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Parallel Programming by Transformation

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Parallel Programming by Transformation

Abstract

The development of efficient software requires the selection of algorithms and optimizations tailored for each target hardware platform. Alternatively, performance portability may be obtained through the use of optimized libraries. However, currently all the invaluable knowledge used to build optimized libraries is lost during the development process, limiting its reuse by other developers when implementing new operations or porting the software to a new hardware platform.

To answer these challenges, we propose a model-driven approach and framework to encode and systematize the domain knowledge used by experts when building optimized libraries and program implementations. This knowledge is encoded by relating the domain operations with their implementations, capturing the fundamental equivalences of the domain, and defining how programs can be transformed by *refinement* (adding more implementation details), *optimization* (removing inefficiencies), and *extension* (adding features). These transformations enable the incremental derivation of efficient and correct by construction program implementations from abstract program specifications. Additionally, we designed an *interpretations* mechanism to associate different kinds of behavior to domain knowledge, allowing developers to *animate* programs and predict their properties (such as performance costs) during their derivation. We developed a tool to support the proposed framework, `ReFlO`, which we use to illustrate how knowledge is encoded and used to incrementally—and mechanically—derive efficient parallel program implementations in different application domains.

The proposed approach is an important step to make the process of developing optimized software more systematic, and therefore more understandable and reusable. The knowledge systematization is also the first step to enable the automation of the development process.

Programação Paralela por Transformação

Resumo

O desenvolvimento de *software* eficiente requer uma selecção de algoritmos e optimizações apropriados para cada plataforma de *hardware* alvo. Em alternativa, a portabilidade de desempenho pode ser obtida através do uso de bibliotecas optimizadas. Contudo, o conhecimento usado para construir as bibliotecas optimizadas é perdido durante o processo de desenvolvimento, limitando a sua reutilização por outros programadores para implementar novas operações ou portar o *software* para novas plataformas de *hardware*.

Para responder a estes desafios, propomos uma abordagem baseada em modelos para codificar e sistematizar o conhecimento do domínio que é utilizado pelos especialistas no desenvolvimento de *software* optimizado. Este conhecimento é codificado relacionando as operações do domínio com as suas possíveis implementações, definindo como programas podem ser transformados por *refinamento* (adicionando mais detalhes de implementação), *optimização* (removendo ineficiências), e *extensão* (adicionando funcionalidades). Estas transformações permitem a derivação incremental de implementações eficientes de programas a partir de especificações abstractas. Adicionalmente, desenhamos um mecanismo de *interpretações* para associar diferentes tipos de comportamento ao conhecimento de domínio, permitindo aos utilizadores *animar* programas e prever as suas propriedades (*e.g.*, desempenho) durante a sua derivação. Desenvolvemos uma ferramenta que implementa os conceitos propostos, `ReFlO`, que usamos para ilustrar como o conhecimento pode ser codificado e usado para incrementalmente derivar implementações paralelas eficientes de programas de diferentes domínios de aplicação.

A abordagem proposta é um passo importante para tornar o processo de desenvolvimento de *software* mais sistemático, e consequentemente, mais perceptível e reutilizável. A sistematização do conhecimento é também o primeiro passo para permitir a automação do processo de desenvolvimento de *software*.

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Chapter 1

Introduction

The increase in computational power provided by hardware platforms in the last decades is astonishing. Increases were initially achieved mainly through higher clock rates, but at some point it was necessary to add more complex hardware features, such as memory hierarchies, non-uniform memory access (NUMA) architectures, multi-core processors, clusters, or graphics processing units (GPU) as coprocessors, to increase computational power.

However, these resources are not "free", *i.e.*, in order to take full advantage of them, the developer has to be careful with program design, and tune programs to use the available features. As Sutter noted, *"the free lunch is over"* [Sut05]. The developer has to choose algorithms that best fit the target platform, he has to prepare a program to use multiple cores/machines, and apply other optimizations specific for the chosen platform. Despite the evolution of compilers, their ability to assist developers is limited as they deal with low-level program's representations, where important information about operations and algorithms used in programs is lost. Different platforms expose different characteristics, and that means the best algorithm, as well as the optimizations to use, is platform-dependent [WD98, GH01, GvdG08]. Therefore, developers need to build and maintain different versions of a program for different platforms. This problem becomes even more important because usually there is no separation between platform-specific and platform-independent code, limiting program reusability

and making program maintenance harder. Moreover, platforms are constantly evolving, thus requiring constant adaptation of programs.

This new reality moves the burden of improving performance of programs from hardware manufacturers to software developers. To take full advantage of hardware, programs must be prepared for it. This is a complex task, usually reserved for application domain experts. Moreover, developers need to have deep knowledge about the platform. These challenges are particularly noticeable in high-performance computing, due to the importance it gives to performance.

A particular type of optimization, which is becoming more and more important due to the ubiquity of parallel hardware platforms, is algorithm parallelization. With this optimization we want to improve program performance making it able to execute several tasks at the same time. This type of optimization receives special attention in this work.

Optimized software libraries have been developed by experts for several domains (*e.g.*, BLAS [LHKK79], FFTW [FJ05], PETSc [BGMS97]), relieving end users from having to optimize code. However, other problems remain. What happens when the hardware architecture changes? Can we leverage expert knowledge to retarget the library to the new hardware platform? And what if we need to add support to new operations? Can we leverage expert knowledge to optimize the implementation of new operations? Moreover, even if the libraries are highly optimized, when used in specific contexts they may often be further optimized for that particular use-case. Again, leveraging expert knowledge is essential.

Typically only the final code of an optimized library is available. The expert knowledge that was used to build and optimize the library is not present in the code, *i.e.*, the series of small steps manually taken by domain experts was lost in the development process. The main problem is the fact that software development, particularly when we talk about the highly optimized code required by current hardware platforms, is more about *hacking* than *science*. We seek an approach that makes the development of optimized software a science, through a systematic encoding of expert knowledge used to produce optimized software. Considering how rare domain experts are, this encoding is critical, so that it can

be understood and passed along to current and next-generation experts.

To answer these challenges, as well as to handle the growing complexity of programs, we need new approaches. *Model-driven engineering (MDE)* is a software development methodology that addresses the complexity of software systems. In this work, we explore the use of model-driven techniques, to mechanize/automate the construction of high-performance, platform-specific programs, much in same way other fields have been leveraging from mechanization/automation since the Industrial Revolution [Bri14].

This work is built upon ideas originally promoted by *knowledge-based software engineering (KBSE)*. KBSE was a field of research that emerged in the 1980s and promoted the use of transformations to map a specification to an efficient implementation [GLB+83, Bax93]. To build a program, the developers would write a specification, and apply transformations to it, with the help of a tool, to obtain an implementation. Similarly, to maintain a program, developers would only change the specification, and then they would replay the derivation process to get the new implementation. In KBSE, developers would work at specification level, *i.e.*, closer to the problem domain, instead of working at code level, where important knowledge about the problem was lost, particularly when dealing with highly-optimized code, limiting the ability to transform the program. KBSE relied on the use of formal, machine-understandable languages to create specifications, and tools to mediate all steps in the development process.

We seek a domain-independent approach, based on high-level, platform independent models and transformations to encode the knowledge of domain experts. It is not our goal to conceive new algorithms or implementations, but rather to distill knowledge of existing programs so that tools can reuse this knowledge for program construction.

Admittedly, this task is enormous; it has been subdivided into two large parallel subtasks. Our focus is to present a conceptual framework that defines how to encode knowledge required for optimized software construction. The second task, which is parallel to our work (and out of the scope of this thesis), is to build an engine that applies encoded knowledge to generate high-performance

software [MBS12, Mar14]. This second task requires a deeper understanding of the peculiarities of a domain, in particular of how domain experts decide whether a design decision is good or not (*i.e.*, whether it is likely to produce an efficient implementation), so that this knowledge can be used by the engine that automates the software generation to avoid having to explore the entire space of valid implementations.

We explore several application domains to test the generality and limitations of the approach we propose. We use *dense linear algebra (DLA)* as our main application domain, as it is a well-known and mature domain, that has always received the attention of researchers concerned with highly optimized software.

1.1 Research Goals

The lack of structure that characterizes the development of efficient programs in domains such as DLA, makes it extraordinarily difficult for non-experts to develop efficient programs and to reuse (let alone understand) knowledge of domain experts.

We aim to address these challenges with an approach that promotes incremental development, where complex programs are built by refining, composing, extending and optimizing simpler building blocks. We believe the key to such an approach is on the definition of a conceptual framework to support the systematic encoding of domain-specific knowledge that is suitable for automation of program construction. MDE has been successful in explaining the design of programs in many domains, thus we intend to continue this line of work with the following goals:

1. Define a high-level framework (*i.e.*, a theory) to encode domain-specific knowledge, namely operations, the algorithms that implement those operations, possible optimizations, and programs architectures. This framework should help non-experts to understand existing algorithms, optimizations, and programs. It should also be easily extensible, to admit new operations, algorithms and optimizations.

2. Develop a methodology to incrementally map high-level specifications to implementations optimized to specific hardware platforms, using previously systematized knowledge. Decisions such as the choice of the algorithm, optimizations, and parallelization should be supported by this methodology. The methodology should help non-experts to understand how algorithms are chosen, and which optimizations are applied, *i.e.*, the methodology should contribute to expose the expert's design decisions to non-experts.

3. Provide tools that allow an expert to define domain knowledge, and that allow non-experts to use this knowledge to mechanically derive optimized implementations for their programs in a correct-by-construction process [Heh84].

This research work is part of a larger project/approach, which we call *Design by Transformation (DxT)*, where the ultimate goal is to fully automate the derivation of optimized programs. Although, as we said earlier, the tool to fully explore the space of all implementations of a specification and to choose the "best" program is *not* the goal of this research work, it is a complementary part of this project, where systematically encoded knowledge is used.

1.2 Overview of the Proposed Solution

To achieve the aforementioned research goals we propose a framework where domain knowledge is encoded as rewrite rules (transformations), which allows the development process to be decomposed into small steps that contributes to make domain knowledge more accessible to non-experts. To ease the specification and understanding of domain knowledge, we use a graphical dataflow notation. The rewrite rules associate domain operations with their possible algorithm implementations, encoding the knowledge needed to refine a program specification into a platform-specific implementation. Moreover, rewrite rules may also relate multiple blocks of computation that provide the same behavior. Indirectly, this knowledge specifies that certain blocks of computation (possibly

inefficient) may be replaced by others (possibly more efficient), which provide the same behavior. Although we want to encode domain-specific knowledge, we believe this framework is general enough to be used in many domains, *i.e.*, it is a domain-independent way to encode the domain-specific knowledge.

The same operation may be available with slightly different sets of features (*e.g.*, a function that can make some computation either in a 2D space or a 3D space). We propose to relate variants of the same operation using extensions. We use extensions to make the derivation process more incremental, as by using them we can start with derivations of simpler variants of a program, and progressively add features to the derivations, until the derivation for the fully-featured specification is obtained.

We will provide methods to associate properties to models, so that properties about programs modeled can be automatically computed (*e.g.*, to estimate program performance).

The basic workflow we foresee has two phases (Figure 1.1): (i) knowledge specification, and (ii) knowledge application. Initially we have a *domain expert* systematizing the domain knowledge, *i.e.*, he starts by encoding the domain operations and algorithms he normally uses. He also associates properties to operations and algorithms, to estimate their performance characteristics, for example. Then, he uses this knowledge to derive (reverse engineer) programs he wrote in the past. The reverse engineering process is conducted defining a high-level specification of the program (using the encoded operations), and trying to use the systematized knowledge (transformations) to obtain the optimized program implementation. While reverse engineering his programs, the domain expert will recall other algorithms he needs to obtain his optimized programs, which he adds to the previously defined domain knowledge. These steps are repeated until the domain expert has encoded enough knowledge to reverse engineering his programs. At this point, the systematized domain knowledge can be made available to other developers (non-experts), that can use it to derive optimized implementations for their programs, and to estimate properties of these programs. Developers also start by defining the high-level specification of their

programs (using the operations defined by domain experts), and then they apply the transformations that have been systematized by domain experts.

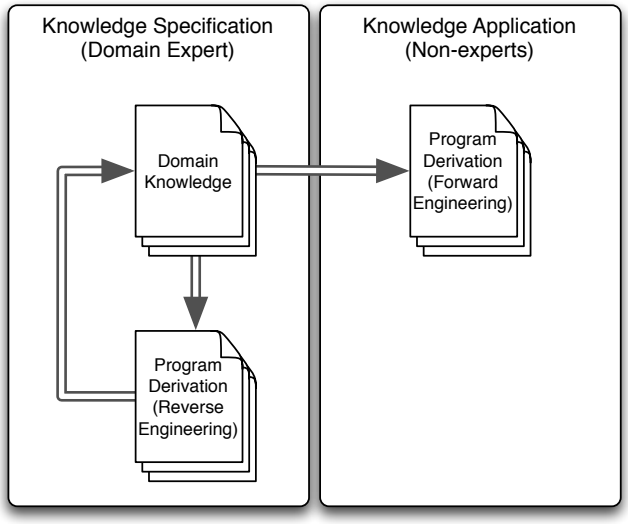


Figure 1.1: Workflow of the proposed solution.

Our research focuses on the first phase. It is our goal to provide tools to mechanically apply transformations based on the systematized knowledge. Still, the user has to choose which transformations to apply, and where. Other tools can be used to automate the application of the domain knowledge [Mar14].

1.3 Document Structure

We start by introducing basic background concepts about MDE and parallel programing, as well as the application domains, in Chapter 2. In Chapter 3 we define the main concepts of the approach we propose, namely the models we use to encode domain knowledge, how this allows the transformation of program specifications by refinement and optimization into correct-by-construction implementations, and the mechanism to associate properties to models. We also present `ReFlO`, a tool that implements the proposed concepts. In Chapter 4 we show how the proposed concepts are applied to derive programs from the relational databases and DLA domains. In Chapter 5 we show how models may be enriched to encode extensions, which specify how a feature is added to models,

and then, in Chapter 6, we show how extensions, together with refinements and optimizations, are used to reverse engineer a fault-tolerant server and molecular dynamics simulation programs. In Chapter 7 we present an evaluation of the approach we propose based on software metrics. Related work is revised and discussed in Chapter 8. Finally, Chapter 9 presents concluding remarks, and directions for future work.

Chapter 2

Background

In this section we provide a brief introduction to the core concepts related to the approach and application domains considered in this research work.

2.1 Model-Driven Engineering

MDE is a software development methodology that promotes the use of models to represent knowledge about a system, and model transformations to develop software systems. It lets the developers focus on the domain concepts and abstractions, instead of implementation details, and relies on the use of systematic transformations to map the models to implementations.

A *model* is a simplified representation of a system. It abstracts the details of a system, making it easier to understand and manipulate, while keeping the ability to provide the stakeholders that are using the model the details about the system they need [BG01].

Selic [Sel03] lists five characteristics that a model should have:

Abstraction. It should be a simplified version of the system, that hides insignificant details (*e.g.*, technical details about languages or platforms), and allows the stakeholders to focus on the essential properties of the system.

Understandability. It should be intuitive and easy to understand by the stakeholders.

Accuracy. It should provide a precise representation of the system, giving to the stakeholders the same answers the system would give.

Predictiveness. It should provide the needed details about the system.

Economical. It should be cheaper to construct than the physical system.

Models conform to a *metamodel*, which defines the rules that the metamodel instances should meet (namely *syntax* and *type* constraints). For example, the metamodel of a language is usually provided by its grammar, and the metamodel of an XML document is usually provided by its XML schema or DTD.

The modeling languages can be divided in two groups. *General purpose modeling languages (GPML)* try to give support for a wide variety of domains and can be extended when they do not fit some particular need. In this group we have languages such as the *Unified Modeling Language (UML)*. On the other hand, *domain-specific modeling languages (DSML)* are designed to support only the needs of a particular domain or system. Modeling languages may also follow different notation styles, such as *control flow* or *data flow*.

Model *transformations* [MVG06] convert one or more source models into one or more target models. They manipulate models in order to produce new artifacts (*e.g.*, code, documentation, unit tests), and allow the automation of recurring tasks in the development process.

There are several common types of transformations. *Refinements* are transformations that add details to models without changing their correctness properties, and can be used to transform a *platform-independent model (PIM)* into a *platform-specific model (PSM)* or, more generally, an abstract specification into an implementation. *Abstractions* do the opposite, *i.e.*, remove details from models. *Refactorings* are transformations that restructure models without changing their behavior. *Extensions* are transformations that add new behavior or features to models. The transformations may also be classified as *endogenous*, when both

the source and the target models are instances of the same metamodel (*e.g.*, a code refactoring), or *exogenous*, when the source and the target models are instances of different metamodels (*e.g.*, the compilation of a program, or a *model to text (M2T)* transformation). Regarding abstraction level, transformations may be classified as *horizontal*, if the resulting model stays at the same abstraction level of the original model, or as *vertical*, if the abstraction level changes as a result of the transformation.

MDE is used for multiple purposes, bringing several benefits to software development. The most obvious is the abstraction it provides, essential to handle the increasing complexity of software systems. Providing simpler views of the systems, they become easier to understand and to reason about, or even to show their correction [BR09]. Models are closer to the domain, and use more intuitive notations, thus even stakeholders without Computer Science skills can participate in the development process. This can be particularly useful in requirements engineering, where we need a precise specification of the requirements, so that developers know exactly what they have to build (natural language is usually too ambiguous for this purpose), expressed in a notation that can be understood by system users, so that they can validate the requirements. Being closer to the domain also makes models more platform independent, increasing reusability and making easier to deploy the system in different platforms.

Models are flexible (particularly when using DSML), giving freedom for users to choose the information they want to express, and how the information should be organized. Users can also use different models and views to express different views of the system.

Models can be used to validate the system or to predict its behavior without having to support the cost of building the entire system, or the consequences of failures in the real systems, which may not be acceptable [IAB09]. They have been used to check for cryptographic properties [JÖ5, ZRU09], to detect concurrency problems [LWL08, SBL08], or to predict performance [BMI04], for example. This allows the detection of problems in early stages of the design process, where they are cheaper to fix [Sch06, SBL09].

Automation is another key benefit of MDE. It dramatically reduces the time needed to perform some tasks, and usually leads to higher quality results than when tasks are performed manually. There are several tasks of the development process that can be automated. Tools can be used to automatically analyze models and detect problems, and even to help the user to fix them [Egy07]. Models are also used to automate the generation of tests [AMS05, Weß09, IAB09]. Code writing is probably the most expensive, tedious and error-prone task in software development. With MDE we can address this problem by building transformations that automatically generate the code (or at least part of it) from models. Empirical studies already showed the benefits of using models in software development [Tor04, ABHL06, NC09].

Some of these tasks (*e.g.*, validation) could also be done using only code. It is important to note that code is also a model.[1] However usually it is not the best model to work with, because of its complexity (as it often contains irrelevant details) and its inability to store all the needed information. For example, code loses information about the operations used in a program, which would be useful if we want to change their implementations (the best implementation for an operation is often platform-specific [GvdG08]). The use of code *annotations* clearly shows the need to provide additional information, *i.e.*, the need to extend the (code) metamodel. Moreover, code is only available in late stages of the development process, which compromises the early detection of problems in the system.

The use of MDE also presents challenges to developers. One of the biggest difficulties when using MDE is the lack of stable and mature tools. This is a very active field of research, and we are seeing tools that exist to help code development being adapted to support models (*e.g.*, version management [GKE09, GE10, Kön10], slicing [LKR10], refactorings [MCH10], generics support [dLG10]), as well as tools that address problems more specific from MDE world (*e.g.*, model migration [RHW+10], graphs layout [FvH10], development of

[1] Although code is also a model, when we use the term *model* we are usually talking about more abstract types of models.

graphical editors [KRA+10]). Standardization is another problem. DSMLs compromise the reuse of tools and methodologies, as well as interoperability. On the other hand, GPMLs are too complex for most of cases [FR07]. The generation of efficient code is also a challenge. However, as Selic noted [Sel03], this was also a problem in the early days of compilers, but eventually they become able to produce code as good as the code that an expert would produce. So we have reasons to believe that, as tools become more mature, this concern will diminish.

2.2 Parallel Computing

Parallel computing is a programming technique where a problem is divided into several tasks that can be executed concurrently by many processing units. By leveraging the use of many processing units to solve the problem, we can make the computation run faster and/or address larger problems. Parallel computing appeared decades ago, and it was mainly used in scientific software. In the past decade it has become essential in all kinds of software applications, due to the difficulties to improve the performance of a single processing unit,[2] making multicore devices ubiquitous.

However, several difficulties arise developing parallel programs, when comparing with developing sequential programs. Additional logic/code is typically required to handle concurrency/coordination of tasks. Sometimes even new algorithms are required, as the ones used in the sequential version of the programs do not perform well when parallelized. Concurrent execution of tasks often make the order of the instruction flow of tasks non-deterministic, making debugging and profiling more difficult. The multiple and/or more complex target hardware platforms may also require specialized libraries and tools (*e.g.*, for debugging or profiling), and contribute to the problem of performance portability.

Flynn's taxonomy [Fly72] provides a common classification for computer architectures, according to the parallelism that can be explored:

[2]Note that even single core CPU may offer instruction-level parallelism. More on this later.

SISD. Systems where a single stream of instructions is applied to one data stream (there is instruction-level parallelism only);

SIMD. Systems where a single stream of instructions is applied to multiple data streams (this is typical in GPUs);

MISD. Systems where multiple streams of instructions are applied to a single data stream; and

MIMD. Systems where multiple streams of instructions are applied to multiple data streams.

One of the most common techniques of exploring parallelism is known as *single program multiple data (SPMD)* [Dar01]. In this case the same program is executed on multiple data streams. Conditional branches are used so that different instances of the program execute different instructions, thus this is a subcategory of MIMD (not SIMD).

The *dataflow computing model* is an alternative to the traditional Von Neumann model. In this model we have operations with inputs and outputs. The operations can be executed when their inputs are available. Operations are connected to each other to specify how data flows through operations. Any two operations that do not have a data dependency among them may be executed concurrently. Therefore this programming model is well-suited to explore parallelism and model parallel programs [DK82, NLG99, JHM04]. Different variations of this model have been proposed over the years [Den74, Kah74, NLG99, LP02, JHM04].

Parallelism may appear at different levels, from fine-grained instruction-level parallelism, to higher-level (*e.g.*, loop-, procedure- or program-level) parallelism. *Instruction-level parallelism (ILP)* takes advantage of CPU features such as multiple execution units, pipelining, out-of-order execution, or speculative execution, available on common CPUs nowadays, so that the CPU can execute several instructions simultaneously. In this research work we do not address ILP. Our focus is on higher-level (loop- and procedure-level) parallelism, targeting shared and distributed memory systems.

In *shared memory systems* all processing units see the same address space, and they can all access all memory data, providing simple (and usually fast) data sharing. However, shared memory systems typically offer a limited scalability as the number of processing units increases. In *distributed memory systems* each processing unit has its own local memory / address space, and the network is used to obtain data from other processing units. This makes sharing data among processing units more expensive, but distributed memory systems typically provide more parallelism. Often both types of systems are mixed, where we have a large distributed memory system, where each of its elements is a shared memory system, allowing programs to benefit from fast data sharing inside the shared memory system, but also taking advantage of the scalability of a distributed memory system.

The *message passing programming model* is typically used in distributed memory systems. In this case, each computing unit (process) controls its data, and other processes can send and receive messages to exchange data. The *message passing interface (MPI)* [For94] is the *de facto* standard for this model. It specifies a communication API, that provides operations to send/receive data to/from other processes, as well as collective communications, to distribute data among processes (*e.g.*, `MPI_BCAST` that copies the data to each processes, or `MPI_SCATTER` that divides data among all processes) and to collect data from all processes (*e.g.*, `MPI_REDUCE` that combines data elements from each processes, or `MPI_GATHER` that receives chunks of data from each process). This programming model is usually employed when implementing SPMD parallelism.

2.3 Application Domains

2.3.1 Dense Linear Algebra

Several sciences and engineering domains face problems where they need to use linear algebra operations to solve them. Due to its importance, the linear algebra domain has received the attention of researchers, in order to develop efficient

algorithms to solve problems such as systems of linear equations, linear least squares, eigenvalue, or singular value decomposition.

This is a mature and well understood domain, with *regular programs*.[3] Moreover, the *basic building blocks* of the domain were already identified, and efficient implementations of these blocks are provided by libraries. This is the main domain studied in this research work.

In this section we provide a brief overview of the field, introducing some definitions and common operations. Developers that need highly optimized software in this domain usually rely on well-known APIs/libraries, which are also presented.

2.3.1.1 Matrix Classifications

We present some common classifications of matrices, that help to understand operations and algorithms of linear algebra.

Identity. A square matrix $\mathtt{A}$ is an *identity* matrix if it has ones on the diagonal, and all other elements are zeros. The $\mathtt{n} \times \mathtt{n}$ identity matrix is usually denoted by $\mathtt{I_n}$ (or simply $\mathtt{I}$ when the size of the matrix is not relevant).

Triangular. A matrix $\mathtt{A}$ is *triangular* if it has all elements above or below the diagonal equal to zero. It is called lower triangular if the zero elements are above the diagonal, and upper triangular if the zero elements are below the diagonal. If all elements on the diagonal are zeros, it is said strictly triangular. If all elements on the diagonal are ones, it is said unit triangular.

Symmetric. A matrix $\mathtt{A}$ is *symmetric* if it is equal to its transpose, $\mathtt{A} = \mathtt{A}^\mathtt{T}$.

Hermitian. A matrix $\mathtt{A}$ is *hermitian* if it is equal to its conjugate transpose, $\mathtt{A} = \mathtt{A}^*$. If $\mathtt{A}$ contains only real numbers, it is hermitian if it is symmetric.

Positive Definite. A $\mathtt{n} \times \mathtt{n}$ complex matrix $\mathtt{A}$ is *positive definite* if for all $\mathtt{v} \neq \mathtt{0} \in \mathbb{C}^\mathtt{n}$, $\mathtt{vAv}^* > \mathtt{0}$ (or $\mathtt{vAv}^\mathtt{T} > \mathtt{0}$, for $\mathtt{v} \neq \mathtt{0} \in \mathbb{R}^\mathtt{n}$ if $\mathtt{A}$ is a real matrix).

[3] DLA programs are regular because (i) they rely on dense arrays as their main data structures (instead of pointer-based data structures, such as graphs), and (ii) the execution flow of programs is predictable without knowing the input values.

Nonsingular. A square matrix $\mathtt{A}$ is *nonsingular* if it is invertible, *i.e.*, if there is a matrix $\mathtt{B}$ such that $\mathtt{AB} = \mathtt{BA} = \mathtt{I}$.

Orthogonal. A matrix $\mathtt{A}$ is *orthogonal* if its inverse is equal to its transpose, $\mathtt{A}^\mathtt{T}\mathtt{A} = \mathtt{A}\mathtt{A}^\mathtt{T} = \mathtt{I}$.

2.3.1.2 Operations

LU Factorization. A square matrix $\mathtt{A}$ can be decomposed into two matrices $\mathtt{L}$, unit lower triangular, and $\mathtt{U}$, upper triangular, such that $\mathtt{A} = \mathtt{LU}$. This process is called *LU factorization* (or *decomposition*).

It can be used to solve linear systems of equations. Given a system of the form $\mathtt{Ax} = \mathtt{b}$ (equivalent to $\mathtt{L}(\mathtt{Ux}) = \mathtt{b}$), we can find $\mathtt{x}$, first solving the system $\mathtt{Ly} = \mathtt{b}$, and then the system $\mathtt{Ux} = \mathtt{y}$. As $\mathtt{L}$ and $\mathtt{U}$ are triangular matrices, any of these systems is "easy" to solve.

Cholesky Factorization. A square matrix $\mathtt{A}$, that is hermitian and positive definite, can be decomposed into $\mathtt{LL}^*$, such that $\mathtt{L}$ is a lower triangular matrix with positive diagonal elements. This process is called *Cholesky factorization* (or *decomposition*).

As LU factorization, it can be used to solve linear systems of equations, providing a better performance. However, it is not as general as LU factorization, as the matrix has to have certain properties.

2.3.1.3 Basic Linear Algebra Subprograms

Basic Linear Algebra Subprograms (BLAS) is a standard API for the DLA domain, which provides basic operations over vectors and matrices [LHKK79, Don02a, Don02b].

The operations provided are divided in three groups. *Level 1* provides scalar and vector operations, *level 2* provides matrix-vector operations, and *level 3* matrix-matrix operations. These operations are the basic building blocks of the linear algebra domain, and upon them, we can build more complex programs.

There are several implementations of BLAS available, developed by the academic community and hardware vendors (such as Intel [Int] and AMD [AMD]), and optimized for different platforms. Using BLAS, the developers are released from having to optimize the basic functions for different platforms, contributing to better performance portability.

2.3.1.4 Linear Algebra Package

The *Linear Algebra Package (LAPACK)* [ABD+90] is a library that provides functions to solve systems of linear equations, linear least squares problems, eigenvalue problems, and singular value problems. It was built using BLAS, in order to provide performance portability.

ScaLAPACK [BCC+96] and PLAPACK [ABE+97] are two extensions to LAPACK that provide implementations for distributed memory systems of some of the functions of LAPACK.

2.3.1.5 FLAME

The *Formal Linear Algebra Methods Environment (FLAME)* [FLA] is a project that aims to make linear algebra computations a science that can be understood by non-experts in the domain, through the development of *"a new notation for expressing algorithms, a methodology for systematic derivation of algorithms, Application Program Interfaces (APIs) for representing the algorithms in code, and tools for mechanical derivation, implementation and analysis of algorithms and implementations"* [FLA]. This project also provides a library, *libflame* [ZCvdG+09], that implements some of the operations provided by BLAS and LAPACK.

The FLAME Notation. The FLAME notation [BvdG06] allows the specification of dense linear algebra algorithms without exposing the array indices. The notation also allows the specification of different algorithms for the same operation, in a way that makes them easy to compare. Moreover, algorithms

Algorithm: $\mathtt{C} := \text{mult}(\mathtt{A}, \mathtt{B}, \mathtt{C})$

Partition $\mathtt{A} \rightarrow \left(\begin{array}{c|c} \mathtt{A_L} & \mathtt{A_R} \end{array} \right)$, $\mathtt{B} \rightarrow \left(\begin{array}{c} \mathtt{B_T} \\ \hline \mathtt{B_B} \end{array} \right)$

where $\mathtt{A_L}$ has 0 columns, $\mathtt{B_T}$ has 0 rows

while $\mathtt{m}(\mathtt{A_L}) < \mathtt{m}(\mathtt{A})$ **do**

Repartition

$$\left(\begin{array}{c|c} \mathtt{A_L} & \mathtt{A_R} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} \mathtt{A_0} & \mathtt{a_1} & \mathtt{A_2} \end{array} \right), \left(\begin{array}{c} \mathtt{B_T} \\ \hline \mathtt{B_B} \end{array} \right) \rightarrow \left(\begin{array}{c} \mathtt{B_0} \\ \hline \mathtt{b_1^T} \\ \hline \mathtt{B_2} \end{array} \right)$$

where $\mathtt{a_1}$ has 1 column, $\mathtt{b_1^T}$ has 1 row

$$\mathtt{C} = \mathtt{a_1 b_1^T} + \mathtt{C}$$

Continue with

$$\left(\begin{array}{c|c} \mathtt{A_L} & \mathtt{A_R} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} \mathtt{A_0} & \mathtt{a_1} & \mathtt{A_2} \end{array} \right), \left(\begin{array}{c} \mathtt{B_T} \\ \hline \mathtt{B_B} \end{array} \right) \leftarrow \left(\begin{array}{c} \mathtt{B_0} \\ \hline \mathtt{b_1^T} \\ \hline \mathtt{B_2} \end{array} \right)$$

endwhile

Figure 2.1: Matrix-matrix multiplication in FLAME notation.

```
function [C] = mult(A, B, C0) {
  C = C0;
  s = size(A,2);

  for i = 1:s
    C = C + A(:,i) * B(i,:);
  end
}
```

Figure 2.2: Matrix-matrix multiplication in Matlab.

expressed using this notation can be easily translated to code using the FLAME API.

We show an example using this notation. Figure 2.1 depicts a matrix-matrix multiplication algorithm using flame notation (the equivalent Matlab code is shown in Figure 2.2).

Instead of using indices, in FLAME notation we start by dividing the matrices in two parts (`Partition` block). In the example, matrix `A` is divided in $\mathtt{A_L}$ (the

left part of the matrix) and $\mathtt{A_R}$ (the right part of the matrix), and matrix B is divided in $\mathtt{B_T}$ (the top part) and $\mathtt{B_B}$ (the bottom part).[4] The matrices $\mathtt{A_L}$ and $\mathtt{B_T}$ will store the parts of the matrices that were already used in the computation, therefore initially these two matrices are empty. Then we have the loop, that iterates over the matrices, while the size of matrix $\mathtt{A_L}$ (given by $\mathtt{m}(\mathtt{A_L})$) is less than the size of A, *i.e.*, while there are elements of matrix A that have not been used in the computation yet. At each iteration, the first step is to expose the values that will be processed in the iteration. This is done in the `Repartition` block. From matrix $\mathtt{A_L}$ we create matrix $\mathtt{A_0}$. The matrix $\mathtt{A_R}$ is divided in two matrices, $\mathtt{a_1}$ (the first column) and $\mathtt{A_2}$ (the remaining columns). Thus, we exposed in $\mathtt{a_1}$ the first column of A that has not been used in the computation. A similar operation is applied to matrices $\mathtt{B_T}$ and $\mathtt{B_B}$ to expose a row of B. Then we update the value of C (the result), using the exposed values. At the end of the iteration, in the `Continue with` block, the exposed matrices are joined with the parts of the matrices that contain the values already used in the computation (*i.e.*, $\mathtt{a_1}$ is joined with $\mathtt{A_0}$ and $\mathtt{b_1^T}$ is joined with $\mathtt{B_0}$). Therefore, in the next iteration the next column/row will be exposed.

For efficiency reasons, matrix algorithms are usually implemented using blocked versions, where at each iteration we process several rows/columns instead of only one. A blocked version of the algorithm from Figure 2.1 is shown in Figure 2.3. Notice that the structure of the algorithm remains the same. When we repartition the matrix to expose the next columns/rows, instead of creating a column/row matrix, we create a matrix with several columns/rows. Using Matlab (Figure 2.4), the indices make code complex (and using language such as C, that does not provide powerful index notations, it would be even more difficult to understand the code).

FLAME API. The `Partition`, `Repartition` and `Continue with` instructions are provided by FLAME API [BQOvdG05], which provides an easy way to translate an algorithm implemented in FLAME notation to code. The FLAME

[4] In this algorithm we divided the matrices in two parts. Other algorithms may require the matrices to be divided in four parts, top-left, top-right, bottom-left and bottom-right.

Algorithm: $\mathtt{C} := \text{mult}(\mathtt{A}, \mathtt{B}, \mathtt{C})$

Partition $\mathtt{A} \rightarrow \left(\begin{array}{c|c} \mathtt{A_L} & \mathtt{A_R} \end{array} \right)$, $\mathtt{B} \rightarrow \left(\begin{array}{c} \mathtt{B_T} \\ \hline \mathtt{B_B} \end{array} \right)$

where $\mathtt{A_L}$ has $\mathtt{0}$ columns, $\mathtt{B_T}$ has $\mathtt{0}$ rows

while $\mathtt{m}(\mathtt{A_L}) < \mathtt{m}(\mathtt{A})$ **do**

Determine block size $\mathtt{b}$

Repartition

$$\left(\begin{array}{c|c} \mathtt{A_L} & \mathtt{A_R} \end{array} \right) \rightarrow \left(\begin{array}{c|c|c} \mathtt{A_0} & \mathtt{A_1} & \mathtt{A_2} \end{array} \right), \left(\begin{array}{c} \mathtt{B_T} \\ \hline \mathtt{B_B} \end{array} \right) \rightarrow \left(\begin{array}{c} \mathtt{B_0} \\ \hline \mathtt{B_1} \\ \hline \mathtt{B_2} \end{array} \right)$$

where $\mathtt{A_1}$ has $\mathtt{b}$ columns, $\mathtt{B_1}$ has $\mathtt{b}$ rows

$$\mathtt{C} = \mathtt{A_1 B_1} + \mathtt{C}$$

Continue with

$$\left(\begin{array}{c|c} \mathtt{A_L} & \mathtt{A_R} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} \mathtt{A_0} & \mathtt{A_1} & \mathtt{A_2} \end{array} \right), \left(\begin{array}{c} \mathtt{B_T} \\ \hline \mathtt{B_B} \end{array} \right) \leftarrow \left(\begin{array}{c} \mathtt{B_0} \\ \hline \mathtt{B_1} \\ \hline \mathtt{B_2} \end{array} \right)$$

endwhile

Figure 2.3: Matrix-matrix multiplication in FLAME notation (blocked version).

```
function [C] = mult(A, B, C0) {
  C = C0;
  s = size(A,2);

  for i = 1:mb:s
    b = min(mb, s-i+1);
    c = c + a(:,i:i+b-1) * b(i+b-1,:);
  end
}
```

Figure 2.4: Matrix-matrix multiplication in Matlab (blocked version).

API is available for C and Matlab languages. The C API also provides some additional functions to create and destroy matrix objects, to obtain information about the matrix objects, and to show the matrix contents.

Figure 2.5 shows the implementation of matrix-matrix multiplication (unblocked version) in Matlab using the FLAME API (notice the similarities between this implementation and algorithm specification presented in Figure 2.1).

```
function [ C_out ] = mult( A, B, C )
  [ AL, AR ] = FLA_Part_1x2( A, ...
                             0, 'FLA_LEFT' );
  [ BT, ...
    BB ] = FLA_Part_2x1( B, ...
                         0, 'FLA_TOP' );

  while ( size( AL, 2 ) < size( A, 2 ) )
    [ A0, a1, A2 ]= FLA_Repart_1x2_to_1x3( AL, AR, ...
                                           1, 'FLA_RIGHT' );
    [ B0, ...
      b1t, ...
      B2 ] = FLA_Repart_2x1_to_3x1( BT, ...
                                    BB, ...
                                    1, 'FLA_BOTTOM' );

    C = C + a1 * b1t;

    [ AL, AR ] = FLA_Cont_with_1x3_to_1x2( A0, a1, A2, ...
                                           'FLA_LEFT' );
    [ BT, ...
      BB ] = FLA_Cont_with_3x1_to_2x1( B0, ...
                                       b1t, ...
                                       B2, ...
                                       'FLA_TOP' );
  end
  C_out = C;
return
```

Figure 2.5: Matlab implementation of matrix-matrix multiplication using FLAME API.

Algorithms for Factorizations Using FLAME Notation. We now show algorithms for LU factorization (Figure 2.6) and Cholesky factorization (Figure 2.7) using the FLAME notation. These algorithms were systematically derived from a specification of the operations [vdGQO08]. Other algorithms exist, see [vdGQO08] for more details about these and other algorithms.

In the algorithms we present here, we do not explicitly define the size of the matrices that are exposed in each iteration (defined by `b`). These algorithms are generic, as they can be used to obtain blocked implementations (for $\texttt{b} > 1$), or unblocked implementations (for $\texttt{b} = 1$).

2.3.1.6 Elemental

Elemental [PMH+13] is a library that provides optimized implementations of DLA operations targeted to distributed memory systems. It follows the SPMD

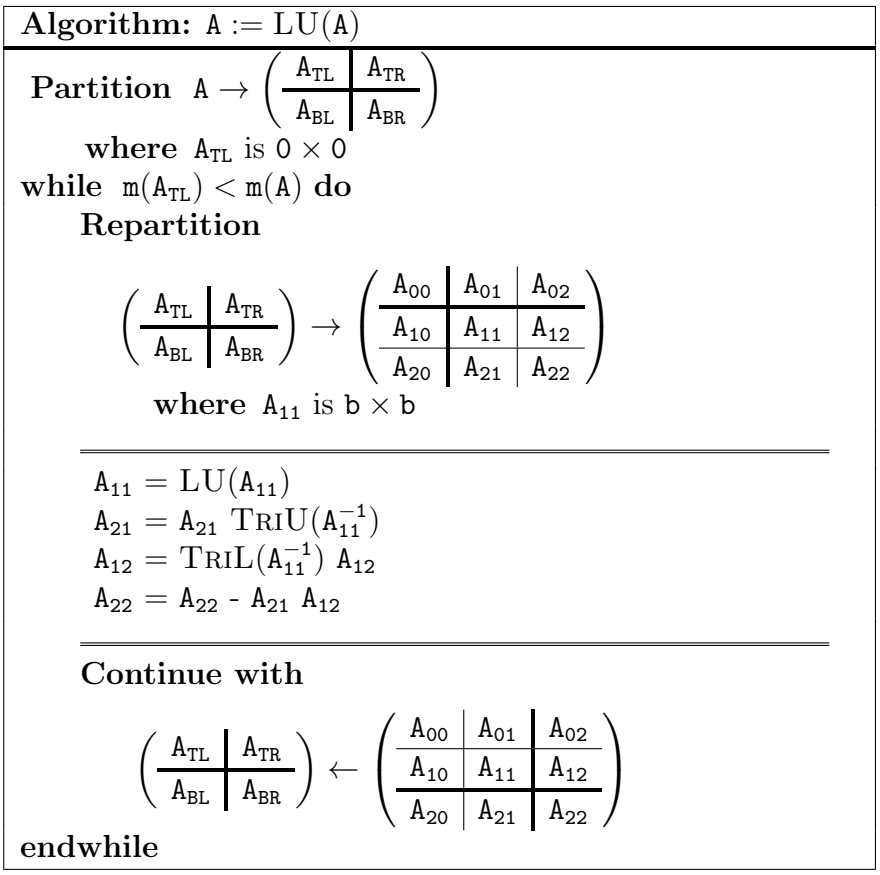


Figure 2.6: LU factorization in FLAME notation.

model, where the different processes execute the same program, but on different elements of the input matrices. On the base of Elemental library there is a set of matrix distributions to a two-dimensional process grid, and redistribution operations that can change the distribution of a matrix using MPI collective communications. To increase programmability, the library implementations *hides* those redistribution operations on assignment instructions.

