7 `SCNs`.

In addition to roles played in the architecture, users may also indicate which parallel hardware architecture (either shared disk or shared nothing) the distributed database will be installed on. We have claimed in Section 5.1 that MySQL Cluster does not support shared disk. However, due to reasons we argued in Section 2.7, we want our solution to be able to run on shared disk hardware architecture. For this, we needed a workaround: each database role (`dn`, `dbs`, and `ndb_mgmd`) runs a process that only accesses a separate and independent directory on the shared disk. The consequences of this workaround may be neglected if users utilize the distributed database in totally in-memory mode. Otherwise, MySQL Cluster continuously writes logs on disk for failure recovery. Even in this scenario, performance should not be significantly impacted since the most important database processing (*i.e.*, queries execution and distributed transaction management) occurs in-memory. If dedicated specialized shared disk hardware (*e.g.*, SAN) is used, this workaround impact can be neglected. We highlight that this discussion is only a concern if the hardware architecture requires shared disk. If, otherwise, shared-nothing clusters or clouds' VMs are used, this discussion may be completely neglected. In this case, user simply needs to set the parameter `is_shared_disk_installation` to *false* in `installation.properties` file. In Figure 13, a typical shared disk installation is shown. In this example, each $\texttt{dn}_i$ saves data in `/root/mysql/nodes/datanode/`<*i*>, where $i = [0..d]$

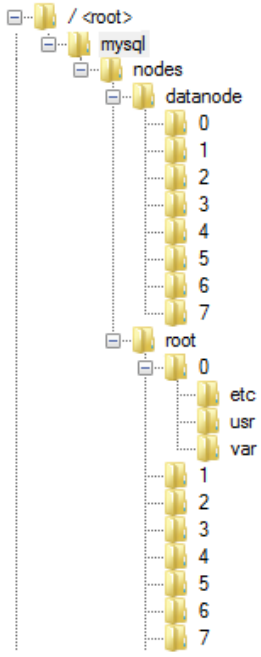


Figure 13 – Example of a directory tree in a shared disk installation

One other important file that users need to be concerned about is MySQL Cluster's initial configuration file (`config.ini`), which is used to define many important configuration parameters[12]. Currently, we specifically determine values for the following parameters (Table 5).

[12] https://dev.mysql.com/doc/refman/5.0/en/mysql-cluster-ndbd-definition.html

Parameter	Meaning
`DataMemory`	It defines the amount of space (in bytes) available for storing database records. The entire amount specified by this value is allocated in memory.
`IndexMemory`	This parameter controls the amount of storage used for hash indexes in MySQL Cluster. Hash indexes are always used for primary key indexes, unique indexes, and unique constraints.
`Diskless`	When set to true, this causes the entire distributed database to operate in diskless mode; hence there will be no disk checkpoints and no logging. Such tables exist only in main memory. As a consequence, the shared disk discussion above may be neglected, but tables would not survive a catastrophic crash and data would be lost after execution if a backup is not saved on disk for *a posteriori* analyses.
`NoOfReplicas`	It defines how many replicas the database will have. Replicas reside in memory. A common value is 2, but if 1 is used, a data node failure causes the entire distributed database to fail. Thus, value 1 is not recommended.
`MaxNoOfExecutionThreads`	Each data node process may handle parallel transactions. This parameter controls the number of threads used by the data node process, up to a maximum of 8 threads. Although this may manually be set by the user, this parameter is automatically set by default to the number of cores defined in d-SCC's XML configuration file.

Table 5 – Important MySQL parameters defined

If these parameters are not set by the user, *SCDBM* will set default values. Two parameters are important to be mentioned. First, `NoOfReplicas` may only assume values from 1 to 4 and it must divide evenly into the number of data nodes in the cluster of data nodes. For example, if there are two data nodes, then `NoOfReplicas` must be equal to either 1 or 2, since 2/3 and 2/4 both yield fractional values; if there are four data nodes, then `NoOfReplicas` must be equal to 1, 2, or 4[13]. Second, `MaxNoOfExecutionThreads` is limited by 8. We commonly set this value to be equal to the number of cores in each machine that host a data node, but if a machine has more than 8 cores, we can only set `MaxNoOfExecutionThreads` to at most 8.

Finally, the file `main-template.sql` contains the main DDL script that will be used to create the database. What is important to mention in this file is the number of partitions of the table that hosts the BoT (`EActivation`). If this parameter is not set by the user, *SCDBM* automatically tries to set it to the number of slaves (σ, as defined in Section 4.1). However, MySQL Cluster limits the number of partitions to

[13] https://dev.mysql.com/doc/refman/5.5/en/mysql-cluster-ndbd-definition.html#ndbparam-ndbd-noofreplicas

$4 * MaxNoOfThreads * (\#dn / NoOfReplicas)$ [14], which is the upper bound limit *SCDBM* defines for the number of partitions.

5.4.2 Initialization Process

After defining all these previous parameters, the distributed database may be initialized. It is known that initiating each role on each machine may be a complex task for humans, especially in a scenario with a huge number of nodes. Yet, depending on the HPC security constraints, it may not be trivial to access each composing machine individually to install the required programs. For this reason, we developed an automatized process that reads all parameters predefined by the user and initialize each role on each machine by running only one Java program (`SCDBM.jar` – The SC Database Manager module) from only one of the machines that is able to access the other composing machines. It is necessary to specify the XML configuration file that contains main properties of the workflow execution and conceptual specification:

```
java –jar SCDBM.jar SC.xml --start
```

This program begins by generating four files. (i) One file is generated based on a template script for creating the main database and its tables. Tables that need to be partitioned based on parameters are resolved at this time. For example, in our current solution, the table that hosts the BoT (`EActivation`) is horizontally partitioned into σ (=number of *SCCore* Nodes) fragments. For this, the number of partitions is explicitly defined in MySQL's DDL scripts. However, in our implementation, σ is derived as explained in Section 5.4.1). Thus, *SCDBM* reads the template script file and correctly writes the number of partitions that will be used in that specific workflow execution; (ii) The second file is based on a template for the `config.ini` file (Section 5.4.1). Currently, two parameters are set at this time by *SCDBM*: `NoOfReplicas` and `MaxNoOfExecutionThreads`, which are set, respectively, to the number of data nodes and to the number of cores that the machines that will host the database nodes have. We note, however, that these values will only be automatically set if the user does not specify them. Otherwise, the effective values will be what the user specified; (iii) The third file lists σ machines which will play `SCN` role, *i.e.*, will effectively run the workflow. This file is generated based on the `machines.conf` file and on discussion on roles accumulation we presented in Section 5.4.1; and finally, (iv) the forth file lists q (number of `dbs` nodes)

[14] https://dev.mysql.com/doc/refman/5.5/en/mysql-cluster-nodes-groups.html#mysql-cluster-nodes-groups-user-partitioning

machines through which the SWfMS will connect to the database cluster. This file is also generated based on the on discussion on roles accumulation we presented in Section 5.4.1.

After generating and correctly placing all these files, *SCDBM* begins the distributed database initialization. It first starts `mgm_ndbd` nodes, then the data nodes, and finally the `dbs` nodes. Following, the database is created using the generated DDL script and a verification is done to check if all database nodes were correctly initialized. If not, users need to check logs which are continuously appended during initialization to look for errors. Finally, when everything is set up, the workflow execution may begin.

The database cluster initialization process takes at least one minute to conclude, for small configurations. This time is going to be greater if a large number of database nodes is used. However, we note that is process should occur only once and many workflow executions may use the initialized distributed database. There is also a convenient shutdown command which safely shuts down all processes that compose the distributed database on all machines hosting it. A common sequence of steps for running a workflow on a cluster environment is:

```
SCDBM --start
SCSetup --create database
SCStarter --start
SCDBM --shutdown
```

In addition, we highlight that during execution, users may interact to the distributed database through one of the `dbs`. By doing this, custom analyses (including merging with domain-specific data), monitoring, and steering may be performed.

5.5 Parallel Data Placement, BoT Fragmentation, and Tasks Scheduling

Recall from the parameters in Table 3, seen in Section 4.5.1, that some parameters need to be adjusted in order to build Architecture II. In our current implementation of such architecture, we fixed some parameters. We highlight that although this makes the concrete architecture implementation simpler, our theoretical Architecture II is supposed to be flexible so these parameters do not need to be fixed or predefined by users. Currently, in our implementation, the parameters are adjusted as shown in Table 6.

Parameter	Brief description	Value
d	#data nodes	Fixed, defined by user (see Section 5.4.1).
q	#dbs nodes	Fixed, defined by user (see Section 5.4.1).
M	#partitions	Fixed σ(#SCN nodes) and σ is derived as explained in Section 5.4.1.
S	#slaves per dbs node	Fixed σ/q

Table 6 – Simplified configuration of Architecture II, as utilized in our current concrete implementation

Mainly as a matter of simplicity, we implemented Architecture II fixing that the number of partitions is equal to the number of `SCN` nodes. By doing this, we reduced the complexity of our solution because choosing an optimal value for M is another problem by itself. We highlight that this may be easily changed by explicitly specifying the number of partitions. If not specified, the *SCDBM* module will set this number to σ. However, although the larger σ, the more we can benefit from parallelism, MySQL Cluster limits the number of partitions[15] by $4 * MaxNoOfExecutionThreads * (d / NoOfReplicas)$. The parameters `MaxNoOfExecutionThreads` and `NoOfReplicas` are explained in Table 5.

Moreover, if σ is large (*e.g.*, in order of hundreds), our solution will take a lot of advantage of parallelism.

To tackle fragmentation, data placement, and initial tasks distribution, as described in Sections 4.5.1 and 4.5.2, MySQL Cluster enables total horizontal fragmentation (partitioning) only based on the primary key[16]. Regarding data placement, MySQL Cluster applies a hash function based on the primary key that places each task on the right partition[17]. For this reason, we changed the schema of the table that hosts the BoT (`EActivation`) by adding the identification of the `SCN` (Section 5.3) to which a task is assigned during initial tasks distribution to compose the primary key. We note that an alternative for this would be defining partitions based on the `SCN` id. By doing this, we could keep all tasks that are assigned to a same `SCN` on a same partition, which could enhance performance. However, since the `SCN` id by itself is not a key in our solution and MySQL Cluster only partitions by key, this alternative is currently not possible.

Initial tasks distribution works in a circular fashion, as described in Section 4.5.2. Nonetheless, for each task in the work queue, the supervisor circularly assigns the *id* of the `SCN` which is supposed to execute the task because we fixed that there will be σ partitions

[15] https://dev.mysql.com/doc/refman/5.5/en/mysql-cluster-nodes-groups.html#mysql-cluster-nodes-groups-user-partitioning

[16] https://dev.mysql.com/doc/refman/5.5/en/partitioning-limitations-storage-engines.html

[17] https://dev.mysql.com/doc/refman/5.6/en/partitioning-key.html

(limited by a value previously explained). After all initial tasks distribution and placement, the actual scheduling begins and it works exactly as described in Section 4.4.2.

5.6 Tasks Scheduling relying on the DBMS, MPI removal, and Barrier

As already explained in Section 3.4, historically, SCC implements its CWQ BoT scheduling based on message passing, utilizing MPI. However, we have argued that one important motivation for a BoT tasks scheduling relying on a DBMS is that it is a specialized system in parallel and concurrency issues; hence, it would be a good idea to outsource our scheduling implementation and take further advantage of the DBMS's features. By doing this, we would alleviate our work to solve these parallel and concurrency issues, which are usually complex, and focus on issues that are inherent to our application (recall from Sections 4.2 and 4.3). For this reason, since MPI in SCC was essentially used to implement tasks scheduling, we were able to completely remove it. As described in details in those mentioned sections, instead of having a master that is the only node that may access the BoT (which was managed by a DBMS in traditional SCC), now, in our solution, all nodes in the cluster may directly retrieve next runnable tasks by directly accessing it. Concurrency issues are resolved by the DBMS.

However, as described in Section 0, one of the dataflow strategies supported by SCC is what is called FAF. Recall that, in FAF, the next activity may only start execution if the previous activity (on which the next activity depends) is completely executed. This is a blocking strategy since, if a node finishes executing activations for an activity, it needs to wait for all other nodes to finish their work so it may continue on the flow. This logic is inherent to our problem, which is essentially centered on dataflows. As we have been arguing, since it is not related to tasks scheduling but, rather, related to our own application logic, we cannot outsource this to the DBMS. Thence, we needed to implement this logic ourselves.

In order to do this, we utilized the classic concept of barrier in parallel programming (Arenstorf and Jordan, 1989). We implemented it in our application as follows. The first node that begins execution of an activity becomes the barrier manager. Within each activity, when a node (including the manager) finishes all activations assigned to it, it notifies the manager that its work has finished and waits. When the manager receives a number of notifications that is equal to the number of slaves, it notifies all waiting nodes so they can keep on working and get activations of the next activity. This is done until all activities finish.

Regarding technology, we need a tool that enables nodes communication. One way to do to this is by making use of a dedicate attribute of a table managed by the DBMS, which is

used as common mean of communication among all nodes. Since it would be only small notification messages, queries would not be complex and the amount of data transmitted would be small. However, nodes would only know that they were notified if they kept querying the database looking for a data change. For example, a *false* value would mean that there is still some node working, so all nodes should wait, and when this value is set to *true*, all nodes may continue. Nodes would only acknowledge this value change if they keep continuously querying the database, which could cause network congestion and downgrade performance.

Alternatively, a message passing library could be used, like MPI. Nevertheless, MPI is a robust library and is common in scenarios of data transmission of complex data types and various data sizes. In our problem, as we argued, we only need to pass notification messages, which are simple and small. In addition, since SCC is written in Java and uses MPJ[18] (known as MPI for Java), its MPI implementation is more limited and does not support fault tolerance if a slave node fails, limiting future work for this. Because we were able to completely remove MPI to implement our tasks scheduling relying on the DDBMS, it is not necessary to use it just for notification message passing. For this reason, we decided to implement the barrier as described before using native Java Remote Method Invocation (RMI)[19] together with Java native synchronization directives (`wait` and `notify` [20]) in our current implementation. Java RMI is known for being simple and easy to use and lightweight, which fits our barrier needs.

5.7 Fault tolerance and load balance

By using an architecture inspired in WQRM (Section 4.1) and using a DDBMS that allows replication of the BoT, we increase the availability of the system. If a machine that hosts a replica of the BoT fails, the entire system does not fail and execution does not stop because we make of use of the replication feature. We highlight that this failure recovery mechanism is outsourced and implemented by the DDBMS – which is acknowledged for being efficient in handling failures (Özsu and Valduriez, 2011) –, and not by our parallel application, which simplifies our solution.

In addition to the distributed database availability, we also mention fault tolerance for nodes that do not compose the distributed database in our theoretical architectures (Chapter 4).

[18] http://mpj-express.org/
[19] http://docs.oracle.com/javase/7/docs/technotes/guides/rmi/
[20] http://docs.oracle.com/javase/8/docs/api/java/lang/Object.html#notify()

Regarding fault tolerance of the supervisor node, we added a secondary supervisor node to remove a single point of failure. Regarding fault tolerance of the slave nodes, we explained that it may be achieved by implementing strategies such as proposed by Anglano *et al*. (2006). However, we did not further explain in details how these strategies would apply hence we did not implement in our current solution. Nevertheless, this is being currently tacked and a more formal description to incorporate fault tolerance on slaves and on supervisors will be provided in future work. Furthermore, we described that it is possible to enhance load balance by verifying whether or not work stealing is advantageous. However, we did not implement it in our current solution and this is also being provided for future work.

6 EXPERIMENTAL EVALUATION

In this chapter, we present the experimental evaluation of our implementation of Architecture II as described in Section 4.5 and in Chapter 5, where we introduced SciCumulus/C on a Distributed Database System (d-SCC).

Regarding hardware, we ran several simulations using Grid5000[21], which is composed of many different clusters distributed in regions in France. In Grid5000, for each region, all clusters share a file system. The hardware specification of each cluster we used is described in Table 7. Regarding software, we implemented our solution using MySQL Cluster version 7.4.6. Specifically, we used a compressed TAR file with binaries for generic Linux 64-bit distribution. We ran most experiments three times and used the average value to present the results.

Cluster / Region	Processors	#Nodes[22]	#Cores per node	Total cores	Memory per node	Network	Storage
Parapide / Rennes	Intel Xeon X5570 2.93GHz/6MB	21	8	**168**	24 GB	InfiniBand	SATA II 7200 RPM (RAID-1 and RAID-5)
Graphene / Nancy	Intel Xeon X3440 2.53 GHz	138	4	**552**	16 GB	InfiniBand	SATA AHCI
Stremi / Reims	AMD Opteron 6164 HE 1.7 GHz/12MB	42	24	**1008**	48 GB	Gigabit Ethernet	SATA AHCI & RAID-5

Table 7 – Hardware specification of clusters in Grid5000

The remainder of this chapter is organized as follows. In Section 6.1, we describe the workflows we experimented. In Section 6.2, we evaluate architecture variations in order to analyze the impact of the many different possibilities to configure our architecture. In Section 6.3, we analyze speedup, scalability, and efficiency for different workflow complexities. In Section 6.4, we show that d-SCC works for a workflow that contains all existing SciWfA operators (Section 3.1) and we also show the efficiency on running a real bioinformatics workflow. Finally, we compare d-SCC with the most recent version of SCC in Section 6.5.

6.1 Workflows case studies

We utilized different workflows to evaluate d-SCC; both synthetic and real workflows were experimented. More specifically, we used the Scientific Workflow Benchmark (SWB)

[21] www.grid5000.fr

[22] The number of available nodes in these clusters may vary mainly depending on hardware health. Our experiments were conducted in May 2015 and those are the available nodes we could use in that time.

(Chirigati *et al*., 2012), a synthetic deep water oil exploration workflow (adapted from (Ogasawara *et al*., 2011), and SciPhy, a real bioinformatics workflow (Ocaña *et al*., 2011).

Most of our tests were run using SWB. In SWB, we can generate synthetic data-centric workflows with a specified number of activities; specify how each activity consumes and generates data; and control the manipulated data. For example, it is possible to specify a 2-activities Map-Reduce workflow: the first activity consumes and produces one tuple at each invocation (*i.e*., it has a Map behavior) and the second activity, dependent on the first activity, consumes many tuples and produces one at each invocation (*i.e*., it has a Reduce behavior). Moreover, we can determine the problem size (*i.e*., the number of tuples that will be consumed) as well as the complexity of each computation (*i.e*., the average elapsed time for each task).

In this work, we generated two SWB workflows and we are going to call them *1-map* (a simple workflow with one Map activity only) and *3-map* (three Map activities, with data dependency in between). Figure 14 Figure 1shows an activity diagram for each of them. For each experiment, we varied both problem size and complexity. Since we only utilized SWB Map activities and each input tuple corresponds to a task that needs to be scheduled and outputs another tuple, we use the term "number of tasks" instead of "number of tuples" when we refer to the problem size of either *1-map* or *3-map* workflows, for readability of this text.

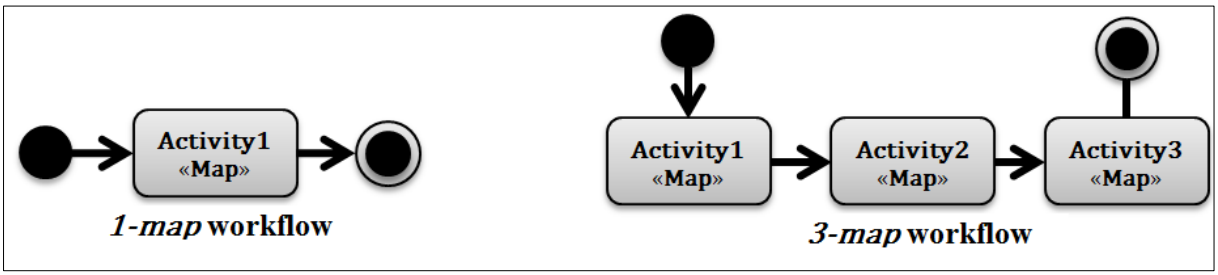


Figure 14 – *1-map* and *3-map* SWB workflows experimented

In addition to the SWB, we experimented a more complex workflow in order to investigate whether or not our solution works for all current SciWfA operators (Section 3.1). The workflow experimented is a synthetic adaptation of a deep water oil exploration workflow specified by Ogasawara et al. (2011) and is illustrated in the activity diagram in Figure 15.

In this workflow, some data files are processed and it has 7 activities, including two that may run in parallel. It is inspired in SWB in the sense that we can control both the problem size and complexity of tasks.