Matrix distributions assume the $\mathtt{p}$ processes are organized as a $\mathtt{p} = \mathtt{r} \times \mathtt{c}$ grid. The default Elemental distribution, denoted by $[\mathtt{M_C}, \mathtt{M_R}]$, distributes the elements of the matrix in a cyclic way, both on rows and columns. Another important distribution is denoted by $[*, *]$, and it stores all elements of the matrix redundantly in all processes. Other distributions are available, to partition the matrix in cyclic way, either on rows or columns only. Table 2.1 (adapted from [Mar14],

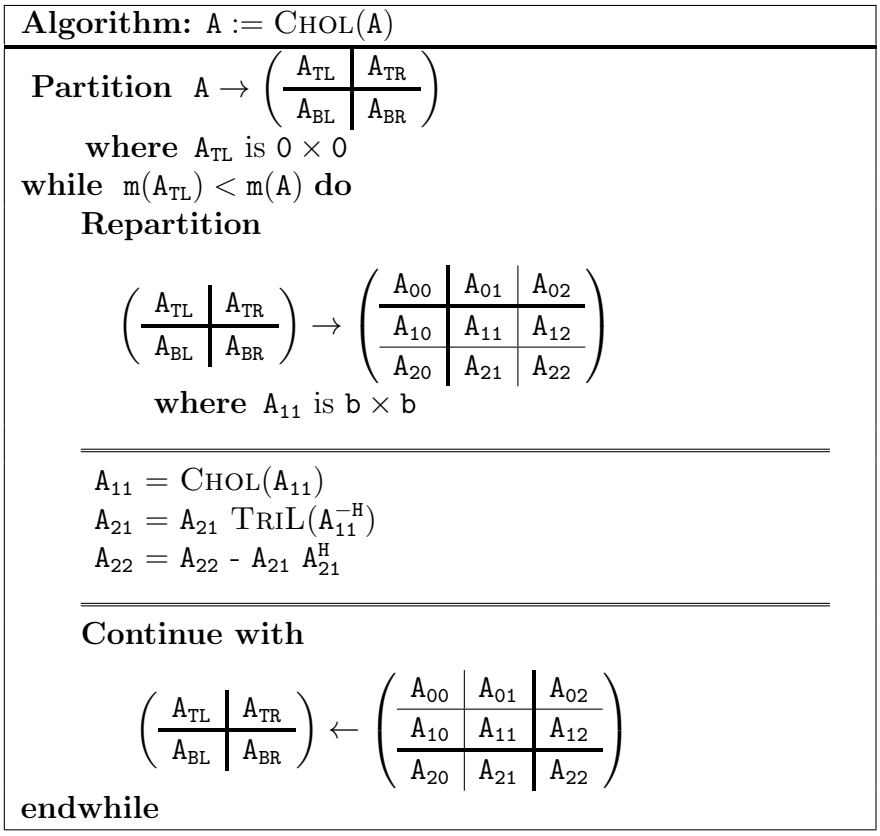


Figure 2.7: Cholesky factorization in FLAME notation.

Distribution	Location of data in matrix
$[*, *]$	All processes store all elements
$[\mathtt{M_C}, \mathtt{M_R}]$	Process $(\mathtt{i}\%\mathtt{r}, \mathtt{j}\%\mathtt{c})$ stores element $(\mathtt{i}, \mathtt{j})$
$[\mathtt{M_C}, *]$	Row $\mathtt{i}$ of data stored redundantly on process row $\mathtt{i}\%\mathtt{r}$
$[\mathtt{M_R}, *]$	Row $\mathtt{i}$ of data stored redundantly on process column $\mathtt{i}\%\mathtt{c}$
$[*, \mathtt{M_C}]$	Column $\mathtt{j}$ of data stored redundantly on process row $\mathtt{j}\%\mathtt{r}$
$[*, \mathtt{M_R}]$	Column $\mathtt{j}$ of data stored redundantly on process column $\mathtt{j}\%\mathtt{c}$
$[\mathtt{V_C}, *]$	Row $\mathtt{i}$ of data stored on process $(\mathtt{i}\%\mathtt{r}, \mathtt{i}/\mathtt{r}\%\mathtt{c})$
$[\mathtt{V_R}, *]$	Row $\mathtt{i}$ of data stored on process $(\mathtt{i}/\mathtt{c}\%\mathtt{r}, \mathtt{i}\%\mathtt{c})$
$[*, \mathtt{V_C}]$	Column $\mathtt{j}$ of data stored on process $(\mathtt{j}\%\mathtt{r}, \mathtt{i}/\mathtt{r}\%\mathtt{c})$
$[*, \mathtt{V_R}]$	Column $\mathtt{j}$ of data stored on process $(\mathtt{j}/\mathtt{c}\%\mathtt{r}, \mathtt{j}\%\mathtt{c})$

Table 2.1: Matrix distributions on a $\mathtt{p} = \mathtt{r} \times \mathtt{c}$ grid (adapted from [Mar14], p. 79).

p. 79), summarizes the different distributions offered by Elemental.

Depending on the DLA operation, different distributions are used so that computations can be executed on each process without requiring communications with other processes. Therefore, before operations, the matrices are redistributed to an appropriate distribution (from the default distribution), and after operations the matrices are redistributed back to the default distribution.

2.3.2 Relational Databases

Relational databases where proposed to abstract the way information is stored on data repositories [Cod70]. We choose this domain to evaluate the approach we propose as it is a well-known domain among computer scientists, and its derivations can be more easily appreciated and understood by others (unlike the other domains considered, where domain-specific knowledge—which typically only computer scientists that work on the domain possess—is required).

The basic entities on this domain are *relations* (*a.k.a.* tables), storing sets tuples that may be queried by users. Thus, a typical program in this domain queries the relations stored in the database management system, producing a new relation. The inputs and outputs of programs are, therefore, relations (or streams of tuples). Queries are usually specified by a composition of relational operations (using the SQL language [CB74]). The functional style used by queries (that transform streams of tuples) makes the programs in this domain well-suited to be expressed using the dataflow computing model, which supports implicit parallelism. Programs in this domain are often parallelized using a map-reduce strategy [DG08].

The main case studies of this domain we use are based on the *equi-join* operation, where tuples of two relations are combined based on an equality predicate. Given a tuple from each relation, the predicate tests whether a certain element of a tuple is equal to a certain element of the other tuple. If they are equal, the tuples are joined and added to the resulting relation.

2.3.3 Fault-Tolerant Request Processing Applications

Request processing applications (RPA) are defined as programs that accept requests from a set of clients, that are then handled by the internal components of the programs, and finally output. These programs may implement a *cylinder* topology, where the outputs are redirected back to the clients. They can be modeled using the dataflow computing model, where the clients and the internal components of the program are the operations. However, RPAs may have state, and in some cases operations may be executed when only part of its inputs are available, which is unusual in the dataflow programing model.

We use UpRight [CKL+09] as a case study in this research work. It is a state-of-the-art fault-tolerant architecture for a stateful server. It implements a simple RPA, where the clients' requests are sent to an abstract server (with state) component, and then the server outputs responses back to the client. Even though the abstract specification of the program implemented is simple, making this specification fault-tolerant and efficient, and considering that the server is stateful, results in a complex implementation [CKL+09]. The complexity of its final implementation motivated us to explore techniques that allowed to decompose the full system as a set of composable features, in order to make the process of modeling the domain knowledge more incremental.

2.3.4 Molecular Dynamics Simulations

Molecular dynamics (MD) simulations [FS01] use computational resources to predict properties of materials. The materials are modeled by a set of particles (*e.g.*, atoms or molecules) with certain properties (*e.g.*, position, velocity, or force). The set of particles is initialized based on some properties such as density and initial temperature. The simulation starts by computing the interactions between the particles, iteratively updating its properties, until the system stabilizes, at which point the properties of the material can be studied/measured. The expensive part of the simulation is the computation of the interactions between all particles, which using a naive implementation has a complexity of $O(N^2)$ (where

`N` is the number of particles). At each step of the iteration additional properties of the simulation are computed, to monitor its state.

The domain of MD simulations is vast. For different materials used and properties to study, different particles and different types of particle interactions are considered. Popular software packages for MD simulations include GROMACS [BvdSvD95], NAMD [PBW+05], AMBER [The], CHARMM [BBM+09], LAMPPS [Pli95], or MOIL [ERS+95].

In our case study we use the Lennard-Jones potential model, as we have previous experience with the implementation of this type of MD simulation (required to be able to extract the domain knowledge needed to implement the simulation). Despite the simplicity of the Lennard-Jones potential model, making the computation of particle interactions efficient may require the addition of certain features to the algorithm, which results in a small product line of MD programs. Thus, this case study allows us to verify how the approach we propose is suitable to model optional program features. The parallelization of the MD simulation is done at loop-level (in the loop that computes the interactions among particles), and follows the SPMD model.

Chapter 3

Encoding Domains: Refinement and Optimization

The development of optimized programs is complex. It is a task usually reserved for experts with deep knowledge about the program domain and target hardware platform. When building programs, experts use their knowledge to optimize the code, but this knowledge is not accessible to others, who can see the resulting program, but can not reproduce the development process, nor apply that knowledge to their own programs. Moreover, compilers are not able to apply several important domain specific optimizations, for example, because the code requires external library calls (that the compiler does not know), or because at the level of abstraction at which the compiler works important information about the algorithm was already lost, making it harder to identify the computational abstractions that may be optimized. We propose to encode the domain knowledge in a systematic way, so that the average user can appreciate programs built by experts, reproduce the development process, and leverage the expert knowledge when building (and optimizing) their own programs. This systematization of the domain knowledge effectively results in a set of transformations that experts apply to their programs to incrementally obtain the optimized implementations, and that can be mechanically applied by tools. This is also the first step to enable automation in the derivation of optimized programs.

In this chapter, we first present concepts used to capture the knowledge of a domain, and the transformations that those concepts encode, which allow us to synthesize optimized program architectures. These concepts are the base for the DxT approach for program development. Then we describe `ReFlO`, a tool suite that we developed to support specification of domain knowledge and the mechanical derivation of optimized program architectures by incrementally transforming a high-level program specification.

3.1 Concepts

A *dataflow graph* is a directed multigraph, where nodes (or boxes) process data, that is then passed to other boxes as specified by the edges (or connectors). Ports specify the different inputs and outputs of a box, and the connectors link an output port to an input port. Input ports are drawn as nubs on the left-side of boxes; output ports are drawn as nubs on the right-side. We obtain a multigraph, as there may exist more than one connector linking different ports of the same boxes.[1] Dataflow graphs provide a simple graphical notation to model program architectures and components, and it is the notation style we use in this work. When referring to a dataflow graph modeling a program architecture, we also use the term *dataflow architecture*.

We do not impose a particular model of computation to our dataflow architectures, *i.e.*, different domains may specify different rules to how a dataflow architecture is to be executed (the dataflow computing model is an obvious candidate to specify the model of computation).

An example of a simple dataflow architecture is given in Figure 3.1, where we have an architecture, called `ProjectSort`, that projects (eliminates) attributes of the tuples of its input stream and then sorts them.

We call boxes `PROJECT` and `SORT` *interfaces*, as they specify only the abstract behavior of operations (their inputs and outputs, and, informally, their semantics). Besides input ports, boxes may have other inputs, such as the attribute to

[1] Instead of a directed multigraph, a dataflow architecture could be a directed hypergraph [Hab92]. A box is a hyperedge, a port is a tentacle, and connectors are nodes.

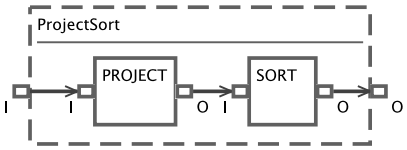


Figure 3.1: A dataflow architecture.

be used as sort key, in the case of the `SORT` interface, or the list of attributes to project, in the case of the `Project` interface, that are not shown in the graphical representation of boxes (in order to make their graphical representation simpler). We follow the terminology proposed by Das [Das95], and we call the former *essential parameters*, and the latter *additional parameters*.

Figure 3.1 is a PIM as it makes no reference to or demands on its concrete implementation. It is a high-level specification that can be mapped to a particular platform or for particular inputs. This mapping is accomplished in DxT by incrementally applying transformations. Therefore, we need to capture the valid transformations that can be applied to architectures in a certain domain.

A transformation can map an interface directly to a *primitive* box, representing a concrete code implementation. Besides primitives, there are other implementations of an interface that are expressed as a dataflow graph, called *algorithms*. Algorithms may reference interfaces. Figure 3.2 is an algorithm. It shows the dataflow graph called `parallel_sort` of a map-reduce implementation of `SORT`. Each box inside Figure 3.2, namely `SPLIT`, `SORT` and `SMERGE` (sorted merge), is an interface which can be subsequently elaborated.

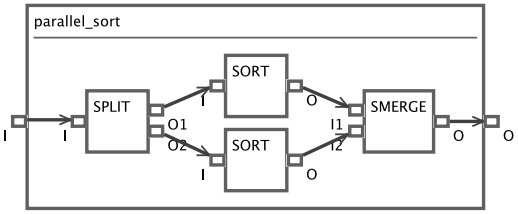
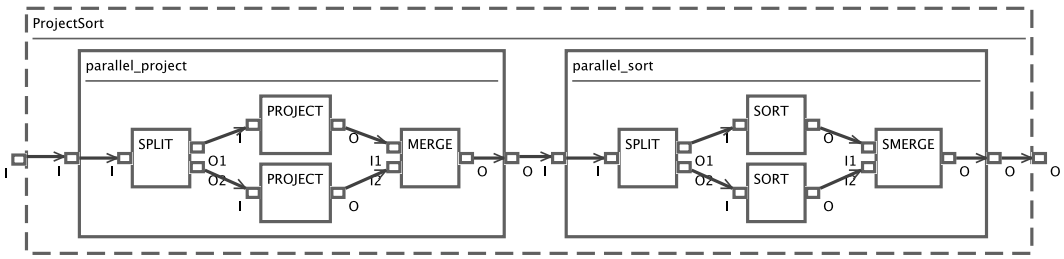


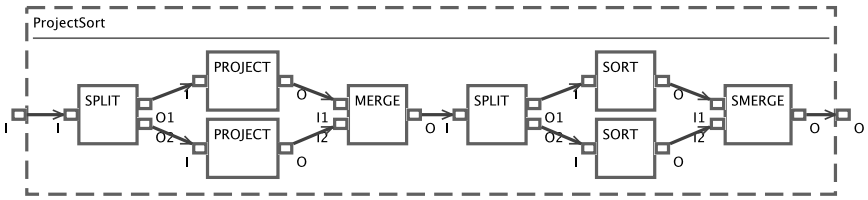
Figure 3.2: Algorithm `parallel_sort`, which implements interface `SORT` using map-reduce.

A *refinement* [Wir71] is the replacement of an interface with one of its implementations (primitive or algorithm). By repeatedly applying refinements,

eventually a graph of wired primitives is produced. Figure 3.1 can be refined by replacing `SORT` with its parallel sort algorithm, and `PROJECT` with a similar map-reduce algorithm. Doing so yields the graph of Figure 3.3a, or equivalently the graph of Figure 3.3b, obtained by removing modular boundaries. Removing modular boundaries is called *flattening*.



(a)



(b)

Figure 3.3: Parallel version of the `ProjectSort` architecture: (a) with modular boundaries and (b) without modular boundaries.

Refinements alone are insufficient to derive optimized dataflow architectures. Look at Figure 3.3b. We see a `MERGE` followed by the `SPLIT` operation, that is, two streams are merged and the resulting stream is immediately split again. Let interface `IMERGESPLIT` be the operation that receives two input streams, and produces two other streams, with the requirement that the union of the input streams is equal to the union of the output streams (see Figure 3.4a). `ms_mergesplit` (Figure 3.4b) is one of its implementations. However, the `ms_identity` algorithm (Figure 3.4c) provides an alternative implementation, that is obviously more efficient than `ms_mergesplit`, as it does not require `MERGE` and `SPLIT` computations.[2]

[2]Readers may notice that algorithms `ms_mergesplit` and `ms_identity` do not produce necessarily the same result. However, both implement the semantics specified by `IMERGESPLIT`,

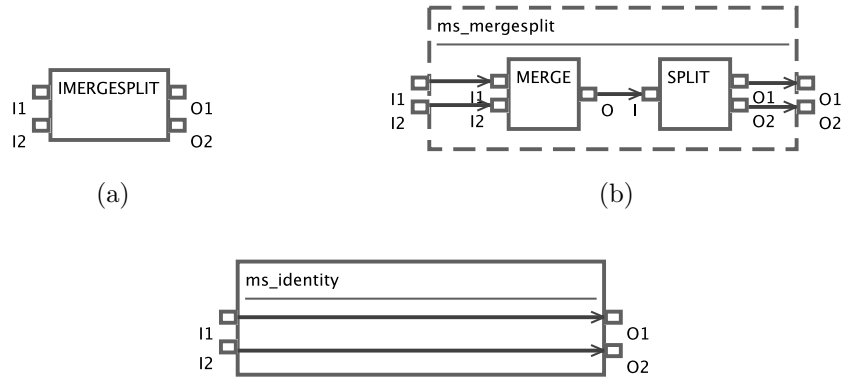


Figure 3.4: `IMERGESPLIT` interface and two possible implementations.

We can use `ms_identity` to optimize `ProjectSort`. The first step is to *abstract* Figure 3.3b with the `IMERGESPLIT` interface, obtaining Figure 3.5a. Then, we refine `IMERGESPLIT` to its `ms_identity` algorithm, to obtain the optimized architecture for `ProjectSort` (Figure 3.5b). We call the action of abstracting an (inefficient) composition of boxes to an interface and then refining it to an alternative implementation an *optimization*.[3] We can also remove the modular boundaries of the `ms_identity` algorithm, obtaining the architecture of Figure 3.5c. After refining each interface of Figure 3.5c to a primitive, we would obtain a PSM for the PIM presented in Figure 3.1, optimized for a parallel hardware platform.

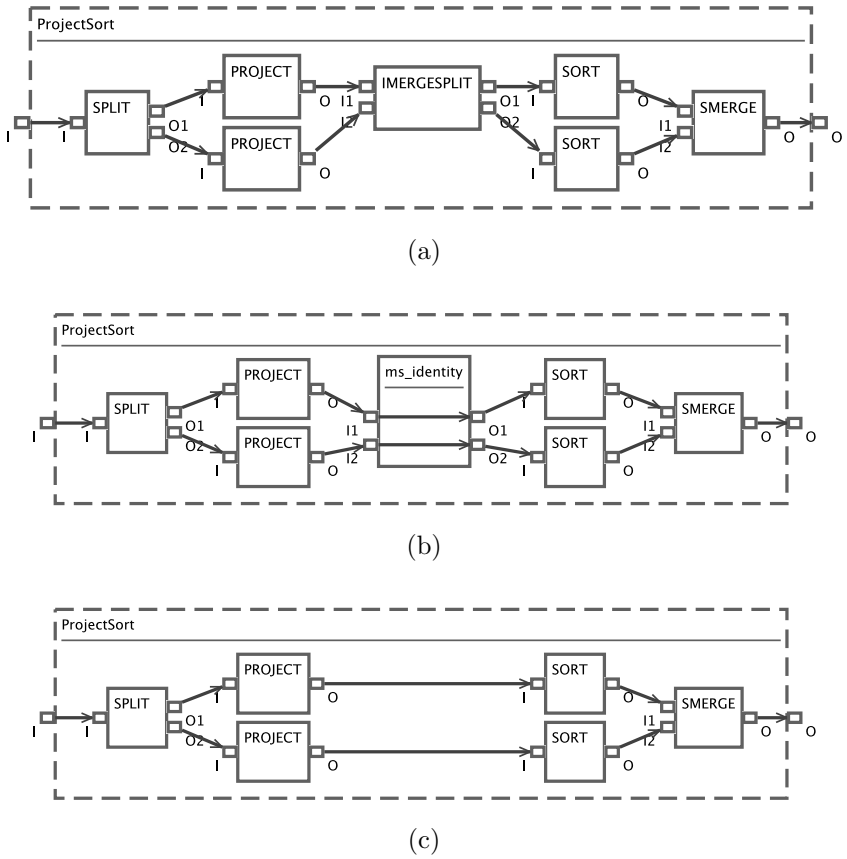
3.1.1 Definitions: Models

In this section we define the concepts we use to model a domain. A simplified view of how the main concepts used relate to each other is shown in Figure 3.6, as a UML class diagram (*a.k.a.* metamodel). Next we explain each type of objects of Figure 3.6, and the constraints that are associated with this diagram.

---

and the result of `ms_identity` is one of the possible results of `ms_mergesplit`, *i.e.*, `ms_identity` removes non-determinism.

[3] Although called optimizations, these transformations do not necessarily improve performance, but combinations of optimizations typically do.



(a)

(b)

(c)

Figure 3.5: Optimizing the parallel architecture of `ProjectSort`.

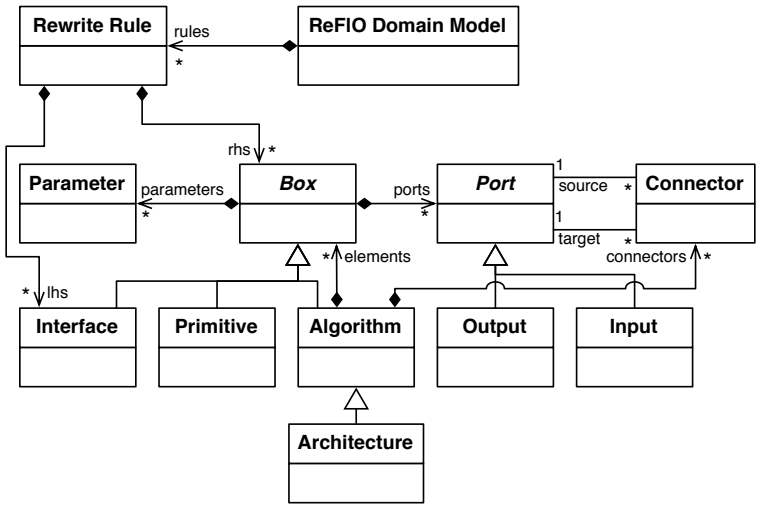


Figure 3.6: Simplified UML class diagram of the main concepts.

A *box* is either an interface, a primitive component, an algorithm, or a dataflow architecture. They are used to encode domain knowledge and/or specify program architectures.

Interface boxes are used to specify (abstract) the operations available in a certain domain.

Definition: An *interface* is a tuple with attributes:

(`name`, `inputs`, `outputs`, `parameters`)

where `name` is the interface's name, `inputs` is the ordered set of input ports, `outputs` is the ordered set of output ports, and `parameters` is the ordered set of additional parameters. The name identifies the interface, *i.e.*, two interfaces modeling different operations must have different names. The operations specified by interfaces may have side-effects (*e.g.*, state).[4]

Operations can be implemented in different ways (using different algorithms or library implementations), which are expressed either using a primitive box or an algorithm box. Primitive boxes specify direct code implementations, whereas algorithm boxes specify implementations as compositions of interfaces.

Definition: A *primitive component* (or simply primitive) is a tuple with attributes:

(`name`, `inputs`, `outputs`, `parameters`)

where `name` is the primitive's name, `inputs` is the ordered set of input ports, `outputs` is the ordered set of output ports, and `parameters` is the ordered set of additional parameters. The name identifies the primitive, *i.e.*, two different primitives (modeling different code implementations) must have different names.

Definition: An *algorithm* is a tuple with attributes:

(`name`, `inputs`, `outputs`, `parameters`, `elements`, `connectors`)

[4]We will use the notation `prop(x)` to denote the attribute `prop` of tuple `x` (*e.g.*, `name(I)` denotes the `name` of interface `I`, and `inputs(I)` denotes the `inputs` of interface `I`.)

where `name` is the algorithm's name, `inputs` is the ordered set of input ports, `outputs` is the ordered set of output ports, `parameters` is the ordered set of additional parameters, `elements` is a list of interfaces, primitives or algorithms, and `connectors` is a list of connectors. The list of elements, together with the set of connectors, encode a dataflow graph that specifies how operations (boxes) are composed to produce the behavior of the algorithm. For all input ports of internal boxes contained in an algorithm,[5] there must be one and only one connector that ends at that port (*i.e.*, there must be a connector that provides the input value, and that connector must be unique). For all output ports of the algorithm, there must be one and only one connector that ends at that port (*i.e.*, there must be a connector that provides the output of the algorithm, and that connector must be unique).

Finally, we have architecture boxes to specify program architectures, which are identical to algorithm boxes.

Definition: A *dataflow architecture* (or simply architecture) is a tuple with attributes:

$$(\texttt{name}, \texttt{inputs}, \texttt{outputs}, \texttt{parameters}, \texttt{elements}, \texttt{connectors})$$

where `name` is the architecture's name, `inputs` is the ordered set of input ports, `outputs` is the ordered set of output ports, `parameters` is the ordered set of additional parameters, `elements` is a list of interfaces, primitives and algorithms, and `connectors` is a list of connectors. The list of elements, together with the set of connectors, encode a graph that specifies how operations are composed to produce the desired behavior. For all input ports of boxes contained in an architecture, there must be one and only one connector that ends at that port (*i.e.*, there must be a connector that specifies the input value, and that connector must be unique). For all output ports of the architecture, there must be one an only one connector that ends at that port (*i.e.*, there must be a connector that

[5] Given an algorithm `A`, we say that `elements(A)` are the internal boxes of `A`, and that `A` is the parent of boxes `b` $\in$ `elements(A)`.

specifies the output of the architecture, and that connector must be unique). All boxes contained in an architecture that have the same name must have the same inputs, outputs, and additional parameters, as they are all instances of the same entity (only the values of additional parameters may be different, as they depend on the context in which a box is used).

As we mentioned before, inputs and outputs of boxes are specified by ports and additional parameters, which we define below.

Definition: A *port* specifies inputs and outputs of boxes. It is a tuple with attributes:

$$(\texttt{name}, \texttt{datatype})$$

where `name` is the port's name, and `datatype` is the port's data type. Each input port of a box must have a unique name (the same must hold for output ports). However, boxes may have an input and an output port with the same name (in case we need to distinguish them, we use the subscripts $_{\texttt{in}}$ and $_{\texttt{out}}$).

Definition: A *parameter* is a tuple with attributes:

$$(\texttt{name}, \texttt{datatype}, \texttt{value})$$

where `name` is the parameter's name, `datatype` the parameter's data type, and `value` the parameter's value. The value of a parameter is undefined for boxes that are not contained in other boxes. For an algorithm or architecture `A`, the values of boxes $\texttt{b} \in \texttt{elements}(\texttt{A})$ may be a constant (represented by a pair $(\mathcal{C}, \texttt{expr})$, where $\mathcal{C}$ is used to indicate the value is a constant, and `expr` defines the constant's value), or the name of a parameter of the parent box `A` (represented by $(\mathcal{P}, \texttt{name})$, where $\mathcal{P}$ is used to indicate the value is a parameter of the parent box and `name` is the name of the parameter). As ports, each additional parameter of a box must have a unique name.

We specify algorithms and architectures composing boxes. Connectors are used to link boxes' ports and define the dataflow graph that expresses how boxes are composed to produce the desired behavior.

Definition: A *connector* is a tuple with attributes:

$$(\texttt{sbox}, \texttt{sport}, \texttt{tbox}, \texttt{tport})$$

where `sbox` is the source box of the connector, `sport` is the source port of the connector, `tbox` is the target box of the connector, and `tport` is the target box of the connector. Connectors are part of algorithms, and connect ports of boxes inside the same algorithm and/or ports of the algorithm. If $(\texttt{b}, \texttt{p}, \texttt{b}', \texttt{p}')$ is a connector of algorithm `A`, then $\texttt{b}, \texttt{b}' \in (\{\texttt{A}\} \cup \texttt{elements}(\texttt{A}))$. Moreover, the following conditions must hold:

- if $\texttt{b} \in \{\texttt{A}\}$, then $\texttt{p} \in \texttt{inputs}(\texttt{b})$
- if $\texttt{b} \in \texttt{elements}(\texttt{A})$, then $\texttt{p} \in \texttt{outputs}(\texttt{b})$
- if $\texttt{b}' \in \{\texttt{A}\}$, then $\texttt{p}' \in \texttt{outputs}(\texttt{b}')$
- if $\texttt{b}' \in \texttt{elements}(\texttt{A})$, then $\texttt{p} \in \texttt{inputs}(\texttt{b}')$

Operations implementations are specified by primitive and algorithm boxes. Rewrite rules are used to associate a primitive or algorithm box to the interface that represents the operation it implements. The set of rewrite rules defines the model of the domain.

Definition: A *rewrite rule* is a tuple with attributes:

$$(\texttt{lhs}, \texttt{rhs})$$

where `lhs` is an interface, and `rhs` is a primitive or algorithm box that implements the `lhs`. The `lhs` and `rhs` must have the same inputs, outputs and additional parameters (same names and data types), *i.e.*, given a rewrite rule `R`:

$$\texttt{inputs}(\texttt{lhs}(\texttt{R})) = \texttt{inputs}(\texttt{rhs}(\texttt{R}))$$

$$\wedge\ \texttt{outputs}(\texttt{lhs}(\texttt{R})) = \texttt{outputs}(\texttt{rhs}(\texttt{R}))$$

$$\wedge\ \texttt{parameters}(\texttt{lhs}(\texttt{R})) = \texttt{parameters}(\texttt{rhs}(\texttt{R}))$$

The `rhs` box must also implement the semantics of the `lhs` interface. When an algorithm `A` is the `rhs` of a rewrite rule, we require that `elements(A)` contains only interfaces. (In Figure 3.12 and Figure 3.13 we show how we graphically represent rewrite rules.)

Definition: A *ReFlO Domain Model (RDM)* is a set of rewrite rules. All boxes contained in an RDM that have the same name encode the same entity, and therefore they must have the same inputs, outputs, and additional parameters (only the values of additional parameters may be different).

3.1.2 Definitions: Transformations

We now present a definition of the transformations we use in the process of deriving optimized program architectures from an initial high-level architecture specification.

As we saw previously, usually the derivation process start by choosing implementations for the interfaces used in the program architecture, which allows users to select an appropriate implementation for a certain target hardware platform, or certain program inputs. This is done using refinement transformations. The possible implementations for an interface are defined by the rewrite rules whose LHS is the interface to be replaced.

Definition: A *refinement* replaces an interface with one of its implementations. Let `P` be an architecture, `(I, A)` a rewrite rule, `I'` an interface present in `P` such that `name(I') = name(I)`, and `B` the box that contains `I'` (*i.e.*, `B` is either the architecture `P` or an algorithm contained in the architecture `P`, such that `I' ∈ elements(B)`). We can refine architecture `P` replacing `I'` with a copy of `A` (say `A'`). This transformation removes `I'` from `elements(B)`, and redirects the connectors from `I'` to `A'`. That is, for each connector `c ∈ connectors(B)` such that `sbox(c) = I'`, `sbox(c)` is updated to `A'` and `sport(c)` is updated to `p`, where `p ∈ outputs(A')` and `name(p) = name(sport(c))`. Similarly, for each connector `c ∈ connectors(B)` such that `tbox(c) = I'`, `tbox(c)` is updated to `A'` and `tport(c)` is updated to `p`,

where $\texttt{p} \in \texttt{inputs}(\texttt{A}')$ and $\texttt{name}(\texttt{p}) = \texttt{name}(\texttt{tport}(\texttt{c}))$. Finally, $\texttt{parameters}(\texttt{A}')$ is updated to $\texttt{parameters}(\texttt{I}')$.

Example: An application of refinement was shown in Figure 3.5.

Refinements often introduce suboptimal compositions of boxes that cross modular boundaries of components (algorithm boxes). These modular boundaries can be removed using the flatten transformation, which enables the optimization of inefficient compositions of boxes present in the architecture.

Definition: The *flatten* transformation removes algorithms' boundaries. Let $\texttt{A}$ be an algorithm, and $\texttt{B}$ an algorithm or architecture that contains $\texttt{A}$. The flatten transformation moves boxes $\texttt{b} \in \texttt{elements}(\texttt{A})$ to $\texttt{elements}(\texttt{B})$. The same is done for connectors $\texttt{c} \in \texttt{connectors}(\texttt{A})$, which are moved to $\texttt{connectors}(\texttt{B})$. Then connectors linked to ports of $\texttt{A}$ are updated. For each connector $\texttt{c}$ such that $\texttt{sport}(\texttt{c}) \in (\texttt{inputs}(\texttt{A}) \cup \texttt{outputs}(\texttt{A}))$, let $\texttt{c}'$ be the connector such that $\texttt{tport}(\texttt{c}') = \texttt{sport}(\texttt{c})$. The value of $\texttt{sport}(\texttt{c})$ is updated to $\texttt{sport}(\texttt{c}')$ and the value of $\texttt{sbox}(\texttt{c})$ is updated to $\texttt{sboc}(\texttt{c}')$. The additional parameters of the internal boxes of $\texttt{A}$ are also updated. For each $\texttt{b} \in \texttt{elements}(\texttt{A})$, each $\texttt{param} \in \texttt{parameters}(\texttt{b})$ is replaced by $\texttt{UpdateParam}(\texttt{param}, \texttt{parameters}(\texttt{A}))$. Lastly, algorithm $\texttt{A}$ is removed from $\texttt{elements}(\texttt{B})$, and connectors $\texttt{c}$ such that $\texttt{tport}(\texttt{c}) \in (\texttt{inputs}(\texttt{A}) \cup \texttt{outputs}(\texttt{A}))$ are removed from $\texttt{connectors}(\texttt{B})$.

Example: An application of the flatten transformation was shown in Figure 3.3.

This transformation has to update the values of additional parameters of boxes contained inside the algorithm to be removed, which is done by the function $\texttt{UpdateParam}$ defined below.

Definition: Let $\texttt{UpdateParam}$ be the function defined below. For a parameter $(\texttt{name}, \texttt{type}, \texttt{value})$ and an ordered set of parameters $\texttt{ps}$:

$$\texttt{UpdateParam}((\texttt{name}, \texttt{type}, \texttt{value}), \texttt{ps}) = (\texttt{name}, \texttt{type}, \texttt{value}')$$

where

$$\texttt{value}' = \begin{cases} \texttt{value} & \text{if } \texttt{value} = (\mathcal{C}, \texttt{x}) \\ \texttt{y} & \text{if } \texttt{value} = (\mathcal{P}, \texttt{x}) \wedge (\texttt{x}, \texttt{type}, \texttt{y}) \in \texttt{ps} \end{cases}$$

After flattening an architecture opportunities for optimization (essentially, inefficient compositions of boxes) are likely to arise. Those inefficient compositions of boxes are encoded by algorithms, and to remove them, we have to first identify them in the architecture, *i.e.*, we have to find a match of the algorithm inside the architecture. Before we define a *match*, we introduce some auxiliary definitions, which are used to identify the internal objects (boxes, ports, parameters and connectors) of an algorithm.

Definition: Let Conns, Params and Ports be the functions defined below. For an algorithm or architecture A:

$$\texttt{Conns}(\texttt{A}) = \{\texttt{c} \in \texttt{connectors}(\texttt{A}) : \texttt{sport}(\texttt{c}) \notin \texttt{inputs}(\texttt{A}) \wedge \texttt{tport}(\texttt{c}) \notin \texttt{outputs}(\texttt{A})\}$$

$$\texttt{Ports}(\texttt{A}) = \bigcup_{\texttt{b} \in \texttt{elements}(\texttt{A})} (\texttt{inputs}(\texttt{b}) \cup \texttt{outputs}(\texttt{b}))$$

$$\texttt{Params}(\texttt{A}) = \bigcup_{\texttt{b} \in \texttt{elements}(\texttt{A})} \texttt{parameters}(\texttt{b})$$

Definition: Let Obj be the function defined below. For an algorithm or architecture A:

$$\texttt{Obj}(\texttt{A}) = \texttt{elements}(\texttt{A}) \cup \texttt{Conns}(\texttt{A}) \cup \texttt{Ports}(\texttt{A}) \cup \texttt{Params}(\texttt{A})$$

Definition: Let P be an architecture or an algorithm contained in an architecture, and A an algorithm. A *match* is an injective map $\texttt{m} : \texttt{Obj}(\texttt{A}) \to \texttt{Obj}(\texttt{P})$, such that:

$$\forall_{\texttt{b} \in \texttt{elements}(\texttt{A})}\ \texttt{name}(\texttt{b}) = \texttt{name}(\texttt{m}(\texttt{b})) \tag{3.1}$$

$$\begin{aligned} \forall_{\texttt{c} \in \texttt{Conns}(\texttt{A})}\ & \texttt{m}(\texttt{sport}(\texttt{c})) = \texttt{sport}(\texttt{m}(\texttt{c})) \\ & \wedge\ \texttt{m}(\texttt{tport}(\texttt{c})) = \texttt{tport}(\texttt{m}(\texttt{c})) \\ & \wedge\ \texttt{m}(\texttt{sbox}(\texttt{c})) = \texttt{sbox}(\texttt{m}(\texttt{c})) \\ & \wedge\ \texttt{m}(\texttt{tbox}(\texttt{c})) = \texttt{tbox}(\texttt{m}(\texttt{c}))) \end{aligned} \tag{3.2}$$

$$\forall_{\mathtt{p}\in\mathtt{Ports(A)}}\ \mathtt{name(p)} = \mathtt{name(m(p))} \\ \wedge\ (\mathtt{p} \in \mathtt{ports(b)} \Leftrightarrow \mathtt{m(p)} \in \mathtt{ports(m(b))}) \tag{3.3}$$

$$\forall_{\mathtt{p}\in\mathtt{Params(A)}}\ \mathtt{name(p)} = \mathtt{name(m(p))} \\ \wedge\ (\mathtt{p} \in \mathtt{parameters(b)} \Leftrightarrow \mathtt{m(p)} \in \mathtt{parameters(m(b))}) \tag{3.4}$$

$$\forall_{\mathtt{p}\in\mathtt{Params(A)}}\ (\mathtt{value(p)} = (\mathcal{C}, \mathtt{e})) \Rightarrow (\mathtt{value(m(p))} = (\mathcal{C}, \mathtt{e})) \tag{3.5}$$

$$\forall_{\mathtt{p}_1,\mathtt{p}_2\in\mathtt{Params(A)}}\ \mathtt{value}(\mathtt{p}_1) = \mathtt{value}(\mathtt{p}_2) \Rightarrow \mathtt{value}(\mathtt{m}(\mathtt{p}_1)) = \mathtt{value}(\mathtt{m}(\mathtt{p}_2)) \tag{3.6}$$

$$\forall_{\mathtt{c}\in\mathtt{connectors(P)}}\ (\mathtt{sport(c)} \in \mathtt{Image(m)} \wedge \mathtt{tport(c)} \notin \mathtt{Image(m)}) \\ \Rightarrow (\exists_{\mathtt{c}'\in\mathtt{connectors(A)}}\ \mathtt{m(sport(c'))} = \mathtt{sport(c)} \\ \wedge\ \mathtt{tport(c')} \notin \mathtt{Obj(A)}) \tag{3.7}$$

$$\forall_{\mathtt{c}_1,\mathtt{c}_2\in\mathtt{connectors(A)}}\ \mathtt{sport}(\mathtt{c}_1) = \mathtt{sport}(\mathtt{c}_2) \\ \Rightarrow (\exists_{\mathtt{c}_1',\mathtt{c}_2'\in\mathtt{connectors(P)}}\ \mathtt{sport}(\mathtt{c}_1') = \mathtt{sport}(\mathtt{c}_2') \\ \wedge\ \mathtt{tport}(\mathtt{c}_1') = \mathtt{m}(\mathtt{tport}(\mathtt{c}_1)) \\ \wedge\ \mathtt{tport}(\mathtt{c}_2') = \mathtt{m}(\mathtt{tport}(\mathtt{c}_2))) \tag{3.8}$$

$\mathtt{Image}(\mathtt{m})$ denotes the subset of $\mathtt{Obj}(\mathtt{P})$ that contains the values $\mathtt{m}(\mathtt{x})$, for any $\mathtt{x}$ in the domain of $\mathtt{m}$, *i.e.*, $\mathtt{Image}(\mathtt{m}) = \{\mathtt{m}(\mathtt{x}) : \mathtt{x} \in \mathtt{Obj}(\mathtt{A})\}$. Conditions (3.1-3.6) impose that the map preserves the structure of the algorithm box being mapped (*i.e.*, the match is a morphism). Condition (3.7) imposes that if an output port in the image of the match is connected to a port that is not, then the corresponding output port of the algorithm (preimage) must also be connected with a port outside the domain of the match.[6] Condition (3.8) imposes that if

[6]This condition is similar to the *dangling condition* in the double-pushout approach to graph transformation [HMP01].

two input ports of the pattern internal boxes are the target of connectors that have the same source, the same must be valid for the matches of those input ports (this is an additional condition regarding preservation of structure).

> **Example:** Figure 3.7 depicts a map that does not meet condition (3.7), and Figure 3.8 depicts a map that does not meet condition (3.8). Therefore, none of them are matches. A valid match is depicted in Figure 3.9.

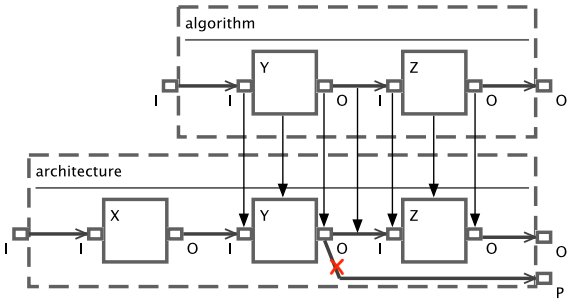


Figure 3.7: Example of an invalid match (connector marked `x` does not meet condition (3.7)).

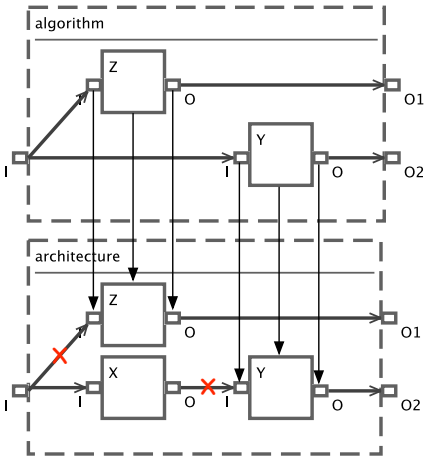


Figure 3.8: Example of an invalid match (connectors marked `x` should have the same source to meet condition (3.8)).

Having a match that identifies the boxes that can be optimized, we can apply an optimizing abstraction to replace the inefficient composition of boxes. This

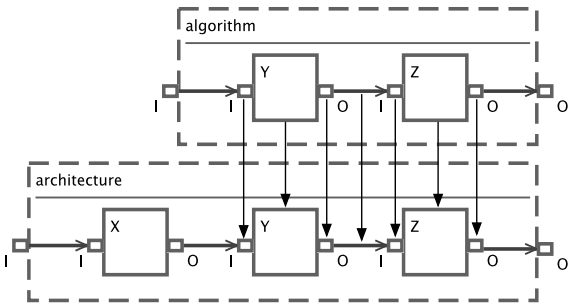


Figure 3.9: A match from an algorithm (on top) to an architecture (on bottom).

transformations is defined next.

Definition: Given an architecture or an algorithm (contained in an architecture) $\mathtt{P}$, a rewrite rule $(\mathtt{I}, \mathtt{A})$ such that $\mathtt{A}$ is an algorithm and

$$\forall_{\mathtt{p}\in\mathtt{inputs(A)}}\ \exists_{\mathtt{c}\in\mathtt{connectors(A)}}(\mathtt{sport(c)} = \mathtt{p}) \wedge (\mathtt{tport(c)} \notin \mathtt{outputs(A)}) \qquad (3.9)$$

and a match $\mathtt{m}$ (mapping $\mathtt{A}$ in $\mathtt{P}$), an *optimizing abstraction* of $\mathtt{A}$ in $\mathtt{P}$ replaces $\mathtt{m(A)}$ with a copy of $\mathtt{I}$ (say $\mathtt{I}'$) in $\mathtt{P}$ according to the following algorithm:

- Add $\mathtt{I}'$ to $\mathtt{elements(P)}$
- For each $\mathtt{p}' \in \mathtt{inputs(A)}$,
  - Let $\mathtt{c}'$ be a connector such that $\mathtt{c}' \in \mathtt{connectors(A)} \wedge \mathtt{sport(c}') = \mathtt{p}' \wedge \mathtt{tport(c}') \notin \mathtt{outputs(A)}$[7]
  - Let $\mathtt{c}$ be a connector such that $\mathtt{c} \in \mathtt{connectors(P)} \wedge \mathtt{tport(c)} = \mathtt{m(tport(c}'))$
  - Let $\mathtt{p}$ be a port such that $\mathtt{p} \in \mathtt{inputs(I}') \wedge \mathtt{name(p)} = \mathtt{name(p}')$
  - Set $\mathtt{tport(c)}$ to $\mathtt{p}$
  - Set $\mathtt{tbox(c)}$ to $\mathtt{I}'$

  (These steps find a connector to link to each input port of $\mathtt{I}'$, and redirect that connector to $\mathtt{I}'$.)