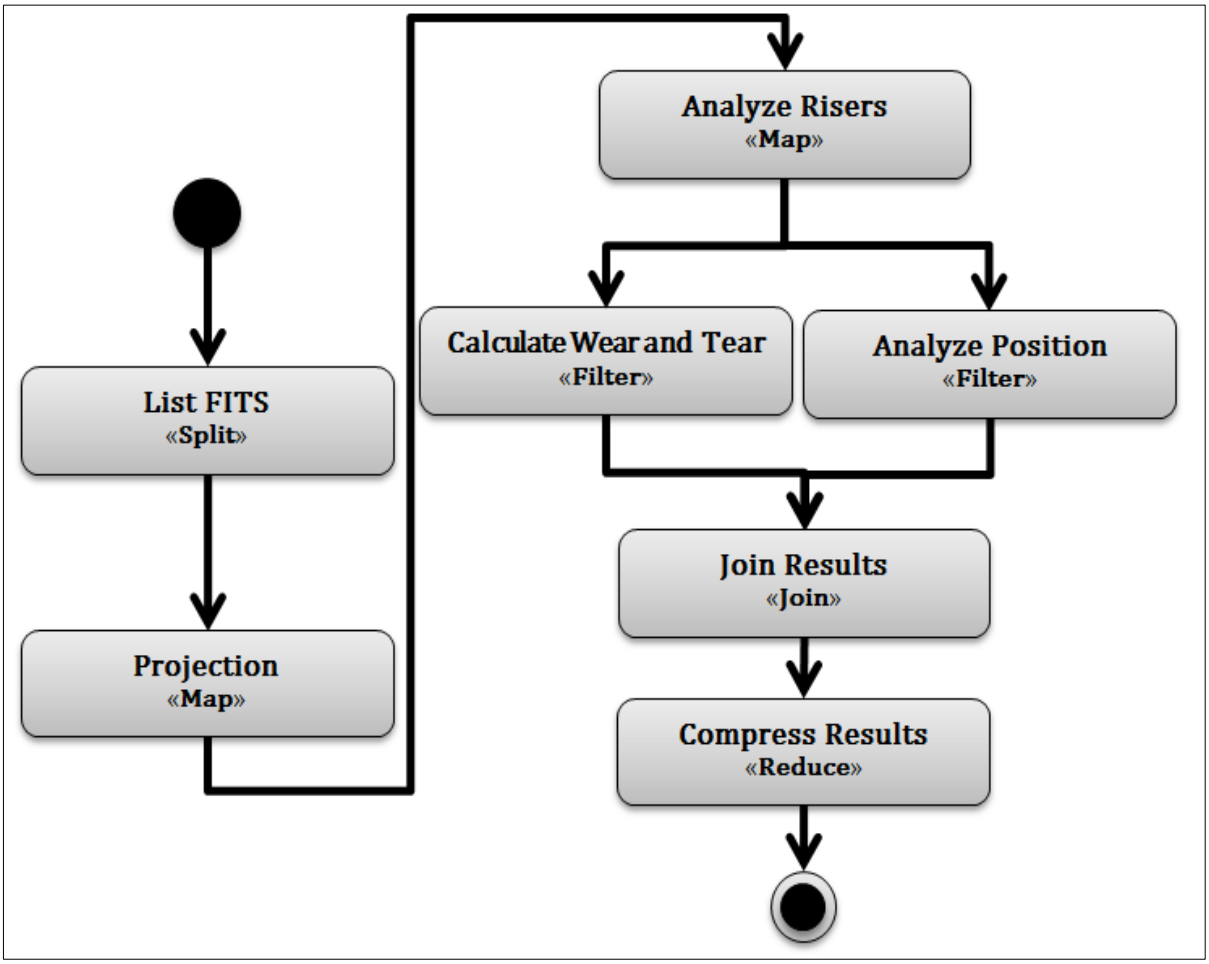


Figure 15 – Deep water oil exploration synthetic workflow (adapted from Ogasawara *et al*., 2011)

Finally, the last workflow we experimented is SciPhy, a bioinformatics workflow for phylogenetic analysis of drug targets in protozoan genomes (Ocaña *et al*., 2011). It also has many big files manipulated and is illustrated in the activity diagram in Figure 16.

6.2 Architecture variations

Our current implementation of d-SCC is composed of four different roles: `dn`, `dbs` `ndb_mgmd`, and `SCN`, as we explained in details in Section 5.3. Moreover, we have argued in Section 5.4.1 that configuring which role each machine will play may directly impact performance. For this reason, in this section, we want to vary the architecture configuration, measure performance impact for each configuration, and try to find the most suitable configuration for a given problem.

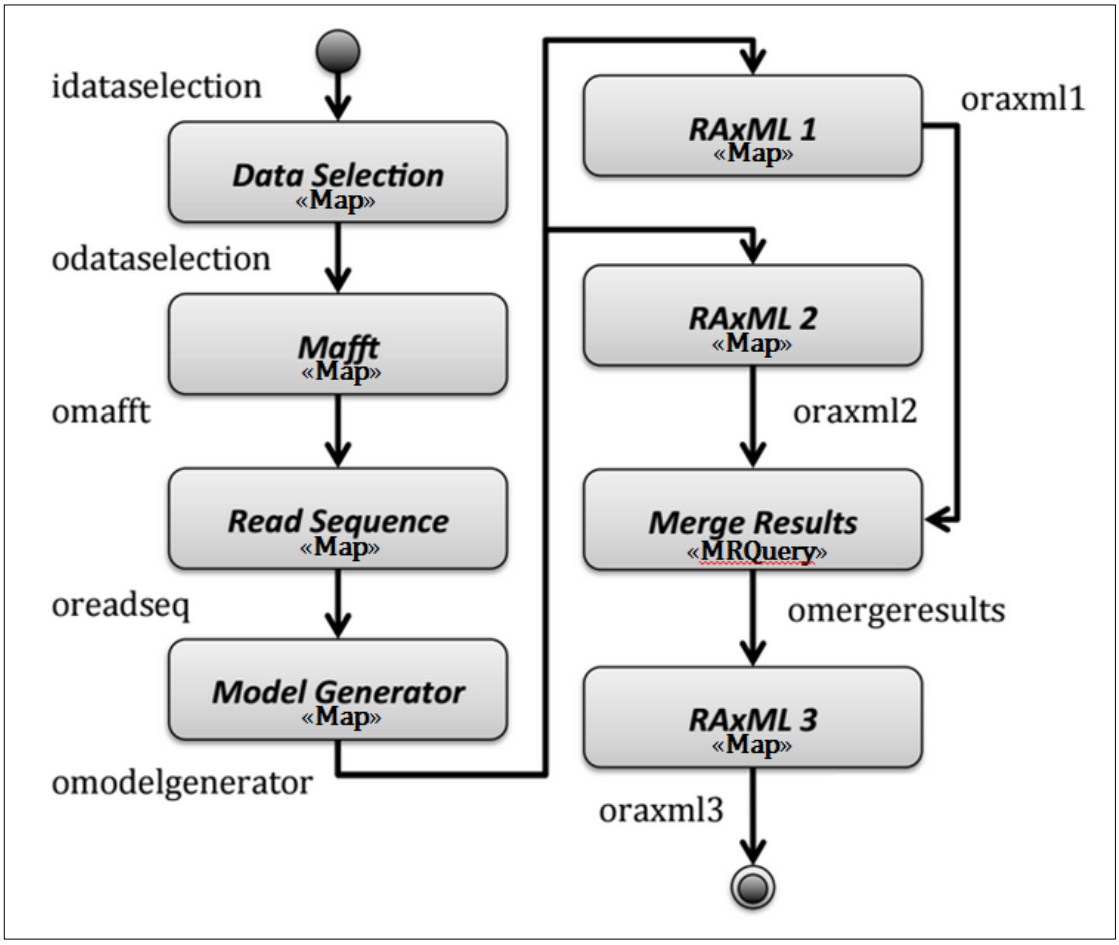


Figure 16 – SciPhy workflow (extracted from Ocaña *et al*., 2011).

Experiment 1. In our first experiment, we want to investigate whether or not we should run, for example, `dn` nodes or `SCN` nodes dedicatedly; or if running them altogether on the same machine has a significant impact. For this, we used the *1-map* workflow setting the problem size to 10 k tasks and average cost to 1 millisecond for tasks. This means that tasks are extremely light and no much computation is needed for each of them. By doing this, we stress the database, since there are many very frequent accesses to it, including reads (get next ready task) and writes (update a completed task status). We only used one node of each role, *i.e*., we used at most 4 machines at the same time. We ran on Parapide cluster, which has 8 cores per machine. However, since we wanted to analyze the behavior when all roles were concurrently running on a same machine, we set the maximum number of threads used both by `SCN` and by `dn`e data node) to 4. We ran five variations of the architecture, as described in Table 8 and the results are shown in Figure 17.

	Description	Number of used machines
I	Each machine dedicatedly runs only one process, for each d-SCC role.	4
II	SCN runs dedicatedly on a machine; DN also runs dedicatedly on another machine; and dbs and ndb_mgmd run together on a third machine.	3
III	SCN and DN processes run concurrently on a same machine; and dbs and ndb_mgmd run on another machine.	2
IV	SCN dedicatedly on one machine; and all other database nodes (dn, dbs, and ndb_mgmd) run together on another machine.	2
V	All four roles run together, concurrently, on a single machine.	1

Table 8 – Description of each run of **Experiment 1**.

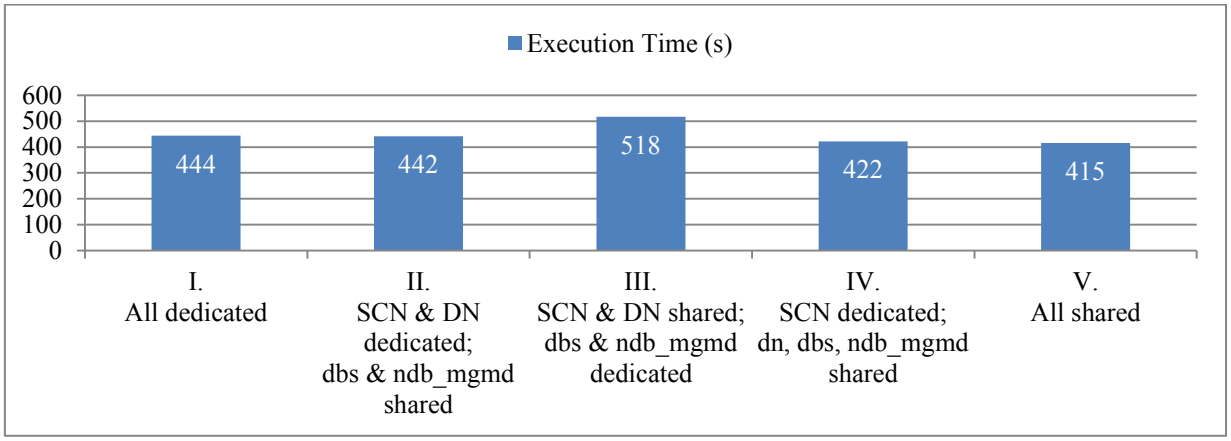


Figure 17 – Results of **Experiment 1**. Varying architecture: shared or dedicated nodes?

From the results, we can see that the variation V showed the best execution time, even though the difference is small. This means that despite having more concurrency in V than in any other variation, the concurrency overhead is lower than the communication overhead. A good conclusion from this result is that the variation with the best execution time required the least number of resources (*i.e.*, only one machine); as a consequence, it points out that we will be able to use more machines to host `SCN` processes without significantly impacting performance, which is the ideal for us. Another important conclusion is related to the idea of data locality. We could expect that having `SCN` and `dn` together on a same machine would improve performance since less communication would be required to access the database. However, the result from variation III contradicts this expectation. Comparing variation III, in which `SCN` and `dn` are located on the same machine, with variations II and IV, in which `SCN` and `dn` are in different machines, we see that III has the worst execution time. However, comparing III with V, in which `SCN` and `DN` are also in the same machine, we see that V has a better performance, suggesting that the communication cost between `SCN` and `dbs` also adds a

non-negligible overhead. Thence, we may conclude that keeping all roles together has the best performance especially due to the lowest communication overhead, even though it has the greatest concurrency overhead. Nevertheless, we need to emphasize that while the machines have 8 cores, we only used at most 4 cores and forced both `SCN` and `dn` to instantiate at most four threads each process, meaning that concurrency overhead is reduced in all these results and we are not using all possible cores for `SCN`. For this reason, we still need more experiments to have better conclusions.

Experiment 2. This experiment aims to analyze the behavior of our solution in a more concurrent scenario. To do this, we ran the same workflow with the same configuration as in **Experiment 1** and we used the variation V of our architecture, that is, only one Parapide (8 cores) machine with all roles sharing this same machine. However, instead of using only four threads at most, we ran two more variations: one with 2 threads (both for the SCN and for the dn) and another one with eight threads. We reused the result obtained in variation V in Figure 17 for four threads. Ideally, when we double the number of threads, the execution time should be divided by two. The results are shown in Figure 18, in which the blue line represents d-SCC's execution time and the red line represents the ideal execution time. The green bars represent how far from the ideal d-SCC achieved, in seconds.

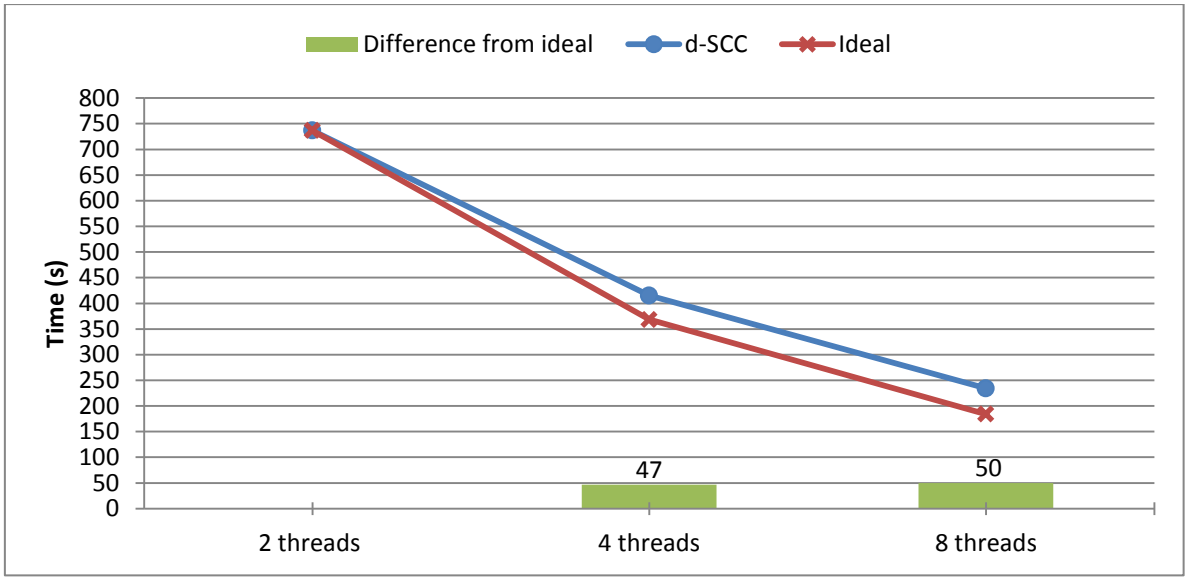


Figure 18 – Results of **Experiment 2**: increasing concurrency

If d-SCC had taken 736 seconds with two threads, the ideal would be if it took 368 seconds (736 * 0.50) with four threads. However, it took 415 seconds (736 * 0.5633), which represents 47 seconds (or 11.2%) of difference from the ideal execution time. With eight threads, the ideal time would be 184 seconds (368 * 0.5), but it took 234 seconds (415 * 0.5643), which represents 50 seconds (or 11.4%) from the ideal time. This difference from

ideal is caused due to parallel management overheads. From these results, we mainly want to show that the overhead caused by concurrency remains close to constant comparing running on four threads with running on eight threads. This means that difference between the overheads with four threads and with eight threads is so small (0.2%) that it can be neglected. In other words, we conclude that we can set the maximum number of threads to be used both by the `SCN` and by the `dn` to be equal to the number of cores in the machine. By doing this, the efficiency should not be significantly impacted, at least for one single machine. Although it cannot be generalized for a greater number of machines, this result is meaningful because we are first mainly interested in finding a good configuration for our architecture rather than running massive experiments to measure speedup and scalability in larger clusters. Moreover, we are going to present a similar experiment running on a 960 cores cluster to measure speedup in next section.

Experiment 3. In this third experiment, we want to analyze the impact of having more database nodes (`dn`, `dbs`, and `ndb_mgmd`) on the system. For this, we ran our tests on Parapide cluster, with 21 nodes and 8 cores each (168 cores total). Each of the 21 nodes hosts a `SCN` process and the database processes are shared. For example, if we configure 2 `dn`, 2 `dbs`, and 2 `mgm_ndbd` (this is the default configuration recommended to remove single points of failure), 3 machines would run 1 `dn`, 1 `dbs`, 1 `mgm_ndbd`, and 1 `SCN` concurrently each; the other 18 machines would only run `SCN` processes, dedicatedly (recall from Section 5.4.1). Regarding the workflow, we used the *1-map* workflow, around 20K tasks with 16 s average task cost. To present the results, we used the real speedup (*Speedup*) metric, as defined in Section 2.8. To calculate the time to execute the workflow with the best (theoretical) sequential program using one processor, we multiplied the approximate number of tasks by the average task cost. The workflow execution takes approximately 3.8 days. We also calculated the difference that each variation has from the best result. The results are shown in Figure 19.

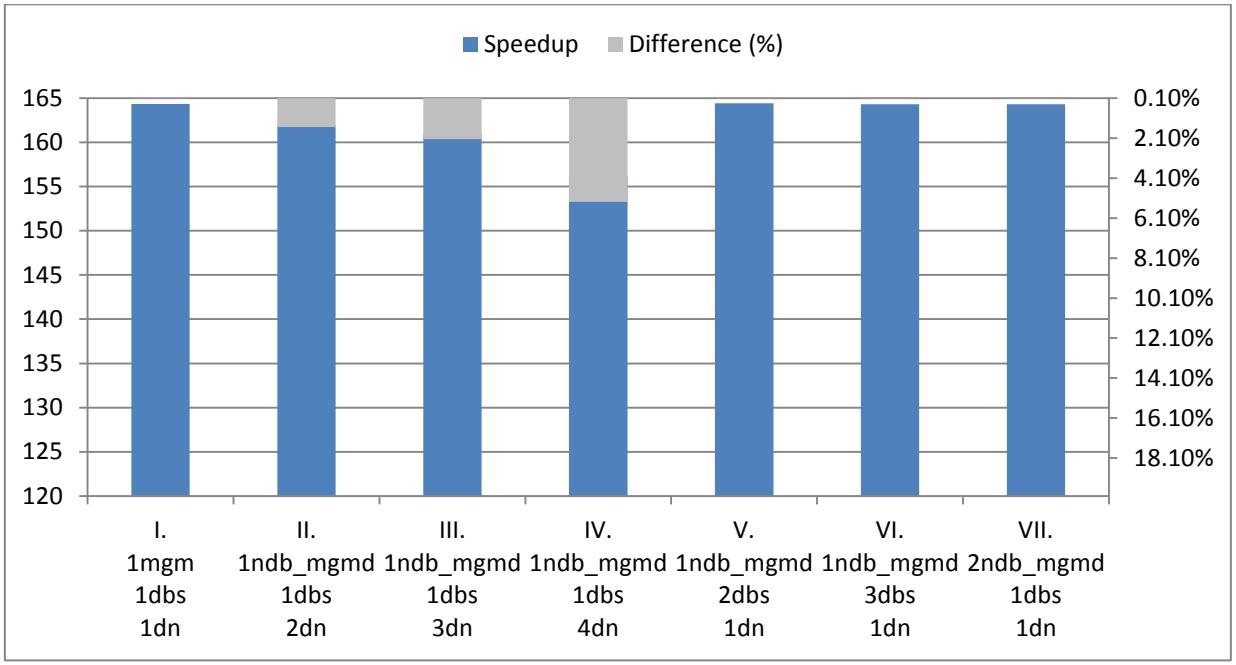


Figure 19 – Results of **Experiment 3**. Varying architecture: changing the number of database nodes.

From the results, comparing the variation I with V, VI, and VII, we can see that varying either the number of `mgm_ndbd` or the number of `dbs` nodes, no much impact is caused on the system's performance. Thus, at least for an experiment with similar characteristics to this **Experiment 3**, changing the number of `mgm_ndbd` or `dbs` has no impact on performance. Since it has no impact on performance, this result enforces the idea that we should use at least two nodes for each of these roles so improve availability and remove single points of failure.