[7]Condition 3.9 guarantees that connector $\mathtt{c}'$ exists.

- For each $\mathtt{c} \in \{\mathtt{d} \in \mathtt{connectors(P)} : \mathtt{sport(d)} \in \mathtt{Image(m)} \wedge \mathtt{tport(d)} \notin \mathtt{Image(m)}\}$
  - Let $\mathtt{c'}$ be a connector such that $\mathtt{c'} \in \mathtt{connectors(A)} \wedge \mathtt{sport(c)} = \mathtt{m(sport(c'))} \wedge \mathtt{tport(c')} \in \mathtt{outputs(A)}$
  - Let $\mathtt{p}$ be a port such that $\mathtt{p} \in \mathtt{outputs(I')} \wedge \mathtt{name(p)} = \mathtt{name(tport(c'))}$
  - Set $\mathtt{sport(c)}$ to $\mathtt{p}$
  - Set $\mathtt{sbox(c)}$ to $\mathtt{I'}$

  (These steps redirect all connectors for which source port (and box) is to be removed to an output port of $\mathtt{I'}$.)

- For each $\mathtt{p} \in \mathtt{parameters(I')}$, if there is a $\mathtt{p'} \in \mathtt{Params(A)}$, such that $\mathtt{value(p')} = (\mathcal{P}, \mathtt{name(p)})$, update $\mathtt{value(p)}$ to $\mathtt{value(m(p'))}$.

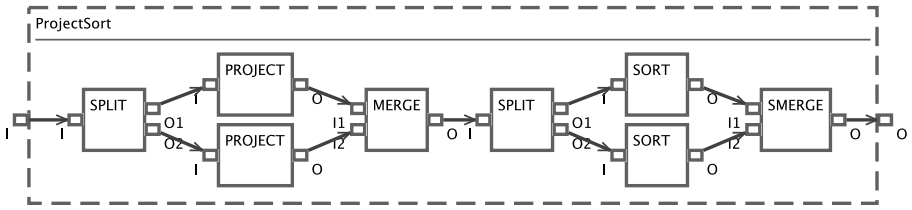
  (This step takes the values of the parameters of boxes to be removed to define the values of the parameters of $\mathtt{I'}$.)

- For each box $\mathtt{b} \in \mathtt{m(elements(A))}$, delete $\mathtt{b}$ from $\mathtt{elements(P)}$
- For each connector $\mathtt{c} \in \mathtt{m(Conns(A))}$, delete $\mathtt{c}$ from $\mathtt{connectors(P)}$
- For each connector $\mathtt{c} \in \mathtt{connectors(P)}$, such that $\mathtt{tport(c)} \in \mathtt{Image(m)}$, delete $\mathtt{c}$ from $\mathtt{connectors(P)}$

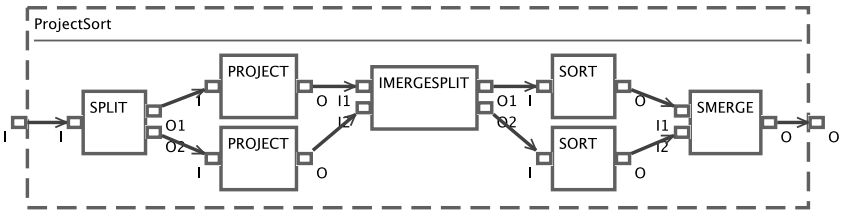
  Example: An application of optimizing abstraction is shown in Figure 3.10 (it was previously shown when transforming Figure 3.3b to Figure 3.5a).

3.1.3 Interpretations

A dataflow architecture P may have many different interpretations. The default is to interpret each box of P as the component it represents. That is, SORT means "sort the input stream". We call this the *standard interpretation* $\mathcal{S}$. The



(a)



(b)

Figure 3.10: An optimizing abstraction.

standard interpretation of box `B` is denoted $\mathcal{S}$(`B`) or simply `B`, *e.g.*, $\mathcal{S}$(`SORT`) is "sort the input stream". The standard interpretation of a dataflow graph `P` is $\mathcal{S}$(`P`) or simply `P`.

There are other equally important interpretations of `P`, which allow us to predict *properties* about `P`, their boxes and ports. $\mathcal{ET}$ interprets each box `B` as a computation that *estimates the execution time* of `B`, given some properties about `B`'s inputs. Thus, $\mathcal{ET}$(`SORT`) is "return an estimate of the execution time to produce `SORT`'s output stream". Each box `B` $\in$ `P` has exactly the same number of inputs and outputs as $\mathcal{ET}$(`B`) $\in$ $\mathcal{ET}$(`P`), but the meaning of each box, as well as the types of each of its I/O ports, is different.

Essentially, an interpretation associates behavior to boxes, allowing the *execution* (or *animation*) of an architecture to compute properties about it.

> **Example:** $\mathcal{ET}$(`ProjectSort`) estimates the execution time of `ProjectSort` for an input `I` whose statistics (tuple size, stream length, etc.) is $\mathcal{ET}$(`I`). An RDM can be used to forward-engineer (*i.e.*, derive) all possible implementations from an high-level architecture specification. The estimated runtime of an architecture `P` is determined by executing $\mathcal{ET}$(`P`). The most efficient architecture de-

rived from an initial architecture specification is the one with the lowest estimated cost.

In general, an interpretation $\mathcal{I}$ of dataflow graph $\mathtt{P}$ is an isomorphic graph $\mathcal{I}(\mathtt{P})$, where each box $\mathtt{B} \in \mathtt{P}$ is mapped to a unique box $\mathcal{I}(\mathtt{B}) \in \mathcal{I}(\mathtt{P})$, and each edge $\mathtt{B}_1 \rightarrow \mathtt{B}_2 \in \mathtt{P}$ is mapped to a unique edge $\mathcal{I}(\mathtt{B}_1) \rightarrow \mathcal{I}(\mathtt{B}_2) \in \mathcal{I}(\mathtt{P})$. Graph $\mathcal{I}(\mathtt{P})$ is identical to $\mathtt{P}$, except that the interpretation of all boxes as computations are different. Usually edges of an interpretation $\mathcal{I}$ have the same direction of the corresponding edge of the architecture. However, we have found cases where to compute some property about an architecture it is convenient to invert the direction of the edges. In that case, an edge $\mathtt{B}_1 \rightarrow \mathtt{B}_2 \in \mathtt{P}$ maps to a unique edge $\mathcal{I}(\mathtt{B}_1) \leftarrow \mathcal{I}(\mathtt{B}_2) \in \mathcal{I}(\mathtt{P})$. We call such interpretations *backward* and the others are *forward*.

The properties of the ports of a box are stored in a *properties map*, which is a map that associates a value to a property name. When computing properties, each box has a map that associates to each input port a properties map, and another map that associates to each output port a properties map. Additionally, there is another properties map, associated with the box itself.

Definition: An interpretation of a box $\mathtt{B}$ is a function that has as inputs the list of additional parameters' values of $\mathtt{B}$, a map containing a properties maps for each input port of $\mathtt{B}$ and a properties map for box $\mathtt{B}$, and returns a map containing the properties maps for each output port of $\mathtt{B}$ and an update properties map for box $\mathtt{B}$. (For backward interpretations, input properties are computed from output properties.)

An interpretation allows the *execution* of an architecture. Given a box $\mathtt{B}$ and an input port $\mathtt{P}$ of $\mathtt{B}$, and let $\mathtt{C}$ be a connector, such that $\mathtt{tport}(\mathtt{C}) = \mathtt{P}$, then the properties map of $\mathtt{P}$ is equal to the properties of $\mathtt{sport}(\mathtt{C})$ (*i.e.*, the properties are shared, and if we change the properties map of $\mathtt{sport}(\mathtt{C})$, we change the properties map of $\mathtt{P}$). A port may be an output port of an interface or primitive (and in that case its properties map is computed by the interpretation), may be an input port of an architecture, or there is a connector that has the port

as target. To compute the properties maps of a port that is the target of a connector, we compute the properties map of the port that is the source of the same connector. In case the port is an input port of an architecture, the properties maps must be provided, as there is no function to compute them, nor connectors that have the port as target (in the case of forward interpretations).

Given an architecture, the properties maps for its input ports, and interpretations for the boxes the architecture contains, properties maps of all ports and boxes contained in the architecture are computed executing the interpretations of the boxes according to their topological order. We do not require acyclic graphs, which means in some cases the graph may not have a topological ordering. In that case, we walk the graph according to the dependencies specified by the dataflow graph, and when we reach a cycle (a point where all boxes have unfulfilled dependencies), we try to find the box that is the *entry point* of the cycle, which is a box that has some of the dependencies already fulfilled. We choose to be executed next the ones that have no direct dependencies on other entry points. If no entry point meets this criteria, we choose to be executed next all the entry points.

3.1.4 Pre- and Postconditions

Boxes often impose requirements on the inputs they accept, *i.e.*, there are some *properties* that inputs and additional parameters must satisfy in order for a box to produce the expected semantics (*e.g.*, when adding two matrices, they must have the same size). The requirements on properties of inputs imposed by boxes define their *preconditions*, and may be used to validate architectures. We want to be able to validate architectures during design time, which means that we need to have the properties needed to evaluate preconditions during design time. Given properties of inputs, we can use those properties not only to evaluate box's preconditions, but also to compute properties about the outputs. Thus, interfaces have associated to them preconditions, predicates of properties of their inputs and additional parameters, which specify when the operation specified by the interface can be used. Additionally, interfaces and primitives have associated

to them functions that compute the properties of their outputs, given properties of their inputs and additional parameters.[8]

The properties of the outputs describe what is known after the execution of a box, and may be seen as box's *postconditions*, *i.e.*, if `f` computes properties of output port `A`, we can say that `properties(A) = f` is a postcondition of `A` (or a postcondition of the box that contains port `A`).

The pre- and postconditions are essentially interpretations of architectures that can be used to semantically validate them (assuming they capture all the expected behavior of a box). We follow this approach, where interpretations are used to define pre- and postconditions, so that we reuse the same framework for different purposes (pre- and postconditions, cost estimates, etc.). Also, this approach simplifies the verification of preconditions (it is done evaluating predicates), and has shown to be expressive enough to model the design constraints needed in the case studies analysed.

Preserving Correctness During Transformations. In Section 3.1.2, we described two main kinds of transformations:

- **Refinement** `I` $\rightarrow$ `A`, where an interface `I` is replaced with an algorithm or primitive `A`; and
- **Optimizing Abstraction** `A` $\rightarrow$ `I`, where the dataflow graph of an algorithm `A` is replaced with an interface `I`.

Considering those transformations, a question arises: under what circumstances does a transformation keep the correction of an architecture, regarding the preconditions of the interfaces it uses? A possible answer is based on the *Liskov Substitution Principle (LSP)* [LW94], which is a foundation of object-oriented design. LSP states that if `S` is a subtype of `T`, then objects of type `S` can be substituted for objects of type `T` without altering the correctness properties of a program. Substituting an interface with an implementing object (component)

[8] Postconditions of algorithms are equivalent to the composition of the postcondition functions of their internal boxes. Thus, algorithms do not have explicit postconditions. The same holds for architectures.

is standard fare today, and is an example of LSP [MRT99, Wik13]. The technical rationale behind LSP is that preconditions for using `S` are not stronger than preconditions for `T`, and postconditions for `S` are not weaker than that for `T` [LW94].

However, LSP is too restrictive for our approach, as we often find implementations specialized to a subset of the inputs accepted by the interface they implement (*nonrobust* implementations [BO92]), and therefore require stronger preconditions. This is a common situation when defining implementations for interfaces: for specific inputs there are specialized algorithms that provide better performance than general ones (*a.k.a. robust* algorithms [BO92]).

Example: Figure 3.11 shows three implementations for `SORT` interface: a map-reduce algorithm, a `quicksort` primitive, and a `do_nothing` algorithm. `do_nothing` says: if the input stream is already in sorted order (a precondition for `do_nothing`), then there is no need to sort. The `SORT` → `do_nothing` violates LSP: `do_nothing` has stronger preconditions than its `SORT` interface.

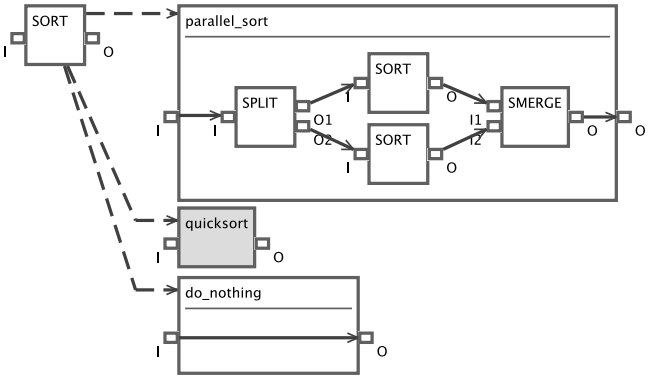


Figure 3.11: Two algorithms and a primitive implementation of `SORT`.

Considering the performance advantages typically associated to nonrobust implementations, it is convenient to allow implementations to have stronger preconditions than their interfaces. In fact, this is the essence of some optimizations

in certain domains, where nonrobust implementations are widely used to optimize an architecture to specific program inputs.

Upward Compatibility and Perry Substitution Principle. There are existing precedences for a solution. Let $\mathtt{B}_1$ and $\mathtt{B}_2$ be boxes, and `pre` and `post` denote the pre- and postconditions of a box. Perry [Per87] defined that $\mathtt{B}_2$ is *upward compatible* with $\mathtt{B}_1$ if:

$$\mathtt{pre}(\mathtt{B}_2) \Rightarrow \mathtt{pre}(\mathtt{B}_1) \tag{3.10}$$

$$\mathtt{post}(\mathtt{B}_2) \Rightarrow \mathtt{post}(\mathtt{B}_1) \tag{3.11}$$

i.e., $\mathtt{B}_2$ requires and provides at least the same as $\mathtt{B}_1$. We call this the *Perry Substitution Principle (PSP)*.

Allowing an interface to be replaced with an implementation with stronger preconditions means that a rewrite rule is *not always applicable* as a refinement. Before any $(\mathtt{I}, \mathtt{A})$ rewrite rule can be applied, we must validate that the `A`'s preconditions hold in the graph being transformed. If not, it cannot be applied.

Rewrite rules to be used in optimizing abstraction rewrites $\mathtt{A} \rightarrow \mathtt{I}$ have stronger constraints. An optimizing abstraction implies that a graph `A` must implement `I`, *i.e.*, $\mathtt{I} \rightarrow \mathtt{A}$. For both constraints to hold, the pre- and postconditions of `A` and `I` must be equivalent:

$$\mathtt{pre}(\mathtt{I}) \Leftrightarrow \mathtt{pre}(\mathtt{A}) \tag{3.12}$$

$$\mathtt{post}(\mathtt{I}) \Leftrightarrow \mathtt{post}(\mathtt{A}) \tag{3.13}$$

These constraints limit the rewrite rules that can be used when applying an optimizing abstraction transformation.

Summary. We mentioned before that interfaces have preconditions associated with them. In order to allow implementation to specify stronger preconditions than its interfaces, we also have to allow primitive and algorithm boxes to have preconditions.[9] We may also provide preconditions for architectures, to restrict

[9] Our *properties* are similar to attributes in an *attributed graph* [Bun82]. Allowing the implementations to have stronger preconditions, we may say that the rewrite rules may have

the inputs we want to accept. As we mentioned before, for algorithms and architectures, postconditions are inferred from the postconditions of their internal boxes, therefore they do not have explicit postconditions. Table 3.1 summarizes which boxes have explicit preconditions and postconditions.

Box Type	Has postconditions?	Has preconditions?
Interface	Yes	Yes
Primitive	Yes	Yes
Algorithm	No	Yes
Architecture	No	Yes

Table 3.1: Explicit pre- and postconditions summary

3.2 Tool Support

In order to support the proposed approach, we developed a tool that materializes the previous concepts, called *ReFlO (REfine, FLatten, Optimize)*, which models dataflow architectures as graphs, domain knowledge as graph transformations, and can interactively/mechanically apply transformations to graphs to synthesize more detailed and/or more efficient architectures. `ReFlO` provides a graphical design tool to allow domain experts to build a knowledge base, and developers to reuse expert knowledge to build efficient (and correct) program implementations.

In this section we describe the language to specify RDMs, the language to specify architectures, the transformations that we can apply to architectures, and how we can define interpretations.

`ReFlO` is an Eclipse [Eclb] plugin. The modeling languages were specified using Ecore [Ecla], and the model editors were implemented using GEF [Graa] and GMF [Grab]. The model transformations and model validation features were implemented using the Epsilon [Eps] family of languages.

We start by describing the `ReFlO` features associated with the creation of an RDM, through which a domain expert can encode and systematize domain

applicability predicates [Bun82] or *attribute conditions* [Tae04], which specify a predicate over the attributes of a graph when a match/morphism is not enough to specify whether a transformation can be applied.

knowledge. Then we describe how developers (or domain experts) can use `ReFlO` to specify their programs architectures, the model validation features, and how to derive an optimized architecture implementation using an RDM specified by the domain expert. Finally we explain how interpretations are specified in `ReFlO`.

3.2.1 ReFlO Domain Models

An RDM is created by defining an interface for each operation, a primitive for each direct code implementation, an algorithm box for each dataflow implementation, and a pattern box for each dataflow implementation that can be abstracted. *Patterns* are a special kind of algorithms that not only implement an interface, but also specify that a subgraph can be replaced by (or abstracted to) that interface, *i.e.*, `ReFlO` only tries to apply optimizing abstractions to subgraphs that match patterns (they model bidirectional transformations: interface to pattern / pattern to interface).[10]

Rewrite rules are specified using *implementations* (an arrow from an interface to a non-interface box), through which we can link an interface with a box that implements it. When an interface is connected to a pattern box, the preconditions/postcondition of the interface and the pattern must be equivalent, to meet the requirements of the Perry Substitution Principle.

> **Example:** Figure 3.12 depicts two rewrite rules, composed by the `SORT` interface, its primitive implementation `quicksort`, and its parallel implementation (algorithm `parallel_sort`), which models one of the rewrite rules that were used to refine the architecture of Figure 3.1. Figure 3.13 depicts two rewrite rules, composed by the `IMERGESPLIT` interface and its implementations (algorithm `ms_identity` and pattern `ms_mergesplit`), which model the rewrite rules used to optimize the architecture of Figure 3.3b.

[10] Graphically, a pattern is drawn using a dashed line, whereas simple algorithms are drawn using a continuous line. We also remind readers that not all algorithms can be pattern: the PSP and equation 3.9, impose additional requirements for an algorithms to be used in an optimizing abstraction.

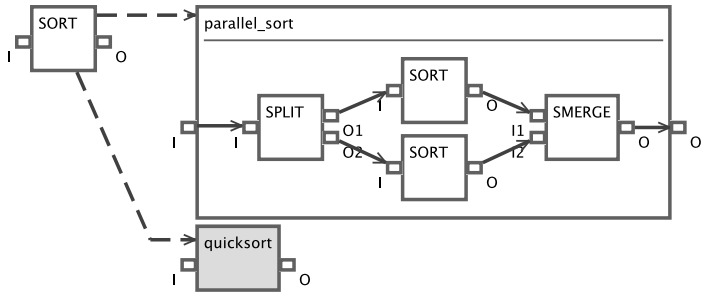


Figure 3.12: `SORT` interface, `parallel_sort` algorithm, `quicksort` primitive, and two implementation links connecting the interface with their implementations, defining two rewrite rules.

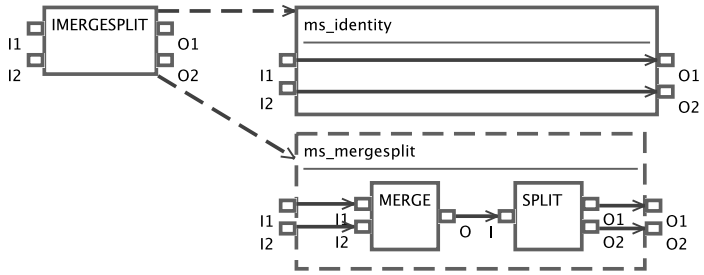


Figure 3.13: `IMERGESPLIT` interface, `ms_identity` algorithm, `ms_mergesplit` pattern, and two implementation links connecting the interface with the algorithm and pattern, defining two rewrite rules.

The rewrite rules are grouped in *layers*. Layers have the attribute *active* to specify whether their implementations (rewrite rules) may be used when deriving an architectures or not (*i.e.*, easily allowing a group of rules to be disabled). Additionally, layers have the attribute *order* that contains an integer value. When deriving an architecture, we can also restrict the rewrite rules to be used to those whose order is in a certain interval, limiting the set of rules that the `ReFlO` tries to apply when deriving architectures, thus improving its performance.[11]

Rewrite rules must be documented so that others who inspect architecture derivations can understand the steps that were used to derive it. Boxes, ports

[11] In some domains it is possible to order layers in such a way that initially we can only apply rewrite rules from the first layer, then we can only apply rules from a second layer, and so on. The *order* attribute allows us to define such an order.

and layers have the *doc* attribute, where domain experts can place a textual description of the model elements. ReFlO provides the ability to generate HTML documentation, containing the figures of boxes, and their descriptions. This ability is essential to describe the transformations and elements of an RDM, thereby providing a form of "documentation" that others could access and explore.

Besides the constraints mentioned in Section 3.1.1, ReFlO adds constraints regarding names of boxes, ports and additional parameters, which must match the regular expression $[a-zA-Z0-9\_]+$. Additionally, a box can only be the target of an implementation link.

Figure 3.14 depicts the UML class diagram of the metamodel for RDMs. The constraints associated with this metamodel have been defined prior to this point.

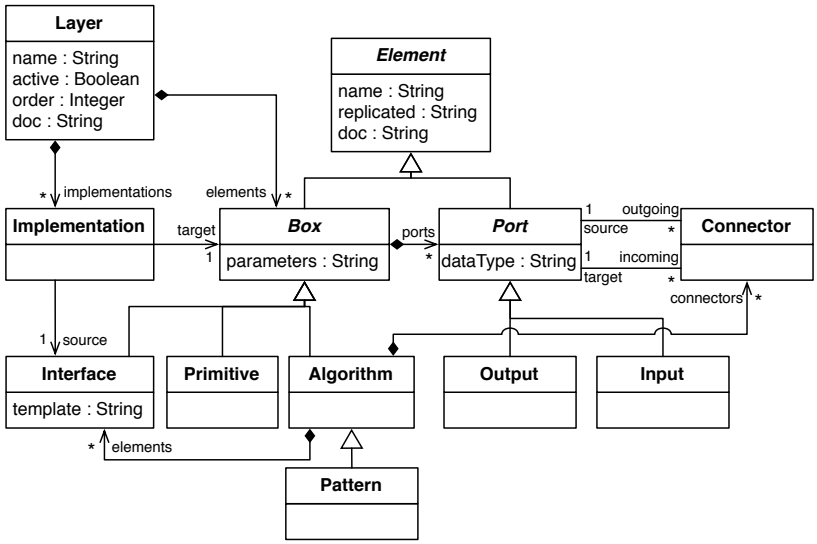


Figure 3.14: ReFlO Domain Models UML class diagram.

Figure 3.15 shows the user interface provided by ReFlO. We have a project that groups files related to a domain, containing folders for RDMs, architectures, interpretations, documentation, etc. When we have an RDM opened (as show in Figure 3.15), we also have a *pallete* on the right with objects and links we can drag to the RDM file to build it. On the bottom we can see a window that allows us to set attributes of the selected object.

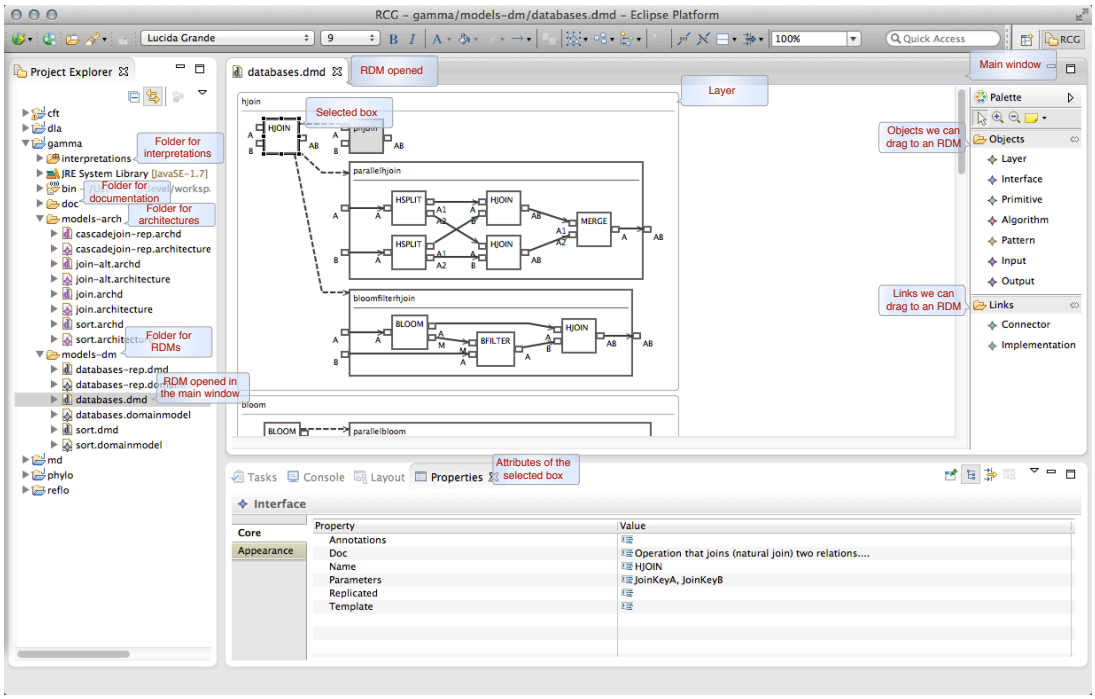


Figure 3.15: `ReFlO` user interface.

3.2.1.1 Additional Parameters

Boxes have the attribute *parameters* to hold a comma-separated list of names, data types and values, which specify their additional parameters. Each element of the list of parameters should have the format `name` : `datatype` (if the parameter's value is undefined), or `name` : `datatype` = `value` (if we want to provide a value). The $ sign is used to specify a value that is a parameter of the parent box (*e.g.*, `x` : `T` = $`y`, where `y` is an additional parameter of the parent box, means that parameter `x`, of type `T`, has the same value as `y`). Additional parameters keep the models simpler (as they are not graphically visible), allowing developers to focus on the essential parts of the model.

> **Example:** Consider the algorithm `parallel_sort`, presented in Figure 3.12. It has an additional parameter, to define the attribute to use as key when comparing the input tuples. It is specified by the expression `SortKey` : `Attribute`. Its internal box `SORT` also has an additional parameter for the same purpose, and which value is equal

to the value of its parent box (`parallel_sort`). Thus, it is specified by the expression `SortKey` : `Attribute` = $`SortKey`.

3.2.1.2 Templates

Templates provide a way to easily specify several different rewrite rules that have a common "shape", and differ only on the name of the boxes. In that case, the name of a particular box present in a rewrite rule denotes a variable, and we use the attribute *template* of the LHS of the rewrite rule to specify the possible instantiations of the variables present in the rewrite rule. Templates provide an elementary form of *higher-order transformations* [TJF+09] that reduces modeling effort.

Example: Consider the boxes of Figure 3.16, where $\mathtt{F}_2 = \mathtt{F}_1^{-1}$. We have the specification of an optimization. Whenever we have a box $\mathtt{F}_1$ followed by a box $\mathtt{F}_2$ (algorithm `IdF1F2`), the second one can be removed (algorithm `IdF1`). A similar optimization can be defined for any pair of boxes $(\mathtt{x}_1, \mathtt{x}_2)$, such that $\mathtt{x}_2 = \mathtt{x}_1^{-1}$.

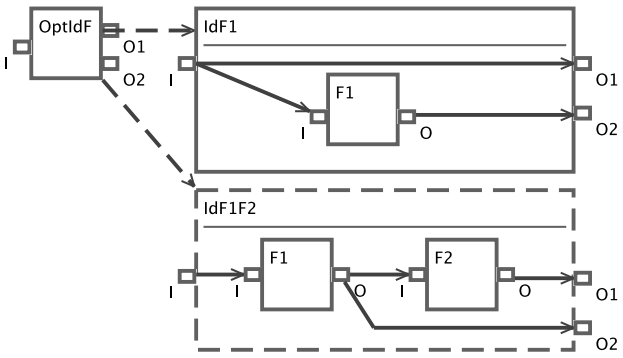


Figure 3.16: Two implementations of the same interface that specify an optimization.

Templates specify all such optimizations with the same set of boxes. Assuming that $\mathtt{G}_2 = \mathtt{G}_1^{-1}$ and $\mathtt{H}_2 = \mathtt{H}_1^{-1}$, we can express the three different optimizations (that remove box $\mathtt{F}_2$, $\mathtt{G}_2$, or $\mathtt{H}_2$) creating the

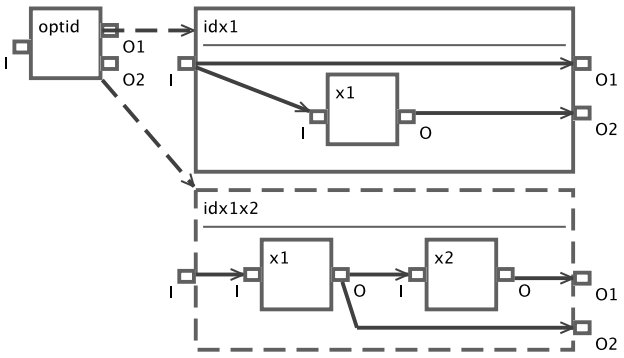


Figure 3.17: Expressing optimizations using templates. The boxes `optid`, `idx1`, `idx1x2`, `x1`, and `x2` are "variables" that can assume different values.

models depicted in Figure 3.17, and setting the attribute *template* of box `optid` with the value

$$
\begin{aligned}
&(\texttt{optid}\ , \texttt{idx1}, \texttt{idx1x2}, \texttt{x1}, \texttt{x2}) \ := \\
&(\texttt{OptIdF}, \texttt{IdF1}, \texttt{IdF1F2}, \texttt{F1}, \texttt{F2}) \mid \\
&(\texttt{OptIdG}, \texttt{IdG1}, \texttt{IdG1G2}, \texttt{G1}, \texttt{G2}) \mid \\
&(\texttt{OptIdH}, \texttt{IdH1}, \texttt{IdH1H2}, \texttt{H1}, \texttt{H2})
\end{aligned}
$$

The left-hand side of := specifies that `optid`, `idx1`, `idx1x2`, `x1`, and `x2` are "variables" (not the box names), which can be instantiated with the values specified on the right-hand side. The symbol | separates the possible instantiations. For example, when instantiating the variables with `OptIdF`, `IdF1`, `IdF1F2`, `F1` and `F2`, we get the optimization of Figure 3.16.

3.2.1.3 Replicated Elements

Figure 3.12 showed a parallel algorithm for `SORT`, the `parallel_sort`, where we execute two instances of `SORT` in parallel. However, we are not limited to two, and we could increase parallelism using more instances of `SORT`. Similarly, the number of output ports of `SPLIT` boxes used in the algorithm, as well as the input ports of `SMERGE`, may vary.

ReFlO allows to express this variability in models, using *replicated elements*. Ports and boxes have an attribute that specifies their replication. This attribute should be empty, in case the element is not replicated, or contain an upper case letter, which is interpreted as a variable that specifies how many times the element is replicated, and that we refer to as *replication variable* (this variable is shown next to the name of the element, inside square brackets).[12] Thus, box B[N] means that there are N instances of box B (B_i, for $i = \{1...N\}$). Similarly for ports.

Example: Using replicated elements, we can express the parallel_sort in a more flexible way, as depicted in Figure 3.18. Output port O of SPLIT, interface SORT, and input port I of SMERGE are replicated N times. Notice that we used the same value (N) in all elements, meaning that they are replicated the same number of times.

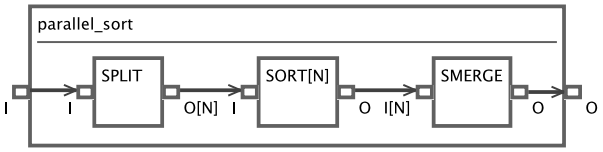


Figure 3.18: parallel_sort algorithm modeled using replicated elements.

Example: We may have elements that can be replicated a different number of times, as in the case of the interface IMERGESPLIT and its implementations, msnm_mergesplit and msnm_splitmerge, depicted in Figure 3.19. Here, the interface has N inputs and M outputs. Inside the patterns we also have some elements replicated N times, and others replicated M times. The scope of these variables is formed by all connected boxes, which means that N and M used in the algorithms are the same used in the interface they implement. This is important in transformations, as we have to preserve these values, *i.e.*, the

[12] These variables can be instantiated when generating code.

replication variables of the elements to remove during a transformation are used to determine the replication variables of the elements to add. More on this in Section 3.2.4.

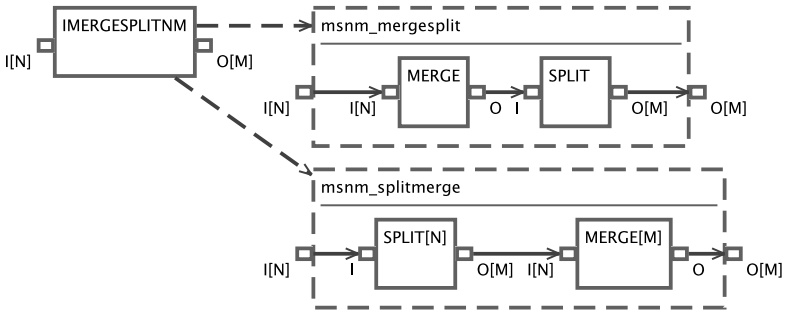


Figure 3.19: `IMERGESPLITNM` interface, and its implementations `msnm_mergesplit` and `msnm_splitmerge`, modeled using replicated elements.

`ReFlO` has specific rules for replicating connectors (*i.e.*, connectors linking replicated ports or ports of replicated boxes). Using the notation `B.P` to represent port `P` of box `B`, given a connector from output port `O` of box `B` to input port `I` of box `C`, the rules are:

- When `O` is replicated `N` times and `B` is not (which implies that either `I` or `C` is also replicated `N` times), connectors link $\texttt{B.O}_\texttt{i}$ to $\texttt{C.I}_\texttt{i}$ or $\texttt{C}_\texttt{i}\texttt{.I}$ (depending on which is replicated), for $\texttt{i} \in \{\texttt{1} \ldots \texttt{N}\}$.
- When `B` is replicated `N` times and `O` is not (which implies that either `I` or `C` is also replicated `N` times), connectors link $\texttt{B}_\texttt{i}\texttt{.O}$ to $\texttt{C.I}_\texttt{i}$ or $\texttt{C}_\texttt{i}\texttt{.I}$ (depending on which is replicated), for $\texttt{i} \in \{\texttt{1} \ldots \texttt{N}\}$.
- When `B` is replicated `N` times and `O` is replicated `M` times (which implies that both `C` and `I` are also replicated), connectors link $\texttt{B}_\texttt{i}\texttt{.O}_\texttt{j}$ to $\texttt{C}_\texttt{j}\texttt{.I}_\texttt{i}$, thereby implementing a *crossbar*, for $\texttt{i} \in \{\texttt{1} \ldots \texttt{N}\}$ and $\texttt{j} \in \{\texttt{1} \ldots \texttt{M}\}$ (this also implies that `C` is replicated `M` times, and `I` is replicated `N` times).

  Example: According to these rules, the pattern `msnm_splitmerge` from Figure 3.19 results in the pattern depicted in Figure 3.20, when

`N` is equal to `2` and `M` is equal to `3`. Notice the crossbar in the middle, resulting from a connector that was linking replicated ports of replicated boxes.

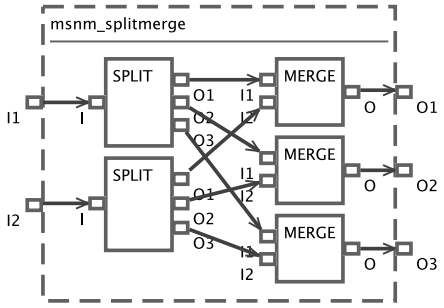


Figure 3.20: `msnm_splitmerge` pattern without replication.

3.2.2 Program Architectures

An architecture models a program that, with the help of an RDM, can be optimized to a specific need (such as a hardware platform). We use a slightly different metamodel to express architectures. Figure 3.21 depicts the UML class diagram of the metamodel for architectures.

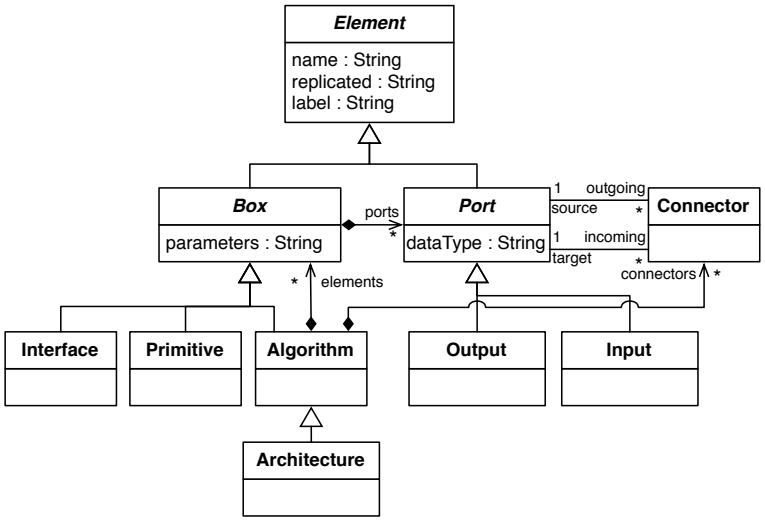


Figure 3.21: Architectures UML class diagram.

To model a program, we start with an architecture box specifying its inputs

and outputs, and a possible composition of interfaces that produces the desired behavior. We may use additional parameters to model some of the inputs of the program. As in RDMs, architectures may contain replicated elements.

> **Example:** Several architectures were previously shown (*e.g.*, Figure 3.1, 3.3a, and 3.5).

3.2.3 Model Validation

`ReFlO` provides the ability to validate RDMs and architectures, checking if they meet the metamodel constraints. It checks whether the boxes have valid names, whether the ports and parameters are unique and have valid names, and whether inherited parameters are valid. Additionally, it also checks whether the ports have the needed connectors, whether the connectors belong to the right box, and whether the replication variables of connected ports and boxes are compatible.

For RDMs, it also checks whether primitives and algorithms implement an interface, and whether they have the same ports and additional parameters of the interface they implement.

3.2.4 Model Transformations

`ReFlO` provides transformations to allow us to map architectures to more efficient ones, optimized for particular scenarios. When creating an architecture, we associate an RDM to it. The RDM specifies the transformations that we are able to apply to the architecture. At any time during the mapping process, we have the freedom to add new transformations to the RDM, which we want to apply, but that are not available yet.

The transformations that can be applied to boxes inside an architecture are described below:

Refine replaces an user selected interface with one of its implementations. `ReFlO` examines the rewrite rules in order to determine which ones meet

the constraints described in Section 3.1.4. Then, a list of valid implementations is shown to the user, for him to choose one (if only one option is available, it is automatically chosen). If either the interface or its ports are replicated, that information is preserved (*i.e.*, the replication variables of the interface are used to define the replication variable of the implementation). If the implementation has replication variables that are not present in the interface being refined, the user is asked to provide a value for the variable.[13]

> **Example:** Using the rewrite rule presented in Figure 3.18 to refine the architecture of Figure 3.1, the user is asked to provide a value for replication variable `N`, and after providing the value `Y`, the architecture of Figure 3.22 is obtained.

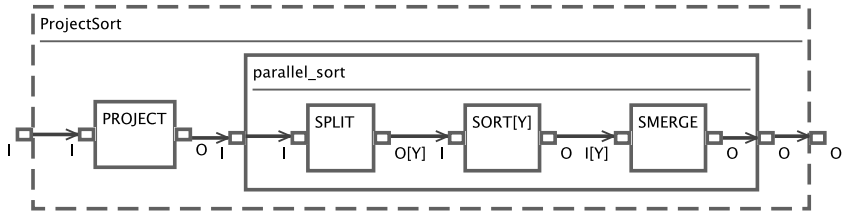


Figure 3.22: Architecture `ProjectSort`, after refining `SORT` with a parallel implementation that use replication.

Flatten removes the modular boundaries of the selected algorithm. If the algorithm to be flattened was replicated, this information is pushed down to its internal boxes.[14]

Find Optimization locates all possible matches for the patterns in the RDM that exist inside a user selected algorithm or architecture. The interfaces that are part of matches are identified setting their attribute *label*, which is shown after their name.

[13] We could also keep the value used in the RDM. However, in some cases we want to use different values when refining different instances of an interfaces (with the same algorithm).

[14] We do not allow the flattening of replicated algorithms that contain replicated boxes, as this would require multidimensional replication.

Example: Applying the find optimization to the architecture of Figure 3.3b results in the architecture of Figure 3.23, where we can see that two boxes are part of a match (of pattern `ms_mergesplit`).

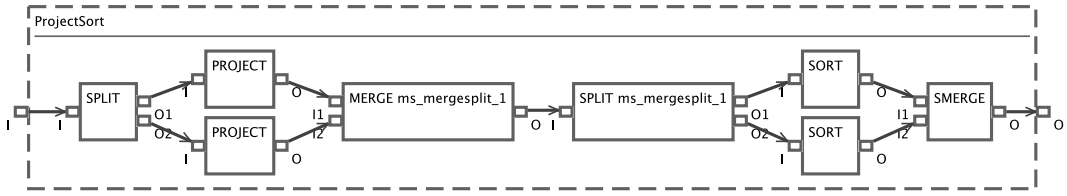
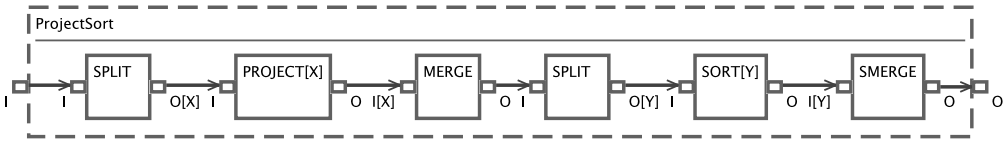


Figure 3.23: Matches present in an architecture: the label shown after the name of boxes `MERGE` and `SPLIT` specifies that they are part of a match of pattern `ms_mergesplit` (the number at the end is used to distinguish different matches of the same pattern, in case they exist).