Nevertheless, comparing I with II, II, and IV, we can verify that the number of `dn` interferes on the system's performance. These results lead us to believe that increasing the number of `dn` decreases performance. However, we note that the difference on performance between variations I, II, III is at most 2.1%, which may be considered small; even the difference in relation to variation IV, which is about 5%, is not very critical. Anyhow, since we were not expecting the performance to decrease when data nodes were added, we further investigate the impact of the number of data nodes on a larger cluster.

Experiment 4. In this experiment, we want to evaluate the impact on varying the number of data nodes (`dn`) using a larger configuration. For this, we used 138 machines in Graphene cluster, each with 4 cores, summing 552 cores. We ran the *1-map* workflow with around 20K tasks with 1 s tasks cost average. We note that the tasks cost in this experiment is considerably lighter than in **Experiment 3**. By doing this, we want to stress the DDBMS with many frequent short queries, with both read and write behavior. Similarly to **Experiment 3**,

we also used the real speedup metric and the best (theoretical) sequential program using one processor would take about 6 hours to run. The results are shown in Figure 20. The blue line represents the speedup varying the number of data nodes when 2 `dbs`, 2 `mgm_ndbd`, and 132 `SCN` were used in a shared way (similarly to **Experiment 3**); the red square shows the speedup when 2 `dn`, 2 `mgm_ndbd`, 132 `SCN`, and 8 `dbs` nodes were used in a shared way; and the difference between each variation and the best result for this experiment is represented in gray bars.

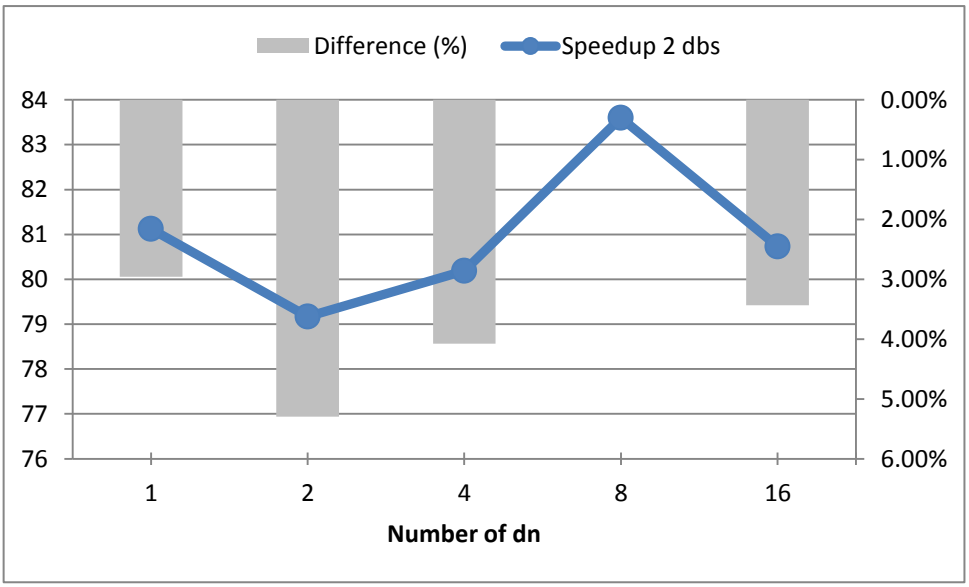


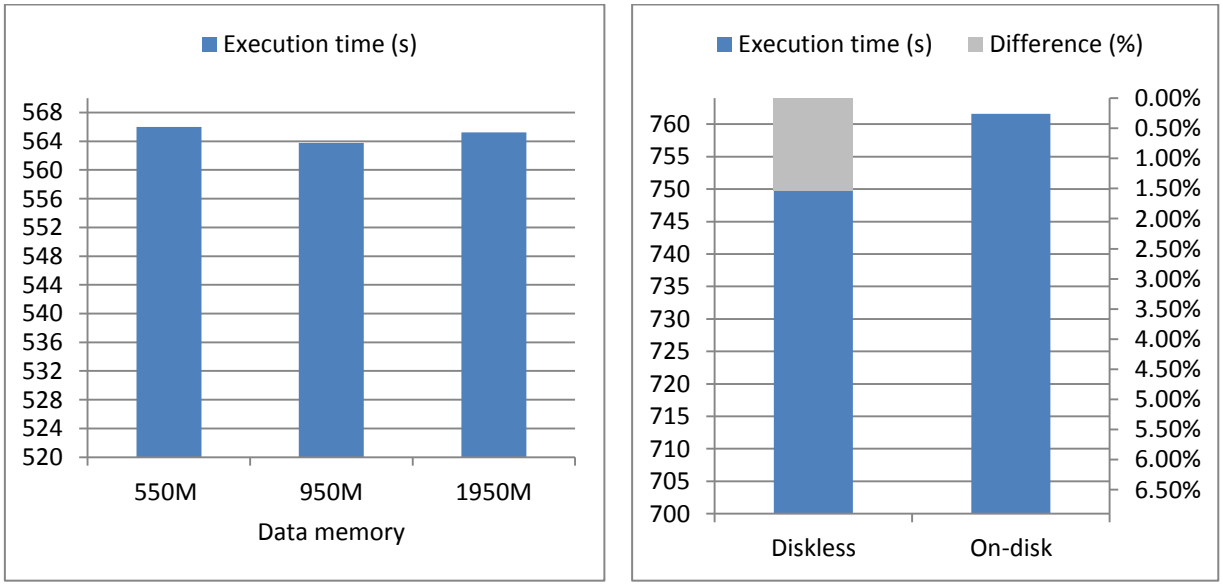
Figure 20 – Results of **Experiment 4**. Varying architecture: increasing number of data nodes.

Conversely, the results of **Experiment 4** show that there is not a clear pattern in relation to adding data nodes as **Experiment 3** suggested. Using two data nodes instead of one resulted in a worse performance, but the difference between these two variations is close to 2%, similarly to **Experiment 3**. However, using 4 data nodes had a better performance than using two and, more surprisingly, using eight data nodes resulted in the best performance. Using 16 data nodes downgraded performance, but the speedup was not very different than when using 1 or 4 data nodes. From these results, we can conclude that when there are multiple short queries (both read and write), using multiple data nodes may alleviate congestion at the DDBMS, leading to better performance than using a low number of data nodes, especially in a large cluster with many machines (*e.g.*, 130 machines). We also highlight that the difference of the performance impact comparing these variations is not very high: about 5% at most. In addition to analyzing the number of data nodes, we also ran a single variation on the number of `dbs` nodes, although it is not presented in Figure 20. We evaluated the utilization of 8 `dbs` instead of 2. We could see that using 8 `dbs` instead of 2 led to a better performance, even though the difference is small (about 1% in relation to using 2

dbs). This happened most likely because congestion is alleviated when using more ports to which the 132 SCNs connect.

Experiment 5. In this last experiment for our architecture variation, we want to analyze differences in relation to the DDBMS configuration. In MySQL Cluster, it is possible to configure the amount of memory will be used to store data. Moreover, another important discussion is related to the fact that we can run MySQL Cluster completely in-memory (recall from the discussion in Section 5.2). Because of these differences, we want to investigate how d-SCC behaves when the DDBMS configuration varies.

We ran two tests, each to analyze different features of the DDBMS. In the first test (I), we analyzed data memory capacities using the *1-map* workflow with approximately 10 k tasks, 1 millisecond average task cost, 3 SCN, 1 dn, 1 dbs, 1 mgm_ndbd, and each of them running dedicatedly (total of 6 machines) on Parapide cluster. In the second test (II), we compared the performance when running in diskless (in-memory) mode with running using on-disk checkpoints. We ran the *1-map* workflow with approximately 50 k tasks, 2 s average task cost, 21 SCN, 1 dn, 1 dbs, 1 mgm_ndbd, in a shared way, on Parapide cluster. We highlight that this was the first time that this amount of tasks was successfully executed in any version of SCC so far. The results are shown in Figure 21.



I. Varying data memory

II. In-memory vs. on-disk

Figure 21 – Results of **Experiment 5**: varying configuration of the DDBMS.

From the results of Figure 21(I), we can see that varying the data memory capacity has no significant impact on performance. The results of Figure 21 (II) show that even though running in diskless mode has 10 s of advantage comparing with on-disk checkpoints mode, the difference is not critical (1.5%). On-disk checkpoints mode has the advantage of

persistence, meaning that if a catastrophic disaster happens or if the energy of the entire cluster fails, the data will remain as long the disk is not damaged. Diskless mode is indeed faster and we usually save a backup of the database when the workflow execution finishes for *a posteriori* data analyses, but if all data nodes fail (*i.e.*, a catastrophic disaster), there will be data loss even if the disk remains intact.

Therefore, from the five experiments we conducted for the architecture variations, we can summarize the following conclusions. Using the all-shared mode has shown to deliver the best performance for the experiments conducted (**Experiment 1**); setting the maximum number of threads as equal to the number of cores in the machine delivers a good performance in a small cluster and more experiments are needed in a larger cluster (**Experiment 2**); the number of `dbs` and `ndb_mgmd` has no significant impact on performance, hence we should use at least two of each to improve availability and remove single points of failure (**Experiment 3**); many data nodes may either downgrade or improve performance, depending on the number of `SCN` and problem complexity (tasks cost) – however, the difference between a lower number and a greater number of `dn` is not very high, hence it is advantageous to use at least two data nodes to remove single points of failure (**Experiment 4**); and data memory variation has no big impact and diskless mode has a slightly better performance than on-disk checkpoints mode (**Experiment 5**). For these reasons, all of our next experiments, unless we specifically state differently, were ran using all-shared mode, number of threads equals to number of cores, at least two database nodes (*i.e.*, 2 `dn`, 2 `dbs`, and 2 `ndb_mgmd`), and diskless mode.

6.3 Scalability, speedup, and efficiency

In this section, we use known performance metrics to evaluate our system. First, we evaluate scalability; then, the speedup varying the number of `SCN`, including different threads per node; and, finally, we measure the efficiency of d-SCC for different problem complexities.

Experiment 6. In this experiment, we measure scalability using *1-map*, 32 s tasks cost average, on Stremi cluster (24 cores per node). We varied from 5 nodes (120 cores) – 2,5 k tasks to 40 nodes (960 cores) – 20 k tasks. The results are shown in Figures Figure 22 and Figure 23.