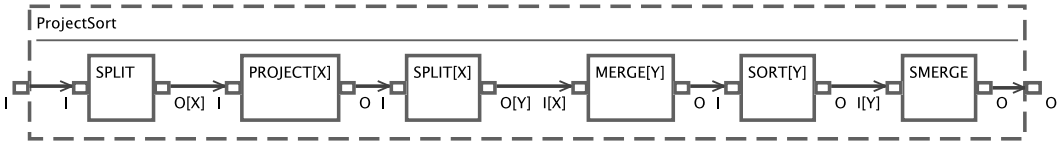
Abstract applies an optimizing abstraction to an architecture, replacing the selected boxes with the interface they implement. If only a box is selected, `ReFlO` checks which interface is implemented by that box, and uses it to replace the selected box. If a set of interfaces is selected, `ReFlO` tries to build a match from the existing patterns in the RDM to the selected boxes. If the selected boxes do not match any pattern, the architecture remains unchanged. If the selected boxes match a pattern, they are replaced with the interface the pattern implements. Otherwise, if more than one pattern is matched, the user is asked to choose one, and the selected boxes are replaced with the interface that the chosen pattern implements. During the transformation, the values of the replication variables of the subgraph are used to define the replication variables of the new interface. Unlike in refinements, no preconditions check is needed to decide whether a pattern can be replaced with the interface. However, to decide whether the selected boxes are an instance of the pattern `A` we need to put the modular boundaries of `A` around the boxes, and verify if `A`'s preconditions are met. That is, it is not enough to verify if the selected boxes have the "shape" of the pattern.

Optimize performs an optimizing abstraction, refinement and flattening as a single step, replacing the selected set of boxes with an equivalent implementation.

> **Example:** Applying the optimize transformation to the architecture of Figure 3.24a, to optimize the composition of boxes `MERGE` – `SPLIT`, using the optimization from Figure 3.19, we get the architecture of Figure 3.24b. Notice that during the transformation the replication variables of the original architecture are preserved in the new architecture, *i.e.*, the boxes being replaced in the original architecture used `X` and `Y` instead of `N` and `M` (see Figure 3.19), therefore the new architecture also uses `X` and `Y` instead of `N` and `M`.



(a)



(b)

Figure 3.24: Optimizing a parallel version of the `ProjectSort` architecture.

Expand expands replicated boxes and ports of an architecture. For each replicated box, a copy is created. For each replicated port, a copy is created, and the suffixes `1` and `2` are added to the names of the original port and its copy, respectively (as two port cannot have the same name). Connectors are copied according to the rules previously defined.

> **Example:** Figure 3.25 depicts the application of the expansion transformation to the architecture of Figure 3.24b.

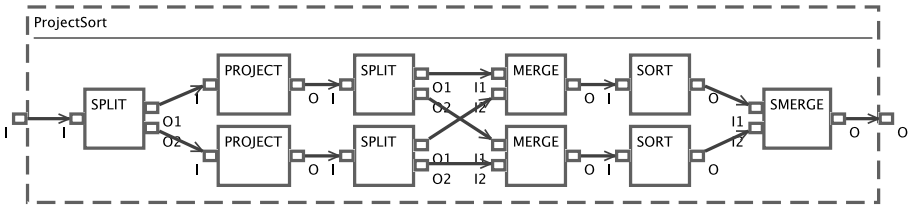


Figure 3.25: Expanding the parallel, replicated version of `ProjectSort`.

3.2.5 Interpretations

Each interpretation is written in Java. For a given interpretation, and a given box, a Java class must be provided by the domain expert. Every interpretation is represented by a collection of classes—one per box—that is stored in a unique Java package whose name identifies the interpretation. Thus if there are `n` interpretations, there will be `n` Java packages provided by the domain expert.

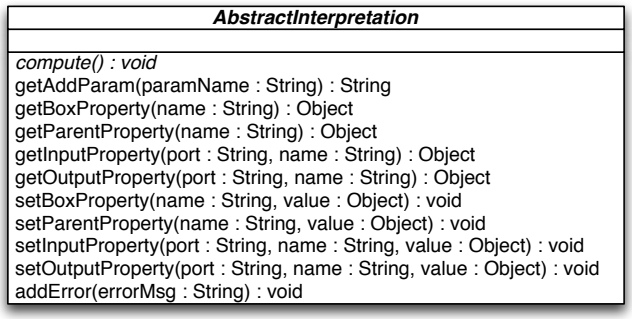
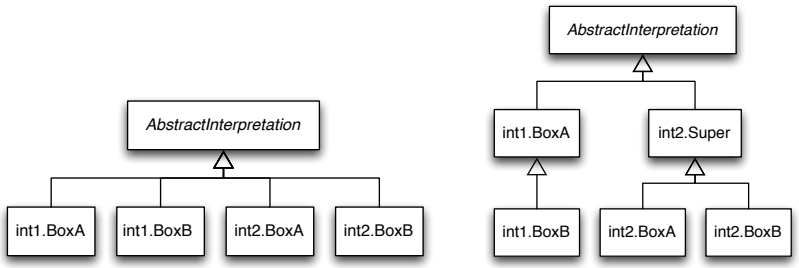


Figure 3.26: The `AbstractInterpretation` class.

Each class has the name of its box, and must extend abstract class `AbstractInterpretation` provided by `ReFlO` (see Figure 3.26). Interpretations grow in two directions: (i) new boxes can be added to the domain, which requires new classes to be added to each package, and (ii) new interpretations can be added, which requires new packages.

The behavior of an interpretation is specified in method `compute`. It computes and stores properties that are associated with its box or ports. For each box/port, properties are stored in a map that associates a value with a property identifier. `AbstractInterpretation` provides `get` and `set` methods for accessing and modifying properties.



(a) (b)

Figure 3.27: Class diagrams for two interpretations `int1` and `int2`.

A typical class structure for interpretations is shown in Figure 3.27a, where all classes inherit directly from `AbstractInterpretation`. Nevertheless, more complex structures arise. For example, one interpretation may inherit from another (this is common when defining preconditions, as an algorithm has the same preconditions of the interface it implements, and possibly more), or there may be an intermediate class that implements part (or all) of the behavior of several classes (usually of the same interpretation), as depicted in Figure 3.27b. Besides requiring classes to extend `AbstractInterpretation`, `ReFlO` allows developers to choose the most convenient class structure for the interpretation at hand. We considered the development of a domain-specific language to specify interpretations. However, by relying in Java inheritance, the presented approach also provides a simple and expressive mechanism to specify interpretations.

Although `ReFlO` expects a Java class for each box, if none is provided, `ReFlO` automatically selects a default class, with an empty `compute` method. That is, in cases where there are no properties to set, no class needs to be provided.

Example: `ReFlO` generates complete executables in $\mathcal{M}2\mathcal{T}$ interpretations; thus interface boxes may have no mappings to code.

Example: Interpretations that set a property of ports usually do not need to provide a class for algorithms, as the properties of their ports are set when executing the `compute` methods of their internal boxes. This is the case of interpretations that compute postconditions, or interpretations that compute data sizes. However, there are

cases where properties of an algorithm cannot be inferred from its internal boxes. A prime example is the `do_nothing` algorithm—it has preconditions, but its internals suggest nothing. (In such cases, a Java class is written for an algorithm to express its preconditions.)

`ReFlO` executes an interpretation in the following way: for each box in a graph, its `compute` method is executed, with the execution order being determined by the topological order of the boxes (in the case of hierarchical graphs, the interpretation of an algorithm box is executed before the interpretations of its internal boxes).[15] After execution, a developer (or `ReFlO` tool) may select any box and examine its properties.

Composition of Interpretations. Each interpretation computes certain properties of a program `P`, and it may need properties that are also needed by other interpretations, *e.g.*, to estimate the execution cost of a box, we may need an estimate of the volume of data output by a box. The same property (volume of data) may be needed for other interpretations (*e.g.*, preconditions). Therefore, it is useful to separate the computation of each property, in order to improve interpretation modularity and reusability.

`ReFlO` supports the composition of interpretations, where two or more interpretations are executed in sequence, and an interpretation has access to the properties computed by previously executed interpretations. For example, an interpretation to compute data sizes ($\mathcal{DS}$) can be composed with one that forms cost estimates ($\mathcal{ET}$) to produce a compound interpretation $(\mathcal{ET} \circ \mathcal{DS})(\texttt{P}) = \mathcal{ET}(\texttt{P}) \circ \mathcal{DS}(\texttt{P})$. The same interpretation $\mathcal{DS}$ can be composed (reused) with any other interpretation that also needs data sizes. $\mathcal{PRE} \circ \mathcal{POST}$ is a typical example where different interpretations are composed. In Section 4.2.4.3 we also show how this ability to compose interpretations is useful when adding new rewrite rules to an RDM.

[15] Backward interpretations reverse the order of execution, that is, a box is executed before its dependencies, and internal boxes are executed before their parent boxes.

Chapter 4

Refinement and Optimization Case Studies

We applied the proposed methodology in different case studies from different application domains, to illustrate how the methodology and tools can be used to help developers deriving optimized program implementations in those domains, and how we can make the derivation process understandable for non-experts by exposing complex program architectures as a sequence of small incremental transformations applied to an initial high-level program architecture.

In this chapter we present case studies from the relational databases and DLA domains. First we describe simple examples, based on the equi-join relational database operation, which is well-known for computer scientists, and therefore can be easily appreciated by others. Then we describe more complex examples from the DLA domain, where we show how we map the same initial architecture (PIM) to architectures optimized for different hardware configurations (PSMs).

4.1 Modeling Database Operations

In this section we show how optimized programs from the relational databases domain are derived. We start by presenting a detailed analysis of the derivation of a Hash Join parallel implementation [GBS14], and its interpretations. Then

we present a more complex variation of the Hash Join derivation.

4.1.1 Hash Joins in Gamma

Gamma was (and perhaps still is) the most sophisticated relational database machine built in academia [DGS+90]. It was created in the late 1980s and early 1990s without the aid of modern software architectural models. We focus on Gamma's join parallelization, which is typical of modern relational database machines, and use `ReFlO` screenshots to incrementally illustrate Gamma's derivations.

4.1.1.1 Derivation

A *hash join* is an implementation of a relational equi-join; it takes two streams of tuples as input (`A` and `B`), and produces their equi-join `A` ⋈ `B` as output (`AB`). Figure 4.1 is Gamma's PIM. It just uses the `HJOIN` interface to specify the desired behavior.

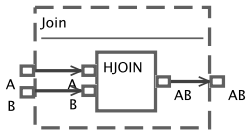


Figure 4.1: The PIM: `Join`.

The derivation starts by refining the `HJOIN` interface with its `bloomfilterhjoin` implementation, depicted in Figure 4.2. The `bloomfilterhjoin` algorithm makes use of *Bloom filters* [Blo70] to reduce the number of tuples to join. It uses two new boxes: `BLOOM` (to create the filter) and `BFILTER` (to apply the filter). Here is how it works: the `BLOOM` box takes a stream of tuples `A` as input and outputs exactly the same stream `A` along with a bitmap `M`. The `BLOOM` box first clears `M`. Each tuple of `A` is read, its join key is hashed, the correspond-

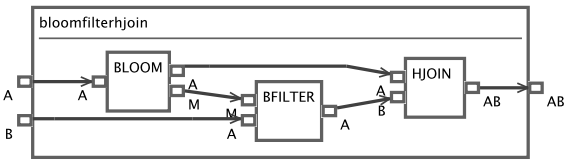


Figure 4.2: `bloomfilterhjoin` algorithm.

ing bit (indicated by the hash) is set in `M`, and the `A` tuple is output. After all `A` tuples are read, `M` is output. `M` is the Bloom filter.

The `BFILTER` box takes Bloom filter `M` and a stream of tuples `A` as input, and eliminates tuples that cannot join with tuples used to build the Bloom filter. The algorithm begins by reading `M`. Stream `A` is read one tuple at a time; the `A` tuple's join key is hashed, and the corresponding bit in `M` is checked. If the bit is unset, the `A` tuple is discarded as there is no tuple to which it can be joined. Otherwise the `A` tuple is output. A new `A` stream is the result.

Finally, output stream `A` of `BLOOM` and output stream `A` of `BFILTER` are joined. Given the behaviors of the `BLOOM`, `BFILTER`, and `HJOIN` boxes, it is easy to prove that `bloomfilterhjoin` does indeed produce $\mathtt{A} \bowtie \mathtt{B}$ [BM11].

After applying the refinement transformation, we obtain the architecture depicted in Figure 4.3. The next step is to parallelize the `BLOOM`, `BFILTER`, and `HJOIN` operations by refining each with their map-reduce implementations.

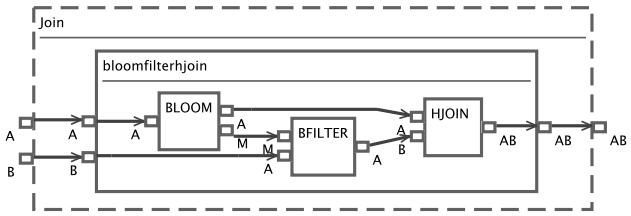


Figure 4.3: `Join` architecture, using Bloom filters.

The parallelization of `HJOIN` is textbook [BFG+95]: both input streams `A`, `B` are hash-split on their join keys using the same hash function. Each stream $\mathtt{A_i}$ is joined with stream $\mathtt{B_i}$ ($\mathtt{i} \in \{1, 2\}$), as we know that $\mathtt{A_i} \bowtie \mathtt{B_j} = \emptyset$ for all $\mathtt{i} \neq \mathtt{j}$ (equal keys must hash to the same value). By merging the joins of $\mathtt{A_i} \bowtie \mathtt{B_i}$ ($\mathtt{i} \in \{1, 2\}$), $\mathtt{A} \bowtie \mathtt{B}$ is produced as output. This parallel implementation of `HJOIN` is depicted in Figure 4.4.

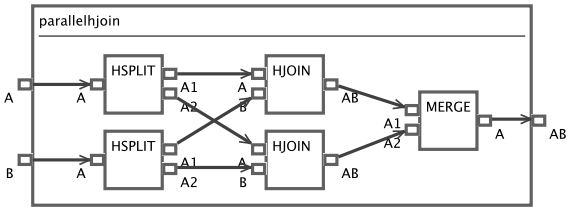


Figure 4.4: `parallelhjoin` algorithm.

The BLOOM operation is parallelized by hash-splitting its input stream A into substreams A_1, A_2, creating a Bloom filter M_1, M_2 for each substream, coalescing A_1, A_2 back into A, and merging bit maps M_1, M_n into a single map M. This parallel implementation of BLOOM is depicted in Figure 4.5.

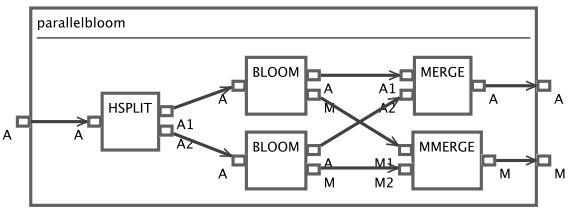


Figure 4.5: parallelbloom algorithm.

The BFILTER operation is parallelized by hash-splitting its input stream A into substreams A_1, A_2. Map M is decomposed into submaps M_1, M_2 and substream A_i is filtered by M_i. The reduced substreams A_1, A_2 output by BFILTER are coalesced into stream A. This parallel implementation of BFILTER is depicted in Figure 4.6.

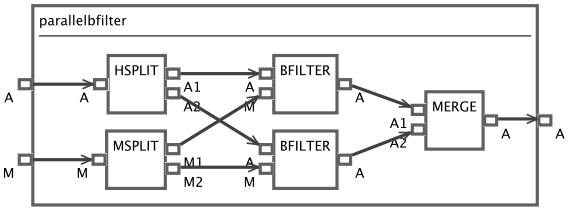


Figure 4.6: parallelbfilter algorithm.

After applying the transformation, we obtain the architecture depicted in Figure 4.7. We reached the point where refinement is insufficient to obtain the Gamma's optimized implementation.

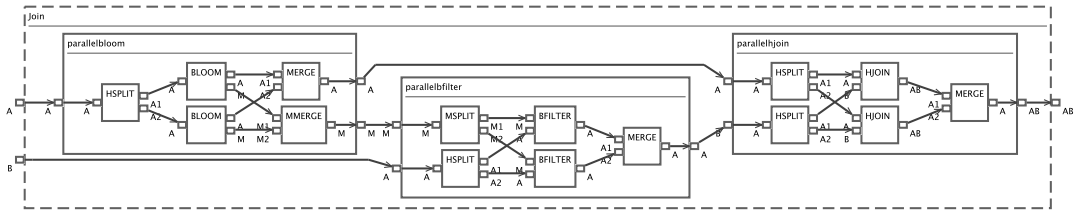


Figure 4.7: Parallelization of Join architecture.

The architecture depicted in Figure 4.7 (after flattened) exposes three *serialization bottlenecks*, which degrade performance. Consider the MERGE of substreams A_1, A_2 (produced by BLOOM) into A, followed by a HSPLIT to reconstruct A_1, A_2. *There is no need to materialize* A: the MERGE – HSPLIT composition can also be implemented by the identity map: $A_i \rightarrow A_i$.

The same applies for the MERGE − HSPLIT composition for collapsing and reconstructing substreams produced by BFILTER. The transformations required to remove these bottlenecks are encoded in the rewrite rules depicted in Figure 4.8. The removal of MERGE − HSPLIT compositions eliminates two serialization bottlenecks.

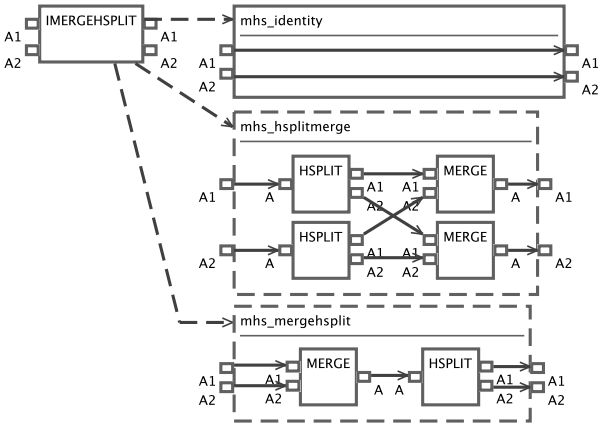


Figure 4.8: Optimization rewrite rules for MERGE − HSPLIT.

The third bottleneck combines maps M_1, M_2 into M, and then decomposes M back into M_1, M_2. The MMERGE − MSPLIT composition can also be implemented by an identity map: $M_i \rightarrow M_i$. This optimization removes the MMERGE − MSPLIT boxes and reroutes the streams appropriately. It is encoded by the rewrite rules depicted in Figure 4.9.

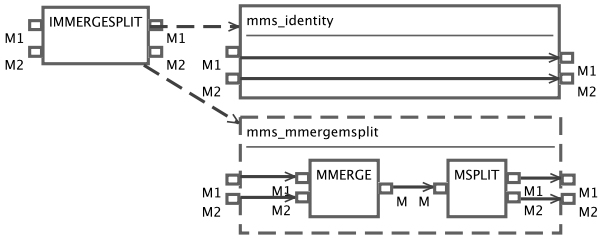


Figure 4.9: Optimization rewrite rules for MMERGE− MSPLIT.

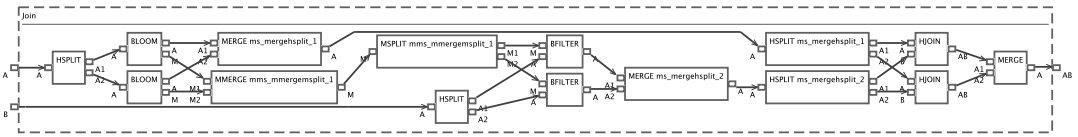


Figure 4.10: Join architecture's bottlenecks.

Using the *Find Optimization* tool available in ReFlO, the bottlenecks are identified, as depicted in Figure 4.10. These bottlenecks can be removed using optimizations, which replace the inefficient compositions of operations by identities. Doing so, we obtain the optimized architecture depicted in Figure 4.11.

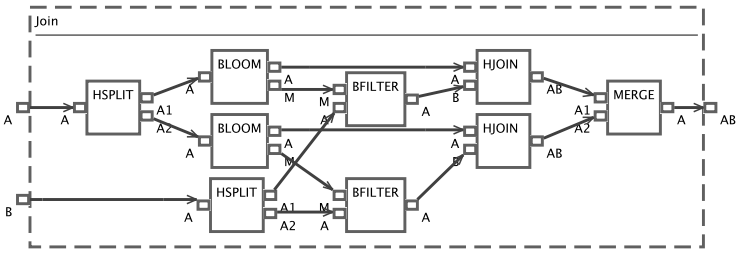


Figure 4.11: Optimized `Join` architecture.

This step finishes the core of the derivation. An additional step is needed. The current architecture is specified using interfaces, thus, we still have to choose the code implementation for each operation, *i.e.*, we have to refine the architecture replacing the interfaces with primitive implementations. This additional step yields the architecture depicted in Figure 4.12, the PSM of Gamma's Hash Join. Later in Section 4.1.2 we show further steps for the derivation of optimized Hash Join implementations in Gamma.

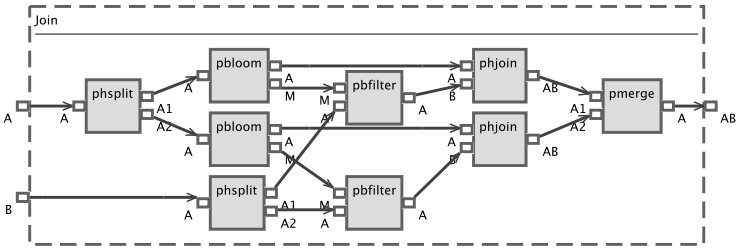


Figure 4.12: The `Join` PSM.

4.1.1.2 Preconditions

In Section 3.1 (Figure 3.13) we shown an optimization for the composition `MERGE` − `SPLIT`. In the previous section we presented a different optimization for composition `MERGE` − `HSPLIT`. The differences between these optimizations go beyond the names of the boxes.

`IMERGESPLIT` interface models an operation that only requires the union of the output streams to be equal to the union of the input streams. This happens as the `SPLIT` interface does not guarantee that a particular tuple will always be assigned to the same output. However, `HSPLIT` always sends the same tuple

to the same output, and it has postconditions regarding the hash values of the tuples of each output, which specify (i) a certain field was used to hash-split the tuples, and (ii) that the outputs of port $\texttt{A}_\texttt{i}$, after being hashed, were assigned to substream of index `i`. The same postconditions are associated with pattern `mhs_mergehsplit`. Also note that pattern `mhs_mergehsplit` needs an additional parameter (`SplitKey`), which specifies the attribute to be used when hash-splitting the tuples (and that is used to define the postconditions).

As required by the PSP, the postconditions of the dataflow graph to be abstracted (pattern `mhs_mergehsplit`) have to be equivalent to the postconditions of the interface it implements, thus, interface `IMERGEHSPLIT` also must provide such postconditions. Through the use of the `HSPLIT` boxes, pattern `mhs_hsplitmerge` provides such postconditions.

`IMERGEHSPLIT` has one more implementation, `mhs_identity`, that implements the interface using identities. The only way to guarantee that the outputs of the identity implementation have the desired postconditions (properties), is to require their inputs to already have them (as properties are not changed internally). Therefore, the `mhs_identity` algorithm needs preconditions. This algorithm can only be used if the input substreams are hash-split using the attribute specified by `SplitKey` (that is also an additional parameter of `mhs_identity`), and if input $\texttt{A}_\texttt{i}$ contains the substream `i` produced by the hash-split operation.

Specifying Postconditions. To specify postconditions, we use the following properties: `HSAttr` is used to store the attribute used to hash-split a stream, and `HSIndex` is used to store the substream to which the tuples were assigned. For each box, we need to specify how these properties are affected. For example, the `HSPLIT` interface sets such properties. On the other hand, `MERGE` *removes* such properties (sets them to empty values). Other boxes, such as `BLOOM` and `BFILTER` preserve the properties of the inputs (*i.e.*, whatever is the property of the input stream, the same property is used to set the output stream). In Figure 4.13 we show the code used to specify these postconditions for some of the boxes used, which is part of the interpretation `hash`.

```
public class HSPLIT extends AbstractInterpretation {
  public void compute() {
    String key = getAddParam("SplitKey");
    setOutputProperty("A1","HSAttr",key);
    setOutputProperty("A2","HSAttr",key);
    setOutputProperty("A1","HSIndex",1);
    setOutputProperty("A2","HSIndex",2);
  }
}

public class MERGE extends AbstractInterpretation {
  public void compute() {
    // by default, properties have the value null
    // thus, no code is needed
  }
}

public class BFILTER extends AbtractInterpretation {
  public void compute() {
    String attr=(String)getInputProperty("A","HSAttr");
    setOutputProperty("A","HSAttr",attr);
    Integer index=(Integer)getInputProperty("A","HSIndex");
    setOutputProperty("A","HSIndex",index);
  }
}
```

Figure 4.13: Java classes for interpretation `hash`, which specifies database operations' postconditions.

Specifying Preconditions. Now we have to specify the preconditions of `mhs_identity`. Here, we have to read the properties of the inputs, and check if they have the desired values. That is, we need to check if the input streams are already hash-split, and if the same attribute was used as key to hash-split the streams. We do that comparing the value of the property `HSAttr` with the value of the additional parameter `SplitKey`. Moreover, we also need to verify if the tuples are associated with the correct substreams. That is, we need to check if the property `HSIndex` of inputs `A1` and `A2` are set to `1` and `2`, respectively. If these conditions are not met, the method `addError` is called to signal the failure in validating the preconditions (it also defines an appropriate error message). In Figure 4.14 we show the code we use to specify the preconditions for the `mhs_identity`, which is part of the interpretation `prehash`.

```
public class mhs_identity extends AbstractInterpretation {
  public void compute() {
    String key=getAddParam("SplitKey");
    String hsAttrA1= (String)getInputProperty("A1","HSAttr");
    String hsAttrA2= (String)getInputProperty("A2","HSAttr");
    Integer hsIndexA1= (Integer)getInputProperty("A1","HSIndex");
    Integer hsIndexA2= (Integer)getInputProperty("A2","HSIndex");
    if(!key.equals(hsAttrA1) || !key.equals(hsAttrA2)
        || hsIndexA1 != 1 || hsIndexA2 != 2) {
      addError("Input streams are not correctly split!");
    }
  }
}
```

Figure 4.14: Java classes for interpretation `prehash`, which specifies database operations' preconditions.

4.1.1.3 Cost Estimates

During the process of deriving a PSM, it is useful for the developers to be able to estimate values of quality attributes they are trying to improve. This is a typical application for interpretations.

For databases, estimates for execution time are computed by adding the execution cost of each interface or primitive present in a graph. The cost of an interface or primitive is computed based on the size of the data being processed. An interface cost is set to that of its most general primitive implementation. It is useful to associate costs to interfaces (even though they do not have direct code implementations), as this allows developers to *estimate execution time costs at early stages of the derivation process.*

Size estimates are used to build a cost expression representing the cost of executing interfaces and primitives. The `size` interpretation takes estimates of input data sizes and computes estimates of output data sizes. We build a string containing a cost symbolic expression, as during design time we do not have concrete values for properties needed to compute costs. Thus, we associate a variable (string) to those properties, and we use those strings to build the symbolic expression representing the costs. `phjoin` is executed by reading each tuple of stream `A` and storing it in a main-memory hash table (`cHJoinAItem` is a constant that represents the cost of processing a tuple of stream `A`), and then

each tuple of stream B is read and joined with tuples of A (cHJoinBItem is a constant that represents the cost of processing a tuple of stream B). Thus, the cost of phjoin is given by $\texttt{size}_\texttt{a} * \texttt{cHJoinAItem} + \texttt{size}_\texttt{b} * \texttt{cHJoinBItem}$. As HJOIN can always be implemented by phjoin, we can use the same cost expression for HJOIN. Figure 4.15 shows the code used to generate a cost estimate for phjoin primitive, which is part of the interpretation costs. The costs interpretation is backward, as the costs of an algorithm are computed from the costs of its internal boxes (*i.e.*, we need to compute costs of internal boxes first). So the costs are progressively sent to their parent boxes, until they reach the outermost box, where the costs of all boxes are aggregated, providing a cost estimate for the entire architecture. Figure 4.16 shows the code used by interpretations of algorithm boxes, which simply add their costs to the aggregated costs stored on their parent boxes.

```
public class phjoin extends AbstractInterpretation {
  public void compute() {
    String sizeA=(String)getInputProperty("A","Size");
    String sizeB=(String)getInputProperty("B","Size");
    String cost="("+sizeA+") * cHJoinAItem + ("
        +sizeB+") * cHJoinBItem";
    setBoxProperty("Cost",cost);
    String parentCost=(String)getParentProperty("Cost");
    if(parentCost==null) parentCost=cost;
    else parentCost="("+parentCost+") + ("+cost+")";
    setParentProperty("Cost", parentCost);
  }
}
```

Figure 4.15: Java classe for interpretation costs, which specifies phjoin's cost.

```
public class Algorithm extends AbstractInterpretation {
  public void compute() {
    String cost=(String) getBoxProperty("Cost");
    String parentCost=(String)getParentProperty("Cost");
    if(parentCost==null) parentCost=cost;
    else parentCost="("+parentCost+") + ("+cost+")";
    setParentProperty("Cost", parentCost);
  }
}
```

Figure 4.16: Java class that processes costs for algorithm boxes.

4.1.1.4 Code Generation

The final step of a derivation is the $\mathcal{M}2\mathcal{T}$ transformation to generate the code from the PSM.

`ReFlO` provides no hard-coded $\mathcal{M}2\mathcal{T}$ capability; it uses a `code` interpretation instead. Figure 4.18 depicts the code that is generated from the architecture of Figure 4.17 (a PSM obtained refining the architecture from Figure 4.3 directly with primitives).

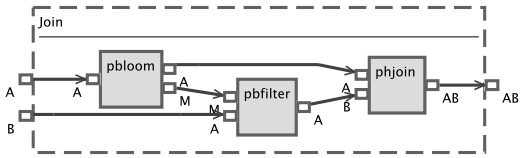


Figure 4.17: `Join` architecture, when using `bloomfilterhjoin` refinement only.

```
import gammaSupport.*;
import basicConnector.Connector;

public class Gamma extends ArrayConnectors implements GammaConstants {
  public Join(Connector inA, Connector inB, int joinkey1, int joinkey2,
      Connector outAB) throws Exception {
    Connector c1 = outAB;
    Connector c2 = inA;
    Connector c3 = inB;
    Connector c4 = new Connector("c4");
    Connector c5 = new Connector("c5");
    Connector c6 = new Connector("c6");
    int pkey1= joinkey1;
    int pkey2= joinkey2;
    new Bloom(pkey1, c2, c5, c4);
    new BFilter(pkey2, c3, c6, c4);
    new HJoin(c5, c6, pkey1, pkey2, c1);
  }
}
```

Figure 4.18: Code generated for an implementation of Gamma.

We use a simple framework, where primitive boxes are implemented by a Java class, which provides a constructor that receives as parameters the input and output connectors, and the additional parameters. Those classes extend interface `Runnable`, and the behavior of the boxes is specified by method `run`. Code generation is done by first using interpretations that associate a unique identifier to each connector, which is then used to define the variables that will

store the connector in the code being generated. Then, each box generates a line of code that calls its constructor with the appropriate connector's variables as parameters (the identifiers previously computed provide this information), and sends the code to its parent box (see Figure 4.19).

```
public class HJOIN extends AbstractInterpretation {
  public void compute() {
    String keyA=getAddParam("JoinKeyA");
    String keyB=getAddParam("JoinKeyB");
    Integer inA=(Integer)getInputProperty("A", "VarId");
    Integer inB=(Integer)getInputProperty("B", "VarId");
    Integer outAB=(Integer)getOutputProperty("AB","VarId");
    String pCode=(String)getParentProperty("Code");
    if(pCode==null) pCode="";
    pCode="\t\tnew HJoin(c" + inA + ", c" + inB + ", p" +
      keyA + ", p" + keyB + ", c" + outAB + ");\n" + pCode;
    setParentProperty("Code", pCode);
  }
}
```

Figure 4.19: Interpretation that generates code for `HJOIN` box.

Similarly to cost estimates, this is a backward interpretation, and the architecture box will eventually gather those calls to the constructors. As a final step, the interpretation of the architecture box is executed, and adds the variable declarations, and the class declaration.

4.1.2 Cascading Hash Joins in Gamma

In the previous section we showed how to derive an optimized implementation for a single Hash Join operation. However, Figure 4.12 is not the last word on Gamma's implementation of Hash Joins. We now show how we can go further, and derive an optimized implementation for cascading joins, where the output of one join becomes the input of another. Moreover, in this derivation we make use of replication, to produce an implementation that offers a flexible level of parallelization. The initial PIM is represented in the architecture of Figure 4.20.

As for the previous derivation, we start by refining `HJOIN` interfaces with its `bloomfilterhjoin` implementation. The next step is again to parallelize the interfaces present in the architecture (`BLOOM`, `BFILTER` and `HJOIN`). This step is,

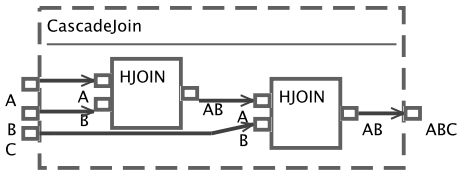


Figure 4.20: The PIM: `CascadeJoin`.

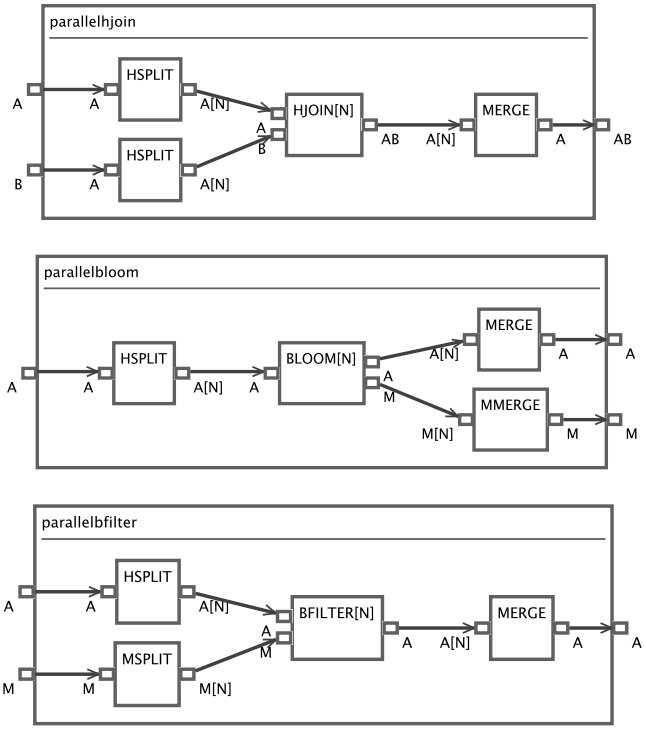


Figure 4.21: Parallel implementation of database operations using replication.

however, slightly different from the previous derivation, as we are going to use replication to define the parallel algorithms. Figure 4.21 shows the new parallel algorithms.

After using these algorithms to refine the architecture, and flattening it, we are again at the point where we need to apply optimizations to remove the serialization bottlenecks. Like in the parallel algorithm implementations, we have to review the optimizations, to take into account replication. Figure 4.22 shows the new rewrite rules that specify replicated variant of the optimizations needed.

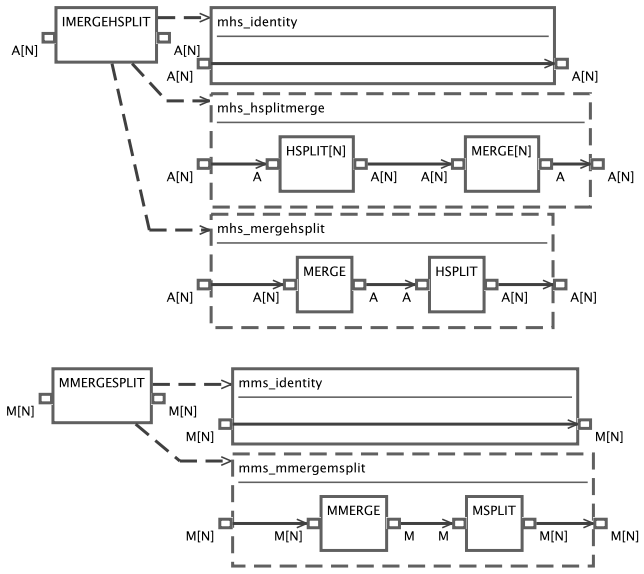


Figure 4.22: Optimization rewrite rules using replication.

This allow us to obtain the architecture depicted in Figure 4.23, which is essentially a composition of two instances of the architecture presented in Figure 4.11 (also using replication).

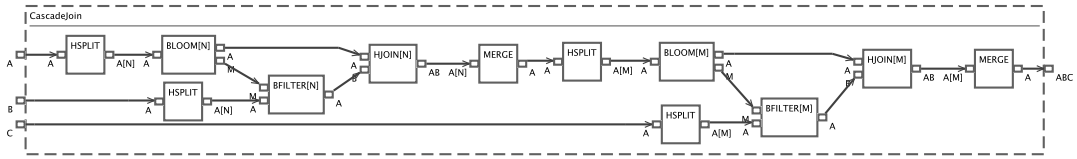


Figure 4.23: `CascadeJoin` after refining and optimizing each of the initial `HJOIN` interface.

This architecture further shows the importance of deriving the architectures, instead of just using a pre-built optimized implementation for the operations present in the initial PIM (in this case, `HJOIN` operations). The use of the optimized implementations for `HJOIN` would have resulted in an implementation equivalent to the one depicted in Figure 4.23. However, when we compose two (or more) instances of `HJOIN`, new opportunities for optimization arise. In this case, we have a new serialization bottleneck, formed by a composition of boxes `MERGE` (that merges the output streams of the first group of `HJOIN`s) and `HSPLIT` (that hash-splits the stream again). Unlike the bottlenecks involving `MERGE` and

HSPLIT previously described, cascading joins use different keys to hash the tuples, so the partitioning of the stream before the merge operation is different from the partitioning after the hash-split operation. Moreover, the number of inputs of merge operation may be different from the number of outputs of hash-split operation (note that two different replication variables are used in the architecture of Figure 4.23), which does not match the pattern mhs_mergehsplit (see Figure 4.22).

Therefore, we need new rewrite rules, to define how this bottleneck can be abstracted and implemented in a more efficient way. We define interface IMERGEHSPLITNM, which models an operation that merges N input substreams, and hash-splits the result in M output substreams, according to a given split key attribute. There are two ways of implementing this interface. We can merge the input substreams, and then hash-split the resulting stream, using the algorithm mhsnm_mergehsplit depicted in Figure 4.24. The dataflow graph used to define this implementation matches the dataflow subgraph that represents the bottleneck we want to remove. An alternative implementation swaps the order in which operations MERGE and HSPLIT are applied, *i.e.*, each input substream is hash-split into M substreams by one of the N instances of HSPLIT, and the resulting substreams are sent to each of the M instances of MERGE. The substreams with the same hash values are then merged. This behavior is implemented by algorithm mhsnm_hsplitmerge, depicted in Figure 4.24.

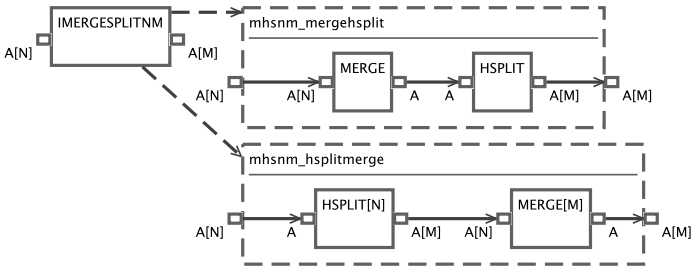


Figure 4.24: Additional optimization's rewrite rules.

After applying this optimization, we obtain the architecture from Figure 4.25. This derivation would be concluded replacing the interfaces with primitive implementations.[1]

[1]For simplification, we will omit this step in this and future derivations.

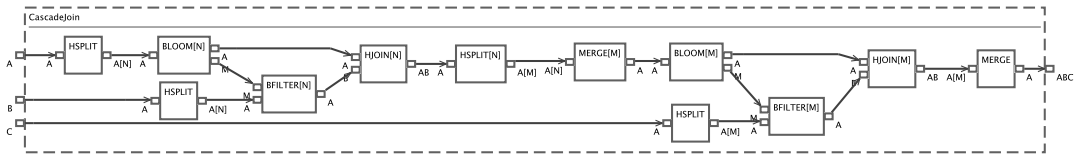


Figure 4.25: Optimized `CascadeJoin` architecture.

Recap. In this section we showed how we used `ReFlO` to explain the design of Gamma's Hash Join implementations. This was the first example of a non-trivial derivation obtained with the help of `ReFlO`, which allow us to obtain the Java code for the optimized parallel hash join implementation. This work has also been used to conduct controlled experiments [FBR12, BGMS13] to evaluate whether a derivational approach for software development, as proposed by DxT, has benefits regarding program comprehension and easy of modification. More on this in Chapter 7.

4.2 Modeling Dense Linear Algebra

In this section we illustrate how DxT and `ReFlO` can be used to derive optimized programs in the DLA domain. We start by showing the derivation of unblocked implementations from high-level specifications of program loop bodies (as they contain the components that we need to transform). We take two programs from the domain (LU factorization and Cholesky factorization), and we start building the RDM at the same time we produce the derivations. We also define the interpretations, in particular pre- and postconditions. At some point, we will have enough knowledge in the RDM to allow us to derive optimized implementations for a given target hardware platform.

Later, we add support for other target platforms or inputs. We keep the previous data, namely the RDM and the PIMs, and we incrementally enhance the RDM to support the new platform. That is, we add new rewrite rules—new algorithms, new interfaces, new primitives, etc.—, we add new interpretations, and we complete the previous interpretations to support the new boxes. The new rewrite rules typically define new implementations specialized for a certain

platform (*e.g.*, implementations specialized for distributed matrices). Preconditions are used to limit the application of rewrite rules when a certain platform is being targeted.

The rewrite rules we use are not proven correct, but, even though they have not been systematized before, they are usually well-known to experts.

In the next section we show the PIMs for LU factorization and Cholesky factorization. We then show how different implementations (unblocked, blocked, and distributed memory) are obtained from the PIMs, by incrementally enhancing the RDM (see Figure 4.26 for the structure of this section).

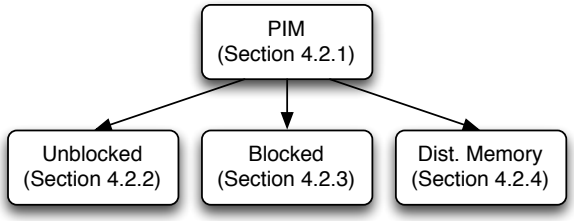


Figure 4.26: DLA derivations presented.

4.2.1 The PIMs

We use the algorithms presented in Section 2.3.1 (Figure 2.6 and Figure 2.7) to define our initial architectures (PIMs). The most important part of these algorithms is their loop body, and it is this part that has to be transformed to adapt the algorithm for different situations. Therefore, the architectures we use express the loop bodies of the algorithms only.

4.2.1.1 LU Factorization

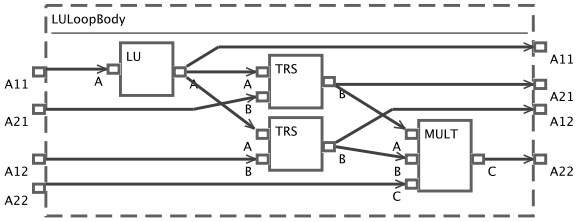


Figure 4.27: The PIM: `LULoopBody`.

Figure 4.27 depicts the architecture `LULoopBody`, the initial architecture for LU factorization (its PIM). The loop body is composed of the following sequence of operations:

- `LU` : $\mathtt{A}_{11} = \mathrm{LU}(\mathtt{A}_{11})$
- `TRS` : $\mathtt{A}_{21} = \mathtt{A}_{21}\ \mathrm{TriU}(\mathtt{A}_{11}^{-1})$
- `TRS` : $\mathtt{A}_{12} = \mathrm{TriL}(\mathtt{A}_{11}^{-1})\ \mathtt{A}_{12}$
- `MULT` : $\mathtt{A}_{22} = \mathtt{A}_{22}$ - $\mathtt{A}_{21}\ \mathtt{A}_{12}$

The `LU` interface specifies an LU factorization. The `TRS` interface specifies an inverse-matrix product $\mathtt{B} = \mathtt{coeff} \cdot \mathtt{op}(\mathtt{A}^{-1}) \cdot \mathtt{B}$ or $\mathtt{B} = \mathtt{coeff} \cdot \mathtt{B} \cdot \mathtt{op}(\mathtt{A}^{-1})$, depending on the value of its additional parameter `side`. `trans`, `tri`, `diag`, and `coeff` are other additional parameters of `TRS`. `trans` specifies whether the matrix is transposed or not ($\mathtt{op}(\mathtt{A}) = \mathtt{A}$ or $\mathtt{op}(\mathtt{A}) = \mathtt{A}^{\mathtt{T}}$). `A` is assumed to be a triangular matrix, and `tri` specifies whether it is lower or upper triangular. Further, `diag` specifies whether the matrix is unit triangular or not. In the case of the first `TRS` operation listed above, for example, the additional parameters `side`, `tri`, `trans`, `diag` and `coeff` have values `RIGHT`, `UPPER`, `NORMAL`, `NONUNIT` and `1`, respectively.

The `MULT` interface specifies a matrix product and sum $\mathtt{C} = \mathtt{alpha} \cdot \mathtt{op}(\mathtt{A}) \cdot \mathtt{op}(\mathtt{B}) + \mathtt{beta} \cdot \mathtt{C}$. Again, `op` specifies whether matrices shall be transposed or not, according to additional parameters `transA` and `transB`. `alpha` and `beta` are also additional parameters of `MULT`. In the case of the `MULT` operation listed above the additional parameters `transA`, `transB`, `alpha` and `beta` have values `NORMAL`, `NORMAL`, -1 and `1`, respectively.

4.2.1.2 Cholesky Factorization

Figure 4.28 depicts the architecture `CholLoopBody`, the initial architecture for Cholesky factorization (its PIM). The loop body is composed of the following sequence of operations:

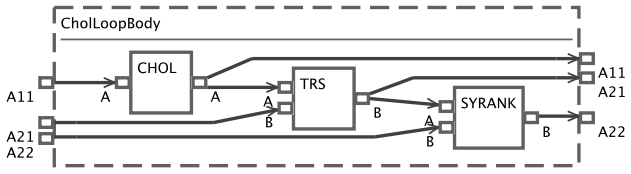


Figure 4.28: The PIM: `CholLoopBody`.

- `CHOL` : $\mathtt{A}_{11} = \textsc{Chol}(\mathtt{A}_{11})$
- `TRS` : $\mathtt{A}_{21} = \mathtt{A}_{21}\ \textsc{TriL}(\mathtt{A}_{11}^{-\mathtt{T}})$
- `SYRANK` : $\mathtt{A}_{22} = \mathtt{A}_{22}$ - $\mathtt{A}_{21}\ \mathtt{A}_{21}^{\mathtt{T}}$

The `CHOL` interface specifies Cholesky factorization. The `TRS` interface was already described. The `SYRANK` interface specifies a symmetric rank update $\mathtt{B} = \mathtt{alpha}\cdot\mathtt{A}\cdot\mathtt{A}^{\mathtt{T}} + \mathtt{beta}\cdot\mathtt{B}$ or $\mathtt{B} = \mathtt{alpha}\cdot\mathtt{A}^{\mathtt{T}}\cdot\mathtt{A} + \mathtt{beta}\cdot\mathtt{B}$, depending on the value of its additional parameter `trans`. `tri`, `alpha` and `beta` are also additional parameters of `SYRANK`. `tri` specifies whether the lower or the upper triangular part of the matrix `C` should be used (that is supposed to be symmetric). In the case of the `SYRANK` operation listed above the additional parameters `tri`, `trans`, `alpha` and `beta` have values `LOWER`, `NORMAL`, -1 and `1`.

4.2.2 Unblocked Implementations

We start by presenting the derivation of unblocked implementations. In this case, input `A11` is a scalar (a matrix of size 1×1), inputs `A21` and `A12` are vectors (matrices of size $\mathtt{n} \times 1$ and $1 \times \mathtt{n}$, respectively), and `A22` is a square matrix of size $\mathtt{n} \times \mathtt{n}$. The derivation of the optimized implementation uses this information to choose specialized implementations for inputs of the given sizes [vdGQO08].

4.2.2.1 Unblocked Implementation of LU Factorization

The first step in the derivation is to optimize `LU` interface (see Figure 4.27) for inputs of size 1×1. In this situation, `LU` operation can be implemented by the identity, which allows us to obtain the architecture depicted in Figure 4.29.

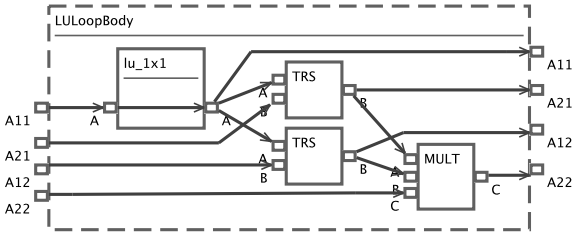


Figure 4.29: `LULoopBody` after replacing `LU` interface with algorithm `LU_1x1`.

We repeat this process for the other boxes, and in the next steps, we replace each interface with an implementation optimized for the input sizes.

For the `TRS` operation that updates `A21`, as input `A` (`A11`) is a scalar, we have `B` (`A21`) being scaled by $\texttt{alpha} \cdot \texttt{1/A}$ (in this case we have $\texttt{alpha} = \texttt{1}$). This can be implemented by algorithm `trs_invscal`, depicted in Figure 4.30. This algorithm starts by scaling `B` by `alpha` (interface `SCALP`), and then it scales the updated `B` by `1/A` (interface `INVSCAL`). After using this algorithm, we obtain the architecture depicted in Figure 4.31b.

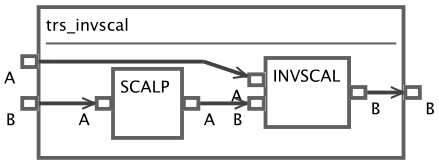
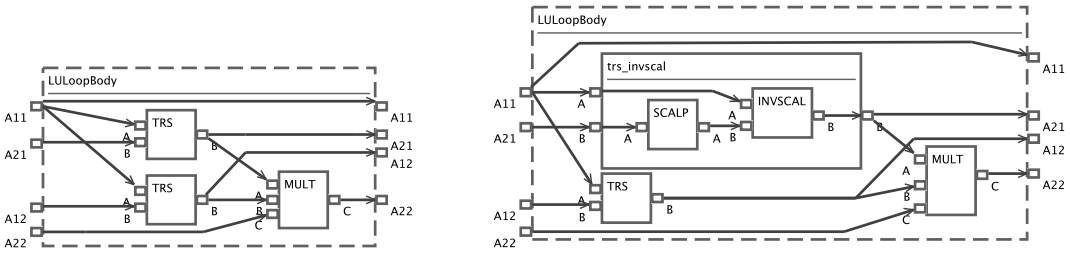


Figure 4.30: `trs_invscal` algorithm.

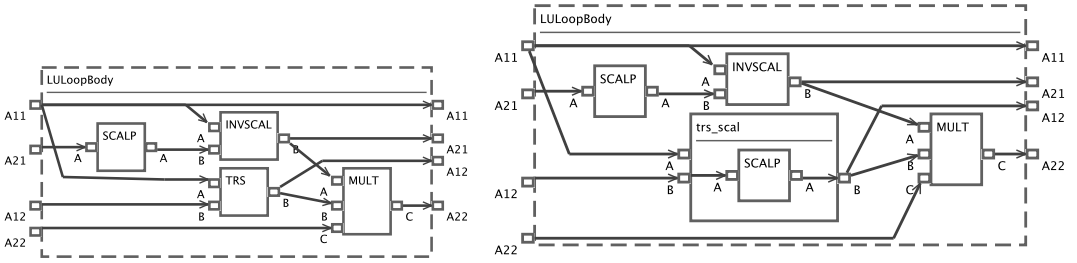


(a) (b)

Figure 4.31: `LULoopBody`: (a) previous architecture after flattening, and (b) after replacing one `TRS` interface with algorithm `trs_invscal`.

Next we proceed with the remaining `TRS` operation that updates `A12`. In this case the lower part of input `A` (`A11`) is used. Moreover, additional parameter `diag` specifies that the matrix is a unit lower triangular matrix, which means that we have `B` (`A12`) being scaled by $\texttt{alpha} \cdot \texttt{1/1}$, or simply by `alpha`. Therefore,

TRS can be implemented by algorithm trs_scal, which uses SCALP interface to scale input B. This allows us to obtain the architecture depicted in Figure 4.32b.



(a) (b)

Figure 4.32: LULoopBody: (a) previous architecture after flattening, and (b) after replacing the remaining TRS interface with algorithm trs_scal.

Finally we have the MULT interface. Inputs A and B are vectors, and C is a matrix, therefore, we use interface GER to perform the multiplication. The algorithm to be used is depicted in Figure 4.33. As MULT performs the operation alpha $\cdot$ A $\cdot$ B + beta $\cdot$ C, and GER, by definition, just performs the operation alpha $\cdot$ A $\cdot$ B + C, we also need to scale matrix C (interface SCALP). After applying this algorithm, we obtain the architecture depicted in Figure 4.34b.

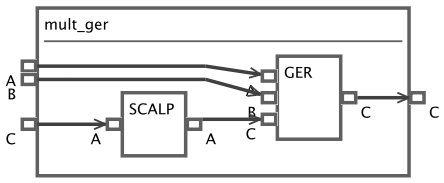
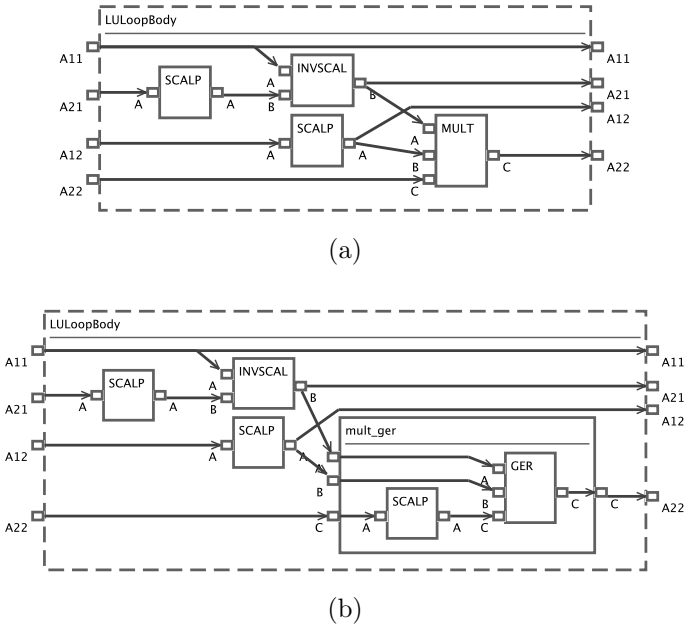


Figure 4.33: mult_ger algorithm.

As the additional parameter alpha used by all SCALP interfaces has the value 1, these interfaces can be implemented by the identity, resulting in the architecture depicted in Figure 4.35b. Figure 4.36 is the final architecture, and expresses an optimized unblocked implementation of LULoopBody. The PSM would be obtained replacing each interface present in the architecture with a primitive implementation.

4.2.2.2 Unblocked Implementation of Cholesky Factorization

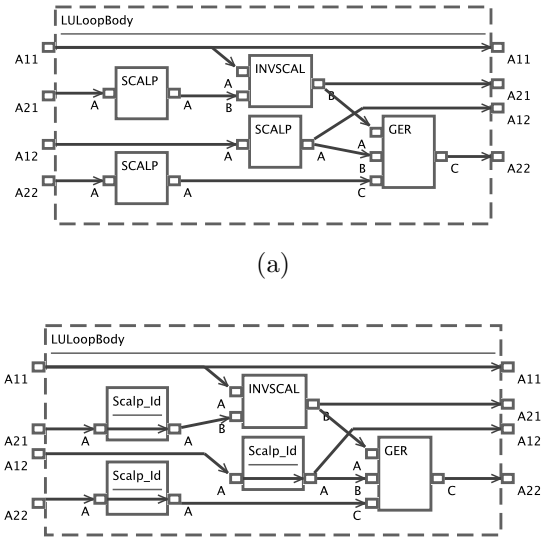
The derivation starts by optimizing CHOL interface (see Figure 4.28) for inputs of size 1 $\times$ 1. In this case, CHOL operation is given by the square root of the input



(a)

(b)

Figure 4.34: `LULoopBody`: (a) previous architecture after flattening, and (b) after replacing one `MULT` interface with algorithm `mult_ger`.



(a)

(b)

Figure 4.35: `LULoopBody`: (a) previous architecture after flattening, and (b) after replacing `SCALP` interfaces with algorithm `scalp_id`.

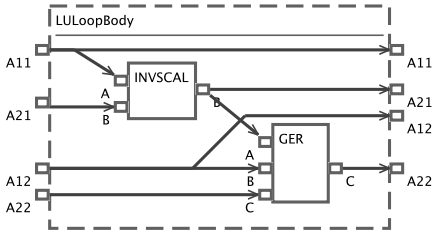


Figure 4.36: Optimized `LULoopBody` architecture.

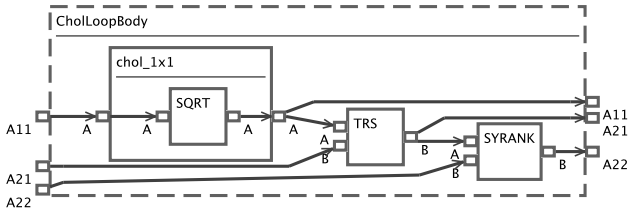


Figure 4.37: `CholLoopBody` after replacing `Chol` interface with algorithm `chol_1x1`.

value, as specified by algorithm `chol_1x1`. Applying this transformation allows us to obtain the architecture depicted in Figure 4.37.

We proceed with the `TRS` operation. Input `A` (`A11`) is a scalar, therefore `B` (`A21`) is scaled by `alpha` $\cdot$ `1/A`, with `alpha` = `1`. This allow us to use algorithm `trs_invscal` (previously depicted in Figure 4.30) to implement `TRS`. After using this algorithm, we obtain the architecture depicted in Figure 4.38b.

We then have the `SYRANK` operation. Input `A` is a vector, and input `B` is a matrix, therefore, we use interface `SYR` to perform the operation. The algorithm to be used is depicted in Figure 4.39. As for `mult_ger` (Figure 4.33), we also need interface `SCALP` to scale matrix `B` by `alpha`. After applying this algorithm, we obtain the architecture depicted in Figure 4.40b.

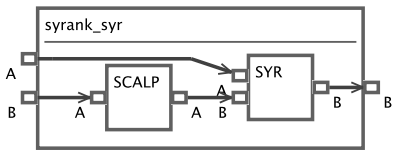
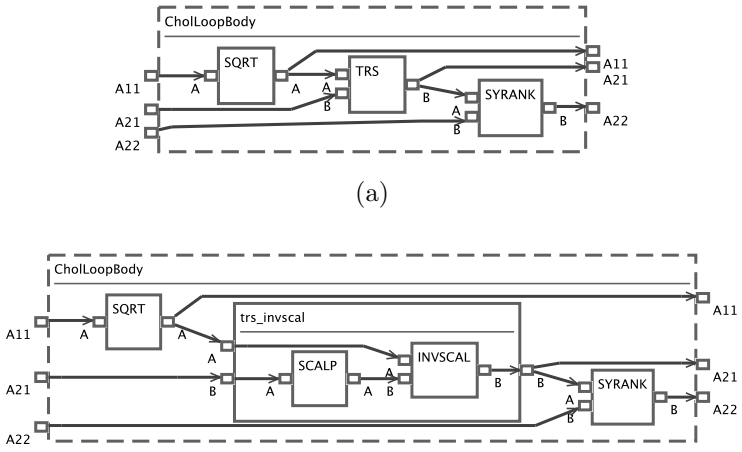


Figure 4.39: `syrank_syr` algorithm.

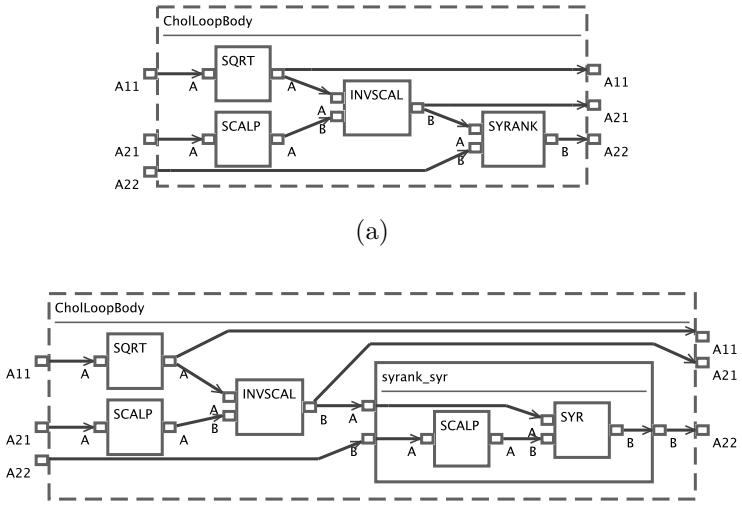
As the additional parameter `alpha` used by all `SCALP` interfaces has the value `1`, these interfaces can be implemented by the identity, resulting in the architecture depicted in Figure 4.41b. Figure 4.42 is the final optimized architecture.



(a)

(b)

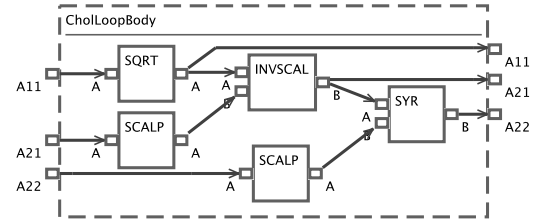
Figure 4.38: `CholLoopBody`: (a) previous architecture after flattening, and (b) after replacing `TRS` interface with algorithm `trs_invscal`.



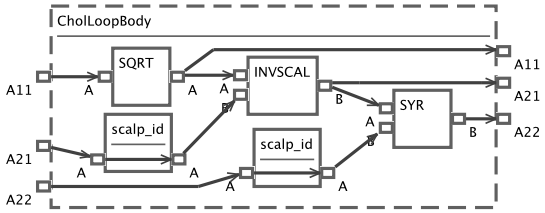
(a)

(b)

Figure 4.40: `CholLoopBody`: (a) previous architecture after flattening, and (b) after replacing `SYRANK` interface with algorithm `syrank_syr`.



(a)



(b)

Figure 4.41: `CholLoopBody`: (a) previous architecture after flattening, and (b) after replacing `SCALP` interfaces with algorithm `scalp_id`.

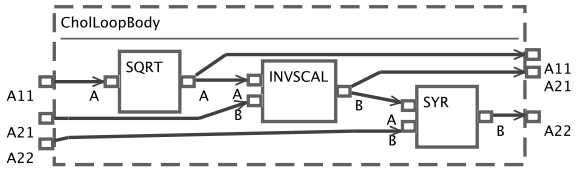


Figure 4.42: Optimized `CholLoopBody` architecture.

4.2.2.3 Preconditions

The derivation of the unblocked implementation of `LULoopBody` was obtained by refining the architecture with interface implementations specialized for the specified input sizes. Consider the rewrite rule (`LU`, `lu_1x1`) (Figure 4.43), which provides an implementation specialized for the case where input matrix `A` of `LU` has size `1x1`. In this case, `LU` operation is implemented by identity (no computation is needed at all). As we saw before, other interfaces have similar implementations, optimized for different input sizes.

The specialized implementations are specified by associating preconditions to rewrite rules, which check properties about the size of inputs. Moreover, postconditions are used to specify how operations affect data sizes. We now

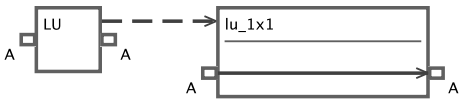


Figure 4.43: (`LU`, `lu_1x1`) rewrite rule.

describe how the pre- and postconditions needed for the derivation of unblocked implementations are specified.[2]

Specifying Postconditions. To specify the postconditions we use the following properties: `SizeM` is used to store the number of rows of a matrix, and `SizeN` is used to store the number of columns of a matrix. Each box uses these properties to specify the size of its outputs. In DLA domain, output size is usually obtained copying the size of one of its inputs. In Figure 4.44 we show the code we use to specify the postconditions for some of the boxes used, which is part of interpretation `sizes`. We define class `Identity11`, which specifies how size is propagated by interfaces with an input and an output named `A`, for which the input size is equal to the output size. Interpretations for boxes such as `LU` or `SCALP` can be defined simply extending this class. Similar Java classes are used to define the `sizes` interpretation for other boxes.

Specifying Preconditions. Preconditions for DLA operations are specified by checking whether the properties of inputs have the desired values. We also have some cases where the preconditions check the values of additional parameters. Figure 4.45 shows some of the preconditions used. Class `AScalar` specifies preconditions for checking whether input `A` is a scalar. It starts by reading the properties containing the input size information, and then it checks whether both sizes are equal to `1`. If not, `addError` method is used to signal a failure validating preconditions. The preconditions for algorithms such as `lu_1x1` or `trs_invscal` are specified simply extending this class. As we mentioned before, other algorithms have more preconditions, namely to require certain values for additional

[2]Later we show how these pre- and postconditions are extended when enriching the RDM to support additional hardware platforms.

```
public class Identity11 extends AbstractInterpretation {
  public void compute() {
    String sizeM = (String) getInputProperty("A", "SizeM");
    String sizeN = (String) getInputProperty("A", "SizeN");
    setOutputProperty("A", "SizeM", sizeM);
    setOutputProperty("A", "SizeN", sizeN);
  }
}

public class LU extends Identity11 {
  // Reuses compute definition from Identity11
}

public class SCALP extends Identity11 {
  // Reuses compute definition from Identity11
}
```

Figure 4.44: Java classes for interpretation `sizes`, which specifies DLA operations' postconditions.

parameters. It is the case of algorithm `trs_scal`, for example, which requires its additional parameter `diag` to have the value `UNIT`, to specify that the input `A` should be treated as a unit triangular matrix. Class `trs_scal` (Figure 4.45) shows how this requirement is specified. In addition to call the `compute` method from its superclass (`AScalar`) to verify whether input `A` is a scalar, it obtains the value of additional parameter `diag`, and checks whether it has the value `UNIT`. Similar Java classes are used to define the preconditions for other boxes.

4.2.3 Blocked Implementations

Most of current hardware architectures are much faster performing computations (namely floating point operations) than fetching data from memory. Therefore, to achieve high-performance in DLA operations, it is essential to make a wise use of CPU caches to compensate the memory access bottleneck [vdGQO08]. This is usually done through the use of blocked algorithms [vdGQO08], having blocks of data—where the number of operations is of higher order than the number of elements to fetch from memory (*e.g.*, cubic *vs.* quadratic)—processed together, which enables a more efficient use of memory by taking advantage of different levels of CPU caches.

In the following we show how loop bodies for blocked variants of programs

```
public class AScalar extends AbstractInterpretation {
  public void compute() {
    String sizeM = (String) getInputProperty("A", "SizeM");
    String sizeN = (String) getInputProperty("A", "SizeN");
    if(!"1".equals(sizeM) || !"1".equals(sizeN)) {
      addError("Input matrix A is not 1x1!");
    }
  }
}

public class lu_1x1 extends AScalar {
}

public class trs_invscal extends AScalar {
}

public class trs_scal extends AScalar {
  public void compute() {
    super.compute();
    String unit = (String) getAddParam("diag");
    if(!"UNIT".equals(unit)) {
      addError("Input matrix A is not unit triangular!");
    }
  }
}
```

Figure 4.45: Java classes for interpretation `presizes`, which specifies DLA operations' preconditions.

are derived from their PIMs. For this version, input `A11` is a square matrix of size `b` × `b` (the block size), inputs `A21` and `A12` are matrices of size `n` × `b` and `b` × `n`, and `A22` is a square matrix of size `n` × `n`. We refine the PIMs to produce implementations optimized for inputs with these characteristics.

4.2.3.1 Blocked Implementation of LU Factorization

We start the derivation by replacing `LU` interface with its general implementation, specified by algorithm `lu_blocked`. This algorithm simply uses `LU_B` interface, which specifies the LU factorization for matrices. This transformation results in the architecture depicted in Figure 4.46.

Next we replace both `TRS` interfaces with algorithm `trs_trsm`, which uses `TRSM` interface to perform the `TRS` operation. These transformations result in the architecture depicted in Figure 4.47b.

Finally, we replace the `MULT` interface with algorithm `mult_gemm`, which uses

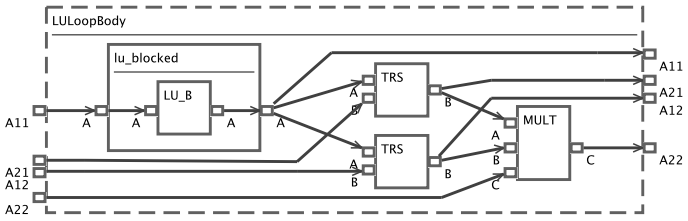
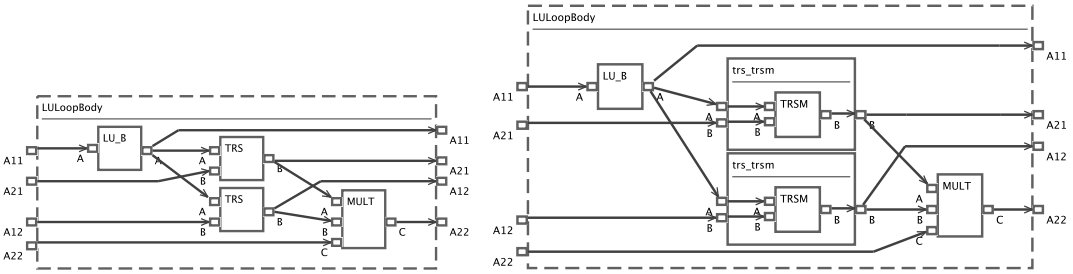
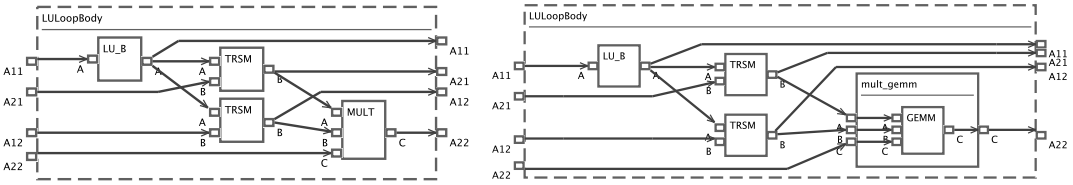


Figure 4.46: `LULoopBody` after replacing `LU` interface with algorithm `lu_blocked`.



(a) (b)

Figure 4.47: `LULoopBody`: (a) previous architecture after flattening, and (b) after replacing both `TRS` interfaces with algorithm `trs_trsm`.



(a) (b)

Figure 4.48: `LULoopBody`: (a) previous architecture after flattening, and (b) after replacing `MULT` interface with algorithm `mult_gemm`.

GEMM interface to perform the MULT operation. After applying this transformation we get the architecture depicted in Figure 4.48b. After flattening, we get the LULoopBody architecture for blocked inputs, depicted in Figure 4.49.

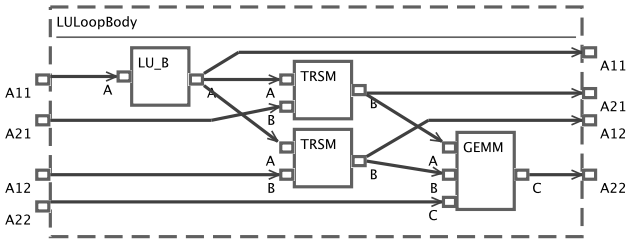


Figure 4.49: Optimized LULoopBody architecture.

4.2.3.2 Blocked Implementation of Cholesky Factorization

We start the derivation by refining CHOL interface with its general implementation, specified by algorithm chol_blocked. It uses CHOL_B interface, which specifies the Cholesky factorization for matrices, resulting in the architecture depicted in Figure 4.50.

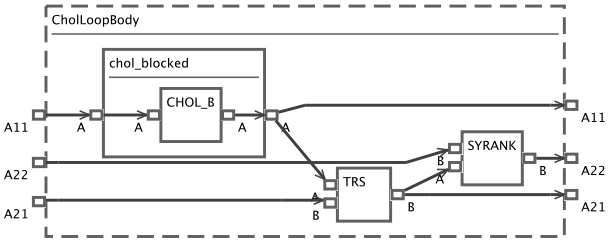
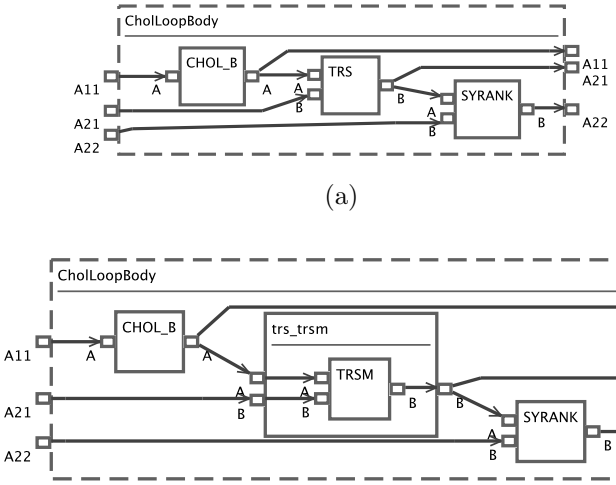


Figure 4.50: CholLoopBody after replacing CHOL interface with algorithm chol_blocked.

We then refine TRS interface with algorithm trs_trsm, which uses TRSM interface to perform the TRS operation. This transformation results in the architecture depicted in Figure 4.51b.

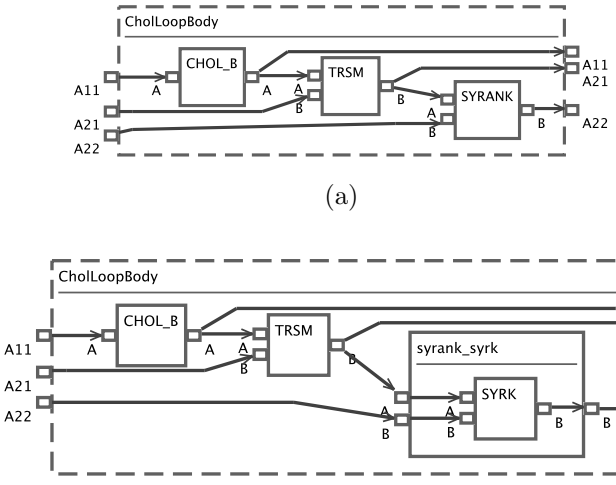
Finally, we refine the SYRANK interface with algorithm syrank_syrk, which uses SYRK interface to perform the operation. After applying this transformation we get the architecture depicted in Figure 4.52b, and after flattening it, we get the CholLoopBody architecture for blocked inputs, depicted in Figure 4.53.



(a)

(b)

Figure 4.51: `CholLoopBody`: (a) previous architecture after flattening, and (b) after replacing both `TRS` interfaces with algorithm `trs_trsm`.



(a)

(b)

Figure 4.52: `LULoopBody`: (a) previous architecture after flattening, and (b) after replacing `MULT` interface with algorithm `syrank_syrk`.

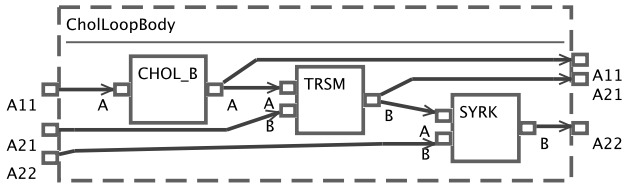


Figure 4.53: Final architecture: `CholLoopBody` after flattening `syrank_syrk` algorithms.

4.2.4 Distributed Memory Implementations

We now show how we can derive distributed memory implementations for DLA programs. We achieve this by adding new rewrite rules. We also add new interpretations to support additional pre- and postconditions required to express the knowledge needed to derive distributed memory implementations. For these derivations, we assume that the inputs are distributed using a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution (see Section 2.3.1.6), and that several instances of the program are running in parallel, each one having a different part of the input (*i.e.*, the program follows the SPMD model). We choose implementations (algorithms or primitives) for each operation prepared to deal with distributed inputs [PMH+13].

4.2.4.1 Distributed Memory Implementation of LU Factorization

The starting point for this derivation is again the PIM `LULoopBody` (see Figure 4.27), which represents the loop body of the program that is executed by each parallel instance of it.

We start the derivation with `LU` operation. We refine `LULoopBody` replacing `LU` interface with its implementation for distributed memory, algorithm `dist2local_lu` (Figure 4.54).

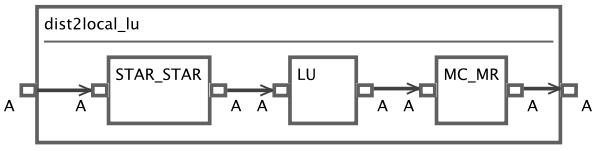


Figure 4.54: `dist2loca_lu` algorithm.

The algorithm implements the operation by first redistributing input `A`. That is, interface `STAR_STAR` represents a redistribution operation, which uses collective communications to obtain the same matrix in a different distribution

(in this case $[*,*]$, which gathers all values of the matrix in all processes).[3] We then call the LU operation on this "new" matrix, and we redistribute the result (interface MC_MR) to get a matrix with a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution so that the behavior of the original LU interface is preserved (it takes a $[\mathtt{M_C}, \mathtt{M_R}]$ matrix, and produces a $[\mathtt{M_C}, \mathtt{M_R}]$ matrix). By applying this transformation, we obtain the architecture from Figure 4.55. Notice that we have again the LU operation in the architecture. However, the input of LU is now a $[*,*]$ distributed matrix, which enables the use of other LU implementations (such as the blocked and unblocked implementations previously described).

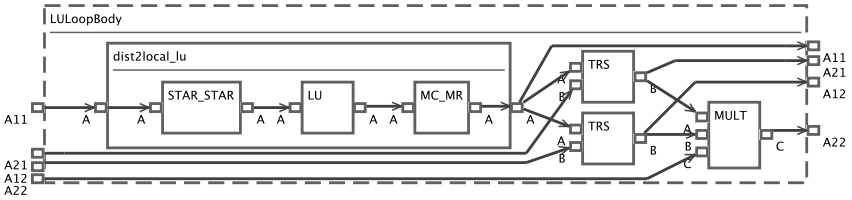


Figure 4.55: LULoopBody after replacing LU interface with algorithm dist2local_lu.

The architecture is then refined by replacing the TRS interface that processes input A21 with a distributed memory implementation. We use algorithm _dist2local_trs (Figure 4.56). The algorithm uses again STAR_STAR to gather all values from input A (initially using a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution). This is a templatized algorithm, where _redist box, which redistributes input matrix B (also initially using a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution), may be a STAR_MC, MC_STAR, STAR_MR, MR_START, STAR_VC, VC_STAR, STAR_VR, VR_STAR, or

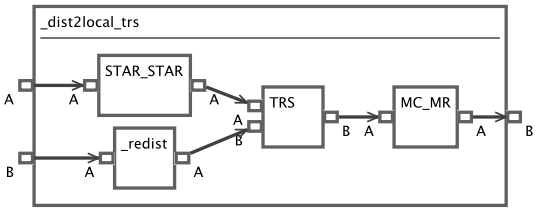


Figure 4.56: _dist2loca_trs algorithm.

[3] We use a_b ($\mathtt{a}, \mathtt{b} \in \{*, \mathtt{M_C}, \mathtt{M_R}, \mathtt{V_C}, \mathtt{V_R}\}$) to denote the redistribution operation that takes a matrix using any distribution, and converts it to a matrix using redistribution $[\mathtt{a}, \mathtt{b}]$. For example, MC_MR converts a matrix to a new one using a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution. By having a single redistribution operation for any input distribution (instead of one for each pair of input and output distributions), we reduce the number of redistribution operations we need to model (one per output distribution), and also the number of rewrite rules we need.

STAR_STAR redistribution. The algorithm has preconditions: STAR_∗ redistributions can only be used when the side additional parameter has value LEFT, and ∗_STAR redistributions can only be used when side has value RIGHT. In this case, side has value RIGHT, and we choose the variant dist2local_trs_r3, which uses MC_STAR redistribution. The redistributed matrices are then sent to TRS, and the output is redistributed by MC_MR back to a matrix using $[M_C, M_R]$ distribution. This transformation yields the architecture depicted in Figure 4.57b. As for the previous refinement, the transformation results in an architecture where the original box is present, but the inputs now use different distributions.

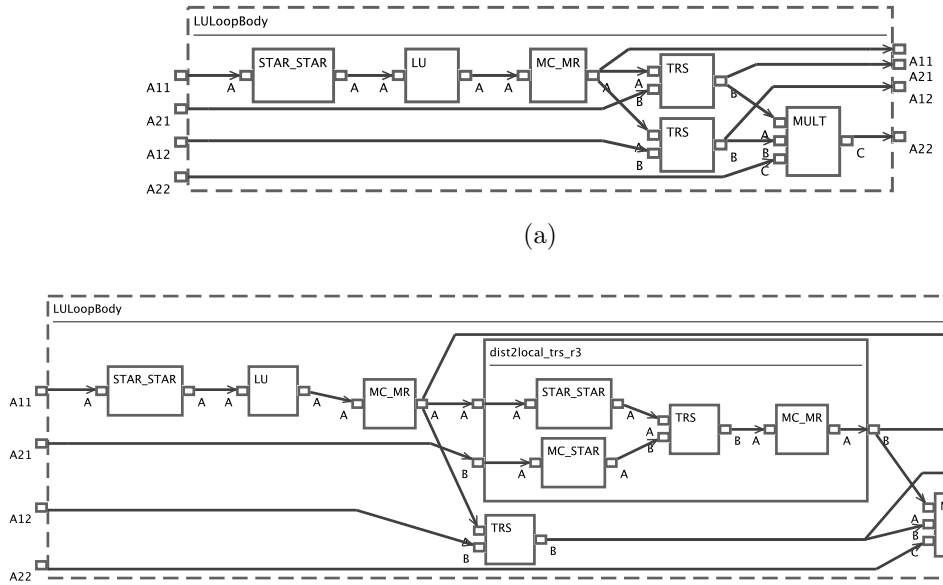
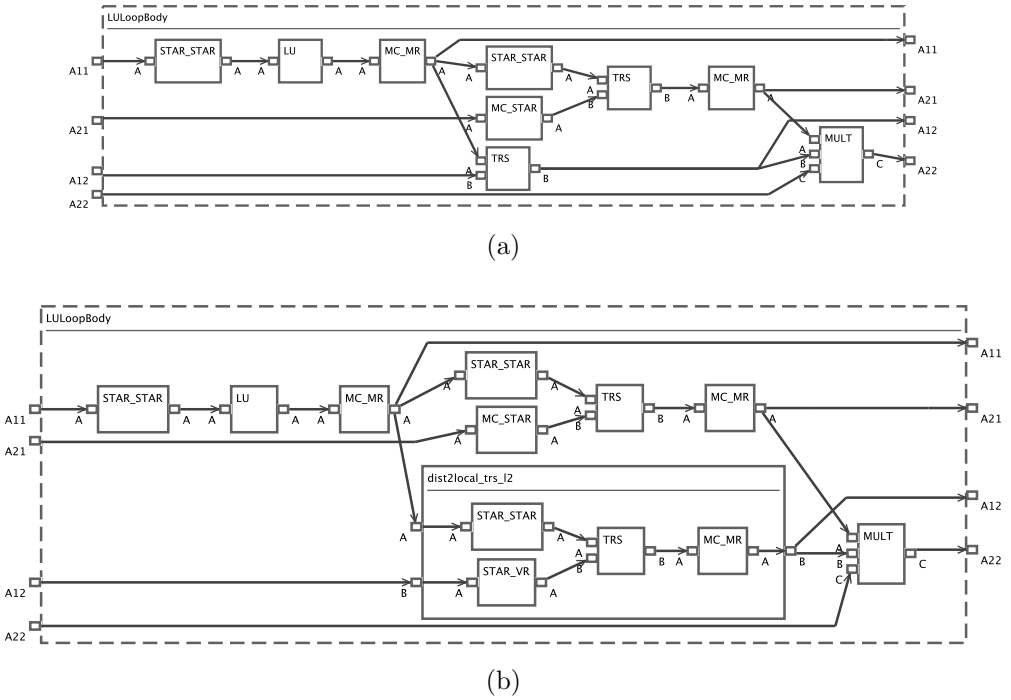


Figure 4.57: LULoopBody: (a) previous architecture after flattening, and (b) after replacing one TRS interface with algorithm dist2local_trs_r3.

Next we refine the architecture replacing the other TRS interface with a similar algorithm. This instance of TRS has the value LEFT for additional parameter side, therefore we use a different variant of the algorithm, dist2local_trs_l2, which uses STAR_VR redistribution. The resulting architecture is depicted in Figure 4.58b.

We now proceed with interface MULT. This operation can be implemented in distributed memory environments by algorithm _dist2local_mult (Figure 4.59).



(a)

(b)

Figure 4.58: `LULoopBody`: (a) previous architecture after flattening, and (b) after replacing `TRS` interface with algorithm `dist2local_trs_l2`.

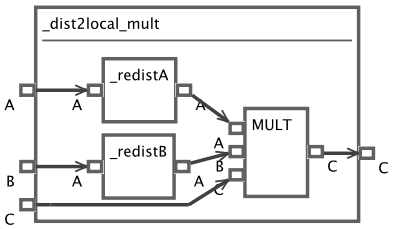
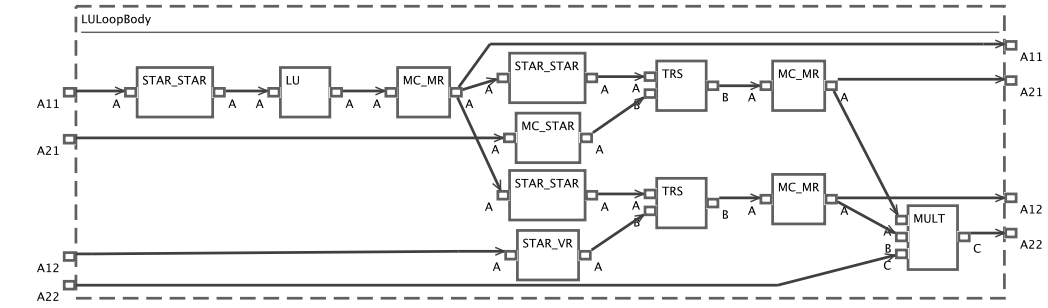
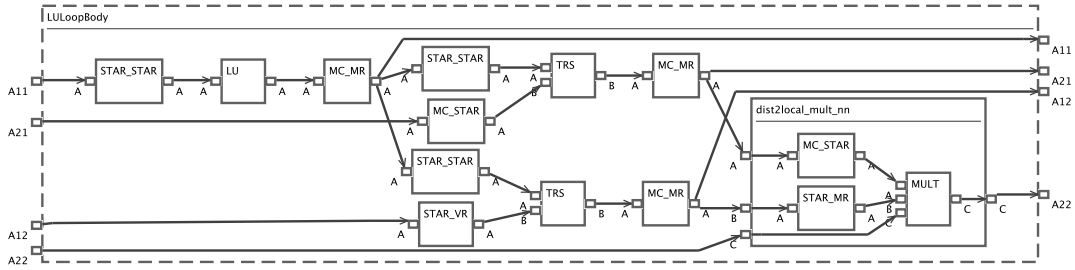


Figure 4.59: `_dist2local_mult` algorithm.