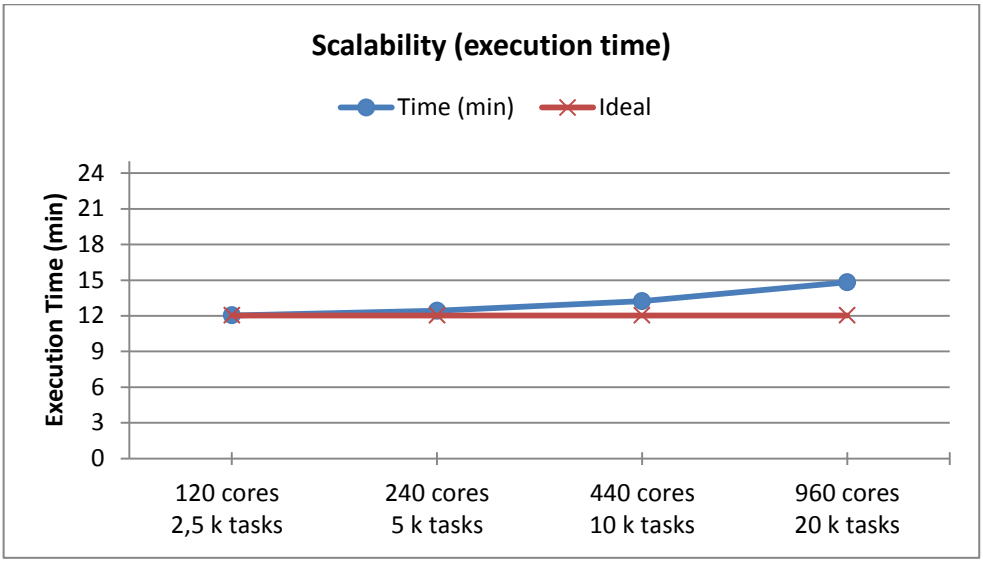


Figure 22 – Results of **Experiment 6**: scalability analyzing execution time.

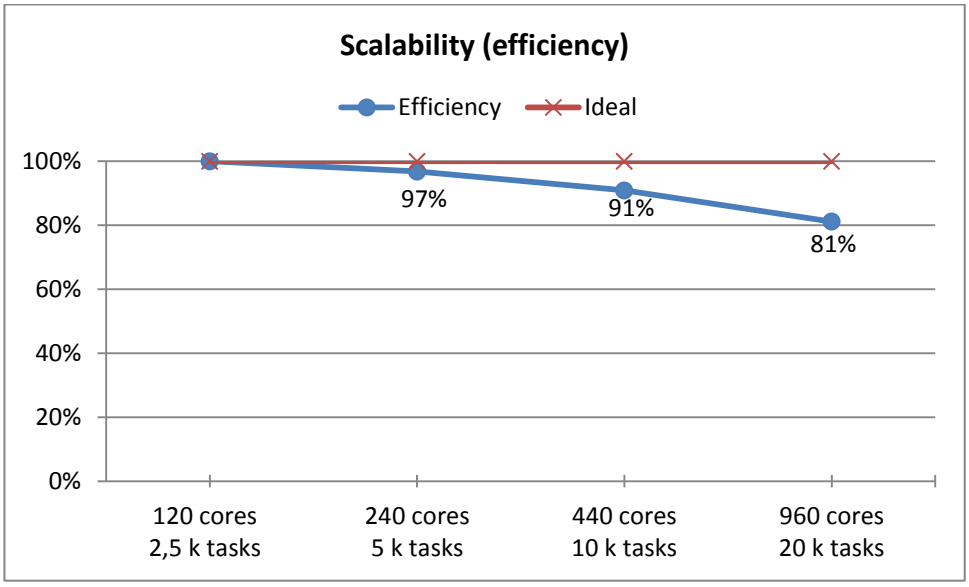


Figure 23 – Results of **Experiment 6**: scalability analyzing efficiency.

The ideal is calculated using the concepts about *scalability* introduced in Section 2.8. From the figures, we can observe a close-to-constant execution time when we double both number of nodes and the problem size. Even though the results were farther from the ideal for 960 cores, the efficiency of the system remained over 80% in all executions. Since the number of cores is relatively large, we consider this a good result.

Experiment 7. To evaluate efficiency when varying complexity (*i.e.*, tasks cost), we used *3-maps* workflow for the first time, with 10 k tasks per map (*i.e.*, 30 k tasks in total). By doing this, we can also investigate a different known inherent overhead of SCC: caused by the FAF dataflow execution strategy (recall from Section 0). Regarding hardware, we used all

available machines in Stremi cluster, summing 1,008 cores. We also highlight that this was the first time that this amount of cores was successfully used to run any version of SCC so far. The results are shown in Figure 24, where the blue line represents our actual execution including a contention overhead, which we will explain next; and the red line represents the efficiency if we removed such overhead.

To measure efficiency, we used the *efficiency* metric, which is based on the real *speedup* metric, as we defined in Section 2.8. To calculate the time to run the workflow running the best (theoretical) sequential program using one processor, we multiplied the approximate number of tasks by the tasks cost average, resulting in approximately 9 hours, 35 hours, 69 hours, 138 hours, and 551 hours for tasks cost average 1 s, 8 s, 16 s, and 65 s, respectively. We highlight that this theoretical sequential time is even farther from reality than in the previous experiments we ran, because it does not include any overhead, which is unrealistic in most large parallel systems, and we have a specific significant overhead are we are going to discuss.

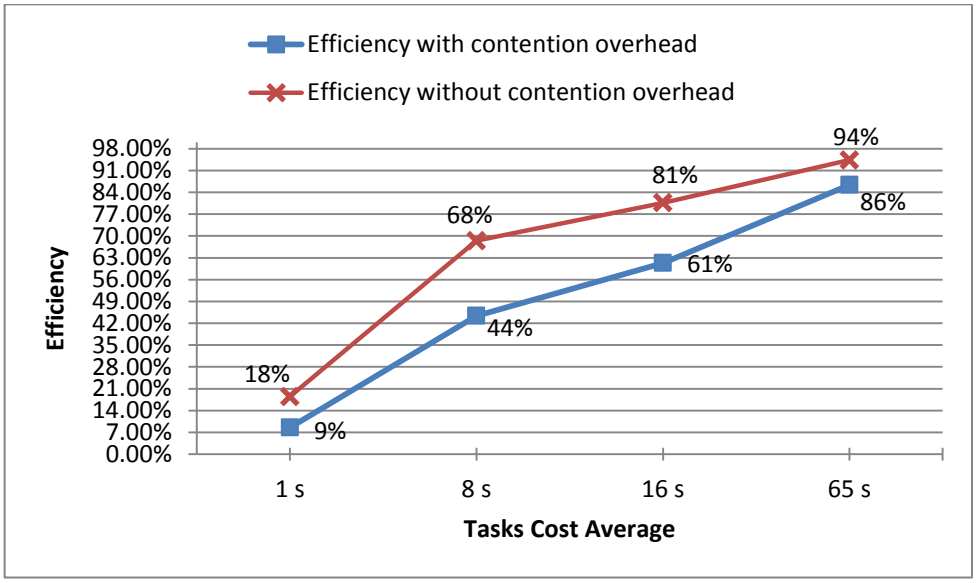


Figure 24 – Results of **Experiment 7**: varying complexity (tasks cost).

The first conclusion we can get from the results analyzing any of the two lines is that the greater the complexity of the problem, the better efficiency d-SCC achieves. This is an expected result and is common in most parallel systems. Indeed, the calculus of efficiency is directly proportional to the sequential execution time, which is directly proportional to the tasks cost average; thus, it is expected to achieve such conclusion. Moreover, Raicu *et al*. mention that tasks in MTC are short, but in the order of seconds or minutes to run (2008). Even though our solution suffers due to overheads when computing many very light tasks,

such as less than 8 seconds in average, in tasks weighting in the order of minutes, we attain excellent efficiencies (frequently over 80% in a 1,000 cores cluster).

In addition, comparing the red line with the blue line in Figure 24, we can see that our system suffers considerably due to the contention overhead caused by the FAF strategy. Specifically, when all nodes finish their tasks for an activity, all nodes remain blocked until the supervisor generates new tasks for the next runnable activity and schedules to all `SCN`, which will only start their execution when all tasks are generated and scheduled. Thence, generating tasks per activity causes a contention in current implementation of our solution, which is more critical for a great number of tasks per activity. This is an inherent overhead in all implementations of SCC for the FAF strategy.

We can measure this overhead because when all nodes finish their tasks for a certain activity, the supervisor marks this activity as "finished" and registers in the provenance database how long this activity took to execute. The `SCNs` will only start executing tasks for the next runnable activity when all tasks for this new runnable activity are generated and scheduled. Thus, the overhead mainly caused by generating and scheduling tasks is given by the difference between the total workflow execution time and the summation of the execution time of all activities, as registered in the provenance database.

The red line in Figure 24 shows the efficiency if this overhead did not exist. This overhead is directly related to the number of tasks rather than the problem complexity; hence, it remains constant even if the problem complexity varies. For greater complexities, the execution time is much greater than the overhead, reducing its impact. For this reason, the difference between the red and blue lines tends to decrease when the complexity increases, meaning that for computationally complex problems, this overhead may be neglected. Anyhow, this conclusion is important because it indicates directions for future improvements in our system. Finally, this overhead may be reduced if tasks were generated in parallel, while other tasks are still running.

Experiment 8. In the last experiment of this section, we measure speedup when the number of cores varies. We used the *1-map* workflow with 30 k tasks and 32 s tasks cost average running on Stremi machines (each machine has 24 cores), varying from 120 cores to 960 cores. In addition, we also want to investigate the impact caused by increasing the concurrency in a larger cluster (recall from the discussion introduced by the results of **Experiment 2**). The metric we used was the *RelativeSpeedup**, *i.e.*, the Equation (3) presented in Section 2.8, where B = 120 cores. The results are presented in Figure 25.

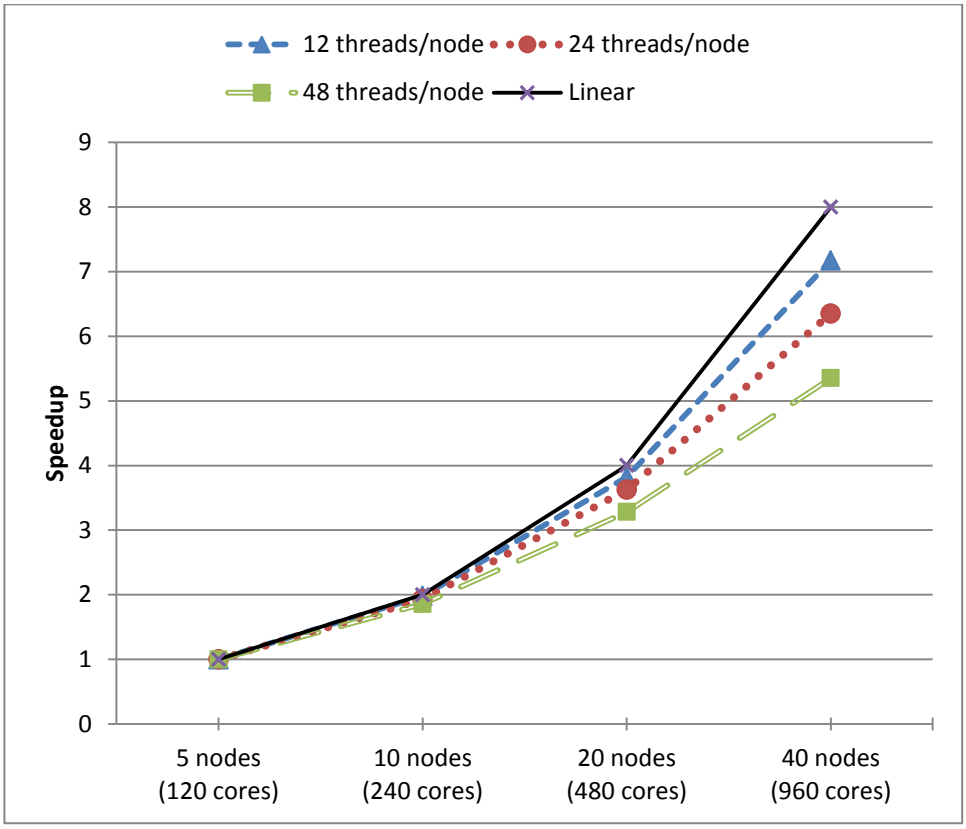


Figure 25 – Results of **Experiment 8**: speedup varying number of cores.

From the results, we can see that speedup attains almost linear until 240 cores. For 480 cores, the speedup was almost linear for 12 and 24 threads and not far from linear for 48 threads. For 960 cores, the speedup attained close to linear using 12 threads per node and 20% away from linear using 24 threads per node. We note that setting the maximum number of threads to be equal to the number of cores gave us a satisfying result (80% of efficiency) in 960 cores.

We can also see that for 48 threads per node, the speedup attained 2.6 points away from the linear speedup, which represents 34% away from the ideal. However, even though with 48 threads per node (*i.e.*, 1920 threads in 960 cores) attained the worst speedup, the execution time is still lower than with 24 threads per node. In fact, the system with 1920 threads ran 1.62 times faster than with 960 threads – the ideal would be 2 times faster.

Analyzing the graph, we can also expect that even with a number of cores greater than 960, the execution time still tends to decrease even with the number of threads twice the number of cores in the cluster. In these experiments, we did not find a limit for which there are no more gains if we add more cores or threads to the system. In other words, apparently, even though the speedup tends to decrease, we will still have gains if we add more cores and

increase the concurrency in each machine by increasing the number of threads. Thus, if we want to find this limit, larger experiments in larger clusters are still needed.

6.4 Oil & Gas and Bioinformatics workflow

So far, we have only experimented SWB workflows, which are mainly used to analyze performance. However, we also need to investigate how d-SCC behaves in more complex dataflows with added semantics in more relevant domains. For this reason, we use two workflows. The first is related to oil and gas domain. The main purpose of running this first workflow is to validate our solution for all current SciWfA operators (Section 3.1). The second workflow is a real bioinformatics workflow and the main purpose of running it is to validate our solution in a real scientific scenario.

Experiment 9. We ran a synthetic workflow from oil and gas domain, inspired in deep water oil exploration scientific applications. Since it is a synthetic workflow, we can predefine the problem complexity by setting tasks cost weight, which is similar to what we can do in relation to setting the average tasks cost in SWB workflows. We ran it on 21 Parapide machines (168 cores in total). Since our main purpose was only to validate d-SCC in a more complex dataflow containing all SciWfA operators, activities that may run in parallel, and file manipulations, we did not evaluate performance of the execution. The execution times for weights 2, 8, and 16 (which just represents complexity; the greater, the more complex) are shown in Figure 26.

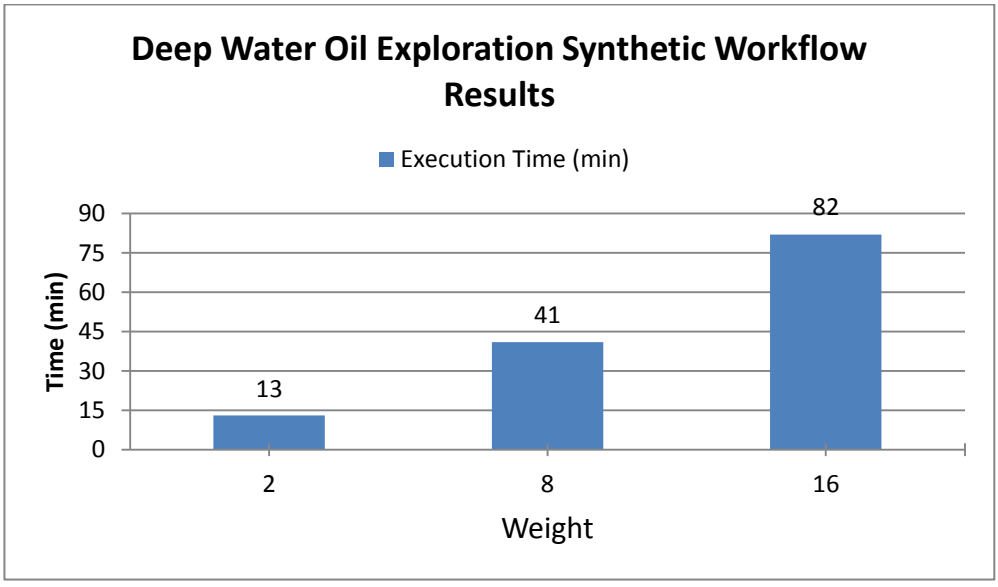


Figure 26 – Execution of **Experiment 9**: Deep water oil exploration synthetic workflow results

Experiment 10. For this experiment, we ran a real bioinformatics workflow, known as SciPhy (recall from Section 6.1). This workflow has 8 activities and some of them are computationally very complex. We ran on 552 cores Graphene cluster. Through queries to the database, we were able to find that tasks of the `Model Generator` activity take more than 30 minutes average each to run. We also found that tasks are considerably balanced. This scenario is suitable for our solution that works better for complex tasks and also for a more balanced workload. Moreover, there are many big files manipulated. The workflow successfully executed in 128 minutes. Through queries to the database, we can estimate a tasks cost average per activity and come up with an estimate sequential time by multiplying the tasks cost average by the total number of tasks. The result is 43.6 days and then, given all this information, we can estimate the real efficiency (`efficiency` as defined in Section 2.8) of d-SCC for running SciPhy on 552 cores: 89%.

Finally, we noted a peculiar occurrence when running SciPhy that did not happen when running any of our previous workflows. When we tried to run using 2 data nodes, as we have been doing in all experiments in sections Section 6.3 and in the previous experiment of this current section (**Experiment 9**), we got an error caused by memory leak. We repeated the same experiment, with same number of cores, and same dataset, but with 4 data nodes instead, and it worked successfully. This most likely has happened because d-SCC stores domain data and SciPhy has data fields with data of significant size. More specifically, phylogenetic trees are stored in the database and they are big. This result motivates us to look for solutions that would recognize that a specific big datum is being stored and an extra data node may be required. Since DDBMSs may implement elastic solutions, such as auto-sharding, which is the case of MySQL Cluster (Oracle, 2015b), we could add or remove data nodes at runtime according to the problem needs. This obviously would impact performance, but the workflow execution would not be interrupted, as happened in our experiment. This, we believe this could be investigated for future work.

6.5 Comparing d-SCC with SCC

In our last experiments, we are going to compare our implementation of d-SCC with the most recent version of SCC so far, which uses an architecture with a centralization point at the master node, as presented in 3 For this, we ran 2 experiments. We ran the exact same experiment – *i.e.*, same workflow with same input data on same hardware – using both solutions (d-SCC and SCC) to compare the results.

Experiment 11. This is a *1-map* workflow on 168 Parapide cores. The results are shown in Figure 27.

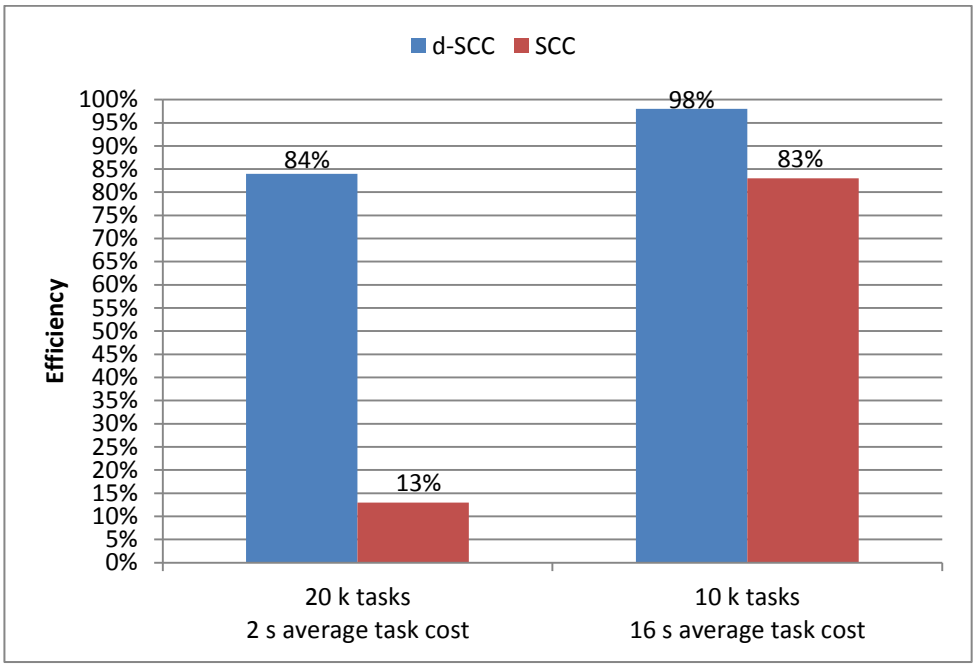


Figure 27 – Results of **Experiment 11**: comparing d-SCC with SCC on 168 cores.