The algorithm is templatized: `_redistA` and `_redistB` can assume several values, which are connected (by preconditions) to the possible values of the additional parameters `transA` and `transB`. `_redistA` interface may be a `MC_STAR` or `STAR_MC` redistribution, depending on whether `transA` is `NORMAL` or `TRANS`, respectively. `_redistB` interface may be a `STAR_MR` or `MR_STAR` redistribution, depending on whether `transB` is `NORMAL` or `TRANS`, respectively. In `LULoopBody`, `MULT` has `transA` = `NORMAL` and `transB` = `NORMAL`, therefore the variant `dist2local_mult_nn` is used, yielding the architecture depicted in Figure 4.60b. Input `A` and `B` (initially using a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution) are redistributed before the `MULT` operation. As input `C` is not redistributed before the `MULT` operation, there is no need to redistribute the output of `MULT`, which always uses a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution in this algorithm.



(a)



(b)

Figure 4.60: `LULoopBody`: (a) previous architecture after flattening, and (b) after replacing `MULT` interface with algorithm `dist2local_mult_nn`.

We refined the architecture to expose the redistributions (communications) needed to perform the computation. That is, at this point, there are implementations for non-redistribution boxes (`LU`, `TRS`, and `MULT`) that do not require any communication. By exposing the redistributions needed by each interface present in the initial PIM, these refinements allow us to optimize the communications, by looking at the compositions of redistribution interfaces that resulted from removing the modular boundaries of the algorithms chosen.

The current `LULoopBody` is shown again, completely flattened, in Figure 4.61. We now show how communications exposed by previous refinements are optimized.

We start analysing the redistributions that follow the `LU` interface. The output of `LU` uses a $[*,*]$ distribution. After `LU`, its output matrix is redistributed to a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution. Before being used by `TRS` interfaces, this matrix is redistributed again to a $[*,*]$ distribution. An obvious

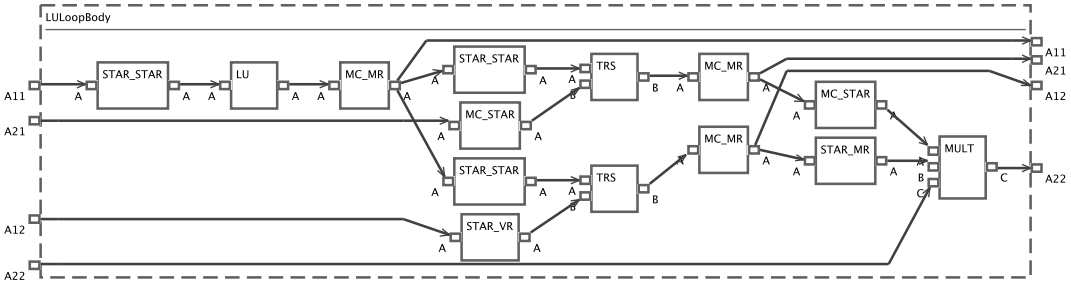


Figure 4.61: `LULoopBody` flattened after refinements.

optimization can be applied, which connects `LU` directly to the `TRS` interfaces, removing the (expensive) redistribution operation `STAR_STAR`. This optimization is expressed by the rewrite rules from Figure 4.62. The algorithm boxes have a precondition that requires the input to use a $[*, *]$ distribution. When this happens, if we redistribute the input to any distribution, and then we redistribute back to a $[*, *]$ distribution (pattern `_inv_ss0`), the `STAR_STAR` interface can be removed (algorithm `_inv_ss1`), as the output of `STAR_STAR` is equal to the original input. These rewrite rules are templatized, as the first redistribution (`_redist`) may be any redistribution interface.

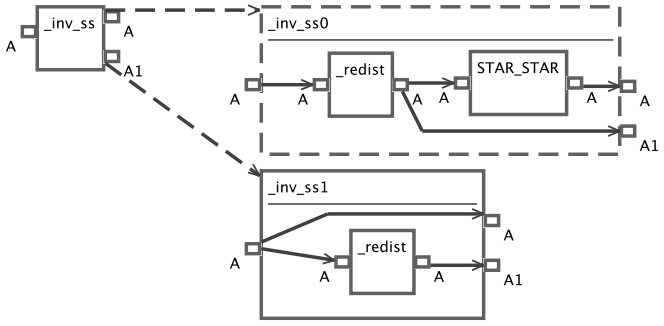


Figure 4.62: Optimization rewrite rules to remove unnecessary `STAR_STAR` redistribution.

By applying the optimization expressed by these rewrite rules twice, we remove both interior `STAR_STAR` redistributions, obtaining the architecture depicted in Figure 4.63.

A similar optimization can be used to optimize the composition of redistributions that follows `TRS` interface that updates `A21`. In this case, the output of `TRS` uses a $[\mathtt{M_C}, *]$ distribution, and it is redistributed to

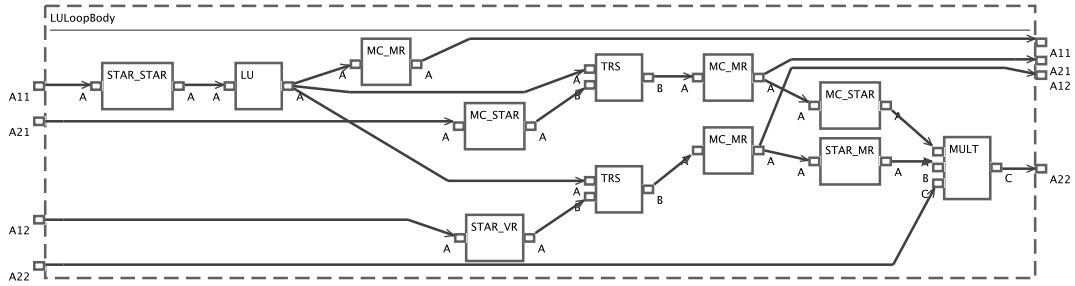


Figure 4.63: `LULoopBody` after applying optimization to remove `STAR_STAR` redistributions.

$[\mathtt{M_C}, \mathtt{M_R}]$, and then back to $[\mathtt{M_C}, *]$, before being used by `MULT`. The rewrite rules depicted in Figure 4.64 (similar to the one previously described in Figure 4.62) express this optimization. Its application yields the architecture depicted in Figure 4.65.

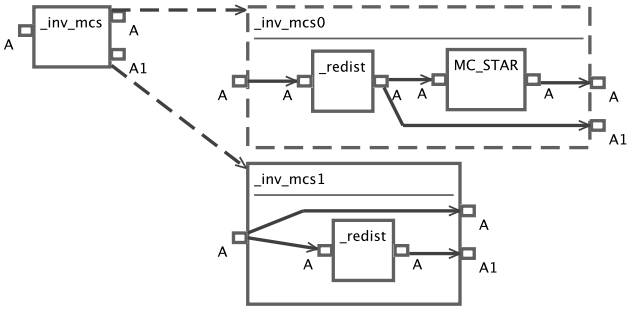


Figure 4.64: Optimization rewrite rules to remove unnecessary `MC_STAR` redistribution.

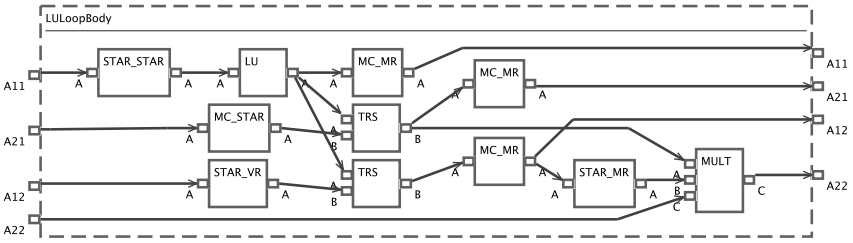


Figure 4.65: `LULoopBody` after applying optimization to remove `MC_STAR` redistributions.

Lastly, we analyse the interfaces that follow `TRS` interface updating matrix `A12`. The output matrix uses a $[*, \mathtt{V_R}]$ distribution, and redistributions `MC_MR` and `STAR_MR` are used to produce $[\mathtt{M_C}, \mathtt{M_R}]$ and $[*, \mathtt{M_R}]$ distributions of the matrix.

However, the same behavior can be obtained inverting the order of the redistributions, *i.e.*, starting by producing $[*, \mathtt{M_C}]$ matrix and then using that matrix to produce a $[\mathtt{M_C}, \mathtt{M_R}]$ distributed matrix. This alternative composition of redistributions is also more efficient, as we can obtain a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution from a $[*, \mathtt{M_C}]$ distribution simply discarding values (*i.e.*, without communication costs). This optimization is expressed by the rewrite rules from Figure 4.66, where two templatized rewrite rules express the ability to swap the order of two redistributions. In this case, `_redistA` is `MC_MR`, and `_redistB` is `STAR_MR`. After applying this transformation, we obtain the optimized architecture depicted in Figure 4.67.

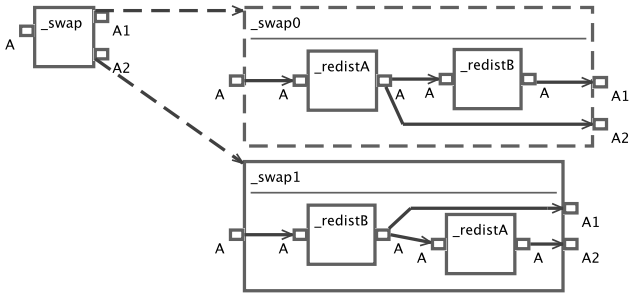


Figure 4.66: Optimization rewrite rules to swap the order of redistributions.

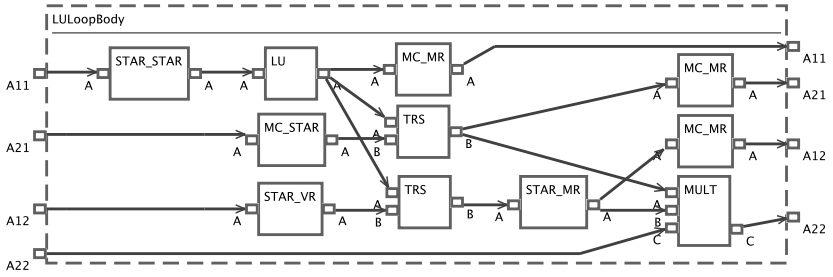


Figure 4.67: Optimized `LULoopBody` architecture.

4.2.4.2 Distributed Memory Implementation of Cholesky Factorization

To derive a distributed memory implementation for Cholesky factorization, we start with the `CholLoopBody` PIM (see Figure 4.28), which represents the loop body of the program that is executed by each parallel instance of it.

The first step of the derivation is to refine the architecture by replacing `CHOL` with an algorithm for distributed memory inputs. We use the `dist2local_chol` algorithm, depicted in Figure 4.68. This algorithm is similar to `dist2local_lu`. It implements the operation by first redistributing input `A` (that initially uses a $[\mathtt{M_C}, \mathtt{MR}]$ distribution), *i.e.*, interface `STAR_STAR` is used to obtain a $[*, *]$ distribution of the input matrix. Then `CHOL` operation is called on the redistributed matrix, and finally we redistribute the result (interface `MC_MR`) to get a matrix with a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution. By applying this transformation, we obtain the architecture depicted in Figure 4.69.

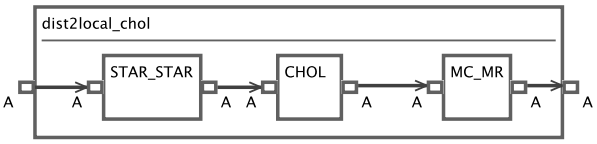


Figure 4.68: `dist2local_chol` algorithm.

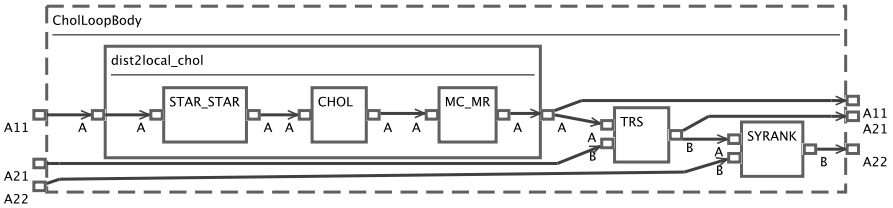
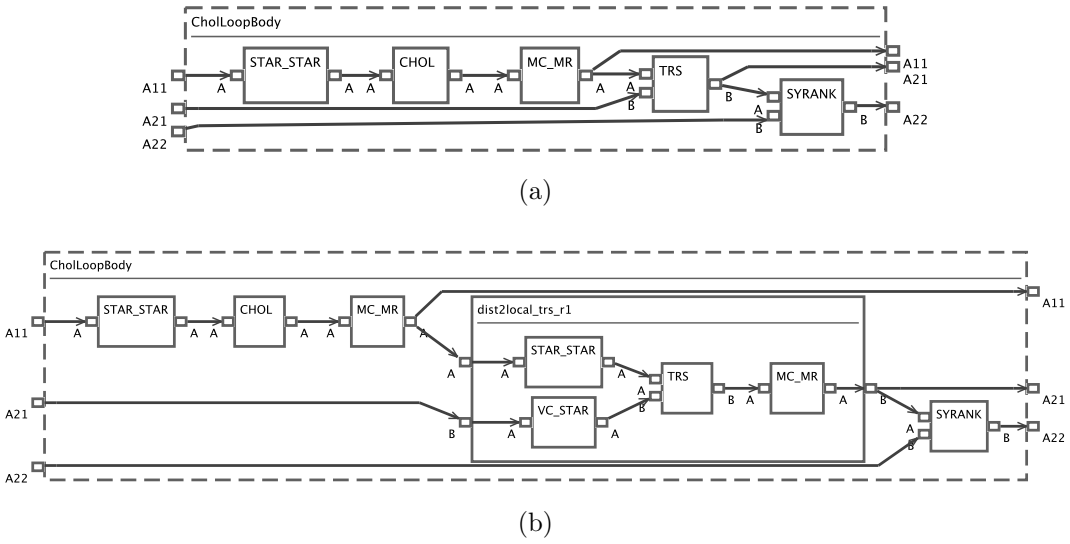


Figure 4.69: `CholLoopBody` after replacing `CHOL` interface with algorithm `dist2local_chol`.

The next step is to refine the architecture by replacing `TRS` interface with a distributed memory implementation. As for `LULoopBody`, we use `_dist2local_trs` templatized implementation (see Figure 4.56). However, in this case we choose algorithm `dist2local_trs_r1`, which uses `VC_STAR` to redistribute input `B`. This transformation yields the architecture depicted in Figure 4.70b.

We proceed with interface `SYRANK`. For this interface, we use algorithm `_dist2local_syrank` (Figure 4.71). This algorithm is templatized: `_redistA` and `_redistB` can assume several values, which are connected (by preconditions) to the possible values of the additional parameter `trans`.



(a)

(b)

Figure 4.70: `CholLoopBody`: (a) previous architecture after flattening, and (b) after replacing `TRS` interface with algorithm `dist2local_trs_r1`.

In this case `trans` = `NORMAL`, therefore variant `dist2local_syrank_n` is used, where `_redistA` is `MR_STAR` and `_redistB` is `MC_STAR`. As input `C` is not redistributed before the `TRRANK` operation, there is no need to redistribute the output of `TRRANK`, which already uses $[\mathtt{M_C}, \mathtt{M_R}]$ distribution. The transformation yields the architecture depicted in Figure 4.72b.

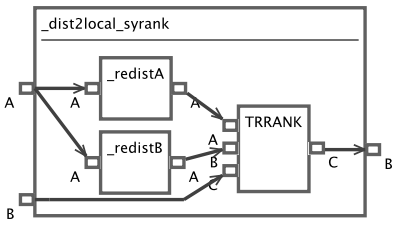


Figure 4.71: `_dist2local_syrank` algorithm.

We reached again the point where we exposed the redistributions needed so that each operation present in the initial PIM can be computed locally. The current `CholLoopBody` is shown again, completely flattened, in Figure 4.73. We proceed the derivation optimizing the compositions of redistributions introduced in the previous steps.

We start analysing the redistributions that follow the `CHOL` interface. It exposes the same inefficiency we saw after `LU` interface in `LULoopBody` (see Figure 4.61). The output of `CHOL` uses a $[*, *]$ distribution, and before the `TRS` interface, this matrix is redistributed to a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution and then back to

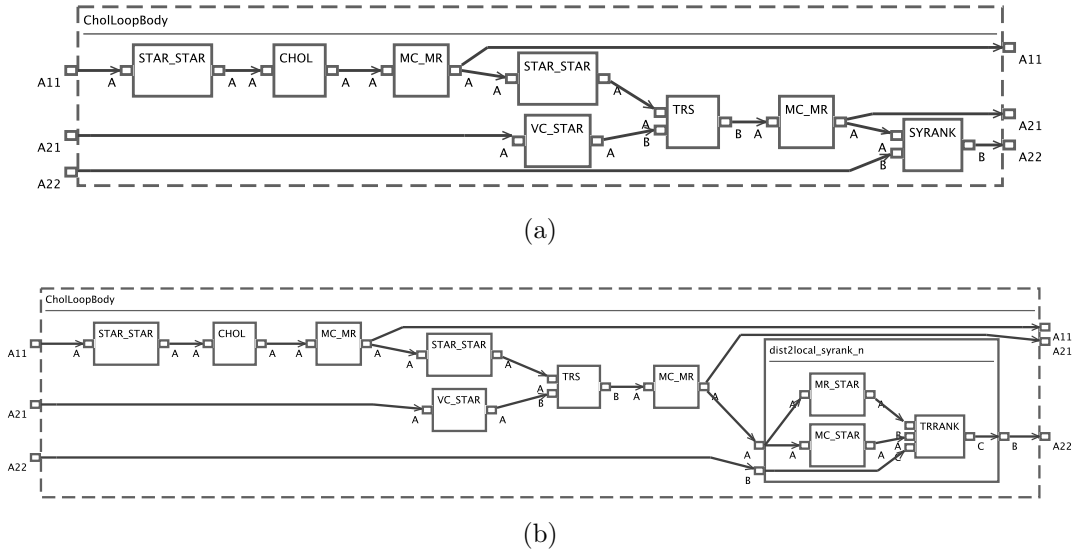


Figure 4.72: `CholLoopBody`: (a) previous architecture after flattening, and (b) after replacing `SYRANK` interface with algorithm `dist2local_syrank_n`.

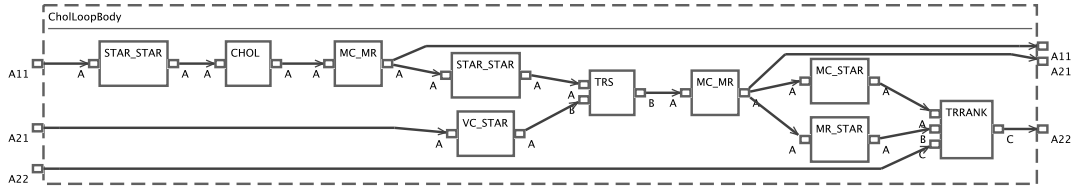


Figure 4.73: `CholLoopBody` flattened after refinements.

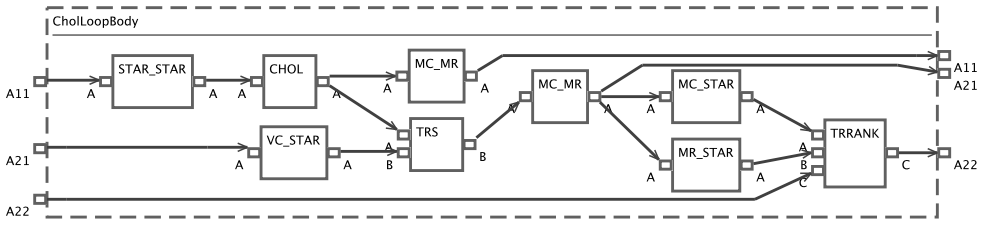


Figure 4.74: `CholLoopBody` after applying optimization to remove `STAR_STAR` redistribution.

a $[*, *]$ distribution. Thus, we can remove redistribution operation `STAR_STAR`, reusing the optimization expressed by the rewrite rules presented in Figure 4.62, which results in the architecture depicted in Figure 4.74.

The next step in the derivation is to refine the architecture expanding some of the redistributions as a composition of redistributions, in order to expose further optimization opportunities. We replace `MC_STAR` with its algorithm `vcs_mcs` (Figure 4.75), which starts by obtaining a $[\mathtt{V_C}, *]$ distribution of the matrix, and only then obtains the $[\mathtt{M_C}, *]$ distribution.

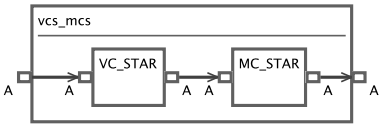


Figure 4.75: `vcs_mcs` algorithm.

We also replace `MR_STAR` with its algorithm `vcs_vrs_mrs` (Figure 4.76), which starts by obtaining a $[\mathtt{V_C}, *]$ distribution of the matrix, then obtains a $[\mathtt{V_R}, *]$ distribution, and finally obtains the $[\mathtt{M_R}, *]$ distribution. These refinements result in the architecture depicted in Figure 4.77.

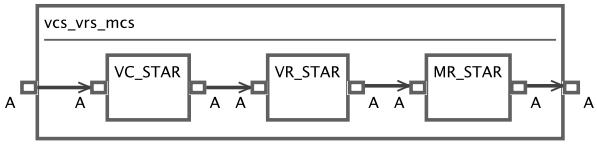


Figure 4.76: `vcs_vrs_mrs` algorithm.

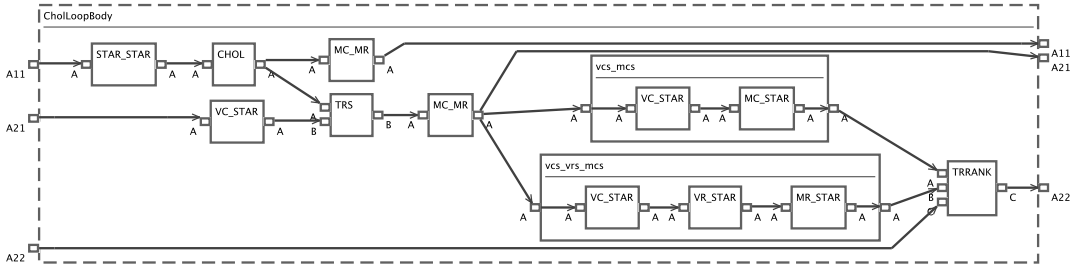


Figure 4.77: `CholLoopBody` after refinements that replaced `MC_STAR` and `MR_STAR` redistributions.

The previous refinements exposed the redistribution `VC_STAR` immediately after the `MC_MR` interface that redistributes the output of `TRS`. But the output of `TRS` is already a matrix using a $[\mathtt{V_C}, *]$ distribution, thus the `VC_STAR` redistributions can be removed. This is accomplished by applying an optimization modeled by similar rewrite rules to the previously presented in Figure 4.62 and Figure 4.64, which yields the architecture depicted in Figure 4.78.

There is one more redistribution optimization. From the output matrix of `TRS`, we are obtaining directly a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution (`MC_MR`) and a

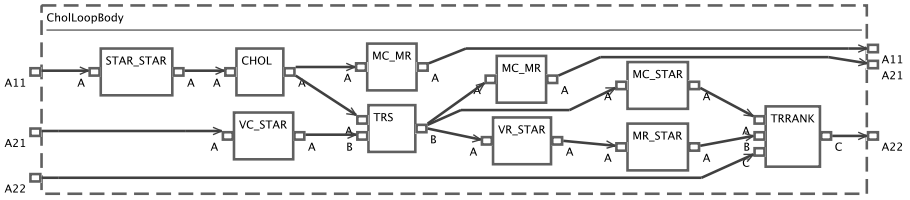


Figure 4.78: `CholLoopBody` after applying optimization to remove `VC_STAR` redistributions.

$[\mathtt{M_C}, *]$ distribution (`MC_STAR`). However, it is more efficient to obtain a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution from a $[\mathtt{M_C}, *]$ distribution than from a $[\mathtt{V_C}, *]$ distribution (used by the output matrix of `TRS`). The former does not require communication at all. The rewrite rules from Figure 4.79 model this optimization. After applying it, we obtain the architecture depicted in Figure 4.80, which finalizes our derivation.

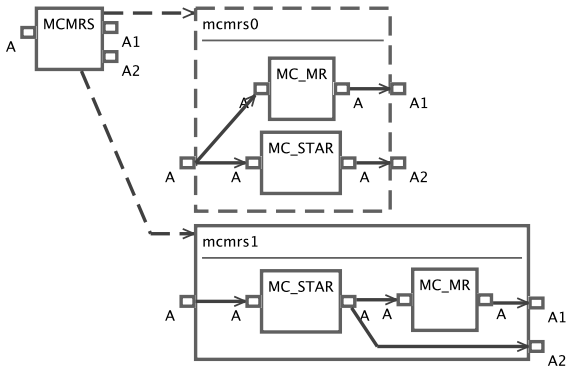


Figure 4.79: Optimization rewrite rules to obtain $[\mathtt{M_C}, \mathtt{M_R}]$ and $[\mathtt{M_C}, *]$ distributions of a matrix.

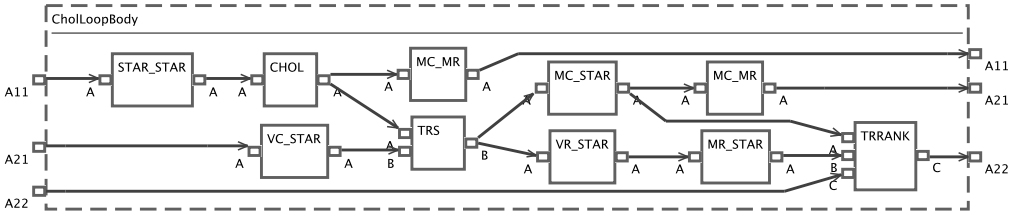


Figure 4.80: Optimized `CholLoopBody` architecture.

4.2.4.3 Preconditions

Previous preconditions for DLA boxes specified requirements of implementations specialized for certain inputs sizes. However, we assumed that all matrices were stored locally. In this section we introduced distributed matrices to allow us to

derive implementations optimized for distributed memory hardware platforms. This required the addition of new rewrite rules. It also requires a revision of pre- and postconditions, which now should also take into account the distribution of input matrices. Due to the ability to compose interpretations provided by `ReFlO`, this can be achieved without modifying the previously defined pre- and postconditions.

Specifying Postconditions. Besides the properties we already defined in interpretation `sizes` (and that we have to specify for the new boxes added to support distributed memory environments), we are going to define a new property (postcondition), called `Dist`, that we use to store the distribution of a matrix. This new postcondition is defined by a new interpretation, called `distributions`. For each interface and primitive, we have to specify how the distribution of its outputs is obtained. For redistribution interfaces, each one determines a specific output's distribution. For example, `STAR_STAR` produces a $[*,*]$ distributed matrix, and `MC_MR` produces a $[\mathtt{M_C},\mathtt{M_R}]$ distributed matrix. For the other boxes, output distribution is usually computed in a similar way to sizes, *i.e.*, it is obtained from the value of the distribution of one of its inputs. Figure 4.81 shows the code we use to specify the `distribution` interpretation for some of the boxes we used. As mentioned before, we also have to define the Java classes of `sizes` interpretation for the new boxes we added. The redistribution interfaces' output matrix size can be obtained from the size of its inputs. For example, for `STAR_STAR` and `MC_MR` it is equal to the input matrix size, thus the `sizes` interpretation for these boxes is defined simply extending the `Identity11` (see Figure 4.44), as shown in Figure 4.81.

Specifying Preconditions. As for postconditions, we are also going to define a new interpretation (`predists`) to specify the additional preconditions required when we allow distributed matrices. For example, algorithms `chol_blocked` or `chol_1x1` require the input matrix to use a $[*,*]$ distribution, or to be a local matrix. Other algorithms have more complex preconditions, where several input distributions are allowed, or where the valid redistributions depend on

```
public class STAR_STAR extends AbstractInterpretation {
  public void compute() {
    setOutputProperty("A", "Dist", "STAR_STAR");
  }
}

public class MC_MR extends AbstractInterpretation {
  public void compute() {
    setOutputProperty("A", "Dist", "MC_MR");
  }
}

public class Identity11 extends AbstractInterpretation {
  public void compute() {
    String dist = (String) getInputProperty("A", "Dist");
    setOutputProperty("A", "Dist", dist);
  }
}

public class LU extends Identity11 {
  // Reuses compute definition from Identity11
}

public class plu_b extends Identity11 {
}

public class SCALP extends Identity11 {
}
```

Figure 4.81: Java classes for interpretation `distributions`, which specifies DLA operations' postconditions regarding distributions.

```
public class STAR_STAR extends Identity11 {
}

public class MC_MR extends Identity11 {
}
```

Figure 4.82: Java classes of interpretation `sizes`, which specifies DLA operations' postconditions regarding matrix sizes for some of the new redistribution interfaces.

the values of additional parameters. For example, algorithm `trs_trsm` requires input matrix `A` to use $[*,*]$ distribution or to be a local matrix, but for input `B` it allows $[*,*]$, $[\mathtt{M_C},*]$, $[\mathtt{M_R},*]$, $[\mathtt{V_C},*]$ or $[\mathtt{V_R},*]$ distribution when additional parameter `side` has value `RIGHT`, or $[*,*]$, $[*,\mathtt{M_C}]$, $[*,\mathtt{M_R}]$, $[*,\mathtt{V_C}]$ or $[*,\mathtt{V_R}]$ distribution when additional parameter `side` has value `LEFT`. During the derivation we also mentioned that the templatized algorithms we presented have precondi-

```
public class chol_blocked extends AbstractInterpretation {
 public void compute() {
  String dist = (String) getInputProperty("A", "Dist");
  if(!"STAR_STAR".equals(dist) && !"LOCAL".equals(dist)) {
   addError("Input matrix A does not use [*,*] distribution nor it is local!");
  }
 }
}
public class chol_1x1 extends AbstractInterpretation {
 public void compute() {
  String dist = (String) getInputProperty("A", "Dist");
  if(!"STAR_STAR".equals(dist) && !"LOCAL".equals(dist)) {
   addError("Input matrix A does not use [*,*] distribution nor it is local!");
  }
 }
}
public class trs_trsm extends AbstractInterpretation {
 public void compute() {
  String distA = (String) getInputProperty("A", "Dist");
  String distB = (String) getInputProperty("B", "Dist");
  String side = (String) getAddParam("side");
  if(!"STAR_STAR".equals(dist) && !"LOCAL".equals(dist)) {
   addError("Input matrix A does not use [*,*] distribution nor it is local!");
  }
  if("RIGHT".equals(side)) {
   if(!"STAR_STAR".equals(distB)&&!"LOCAL".equals(dist)&&!"MC_STAR".equals(distB)&&
     !"MR_STAR".equals(distB)&&!"VC_STAR".equals(distB)&&!"VR_STAR".equals(distB)) {
    addError("Input matrix B does not use a valid distribution!");
   }
  }
  else if("LEFT".equals(side)) {
   if(!"STAR_STAR".equals(distB)&&!"LOCAL".equals(dist)&&!"STAR_MC".equals(distB)&&
     !"STAR_MR".equals(distB)&&!"STAR_VC".equals(distB)&&!"STAR_VR".equals(distB)) {
    addError("Input matrix B does not use a valid distribution!");
   }
  }
 }
}
public class dist2local_trs_r3 extends AbstractInterpretation {
 public void compute() {
  String distA = (String) getInputProperty("A", "Dist");
  String distB = (String) getInputProperty("B", "Dist");
  String side = (String) getAddParam("side");
  if(!"MC_MR".equals(distA)) {
   addError("Input matrix A does not use [Mc,Mr] distribution!");
  }
  if(!"MC_MR".equals(distB)) {
   addError("Input matrix B does not use [Mc,Mr] distribution!");
  }
  if(!"RIGHT".equals(side)) {addError("Additional parameter side is not 'RIGHT'!");}
 }
}
```

Figure 4.83: Java classes of interpretation `predists`, which specifies DLA operations' preconditions regarding distributions.

tions regarding the additional parameters. For example, the `dist2local_trs_r3` algorithm used during the derivation of `LULoopBody` can only be used when additional parameter `side` has value `RIGHT`. Moreover, the `dist2local_*` algorithms assume the input matrices use a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution. In Figure 4.83 we show the Java classes we use to specify these preconditions. By composing interpretations `predist` ∘ `presizes` ∘ `distributions` ∘ `sizes` we are able to evaluate the pre- and postconditions of architectures. This ability to compose interpretations was essential to allow us to add new preconditions to existing boxes without having to modify previously defined classes.

4.2.5 Other Interpretations

4.2.5.1 Cost Estimates

Cost estimates are obtained adding the costs of each box present in an architecture. As for databases, we build a string containing a symbolic expression. Constants denoting several runtime parameters, such as network latency cost (`alpha`), the network transmission cost (`beta`), the cost of a floating point operation (`gamma`), or the size of the grid of processors (`p`, `r`, `c`) are used to define the cost of each operation. The costs of the operations depends on the size of the data being processed. Thus, we reuse the `sizes` interpretation. Moreover, it also depends on the distribution of the input, and therefore `distributions` interpretation is also reused.

Figure 4.84 shows examples of cost expressions for `pchol_b` primitive, and for `STAR_STAR` interface and `pstar_star` primitive box, implemented by `costs` interpretation. For `pchol_b`, the cost is given by $\mathtt{1/3{*}size_M^3{*}gamma}$, where $\mathtt{size_M}$ is the number of rows (or the number of columns, as the matrix is square) of the input matrix. As `pchol_b` requires a `STAR_STAR` distributed matrix, or a local matrix, the cost does not depend on the input distribution. For `STAR_STAR`, the cost depends on the input distribution. In the case the input is using a $[\mathtt{M_C}, \mathtt{M_R}]$ distribution, the `STAR_STAR` redistribution requires an *AllGather* communication operation [CHPvdG07]. We use method `Util.costAllGather` to provide us the

cost expression of an *AllGather* operation for a matrix of size $\texttt{size}_{\texttt{M}} * \texttt{size}_{\texttt{N}}$, and using `p` processes. The cost of primitive `pstar_star` is the same of the interface it implements, therefore its Java class simply extends class `STAR_STAR`. The `costs` interpretation is backward, as the costs of an algorithm are computed from the costs of its internal boxes. Thus, the costs are progressively sent to their parent boxes, until they reach the outermost box, where the costs of all boxes are aggregated. (This is done in the last four lines of code of each `compute` method.) The $\mathcal{COSTS}$ interpretation is the result of the composition of interpretations `costs` ∘ `distributions` ∘ `sizes`.

```
public class pchol_b extends AbstractInterpretation {
  public void compute() {
    String sizeM = (String) getInputProperty("A", "SizeM");
    String cost = "1/3 * (" + sizeM + ")^3 * gamma";
    setBoxProperty("Cost", cost);
    String parentCost = (String) getParentProperty("Cost");
    if(parentCost == null) parentCost = cost;
    else parentCost = "(" + parentCost + ") + (" + cost + ")";
    setParentProperty("Cost", parentCost);
  }
}

public class STAR_STAR extends AbstractInterpretation {
  public void compute() {
    String sizeM = (String) getInputProperty("A", "SizeM");
    String sizeN = (String) getInputProperty("A", "SizeN");
    String dist = (String) getInputProperty("A", "Dist");
    String cost = "";
    if("MC_MR".equals(dist)) {
      cost = Util.costAllGather("(" + sizeM + ") * (" + sizeN + ")", "p");
    }
    else {
      // costs for other possible input distributions
    }
    setBoxProperty("Cost", cost);
    String parentCost = (String) getParentProperty("Cost");
    if(parentCost == null) parentCost = cost;
    else parentCost = "(" + parentCost + ") + (" + cost + ")";
    setParentProperty("Cost", parentCost);
  }
}

public class pstar_star extends STAR_STAR {
}
```

Figure 4.84: Java classes of interpretation `costs`, which specifies DLA operations' costs.

4.2.5.2 Code Generation

`ReFlO` generates code (in this case, C++ code for the Elemental library [PMH+13]) using interpretations. For this purpose, we rely on three different interpretations. Two of them are used to determine the names of variables used in the program loop body. The variable's name is determined by the architecture input variable name, and by the distribution. Thus, one of the interpretations used is `distributions` (that we also used to compute preconditions and costs). The other one propagates the names of variables, *i.e.*, it takes the name of a certain input variable and associates it to the output. We named this interpretation `names`, and some examples of Java classes used to specify this interpretation are shown in Figure 4.85.

```
public class Identity11 extends AbstractInterpretation {
  public void compute() {
    String name = (String) getInputProperty("A", "Name");
    setOutputProperty("A", "Name", name);
  }
}

public class Identity21 extends AbstractInterpretation {
  public void compute() {
    String name = (String) getInputProperty("B", "Name");
    setOutputProperty("B", "Name", name);
  }
}

public class plu_b extends Identity11 {
}

public class ptrsm extends Identity21 {
}

public class STAR_STAR extends Identity11 {
}
```

Figure 4.85: Java classes of interpretation `names`, which specifies DLA operations' propagation of variables' names.

Lastly, we have interpretation `code`, which takes the variable's names and distributions, and generates code for each primitive box. Figure 4.86 shows Java classes specifying how code is generated for `plu_b` (a primitive that implements `LU_B`), and `pstar_star` (a primitive that implements `STAR_STAR`). For `plu_b`, function `LU` is called with the input matrix (that is also the output matrix).

(Method `Util.nameDist` is used to generate the variable name, and to append a method call to it to obtain the local matrix, when necessary.) Code for other DLA operations is generated in a similar way. For `pstar_star`, we rely on = operator overload provided by Elemental, therefore the generated code is of the type < `inputname` >=< `outputname` >;.

```
public class plu_b extends AbstractInterpretation {
  public void compute() {
    String dist = (String) getInputProperty("A", "Dist");
    String name = (String) getInputProperty("A", "Name");
    String nameDist = Util.nameDist(name, dist, false);
    String pCode = (String) getParentProperty("Code");
    if(pCode==null) pCode="";
    pCode = "LU(" + nameDist + ");\n" + pCode;
    setParentProperty("Code", pCode);
  }
}

public class pstar_star extends AbstractInterpretation {
  public void compute() {
    String dist = (String) getInputProperty("A", "Dist");
    String name = (String) getInputProperty("A", "Name");
    String nameDist = Util.nameDist(name, dist, false);
    String pCode = (String) getParentProperty("Code");
    if(pCode==null) pCode="";
    pCode = name + "_STAR_STAR = " + nameDist";\n" + pCode;
    setParentProperty("Code", pCode);
  }
}
```

Figure 4.86: Java classes of interpretation `names`, which specifies DLA operations' propagation of variables' names.

The $\mathcal{M}2\mathcal{T}$ interpretation is therefore the result of the composition of interpretations `code` ∘ `names` ∘ `distributions`. It allows us to generate the code for an architecture representing the loop body of a program. An example of such code is depicted in Figure 4.87.

Recap. In this section we showed how we use `ReFlO` to explain the derivation of optimized DLA programs. We illustrated how optimized implementations for different hardware platforms (PSMs) can be obtained from the same initial abstract specification (PIM) of the program. Moreover, we showed how `ReFlO` allows domain experts to incrementally add support for new hardware platforms in an RDM. By encoding the domain knowledge, not only we can recreate (and

```
A11_STAR_STAR = A11;
LU(A11_STAR_STAR);
A11 = A11_STAR_STAR;
A21_MC_STAR = A21;
Trsm(RIGHT, UPPER, NORMAL, NON_UNIT, F(1), A11_STAR_STAR.LockedMatrix(),
        A21_MC_STAR.Matrix());
A21 = A21_MC_STAR;
A12_STAR_VR = A12;
Trsm(LEFT, LOWER, NORMAL, UNIT, F(1), A11_STAR_STAR.LockedMatrix(),
        A12_STAR_VR.Matrix());
A12_STAR_MR = A12_STAR_VR;
Gemm(NORMAL,NORMAL, F(-1), A21_MC_STAR.LockedMatrix(), A12_STAR_MR.LockedMatrix(),
        F(1), A22.Matrix());
A12 = A12_STAR_MR;
```

Figure 4.87: Code generated for the architecture of Figure 4.67 (after replacing interfaces with blocked implementations, and then with primitives).

explain) expert's created implementations, but also allow other developers to use expert knowledge when optimizing their programs. Further, `ReFlO` can export an RDM to C++ code that can be used by an external tool to automate the search for the best implementation (according to some cost function) for a certain program [MPBvdG12].

Chapter 5

Encoding Domains: Extension

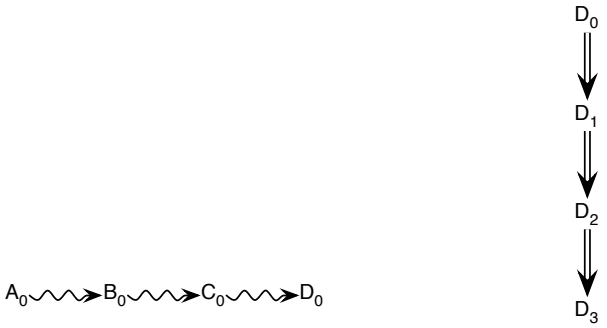
In Chapter 3 we explained how we encode knowledge to derive an optimized implementation from a high-level architecture (specification). Using refinements and optimizations, we incrementally transformed an initial architecture, preserving its behavior, until we reached another architecture with the desired properties regarding, for example, efficiency or availability.

The derivation process starts with an initial architecture (*i.e.*, abstract specification or PIM). This initial architecture could be complicated and not easily designable from scratch. A way around this is to "derive" this initial architecture from a simpler architecture that defined only part of the desired behavior. To this simpler architecture, new behavior is added until we get an architecture with desired behavior. Adding behavior is the process of *extension*; the behavior (or functionality) that is added is called a *feature*.

In its most basic form, an extension maps a box `A` without a functionality to a new box `B` that has this functionality *and* the functionality of `A`. Like refinements and optimizations, extensions are transformations. But unlike refinements and optimizations, extensions change (enhance) the behavior of boxes. We use $\texttt{A} \rightsquigarrow \texttt{B}$ to denote that box `B` extends box `A` or $\texttt{A} \rightsquigarrow \texttt{f.A}$, where `f.A` denotes `A` extended with feature `f`.

Extensions are not new. They can be found in classical approaches to software development [Spi89, Abr10]. Again, one starts with a simple specification $\texttt{A}_0$ and

progressively extends it to produce the desired specification, say $\mathtt{D}_0$. This process is $\mathtt{A}_0 \rightsquigarrow \mathtt{B}_0 \rightsquigarrow \mathtt{C}_0 \rightsquigarrow \mathtt{D}_0$ in Figure 5.1a. The final specification is then used as the starting point of the derivation, using refinements and optimizations, to produce the desired implementation $\mathtt{D}_4$. This derivation is $\mathtt{D}_0 \Rightarrow \mathtt{D}_1 \Rightarrow \mathtt{D}_2 \Rightarrow \mathtt{D}_3$ in Figure 5.1b. Alternative development paths can be explored to make this development process more practical [RGMB12].



(a) (b)

Figure 5.1: Extension *vs.* derivation.

There are rich relationships among extensions, rewrite rules, derivations, dataflow graphs, and *software product lines (SPLs)* [CN01]. This chapter is dedicated to the exploration of these relationships, to obtain a practical methodology to show how to extend dataflow graphs and rewrite rules, and an efficient way to encode this knowledge in the `ReFlO` framework/tool. We also explore the use of extensions to enable the derivation of product lines of program architectures, which naturally arise when extensions express optional features. We start by motivating examples of extensions.

5.1 Motivating Examples and Methodology

5.1.1 Web Server

Consider the `Server` dataflow architecture (PIM) in Figure 5.2 that besides projecting and sorting a stream of tuples (as in the `ProjectSort` architecture,

previously shown in Section 3.1), formats them to be displayed (box `WSERVER`), and outputs the formatted stream.

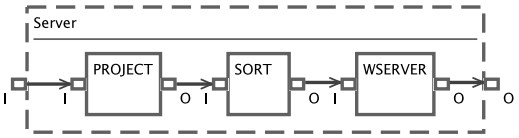


Figure 5.2: The `Server` architecture.

Suppose we want to add new functionality to the `Server` architecture. For example, suppose we want `Server` to be able to change the sort key attribute at runtime. How would this be accomplished? We would need to extend the original PIM with feature `key` (labeled `K`): `Server` $\rightsquigarrow$ `K.Server`, resulting in the PIM depicted in Figure 5.3.

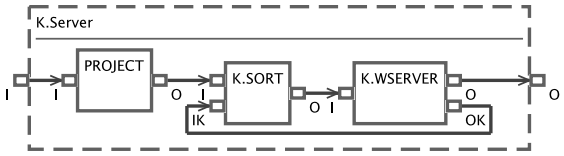


Figure 5.3: The architecture `K.Server`.

Methodology. This mapping is accomplished by a simple procedure. Think of `K` (or `key`) as a function that maps each element `e`—where an element is a box, port or connector—to an element `K.e`. Often `K.e` is an extension of `e`: a connector may carry more data, a box has a new port, or its ports may accept data conforming to an extended data type.[1] Sometimes, `K` deletes or removes element `e`. What exactly the outcome should be is known to an expert—it is not always evident to non-experts. For our `Server` example, the effect of extensions are not difficult to determine.

The first step of this procedure is to perform the `K` mapping. Figure 5.4 shows that the only elements that are changed by `K` are the `SORT` and `WSERVER` boxes. Box `K.SORT`, which `k`-extends `SORT`,

[1]In object oriented parlance, `E` is an extension of `C` iff `E` is a subclass of `C`.

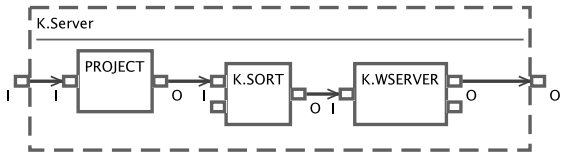


Figure 5.4: Applying `K` to `Server`.

has sprouted a new input (to specify the sort key parameter), and `K.WSERVER` has sprouted a new output (that specifies a sort key parameter). The resulting architecture (Figure 5.4) is called *provisional*—it is not yet complete.

The last step is to complete the provisional architecture: the new input of `K.SORT` needs to be provided by a connector, and an expert knows that this can be achieved by connecting the new output of `K.WSERVER` to the new input of `K.SORT`. This yields Figure 5.3, and the `Server` $\rightsquigarrow$ `K.Server` mapping is complete.

Now suppose we want `K.Server` to change the list of attributes that are projected at runtime. We would accomplish this with another extension: `K.Server` $\rightsquigarrow$ `L.K.Server` (`L` denotes feature `list`). This extension would result in the PIM depicted in Figure 5.5.

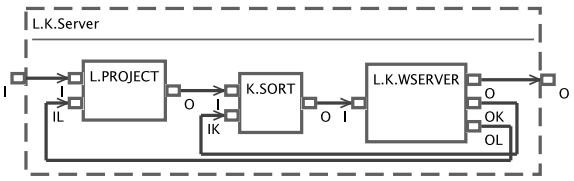


Figure 5.5: The architecture `L.K.Server`.

Methodology. The same methodology is applied as before. `L` maps each element `e` $\in$ `K.Server` to `L.e`. The `L` mapping is similar to that of `K`: box `L.PROJECT` sprouts a new input port (to specify the list of attributes to project) and `L.K.WSERVER` sprouts a new output port (to provide that list of attributes). This results in the provisional architecture of Figure 5.6.

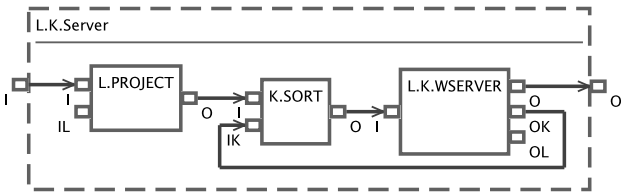


Figure 5.6: Applying `L` to `K.Server`.

> The next step is, again, to complete Figure 5.6. The new input of `L.Project` needs to be provided by a connector, and an expert knows that the source of the connector is the new output of `L.K.Server`. This yields Figure 5.5, which completes the `K.Server` $\rightsquigarrow$ `L.K.Server`.

Considering the two features just presented, we have defined three PIMs: `Server`, `K.Server`, and `L.K.Server`. Another PIM could also be defined, taking our initial `Server` architecture, and extending it with just the `list` feature.

Figure 5.7 depicts the different PIMs we can build. Starting from `Server`, we can either extend it with feature `key` (obtaining `K.Server`) or with feature `list` (obtaining `L.Server`). Taking any of these new PIMs, we can add the remaining feature (obtaining `L.K.Server`). That is, we have a tiny product line of `Server`s, where `Server` is the base product, and `key` and `list` are optional features.

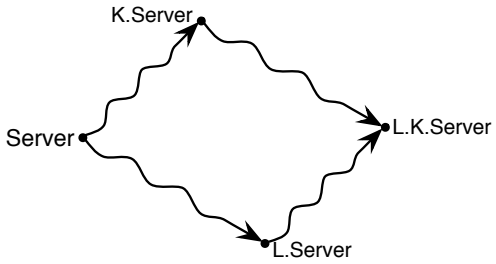


Figure 5.7: A `Server` Product Line.

Henceforth, we assume the order in which features are composed is irrelevant: `L.K.Server` = `K.L.Server`, *i.e.*, both mean `Server` is extended with features `list` and `key`. This is a standard assumption in the SPL literature, where a product is identified by its set of features. Of course, dependencies among features can exist, where one feature requires (or disallows) another [ABKS13, Bat05]. This

is not the case for our example; nevertheless, the approach we propose does not preclude such constraints.

PIMs are abstract specifications that are used as the starting point for the derivation of optimized program implementations. We can use the rewrite rules presented in Section 3.1 to produce an optimized implementation (PSM) for the `Server` PIM. Similar derivations can be produced for each of the extended PIMs. The question we may pose now is: what is the relationship among the derivations (and the rewrite rules they use) of the different PIMs obtained through extension?

5.1.2 Extension of Rewrite Rules and Derivations

Taking the original `Server` PIM, we can use the rewrite rules presented in Section 3.1 and produce an optimized parallel implementation for it. We start by using algorithm `parallel_sort` (we denote it by $\mathtt{t}_1$) and `parallel_project` (we denote it by $\mathtt{t}_2$) to refine the architecture. Then, we use `ms_mergesplit` ($\mathtt{t}_3$) and `ms_identity` ($\mathtt{t}_4$) algorithms to optimize the architecture. That is, we have the derivation $\mathtt{Server}_0 \overset{\mathtt{t}_0}{\Rightarrow} \mathtt{Server}_1 \overset{\mathtt{t}_1}{\Rightarrow} \mathtt{Server}_2 \overset{\mathtt{t}_3}{\Rightarrow} \mathtt{Server}_3 \overset{\mathtt{t}_4}{\Rightarrow} \mathtt{Server}_4$ (the `Server` indexes denote the different stages of the derivation, where $\mathtt{Server}_0$ is the PIM, and $\mathtt{Server}_4$ is the PSM). This derivation results in the PSM depicted in Figure 5.8.

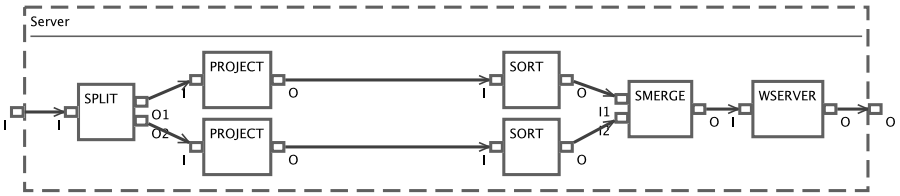


Figure 5.8: The optimized `Server` architecture.

We showed in the previous section how to extend the `Server` PIM to support additional features. However, we also want to obtain the extended PSMs for these PIMs. To extend the PIM, we extended the interfaces it used. Therefore, to proceed with the PSM derivation of the extended PIMs, we have to do the same with the implementations of these interfaces. Effectively, this means we are

extending the rule set $\{\mathtt{t}_1, \mathtt{t}_2, \mathtt{t}_3, \mathtt{t}_4\}$. Figure 5.9 shows $(\mathtt{SORT}, \mathtt{parallel\_sort}) \rightsquigarrow (\mathtt{K.SORT}, \mathtt{K.parallel\_sort})$, *i.e.*, how the rewrite rule $(\mathtt{SORT}, \mathtt{parallel\_sort})$ (or $\mathtt{t}_1$) is extended to support the `key` feature.

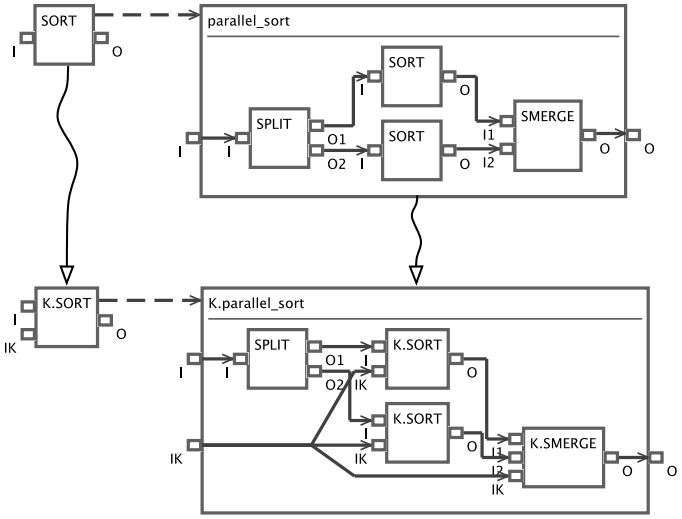


Figure 5.9: Extending the $(\mathtt{SORT}, \mathtt{parallel\_sort})$ rewrite rule.

> **Methodology**. Extending rules is no different than extending architectures. To spell it out, a rewrite rule $(\mathtt{L}, \mathtt{R})$ has an LHS box `L` and an RHS box `R`. If `K` is the feature/extension to be applied, `L` is mapped to a provisional `K.L`, and `R` is mapped to a provisional `K.R`. These provisional architectures are then completed (by an expert) yielding the non-provisional `K.L` and `K.R`. From this, rule extension follows: $(\mathtt{L}, \mathtt{R}) \rightsquigarrow (\mathtt{K.L}, \mathtt{K.R})$.

The rewrite rule $(\mathtt{PROJECT}, \mathtt{parallel\_project})$ can be extended in a similar way to support the `list` feature. We also have the extension of $(\mathtt{SORT}, \mathtt{parallel\_sort})$ by the `list` feature, and the extension of $(\mathtt{PROJECT}, \mathtt{parallel\_project})$ by the `key` feature. Both extensions are identity mappings, *i.e.*:

$$(\mathtt{SORT}, \mathtt{parallel\_sort}) = (\mathtt{L.SORT}, \mathtt{L.parallel\_sort})$$

$$(\mathtt{PROJECT}, \mathtt{parallel\_project}) = (\mathtt{K.PROJECT}, \mathtt{K.parallel\_project})$$

The same happens with the optimization rewrite rules, because they are not affected by these extensions. Moreover,

$$(\texttt{K.SORT}, \texttt{K.parallel\_sort}) \rightsquigarrow (\texttt{L.K.SORT}, \texttt{L.K.parallel\_sort})$$

$$(\texttt{L.PROJECT}, \texttt{L.parallel\_project}) \rightsquigarrow (\texttt{L.K.PROJECT}, \texttt{L.K.parallel\_project})$$

are also identity mappings.

With these extended rewrite rules, we can now obtain derivations:

- $\texttt{K.Server}_0 \overset{\texttt{K.t}_0}{\Longrightarrow} \texttt{K.Server}_1 \overset{\texttt{K.t}_1}{\Longrightarrow} \texttt{K.Server}_2 \overset{\texttt{K.t}_3}{\Longrightarrow} \texttt{K.Server}_3 \overset{\texttt{K.t}_4}{\Longrightarrow} \texttt{K.Server}_4$,
- $\texttt{L.Server}_0 \overset{\texttt{L.t}_0}{\Longrightarrow} \texttt{L.Server}_1 \overset{\texttt{L.t}_1}{\Longrightarrow} \texttt{L.Server}_2 \overset{\texttt{L.t}_3}{\Longrightarrow} \texttt{L.Server}_3 \overset{\texttt{L.t}_4}{\Longrightarrow} \texttt{L.Server}_4$, and
- $\texttt{L.K.Server}_0 \overset{\texttt{L.K.t}_0}{\Longrightarrow} \texttt{L.K.Server}_1 \overset{\texttt{L.K.t}_1}{\Longrightarrow} \texttt{L.K.Server}_2 \overset{\texttt{L.K.t}_3}{\Longrightarrow} \texttt{L.K.Server}_3 \overset{\texttt{L.K.t}_4}{\Longrightarrow} \texttt{L.K.Server}_4$

which produce the PSMs for the different combinations of features.

Considering that rewrite rules express transformations, and that extensions are also transformations, extensions of rewrite rules are higher-order transformations, *i.e.*, transformations of transformations.

5.1.2.1 Bringing It All Together

We started by extending our `Server` PIM, which lead to a small product line of servers (Figure 5.7). We showed how the rewrite rules used in the derivation of the original PIM can be extended. Those rewrite rules were then used to obtain the derivations for the different PIMs, and allowed us to obtain their optimized implementations. That is, by specifying the different extensions mappings (for PIMs, interfaces, implementations), we can obtain the extended derivations (and the extended PSMs), as show in Figure 5.10a. Our methodology allows us to relate extended PSMs in the same way as their PIMs (Figure 5.10b).

Admittedly, `Server` is a simple example. In more complex architectures, obtaining extended derivations may require additional transformations (not just the

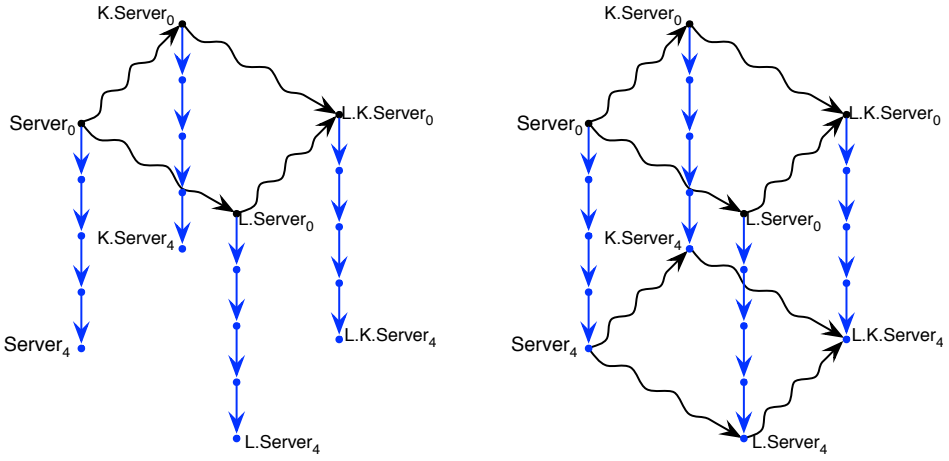


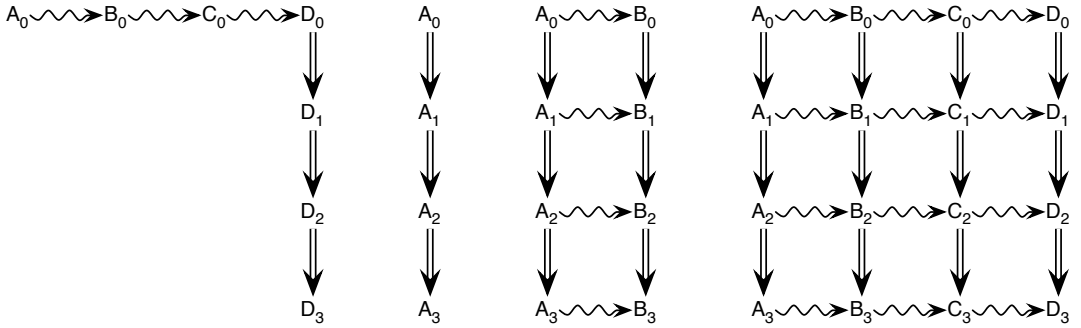
Figure 5.10: Extending derivations and PSMs.

extended counterparts of previous transformations), or previously-used transformations to be dropped. Such changes we cannot automate—they would have to be specified by a domain-expert. Nevertheless, a considerable amount of tool support can be provided to users and domain-experts in program derivation, precisely because the basic pattern of extension that we use is straightforward.

5.1.3 Consequences

We now discuss something fundamental to this approach. When we extend the rewrite rules and add extra functionality, we make models slightly more complex. Extended rewrite rules are used to produce extended PSMs. *We have observed that slightly more complex rewrite rules typically result in significantly more complex PSMs.*

To appreciate the (historical) significance of this, recall that a tenet of classical software design is to start with a simple specification (architecture) $\mathtt{A}_0$ and progressively extend it to the desired (and much more complex spec) $\mathtt{D}_0$. At this time, refinements and optimizations are applied to derive the implementation $\mathtt{D}_3$ of $\mathtt{D}_0$ (Figure 5.11a). This additional complexity added by successive extensions often makes it impractical to discover the refinements and optimizations required to obtain to final implementation [RGMB12].



(a) (b) (c) (d)

Figure 5.11: Derivation paths.

This lead us to explore an alternative, more incremental approach, based on extensions. Instead of starting by extending the specification, we start by obtaining an implementation for the initial specification. That is, considering the initial specification $\mathtt{A}_0$, we build its derivation $\mathtt{A}_0 \Rightarrow \mathtt{A}_1 \Rightarrow \mathtt{A}_2 \Rightarrow \mathtt{A}_3$, to obtain implementation $\mathtt{A}_3$ (Figure 5.11b). Next, we extend the specification, producing a new one ($\mathtt{B}_0$), closer to the desired specification, from which we produce a new derivation $\mathtt{B}_0 \Rightarrow \mathtt{B}_1 \Rightarrow \mathtt{B}_2 \Rightarrow \mathtt{B}_3$ (Figure 5.11c). We repeat the process until we get to the final (complete) specification $\mathtt{D}_0$, from which we build the derivation that produces the desired implementation $\mathtt{D}_3$ (Figure 5.11d).

This alternative approach makes a derivation process more incremental [RGMB12]. It allows us to start with a simpler derivation, which uses refinements and optimizations easier to understand and explain. Then, each new derivation is typically obtained with rewrite rules similar to the ones used in the previous derivation. By leveraging the relationships among the different derivations, and among the rewrite rules required for each derivation, we can improve the development process, providing tool support to capture additional knowledge, and making it easier to understand and explain. (Chapter 7 is devoted to an analysis of the complexity of commuting diagrams like Figure 5.11d.)

The need to support extensions first appeared when reverse engineering UpRight [CKL+09]. Extensions allowed us to conduct the process incrementally, by starting with a simple PIM to PSM derivation, which was progressively en-

hanced until we got a derivation that produced the desired PSM [RGMB12]. Later, when analyzing other case studies, we realized that the ability to model feature-enhanced rewrite rules was useful even to just produce different PSMs (that only differs in non-functional properties) for the same PIM. This happens as we add features to boxes that are not visible externally (*i.e.*, when looking to the entire architecture, no change on functional properties is noticed).

Road Map. In the remainder of this chapter, we outline the key ideas needed to encode extension relationships. We explain how we capture the extension relationships in RDMs (so that they effectively express product lines of RDMs), and how we can leverage from the extension relationships and the methodology proposed to provide tools support to help developers to derive product lines of PSMs.

5.2 Implementation Concepts

5.2.1 Annotative Implementations of Extensions

There are many ways to encode extensions. At the core of `ReFlO` is its ability to store rewrite rules. For each rule, we want to maintain a (small) product line of rules, containing a base rule and each of its extensions. For a reasonable number of features, a simple way to encode all these rules is to form the union of their elements, and annotate each element to specify when that element is to appear in a rule for a given set of features.

We follow Czarnecki's *annotative approach* [CA05] to encode product lines. With appropriate annotations we can express the elements that are added/removed by extensions, so that we can "project" the version of a rule (and even make it disappear if no "projection" remains) for a given set of features. So in effect, we are using an annotative approach to encode extensions and product lines of RDMs, and this allows us to project an RDM providing a specific set of features.

Model elements are annotated with two attributes: a feature predicate and a feature tags set. The *feature predicate* determine when boxes, ports, or connectors are part of an RDM for a given set of features. The *feature tags set* is used to determine how boxes are tagged/labeled (*e.g.*, `K` is a tag for feature `key`).

> **Methodology.** A user starts by encoding an initial RDM $\mathcal{R}$ that allows him to derive the desired PSM from a given PIM. Then, for each feature $\mathtt{f} \in \mathcal{F}$, the user considers each $\mathtt{r} \in \mathcal{R}$, adds the needed model elements (boxes, ports, connectors), and annotates them to express the `f`-extension of `r`. Doing so specifies how each rewrite rule `r` evolves as each feature `f` is added to it. This results in a product line of rewrite rules centered on the initial rule `r` and its extensions. Doing this for all rules $\mathtt{r} \in \mathcal{R}$ creates a product line of RDMs.
>
> Of course, there can be $2^{\mathtt{n}}$ distinct combinations of `n` optional features. Usually, when an `f`-extension is added, the user can take into account all combinations of `f` with previous features. The rule bases are not always complete though. Occasionally, the user may later realise he needs additional rules for a certain combination of features.

5.2.2 Encoding Product Lines of RDMs

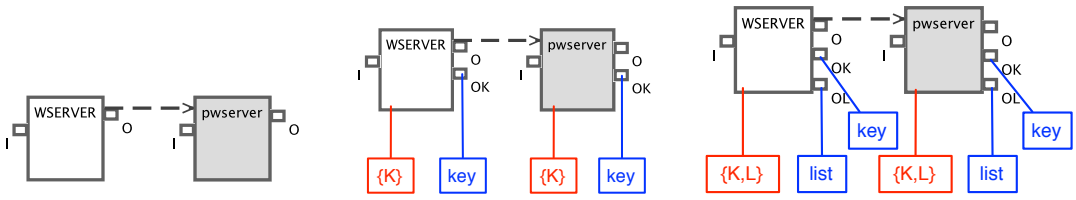
All RDMs of a product line are superimposed into a single artifact, which we call an *eXtended `ReFlO` Domain Model (XRDM)*. The structure of an XRDM is described by the same UML class diagram metamodel previously shown (Figure 3.6). However, some objects of the XRDM have additional attributes described below.

Boxes, ports, and connectors receive a new `featuresPredicate` attribute. Given a subset of features $\mathcal{S} \subseteq \mathcal{F}$, and a model element with predicate $\mathtt{P} : \mathcal{P}(\mathcal{F}) \rightarrow \{\mathtt{true}, \mathtt{false}\}$ (where $\mathcal{P}$ denotes the power set), $\mathtt{P}(\mathcal{S})$ is true if and only if the element is part of the RDM when $\mathcal{S}$ are the enabled features. We use a propositional formula to specify `P`, where its atoms represent the features of the domain. $\mathtt{P}(\mathcal{S})$ is computed evaluating the propositional formula associating

`true` to the atoms corresponding to features in $\mathcal{S}$, and associating `false` to the remaining atoms.

Boxes have another new attribute, `featuresTags`. It is a set of abbreviated features names that determines how a box is tagged. A tag is a prefix that is added to a box name to identify the variant of the box being used (*e.g.*, `L` and `K` are tags of box `L.K.WSERVER`, specifying that this box is a variant of the `WSERVER` with features `L(ist)` and `K(ey)`).[2]

> **Example:** Recall our web server example. We initially defined rewrite rule (`WSERVER`, `pwserver`) to specify a primitive implementation for `WSERVER` (see Figure 5.12a). Then we add feature `key` (abbreviated as `K`) to this rewrite rule, which means adding a new port (`OK`) to each box. As this port is only present when feature `key` is enabled, those new ports are annotated with predicate `key`. Moreover, the boxes now provide extra behavior, therefore we need to add `K` tag to each box. The result is depicted in Figure 5.12b (red boxes show tags sets, and blue boxes show predicates). Finally, we add feature `list` (abbreviated as `L`), which requires another port (`OL`) in each box. Again, the new ports are annotated with a predicate (in this case, `list` specifies the ports are only part of the model when feature `list` is enabled). The set of tags of each box also receives an additional tag `L`. The final model is depicted in Figure 5.12c.



(a) (b) (c)

Figure 5.12: Incrementally specifying a rewrite rule.

[2]Connectors are not named elements, neither have behavior associated with them, therefore they do not need to be tagged.

This provides sufficient information to project the RDM for a specific set of features from the XRDM. The XRDM itself also has an additional attribute, `featureModel`. It expresses the valid combinations of features, capturing their dependencies and incompatibilities, and it is specified using GuiDSL's grammar notation [Bat05].

5.2.3 Projection of an RDM from the XRDM

A new transformation is needed to map an XRDM to an RDM with the desired features enabled. This transformation takes an XRDM, and a given list of active features, and *projects* the RDM for that set of features. The projection is done by walking through the different model elements, and hiding (or making inactive) the elements for which its predicate is evaluated to `false` for the given list of features. To simplify the predicates we need to specify, there are implicit rules that determine when an element must be hidden regardless of the result of evaluating its predicate. The idea is that when a certain element is hidden, its dependent elements must also be hidden. For example, when a box is hidden, all of its ports must also be hidden. A similar reasoning may be applied in other cases. The implicit rules used are:

- if the `lhs` of a rewrite rule is hidden, the `rhs` is also be hidden;
- if a box is hidden, all of its ports are also be hidden;
- if an algorithm is hidden, its internal boxes and connectors are also hidden;
- if a port is hidden, the connectors linked to that port must also be hidden.

These implicit rules greatly reduce the amount of information we have to provide when specifying an XRDM, as we avoid the repetition of formulas. Taking into account the implicit rules, the projection transformation uses the following algorithm:

- For each rewrite rule:

- If the predicate of its `lhs` interface box is evaluated to `false`, hide the rewrite rule;
- For each port of the `lhs` interface, if the predicate of the port is evaluated to `false`, hide the port;
- If the predicate of the `rhs` box is evaluated to `false`, hide the `rhs` box;
- For each port of the `rhs` box, if the predicate of the port is evaluated to `false`, hide the port;
- If the `rhs` is an algorithm, for each connector of the `rhs` algorithm:
  - If the predicate of the connector is evaluated to `false`, hide the connector;
- If the `rhs` is an algorithm, for each internal box of the `rhs` algorithm:
  - If the predicate of the internal box is evaluated to `false`, hide the internal box;
  - For each port of the internal box, if the predicate of the port is evaluated to `false`, hide the port and the connectors linked to the port.

During projection, we also have to determine which tags are attached to each box. Given the set $\mathcal{F}$ of feature to project, and given a box `B` with features tags set `S`, the tags of `B` after the projection are given by $\mathtt{S} \cap \mathcal{F}$. That is, `S` specifies the features that change the behavior of `B`, but we are only interested in the enabled features (specified by $\mathcal{F}$).

Example: Considering the rewrite rule from Figure 5.12c, and assuming we want to project feature `K` only, we would obtain the model from Figure 5.13. Ports `OK`, which depend on feature `K`, are present. However, ports `OL`, which depend on feature `L`, are hidden. Additionally, boxes are tagged with `K` ($\{\mathtt{K}\} = \{\mathtt{K}, \mathtt{L}\} \cap \{\mathtt{K}\}$).

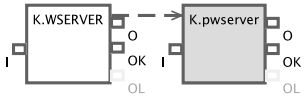


Figure 5.13: Projection of feature `K` from rewrite rule (`WSERVER`, `pwserver`) (note the greyed out `OL` ports).

5.3 Tool Support

`ReFlO` was adapted to support XRDM and extensions. Besides minor changes to the metamodels, and the addition of the RDM projection transformation, other functionalities were added to `ReFlO`, namely to provide better validation, and to help developers to replay a derivation after adding features to the RDM.

5.3.1 eXtended ReFlO Domain Models

When using extensions, we start defining an XRDM as if it was an RDM, *i.e.*, we specify the rewrite rules for the base (mandatory) features. Then, new elements and annotations are incrementally added to the initial model, in order to support other features. Typically, the new elements are annotated with a predicate that requires the presence of the feature being defined for the element be present. Boxes that receive new elements are also tagged. Occasionally elements previously added have their predicate changed, for example to specify they should be removed in the presence a certain features.

Predicates are provided in `featuresPredicates` attribute of boxes, ports and connectors, and are specified using a simple language for propositional formulas that provides operators `and` (logical conjunction), `or` (logical disjunction), `implies` (implication), and `not` (negation). An empty formula means `true`.

Tags are specified in attribute `featuresTags`, by providing a comma-separated list of names. To make the tags more compact (improving the visualization of models), we allow the specification of alias that associate a shorter tag name to a feature. Those alias are specified in attribute `featuresTagsMap` of the XRDM, using a comma-separated list of pairs `featurename` : `tagname`.

The XRDM has another extra attribute, `featureModel`, that is used to spec-

ify the feature model of the XRDM, *i.e.*, the valid combinations of features the XRDM encodes. As we mentioned previously, the feature model is specified using the language from GuiDSL [Bat05].

Given an XRDM, users can select and project the RDM for a desired set of features. `ReFlO` checks whether the selected combination of features is valid (according to the feature model), and if it is, it uses the algorithm described in Section 5.2.3 to project the XRDM into the desired RDM.

5.3.2 Program Architectures

Developers that use `ReFlO` start by providing a PIM, which is progressively transformed until a PSM with the desired properties is obtained. Given the XRDM, the developers have to select the set of features of the RDM they want to use to derive the PSM. Moreover, they also provide the PIM with the desired features (often all PIMs are expressed by the same graph, where only the box tags vary, according to the desired set of features).

Most of the variability is stored at XRDM, and when deriving a PSM, there is already a fixed set of features selected. This means the only additional information we have to store in architectures to support extensions are box tags. Therefore, the metamodel of architectures is modified to store this information, *i.e.*, boxes now have a new attribute `tags`.

5.3.3 Safe Composition

Dataflow models must satisfy constraints in order to be syntactically valid. `ReFlO` already provided dataflow model constraint validation. Before the introduction of extensions, it would simply assume all elements were part of the model, and apply its validation rules (see Section 3.2.3). With extensions, the validation function was changed to check only whether the active elements form a valid RDM. A more important question is whether all the possible RDMs obtained from projecting subsets of features form a valid RDM. When annotating models,

designers sometimes forget to annotate some model elements, leading to errors that would be difficult to detect without proper tool support.[3]

`ReFlO` provides a mechanism to test if there is some product (or RDM) expressed by the SPL (XRDM) that is syntactically invalid. The implemented mechanism is based on *safe composition* [CP06, TBKC07]. Constraints are defined by the propositional formulas described below (built using the propositional formulas of the model elements):[4]

- An implementation, if active, must have the same ports of its interface. Let `i1` be the propositional formula of the interface, and `p1` be the propositional formula of one of its ports. We know that `p1` $\Rightarrow$ `i1`. Let `a` the propositional formula of the implementation, and `p2` be the propositional formula of the equivalent port in the implementation. The propositional formula `a` $\Rightarrow$ (`p1` $\Leftrightarrow$ `p2`) must be true.

- An interface used to define an active algorithm must be defined (*i.e.*, it has to be the LHS of a rewrite rule). Let `i2` be the propositional formula of the interface used to define the algorithm, and `i1` be the propositional formula of the interface definition. The propositional formula `i2` $\Rightarrow$ `i1` must be true.

- An algorithm must have the same ports as its interface (*i.e.*, the LHS and RHS of a rewrite rule must have the same ports). Let `p3` be the propositional formula of a port of an interface used to define an algorithm, `i2` be the propositional formula of the interface, and `p1` be the propositional formula of the same port in the interface definition. The propositional formula `i2` $\Rightarrow$ (`p1` $\Leftrightarrow$ `p3`) must be true.

- The input ports of interfaces used to define an algorithm must have one and only one incoming connector. Let `p3` be the propositional formula of

[3] In our studies, we noticed that we sometimes forget to annotate ports that are added for a specific feature.

[4] We refer to the explicit propositional formula defined in the model elements in conjunction with their implicit propositional formulas, as defined in Section 5.2.3.

an input port of an interface used to define an algorithm, and c1, . . . , cn be the propositional formulas of its incoming connectors. The propositional formula p3 ⇒ choose1(c1, . . . , cn)[5] must be true.

- The output ports of an algorithm must have one and only one incoming connector. Let p4 be the propositional of an output port of an algorithm, and c1, . . . , cn be the propositional formulas of its incoming connectors. The propositional formula p4 ⇒ choose1(c1, . . . , cn) must be true.

Let fm be the feature model propositional formula. To find combinations of features that originate an invalid RDM, for each of the propositional formulas p described above, and for each model element it applies to, we test the propositional formula fm∧¬p with a SAT solver.[6] If there is a combination of features for which one of those predicates is true, then that combination of features reveals an invalid RDM. ReFlO safe composition test tells the developer if there is such combination, and, in case it exists, the combination of features and the type of problem detected. Given a combination that produces the invalid RDM, the developer may use ReFlO to project that features and validate the obtained RDM (doing this, the developer obtains more precise information about the invalid parts of the RDM, which allows him to fix them).

In addition, ReFlO can also detect *bad smells*, *i.e.*, situations that, although do not invalidate an RDM, are uncommon and likely to be incorrect. The two case we detect are:

- The input of an algorithm is not used (*i.e.*, a *dead input*). Let p be the propositional formula of an input port of an algorithm, and c1, . . . , cn be the propositional formulas of its outgoing connectors. The propositional formula p ⇒ choose(c1, . . . , cn) must be true.

[5] choose(e1, . . . , en) means at least one of the propositional formula e1, . . . , en is true, and choose1(e1, . . . , en) means exactly one of the propositional formulas e1, . . . , en is true [Bat05].

[6] Although SAT solvers may imply a significant performance impact in certain uses, in this particular kind of application, for the most complex case study we modeled (with 4 different features, and about 40 rewrite rules) the test requires less than 2 seconds to run.

- The output of an interface in an algorithm is not used (*i.e.*, a *dead output*). Let `p` be the propositional formula of an output port of an interface used to define an algorithm, and `c1`, ..., `cn` be the propositional formula of its outgoing connectors. The propositional formula `p` ⇒ `choose(c1, ..., cn)` must be true.

In case there is a combination of features where a bad smell is detected, the developer is warned, so that he can further check if the XRDM is correct.

5.3.4 Replay Derivation

When reverse engineering existing programs using `ReFlO` extensions, we start with a minimal PIM and an RDM with minimal features, and the PIM is mapped to a PSM. Later, an RDM and PIM with additional features is used, to produce a new derivation of a PSM that is closer to the desired implementation. This new derivation usually reuses the same transformations (or rather their extended counterparts) to produce the PSM. Sometimes new transformations are also required, or previously used transformations are not needed anymore.

Therefore, it is important to keep track of the sequence of transformations used in a derivation, as it can be used to help producing a new derivation. `ReFlO` stores the list of transformations used in a derivation. In this way, when trying to obtain a derivation of PIM with a different set of features, developers can ask `ReFlO` to replay the derivation. The user should select both the new PIM and the previously derived PSM. `ReFlO` reads the transformations used in the previously derived PSM, and tries to reapply the same sequence of transformation to the new PIM.[7] As mentioned earlier, new transformations may be needed (typical when we added features to the PIM), or certain transformations may not be applicable anymore (typical when we remove features from the PIM). `ReFlO` stops the replay process if it reaches a transformation it cannot successfully reapply, either because is not needed anymore, or because an entirely new transformation is required in the middle of the derivation. After this point, the developer

[7]Box names do not change, they are only tagged. In this way it is easy to determine the extended counterpart of a transformation used in a previous derivation.

has to manually apply the remaining transformations, in case there are more transformations needed to finish the derivation.

Chapter 6

Extension Case Studies

To validate our approach to encode extensions and product lines, we used `ReFlO` on different case studies. This chapter is dedicated to two of those case studies. We start with a case study where a fault-tolerant server architecture is reverse-engineered using extensions and our incremental approach. Later we show another case study where different variants of an MD simulation program are derived with the help of extensions.

6.1 Modeling Fault-Tolerant Servers

UpRight [CKL+09] is a state-of-the-art fault-tolerant server architecture. It is the most sophisticated case study to which we applied extensions, and its complexity drove us to develop its architecture incrementally, using extensions, thereby creating a small product line of UpRight designs. The initial architecture `SCFT` defines a vanilla RPA. Using refinements and optimizations, we show how this initial program architecture is mapped to a PSM that is fault-tolerant. Later, extensions (features) are added to provide recovery and authentication support. Figure 6.1 shows the diagram of the product line that is explored in this section.

We start with the initial PIM of UpRight.

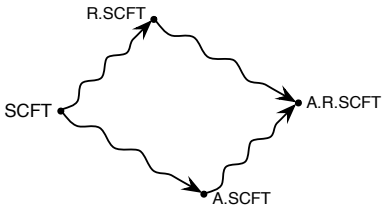
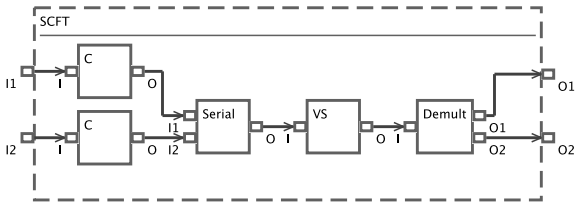


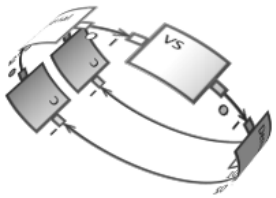
Figure 6.1: The UpRight product line.

6.1.1 The PIM

The initial PIM for this architecture is depicted in Figure 6.2a. It contains clients (`C` boxes) that send requests to a server.[1] The requests are first serialized (`Serial` box), and then sent to the server (`VS` box). The server processes each request in order (which involves updating the server's state, *i.e.*, the server is stateful), and outputs a response. The response is demultiplexed (`Demult` box) and sent back to the client that originated the request. The program follows a cylinder topology, and the initial PIM is in fact the result of unrolling the cylinder depicted in Figure 6.2b.



(a)



(b)

Figure 6.2: The PIM.

6.1.2 An SCFT Derivation

The simplest version of UpRight implements a *Synchronous Crash-Fault Tolerant (SCFT)* server, which has the ability to survive to failures of some components. The design removes *single points of failure (SPoF)*, *i.e.*, boxes that if they failed (stopped processing requests altogether), they would make the entire server ab-

[1] For simplicity, we have only two clients in the PIM. There may exist any number of clients; our approach/tools supports its representation using replication.

straction fail. For example, in the PIM, boxes `Serial`, `VS` and `Demult` are SPoF. In this derivation, we show how SPoF are eliminated by replication [Sch90].

The derivation starts by refining the `VS` box, to expose a network queue in front of the server. The `list` algorithm, depicted in Figure 6.3, is used. This refinement places an `L` box (list or queue) between the clients and the server, which collects the requests sent by clients, and passes them to the server, one at the time. The architecture obtained is depicted in Figure 6.4.

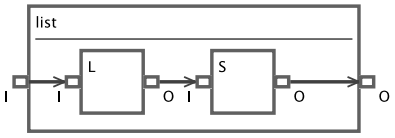


Figure 6.3: `list` algorithm.

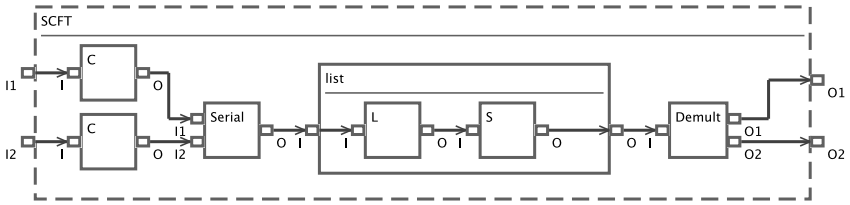


Figure 6.4: `SCFT` after `list` refinement.

Next, the network queue and the server are replicated, using a map-reduce strategy, to increase resilience to crashes of those boxes. The `paxos` algorithm (Figure 6.5) replicates the network queue [Lam98]. This algorithm forwards the input requests to different agreement boxes `A`, that decide which request should be processed next.[2] The requests are then serialized and sent to the quorum box (`Qa`), which outputs the request as soon as it receives it from a required number of agreement boxes.

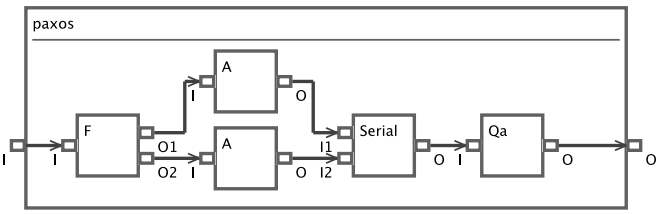


Figure 6.5: `paxos` algorithm.

[2] As for clients, we use only two replicas for simplicity. The number of replicas depends on the number of failures to tolerate. The number of clients, agreement boxes and servers is not necessarily the same.

The `reps` algorithm (Figure 6.6) replicates the server. The algorithm reliably broadcasts (`RBcast`) requests to the server replicas. For correctness, it is important to guarantee that all servers receive each request in synchrony, thus the need for the *reliable* broadcasts. The servers receive and process the requests in lock step, their responses are serialized and sent to the quorum box (`Qs`) that outputs the response as soon as it receives the same response from a required number of servers. The architecture obtained is depicted in Figure 6.7.

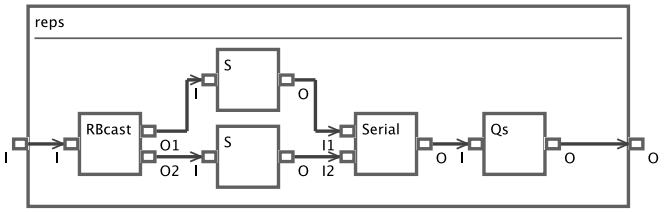


Figure 6.6: `reps` algorithm.