From the results, we can see that, like d-SCC, SCC also has a better efficiency (`efficiency` as defined in Section 2.8) for more complex tasks than for short tasks. Moreover, analyzing the 2 s results (very frequent short queries), we can see that the centralized architecture suffers considerably more than our distributed architecture that relies on a DDBMS. d-SCC showed a gain of 71% over SCC. However, for more complex tasks (16 s average), the `SCN`s spend more time with local processing and congestion at centralized points (*e.g.*, master node and database) is alleviated. In this second scenario, d-SCC almost achieved a perfect efficiency – we highlight that we used the theoretical real efficiency rather than the relative efficiency, which would give us an even greater result. The gain over SCC was 15%, which is considerably lower than those 71% for short tasks. This means that at least for 168 cores and for more complex problems, SCC is still a good solution.

Experiment 12. This is our last experiment. We ran the *3-map* workflow, 10 k tasks per map, on 1008 Stremi cores. By using the *3-map* workflow, we can see performance loss caused by the contention due to the need of waiting for the tasks to be generated and scheduled.

Efficiency is calculated using the `efficiency` metric, which is based on a sequential theoretical time, as defined in Section 2.8. As we discussed in **Experiment 7**, this efficiency tends to be farther from reality because it does not include any overhead, which is unrealistic

in large parallel systems, and it tends to be unfair due to inherent overheads caused by contentions due to FAF usage. We could not use the *RelativeEfficiency** in this experiment because running on a smaller number of cores was taking too long and, more importantly, our main purpose in this experiment was just to see how different the performance between SCC and d-SCC is. The results are shown in Figure 28.

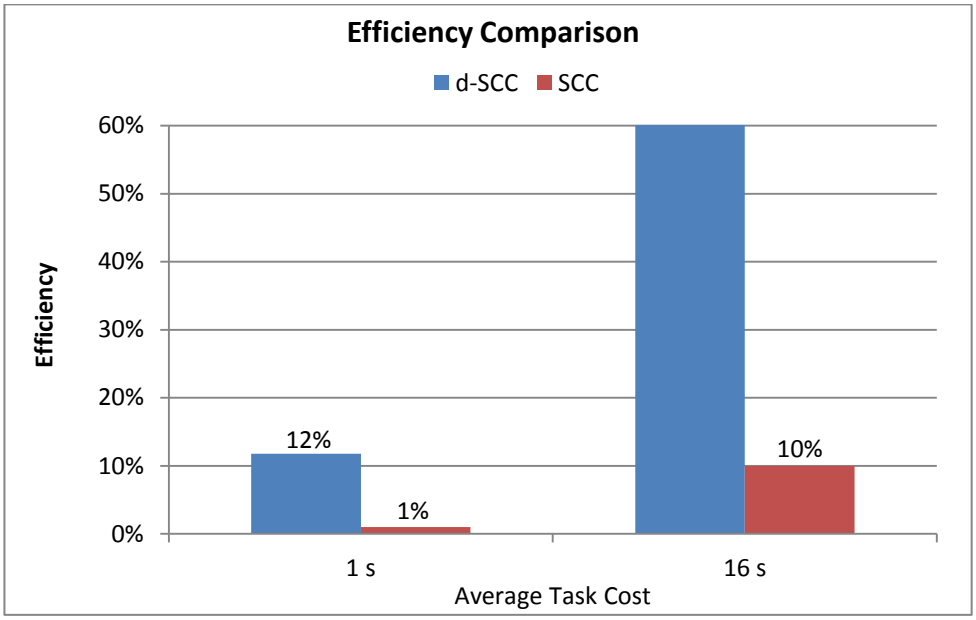


Figure 28 – Results of **Experiment 12**: comparing d-SCC with SCC on 1008 cores.

For 1,008 cores, for only 1 s tasks cost average, we can see that both solutions do not show a good performance. The tasks are so short that generating and scheduling 10 k tasks for each activity, for all cores, take longer than actually running them. We note that SCC performs very poorly, considerably worse than d-SCC. For the 16 s experiment, d-SCC achieves a better performance (more than 51% of gains over SCC), whereas SCC attains at most 10% of efficiency. Therefore, in all experiments we ran comparing d-SCC with the most recent version of SCC, we could see significant gains.

7 CONCLUSIONS

This work is inserted in the context of systems that support large-scale computer-based scientific simulations. Such simulations may be modeled as data-centric scientific workflows, require HPC, and manipulate a lot of data that need to be carefully managed. We argued that the control of this data management should not be centralized so performance can be improved and the HPC environment can be utilized more efficiently. This is an open problem because current solutions either use a centralized DBMS or use a distributed data control based on files. The limitations of file-based solutions are mainly due to lack of provenance storing at runtime, restrictions in analyzing the control information distributed in flat files and also limitations on provenance generation in the end of execution. To show our points, we developed a system that not only manages a large volume of data using a distributed database system, but also relies on such database system to take advantage of its distributed concurrency control and fault tolerance mechanisms to aid parallel execution of scientific workflows and remove single points of failure and contention.

Our main contribution is the development of SciCumulus on a Distributed Database System (d-SCC) built upon Architecture II. Architecture II is a high level architecture in the sense that it is technology independent – as long as there is a reliable distributed database system and a parallel workflow management system. It also considers many important aspects of a large-scale parallel execution of workflows, such as dynamic load balancing and fault tolerance, taking advantage of a distributed database system.

We concluded that most of the effort spent on developing the tasks scheduling based on a master-slave architecture was relieved due to using the DDBMS; thence, we could remove message passing communications that were only being used for tasks' scheduling and this facilitated removing a centralized scheduler master. However, we note that a supervisor node is still necessary for special responsibilities, such as initial tasks distribution, load balancing, and fault tolerance. Since communication between nodes is needed for this, we still need to investigate whether it is advantageous not to use other communication strategy rather than relying on the DDBMS, as we found that using Java RMI would be faster than using the DDBMS to implement FAF (*i.e.*, a blocking or non-pipeline, recall from Section 0) strategy.

We conducted several experiments to evaluate our implementation of d-SCC. First, we tried different variations of our architecture to choose the best one to use in most of our latter experiments. Then, we analyzed scalability and we found that the execution time remains close to constant when we double the number of cores and the problem size, even running on

over 960 cores. We measured speedup and found that by using the number of threads equal to half of the number of cores, we obtained a speedup very close to linear. Using the number of threads equal to double of the number of cores, we found that the execution time still tends to decrease when we increase number of cores, even though speedup was farther from linear. We did not find a limit for which the execution time stops decreasing when we increase the number of cores, at least until 960 cores. We also found that the efficiency of our system is high especially when the problem is complex (*i.e.*, average task cost is high), by frequently obtaining efficiencies over 80% even on a 1 k cores cluster. We highlight that this was the first time a system based on SCC ran on such scale of cores and for such problem size (over 50 k tasks). Before that, the centralized solution presented severe limitations to go beyond 500 cores. Moreover, we also experimented our solution in more complex workflows and in a real bioinformatics workflow. In the end, our last experiments compared d-SCC with SCC and we found that our solution significantly outperforms the most recent version of SCC, especially in a 1,000 cores cluster.

This work introduces a first prototype of a distributed architecture to control the parallel execution of data-centric workflows relying on a DDBMS. We implemented it using open software (MySQL Cluster), yet scaling up to a considerably large number of cores. Based on the many good results obtained, we see a lot of opportunities for potential improvements, in addition to some services that are not currently fully operational. In the following paragraphs, we point out directions on how our system may be improved and extended.

We have been claiming that although the underlying d-SCC's architecture (*i.e.*, Architecture II) was theoretically proposed considering many relevant aspects of parallel execution of large-scale workflows, we did not implement a few parts of this architecture. The specific parts we proposed and we did not implement are related to dynamic load balancing through task stealing or any other more sophisticated strategy and failure recovery mechanisms when either a slave node or the supervisor node faces a hardware failure. Therefore, this should be implemented in future work. Moreover, the impact on performance of the solutions for both problems needs to be analyzed.

Furthermore, we argued that the database recovery in case of failure of a database node is responsibility of the DDBMS. Although we tested our executions forcing a data node to fail and we found that the execution is indeed not interrupted, this failure recovery mechanism has impacted the performance of the workflow execution. Thus, we verified that the single point of failure introduced by a centralized DBMS is removed when a DDBMS is

used, but we did not evaluate the impact on performance when a database node fails. This is an ongoing work jointly with an undergrad student.

In addition to database node failure recovery, one other important aspect to consider is real time adaptive sharding. This means that when the system acknowledges that too much data is being stored, an extra data node could be automatically added to the DDBMS so the execution would not stop. We perceived this necessity when we ran SciPhy, which requires a lot of domain data to be stored in the database, and the execution of d-SCC was interrupted by an error and we had to add extra node nodes so it could work (Section 6.4). Thus, implementing automatic adaptive sharding on d-SCC and analyzing its impact on performance would be appreciated.

Moreover, we found that the way FAF (Section 3.2) is currently implemented introduces a significant overhead, especially when dealing with a large MTC problem. The fact that all processing nodes remain blocked until the supervisor generates tasks and schedules them so the execution can continue to the next activity (when there is more than one activity) downgraded performance severely, mainly when the problem's complexity is small. Also, FTF (*i.e.*, pipelining) needs to be implemented in d-SCC, which would not introduce such blocking barrier overhead. The implementation of FTF and improvements on FAF need to be tackled in future work and this is essential if we want to be able to handle even larger problems (*e.g.*, millions of tasks), which is currently not viable due to very long waiting time. Additionally, in Section 2.4.1, we mentioned that determining a good number value of the chunk size in a BoT may be complex, but may lead to performance improvements and we could take advantages of the provenance database since we store a lot of relevant execution data in it. This could be analyzed more deeply in future work. Furthermore, workflows executed in d-SCC commonly manipulate many big files and we still need significant improvements on dealing with large domain data files in order to enhance performance. This is actually being tackled in current work and, for future work, these efficient domain data management techniques need to be merged into d-SCC.

Finally, d-SCC mainly uses its database with OLTP usage characteristics. Currently, the DDBMS we chose to implement our architecture is an in-memory database, which delivered good advantages related to performance. We also showed that using it completely in-memory, with no checkpoints to the disk, performs considerably well. However, its storage is limited to the memory of the nodes that compose the DDBMS, which is not a problem when executing and analyzing one workflow run. Since we want to enable joint rich analyses of historical big data combining with data of many workflows or workflow executions, we

need to load the data from the in-memory database into an on-disk data warehouse. This should also be tackled in future work.

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