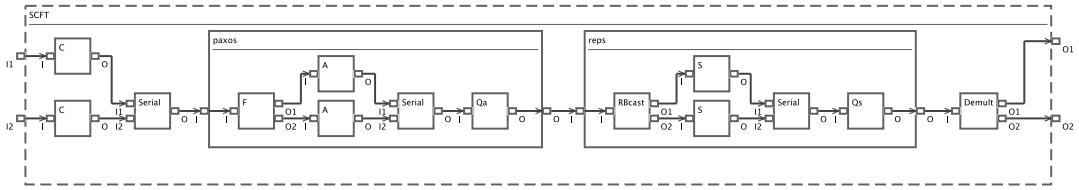


Figure 6.7: `SCFT` after replication refinements.

At this point, although we improved the resilience to crashes of the server, the entire system contains even more SPoF than the original (there were originally 3 SPoF, and now we have 8 SPoF). We rely on optimizations to remove them. Rotation optimizations, which swap the order in which two boxes are composed, remove SPoF.

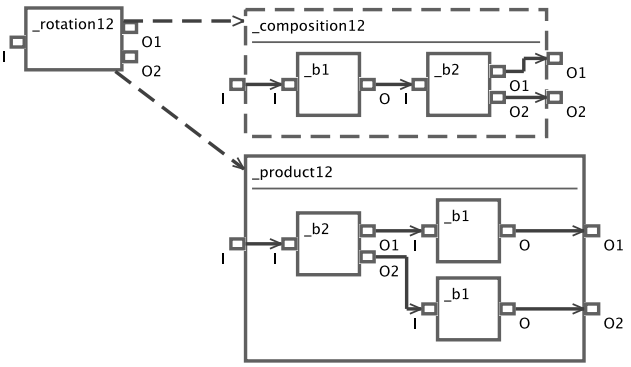


Figure 6.8: Rotation optimization.

The rewrite rules that express the optimizations needed are depicted in Figure 6.8 and Figure 6.9. These are templatized rewrite rules, where `_b1` and `_b2` can be replaced with concrete boxes. In the case of Figure 6.9 both boxes `_b1` and `_b2` are replicated as a result of the rotation, thus the optimization removes the SPoF associated with `_b1` and `_b2`. In the case of Figure 6.8 only box `_b1` is replicated as a result of the rotation, which means that this optimization alone is not enough to remove the SPoF. As we show below, we sometimes have to apply more than one optimization to remove all SPoF.

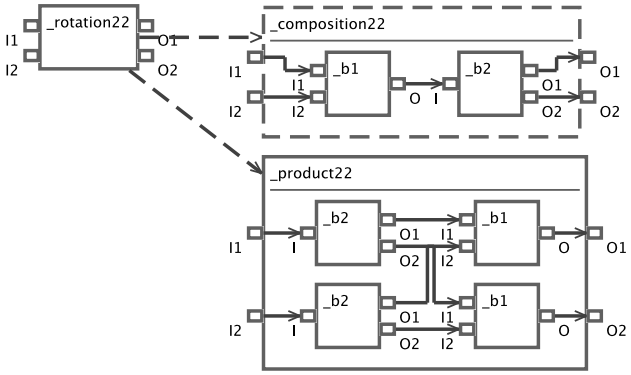


Figure 6.9: Rotation optimization.

As an example of instantiation of these rewrite rules, in Figure 6.9, `_b1` may be `Serial` and `_b2` may be `F` (Figure 6.10). This instantiation would remove the SPoF for the composition `Serial`−`F` present immediately after the client boxes. Applying the same optimization at other points, as well as its variant depicted in Figure 6.8, allows us to completely remove SPoF from the system. For `Serial` − `Qa` − `RBcast`, we first rotate `Qa` − `RBcast`, and then `Serial` − `RBcast`. For `Serial` − `Qs` − `Demult`, we follow a similar process. In this way, we obtain the architecture from Figure 6.11.

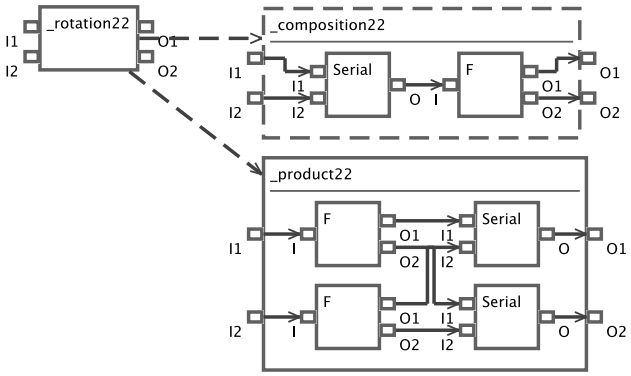


Figure 6.10: Rotation instantiation for `Serial` and `F`.

An additional optimization is needed. It is well-known to the distributed

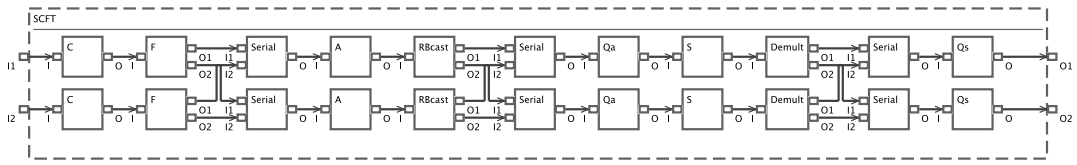


Figure 6.11: `SCFT` after rotation optimizations.

systems community that reliable broadcast is expensive, and therefore should be avoided. As quorums are taken from the requests broadcast, reliable broadcasts can be replaced by simple (unreliable) broadcasts. (Although this step may not be obvious for readers, it is common knowledge among domain experts.) After this step, we obtain the desired SCFT architecture, depicted in Figure 6.12. This is the "big-bang" design that was extracted by domain experts from UpRight's implementation.

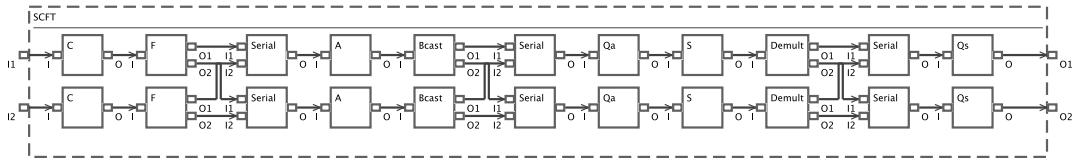


Figure 6.12: The `SCFT` PSM.

6.1.3 Adding Recovery

There are other features we may want to add to our initial PIM. The SCFT implementation previously derived improved resilience to failures. Still, a box failure would be permanent, thus, after a certain amount of failures, the entire system would fail.

The resilience to failures can be further improved adding recovery capabilities, so that the system can recover from occasional network asynchrony (*e.g.*, box failures). We now show how the RDM used in the SCFT can be extended so that an enhanced implementation of the SCFT with recovery capabilities, called *Asynchronous Crash-Fault Tolerant (ACFT)*, can be derived.

The first step is to R*ecovery*-extend the SCFT PIM to the ACFT PIM. That is, we want to show `SCFT` $\rightsquigarrow$ `R.SCFT`, where `ACFT` = `R.SCFT`. The ACFT PIM is

shown in Figure 6.13. Our goal is to map it to its PSM by replaying the SCFT derivation using R*ecovery*-extended rewrite rules.

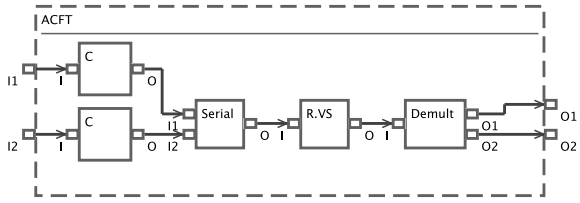


Figure 6.13: The `ACFT` PIM.

As for SCFT, the first step in the ACFT derivation is a refinement that exposes a network queue in front of the server. The algorithm has to be extended to account for recovery. Boxes `L` and `S` are both extended so that `S` can send recovery information to `L`. Thus, tag `R` is added to the tags set of both boxes. `S` gets a new output port that produces recovery information, and `L` gets a new input port that receives this information. Moreover, a new connector is added in algorithm `list`, linking the new ports of `S` and `L`. The new ports are annotated with the predicate `Recovery`, as they are only part of the RDM when we want the recovery property. The result is the algorithm depicted in Figure 6.14.[3] Using the extended algorithm to refine the initial specification, we obtain the architecture shown in Figure 6.15.

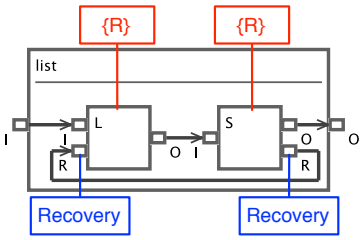


Figure 6.14: `list` algorithm, with recovery support.

The next transformations in the ACFT derivation are the replication of boxes `L` and `S`. Again, the algorithms previously used have to be extended to account for recovery.

[3] *Tags sets* are not graphically visible in an XRDM. This happens as the XRDM expresses all combinations of features, and the tags sets contains tags for features that change the behavior of a box, namely for feature that may not be "enabled" in a particular derivation. Architectures, on the other hand, have a fixed set of features, therefore tags are graphically visible. In the figures of XRDM boxes, we use red boxes to show tags sets attribute, and blue boxes to show predicates attribute.

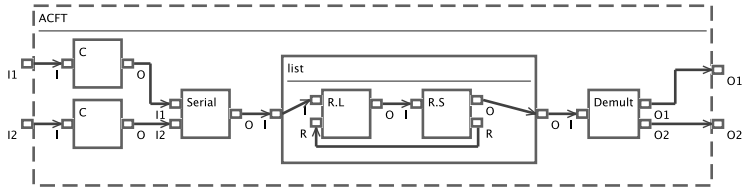


Figure 6.15: `ACFT` after `list` refinement.

For `paxos`, a new input port is added (to match interface `L`). The `A` boxes are also extended with an equivalent input port. Thus, tag `R` is added to the tags set of box `A`. Additionally, a new `RBcast` box is added, as well as the appropriate connectors, to broadcast the value of the new input port of `paxos` to the new inputs ports of `A`. The new ports of `paxos` and `A`, as well as box `RBcast`, are annotated with predicate `Recovery`. The extended algorithm is depicted in Figure 6.16.

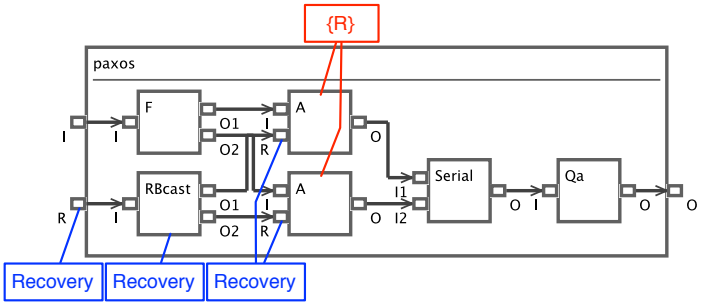


Figure 6.16: `paxos` algorithm, with recovery support.

For `reps`, a new output port is added to the algorithm box. As mentioned earlier, `S` also has an additionally output port that provides the values for the new output port of the algorithm. The values are first serialized (`Serial`), and then sent to a quorum box (`Qr`), before being output. The new ports of `reps` and `S`, and boxes `Serial` and `Qr` are annotated with predicate `Recovery`. The appropriate connectors are also added. Tag `R` is added to the tags set of box `S`. The extended algorithm is depicted in Figure 6.17.

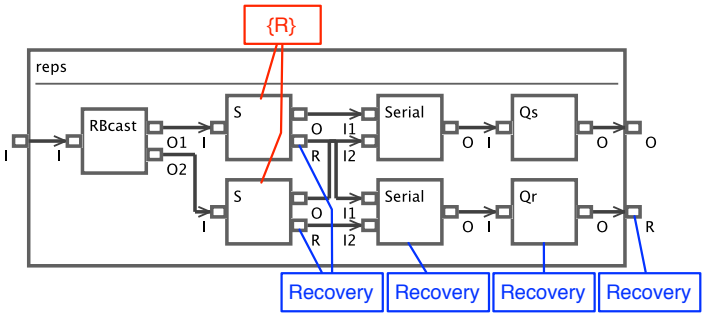


Figure 6.17: `rreps` algorithm, with recovery support.

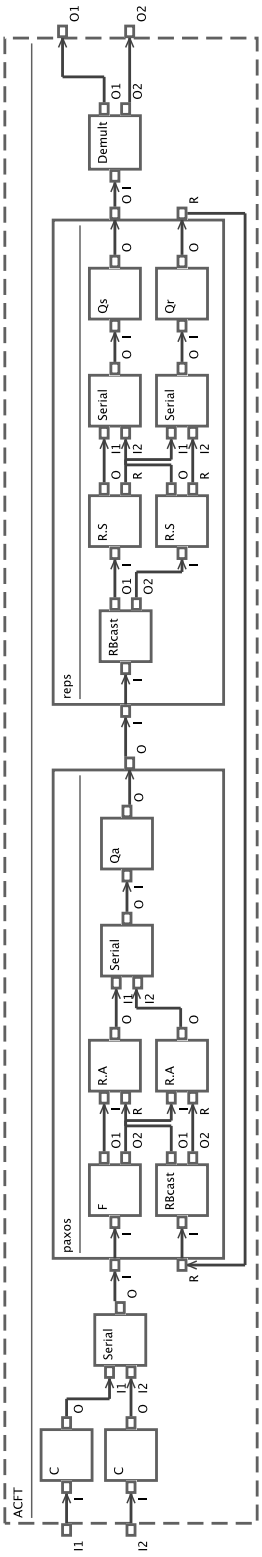


Figure 6.18: `ACFT` after replication refinements.

Note that interface `Qr` did not exist before. This is an example of a case where new rewrite rules need to be added to the RDM, as part of an extension, to handle new interfaces. Applying the refinements again, we obtain the program depicted in Figure 6.18.

We have now reached the point where we have to use optimizations to remove SPoF. Optimizations do not affect extended boxes, and therefore the optimization rewrite rules do not need to be extended. We can just reapply their previous definitions. Doing so, we obtain the architecture depicted in Figure 6.19.

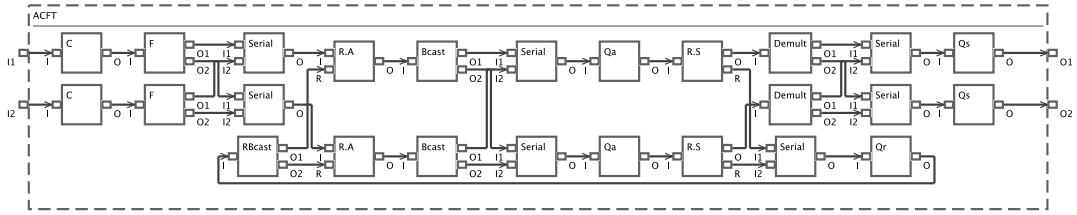


Figure 6.19: `ACFT` after replaying optimizations.

Nevertheless, in this case previous optimizations are not enough. We need to apply additional optimizations to the composition of boxes `Serial`−`Qr`−`RBcast`, which are still SPoF in the architecture of Figure 6.19. The aforementioned composition of boxes can optimized also using rotations, similarly to the optimization of `Serial` − `Qa` − `RBcast`. After these optimizations we obtain the architecture depicted in Figure 6.20, with no SPoF, *i.e.*, the PSM for the ACFT program.

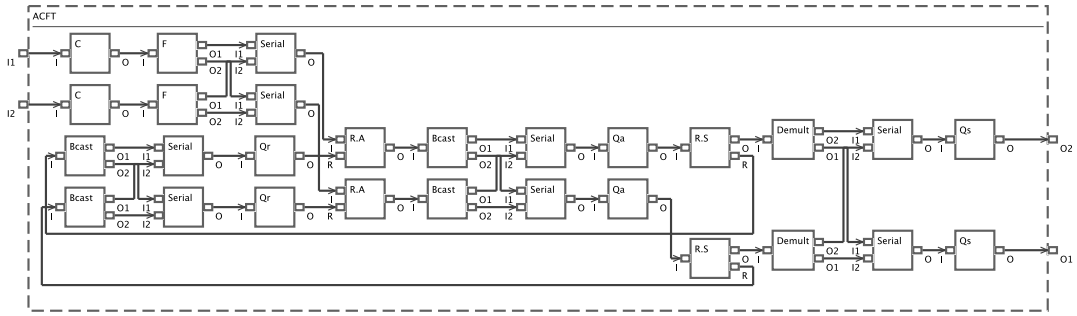


Figure 6.20: The `ACFT` PSM.

6.1.4 Adding Authentication

We saw earlier how the recovery feature mapped UpRight's SCFT design, its derivation and rewrites to UpRight's ACFT design, its derivation and rewrites. We now show how the ACFT server can be extended with another property, A*uthentication*, which is the next stage in UpRight's design. This new system, called AACFT (`AACFT` = `A.R.SCFT`), changes the behavior of the system by checking the requests and accepting only those from valid clients. That is, the server has now also validation capabilities, and therefore box `R.VS` receives a new tag to express this new feature (producing box `A.R.VS`). The initial PIM for this new derivation is shown in Figure 6.21.

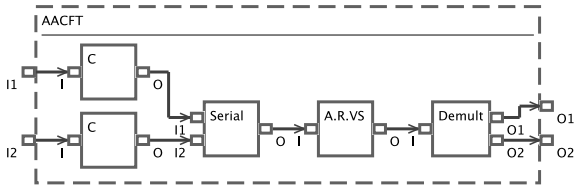


Figure 6.21: The `AACFT` PIM.

We now replay the ACFT derivation to obtain the desired implementation (PSM). The `list` algorithm is `A`-extended, to support authentication (Figure 6.22). This extension of `list` requires a box `V`, which validates and filters requests, to be added before the network queue. The new box is annotated with predicate `Authentication`. This also means the previous connector that links input `I` of `list` to input `I` of `L` is not present when authentication is being used (thus, it is annotated with predicate `not Authentication`). After performing this refinement, the architecture from Figure 6.23 is produced.

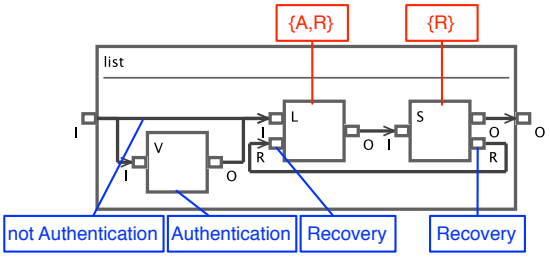


Figure 6.22: `list` algorithm, with recovery and authentication support.

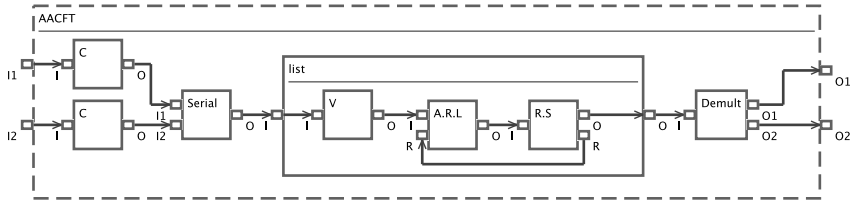


Figure 6.23: `AACFT` after `list` refinement.

The previous replication algorithms are not affected by this new feature. However, a new replication refinement is needed, to handle the new box `V`. For that purpose, we use the algorithm `repv` (Figure 6.24) to replicate `V` boxes using a map-reduce strategy, similar to the algorithm `reps`. That is, input requests are broadcast, and after being validated in parallel, they are serialized, and a quorum is taken. The resulting architecture is depicted in Figure 6.25.

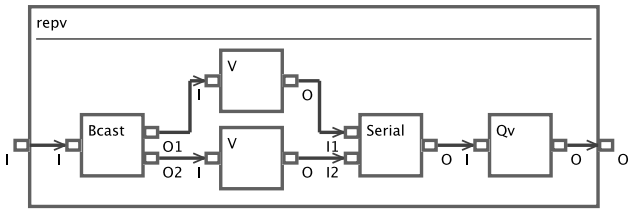


Figure 6.24: `repv` algorithm.

For the optimization step, we replay the optimizations used in the ACFT derivation. However, the sequential composition of boxes $\texttt{Serial} - \texttt{F}$ is no longer present, which means the optimization that removes these SPoF is not applicable anymore. Instead, we have two new groups of boxes forming SPoF: (i) $\texttt{Serial} - \texttt{Bcast}$, and (ii) $\texttt{Serial} - \texttt{Qv} - \texttt{F}$ (Figure 6.26). Rotations are once again used to remove these SPoF, allowing us to produce the desired PSM, depicted in Figure 6.27.

6.1.5 Projecting Combinations of Features: SCFT with Authentication

We have enhanced the XRDM specifying extensions to support recovery and authentication, besides the base fault-tolerance property. With only the information already provided in the XRDM, there is yet another implementation we can derive: SCFT with authentication, or $\texttt{ASCFT} = \texttt{A.SCFT}$. We can project

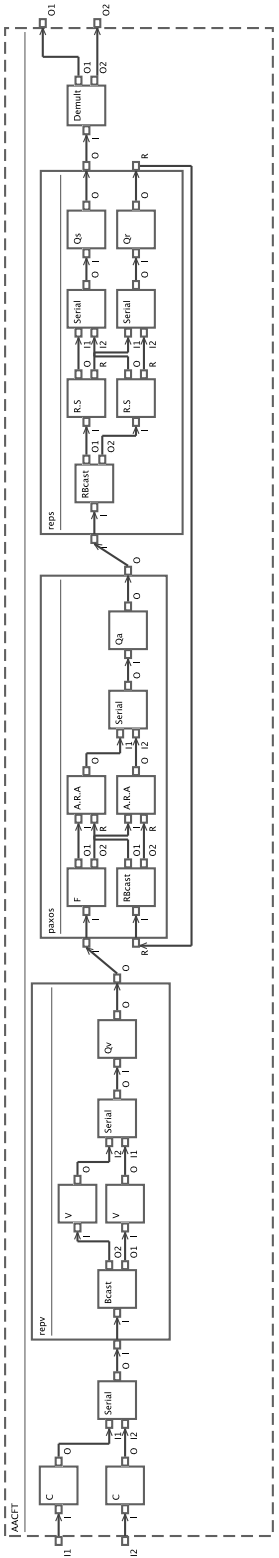


Figure 6.25: AACFT after replication refinements.

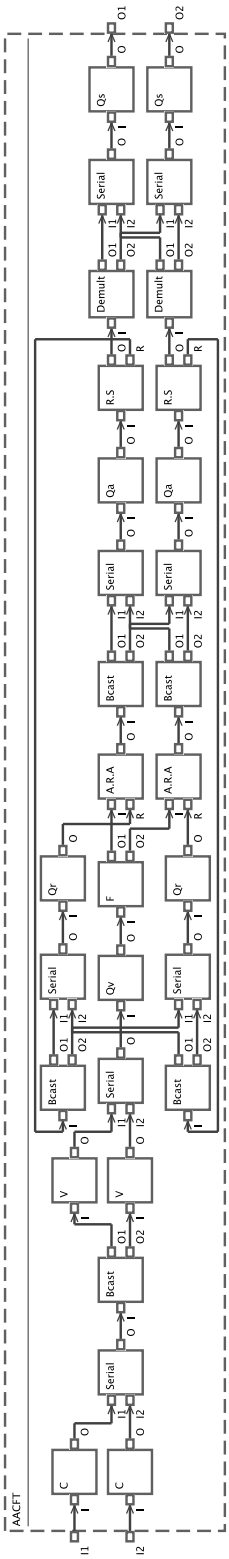


Figure 6.26: AACFT after replaying optimizations.

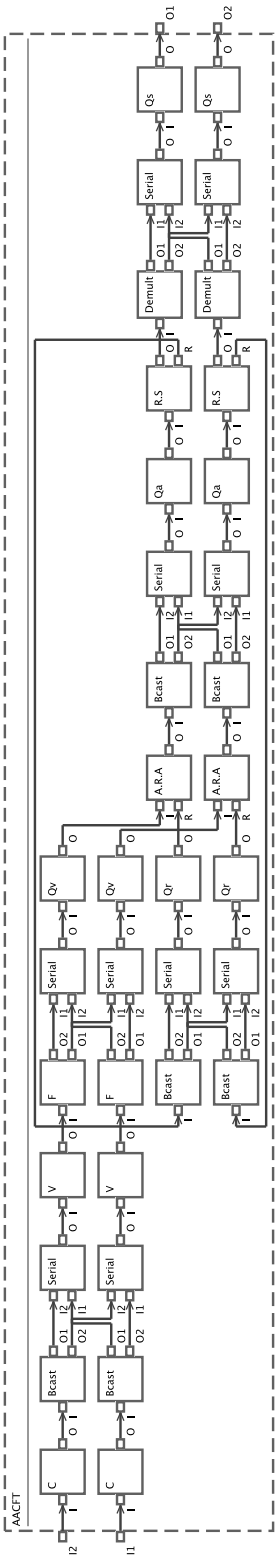


Figure 6.27: The AACFT PSM.

the RDM that expresses the desired features, and replay the derivation to obtain the implementation of ASCFT. The rewrite rules used for refinements, after projected, result in the graphs depicted in Figure 6.28.

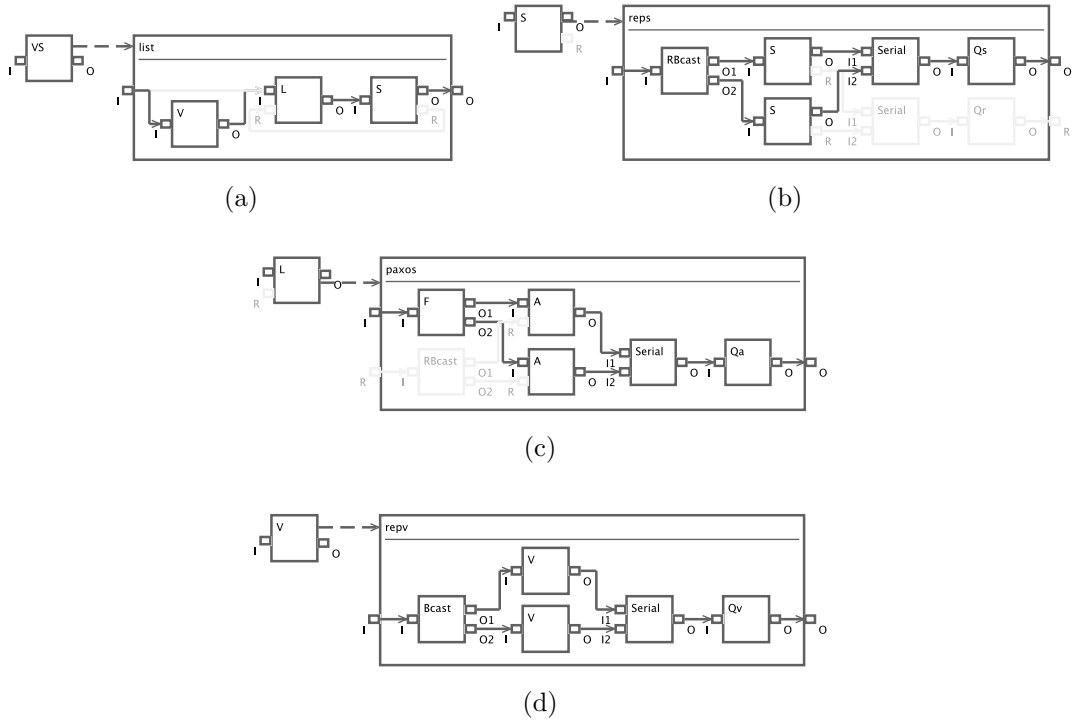


Figure 6.28: Rewrite rules used in initial refinements after projection (note the greyed out hidden elements, which are not part of the model for the current combination of features).

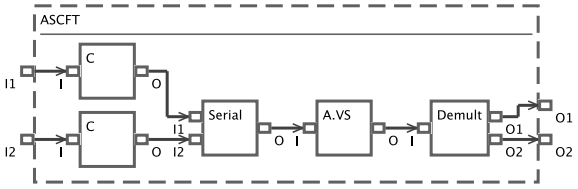


Figure 6.29: The `ASCFT` PIM.

Given the initial PIM for `ASCFT` (Figure 6.29), `ReFlO` is able to replay the derivation automatically (this derivation requires only a subset of the transformations used for the AACFT derivation), and produce the desired implementation, depicted in Figure 6.30.

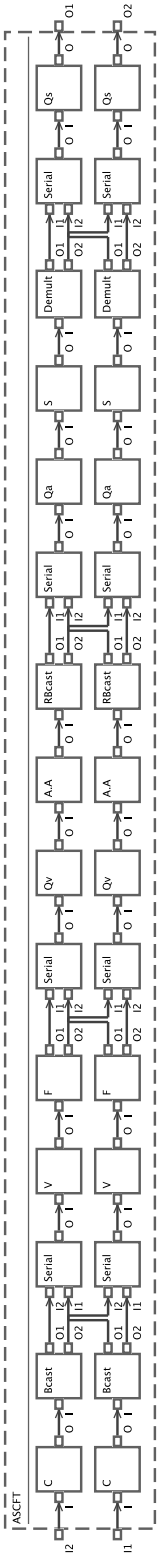


Figure 6.30: The ASCFT PSM.

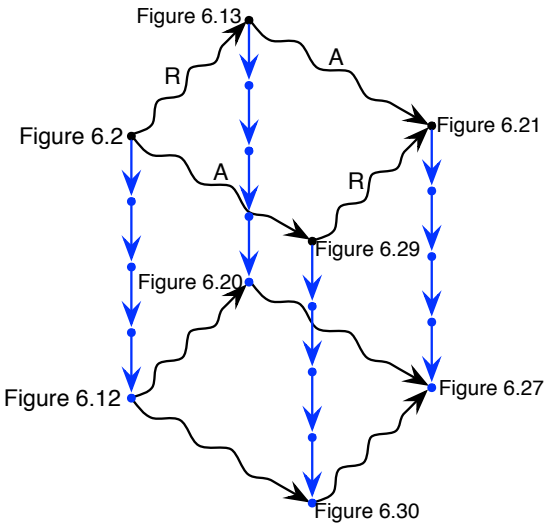


Figure 6.31: UpRight's extended derivations.

Recap. We showed how different designs of UpRight were obtained using the approach we propose. By using extensions we were able to encode and expose deep domain knowledge used to build such designs. We derived an optimized implementation that provides fault-tolerance. Later we improved fault-tolerance by adding recovery capabilities, and we also added authentication support. For the different combinations of features, we were able to reproduce the derivation. Figure 6.31 illustrates the different derivations covered in this section.

6.2 Modeling Molecular Dynamics Simulations

Another case study we explored to validate our work was MD simulations. The base implementation was the Java Grande Forum benchmark implementation [BSW+99], to which several other improvements are applied [SS11]. This implementation provides the core functionality of the most computationally intensive part of an MD simulation.

In this section we show how we can model a small product line of MD programs. The base PIM is mapped to optimized parallel implementations. Extensions are used to add further improvements, such as N*eighbors*, B*locking*, and C*ells* [SS11]. Figure 6.32 shows the diagram of the product line that is explored

in this section (note that the C*ells* feature requires the B*locks* feature).

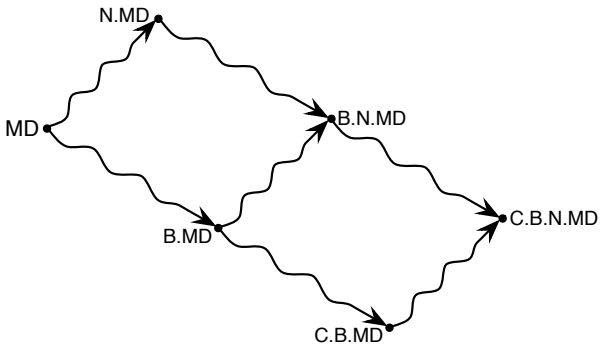


Figure 6.32: The MD product line.

6.2.1 The PIM

MD simulations are typically implemented by an iterative algorithm. A list of particles is updated at each iteration, until the particles stabilize, and some computations are then done using the updated list of particles. The architecture for the loop body of the program used is depicted in Figure 6.33, where we have the `UPDATEP` that updates the particles (input/output `p`), and some other additional operations to compute the status of the simulation.

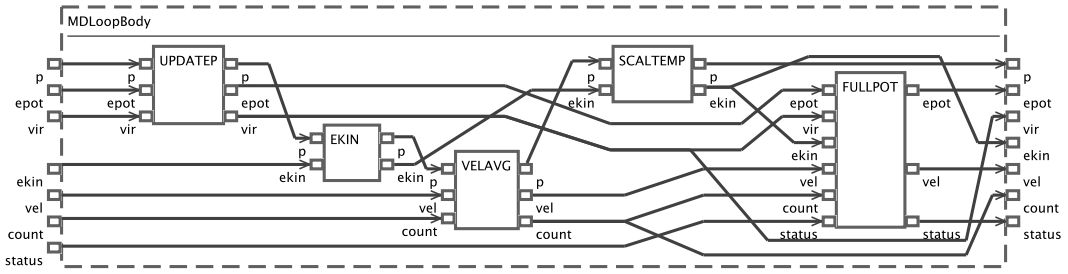


Figure 6.33: MD loop body.

The most important part of the algorithm is the update of particles, as it is computationally intensive, and contains the boxes that are affected by transformations. Therefore, in this section we use the architecture depicted in Figure 6.34 (that we call `MDCore`) as PIM. Besides input/output `p`, we also have input/output `epot` (potential energy) and `vir` (virial coefficient).

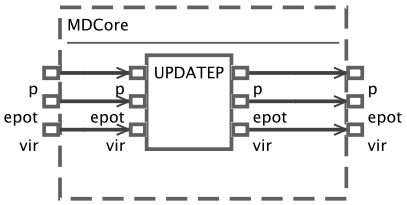


Figure 6.34: The `MDCore` PIM.

6.2.2 MD Parallel Derivation

We start by showing the derivation that maps the initial PIM to a parallel implementation. Different choices of algorithms can be used to target the PIM to different platforms, namely shared memory, distributed memory, or both. We obtain the implementation that uses both shared and distributed memory parallelization at the same time (the other two implementations can be obtained removing one of the refinements used). The distributed memory parallelization follows the SPMD model, where replicas of the program run on each processes. All data is replicated in all processes, but each process only deals with a portion of the total computation.

The derivation starts by applying a refinement that exposes the two steps of updating the list of particles. The algorithm used (depicted in Figure 6.35), shows how the two steps are composed. First the particles are moved (box `MOVE`), based on the current forces among the particles. Then the forces are recomputed based on the new positions of the particles (box `FORCES`). This results in the architecture depicted in Figure 6.36.

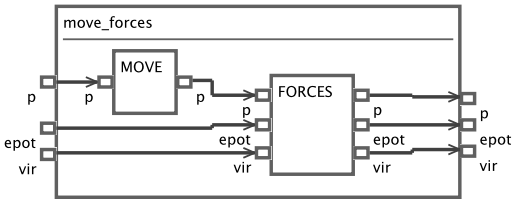


Figure 6.35: `move_forces` algorithm.

The next step is to parallelize the operation `FORCES` for distributed memory platforms, as shown in the algorithm depicted in Figure 6.37. The algorithm starts by dividing the list of particles, so that each process (program replica) only computes a subset of the forces [BSW+99]. This is done by box `PARTITION`, which takes the entire set of particles, and outputs a different (disjoint) subset on each program replica. In fact, the division of particles is only logical, and all particles

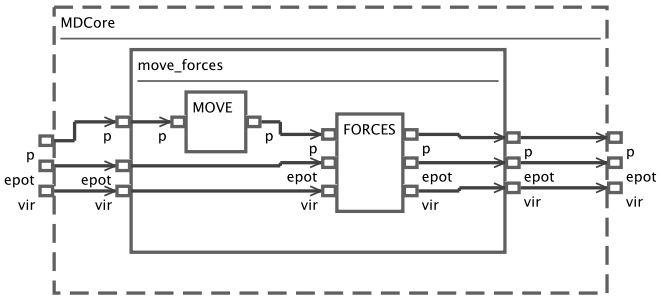


Figure 6.36: `MDCore` after `move_forces` refinement.

stay at all processes, as each process computes the forces between a subset of the particles and all other particles. Thus, during this process all particles may be updated, which requires reduction operations at the end. This is done by boxes `ALLREDUCEF` and `ALLREDUCE`. The former is an *AllReduce* operation [For94] specific to the list of particles, which only applies the reduction operation to the forces of each particle. The latter is a generic *AllReduce* operation, in this case being applied to scalars. This transformation results in the architecture depicted in Figure 6.38.

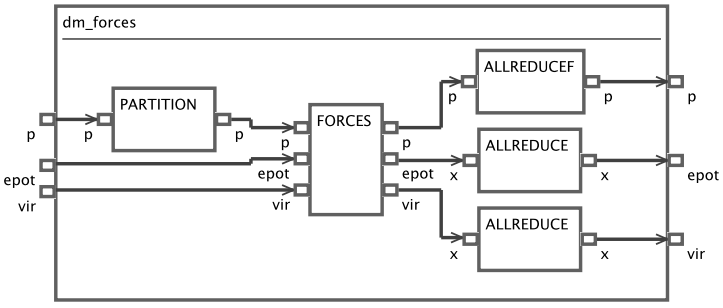


Figure 6.37: `dm_forces` algorithm.

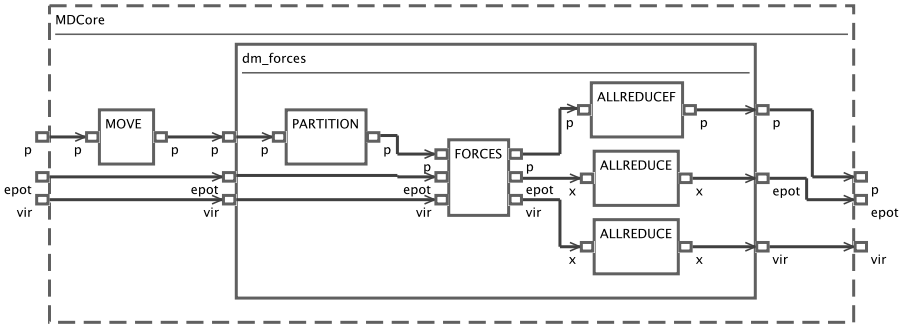


Figure 6.38: `MDCore` after distributed memory refinement.

The derivation is concluded with parallelization of `FORCES` for shared memory platforms, using the algorithm depicted in Figure 6.39. This parallelization is similar to the one used before for distributed memory. It also starts by dividing the list of particles. However, in this case, the forces of particles are physically copied to a different memory location, specific to each thread. This is done by box `SMPARTITION`. As the data is moved, the forces computation has to take into account the new data location, thus a different `SMFORCES` operation is used. Additionally, this operation also has to provide proper synchronization when updating `epot` and `vir` values (that store the global potential energy and virial coefficient of the simulation), which are shared among all threads. In the end, the data computed by the different threads has to be joined, and moved backed to the original location. This is done by box `REDUCEF`, which implements a *Reduce* operation. `epot` and `vir` do not need to be reduced, as their values are shared among all threads. This transformation results in the architecture depicted in Figure 6.40, or equivalently the flattened architecture in Figure 6.41.

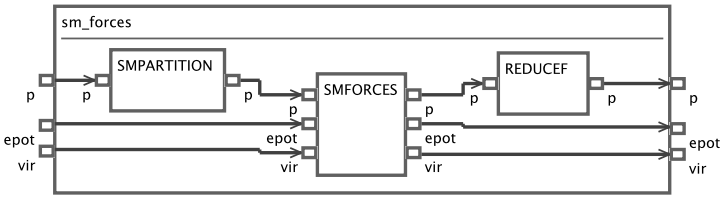


Figure 6.39: `sm_forces` algorithm.

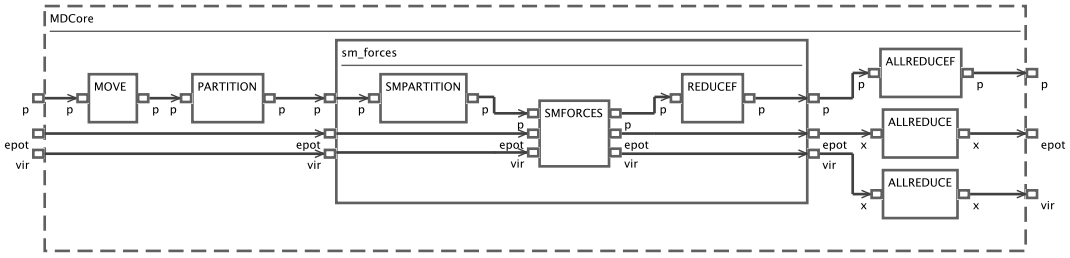


Figure 6.40: `MDCore` after shared memory refinement.

6.2.3 Adding Neighbors Extension

One common optimization applied to MD simulations consists in pre-computing (and caching) the list of particles that interact with any other particle [Ver67].

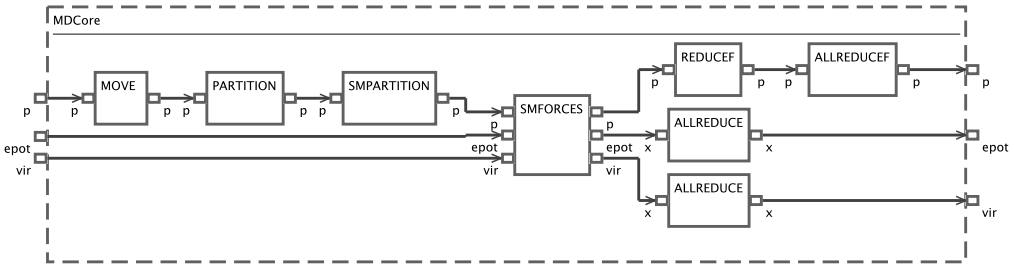


Figure 6.41: The `MDCore` PSM.

This improves performance as forces between particles that are not spatially close can be ignored, therefore by caching the pairs that interact we can reduce the $\mathtt{O}(\mathtt{N}^2)$ complexity. We call this optimization N*eighbors*, as this pre-computation essentially determines the neighbors of each particle. This optimization may or may not change the behavior of the simulation,[4] but we still use extensions to model this optimization, as it requires the extension of the behavior of the internal boxes used by the program.

The starting point for this derivation is the N*eighbors*-extended PIM (called `NMDCore`), depicted in Figure 6.42, which uses the tagged `UPDATEP` operation.

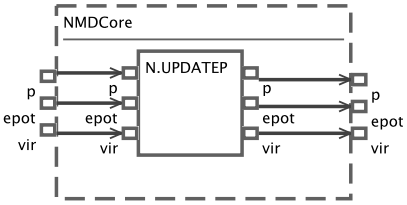


Figure 6.42: The `NMDCore` PIM.

From this PIM, we replay the previous derivation, starting with the `move_forces` algorithm. The algorithm is extended as shown in Figure 6.43, in order to support the N*eighbors* feature. Box `NEIGHBORS`, which does the pre-computation, is added. Box `FORCES` is extended to take into account the data pre-computed by `NEIGHBORS`, and receives a new input port (`N`). The appropriate connectors are also added, to provide the list of particles to `NEIGHBORS`, and to provide the neighbors data to `FORCES`.

[4] If we "relax" the correction criteria of the simulation (and therefore change the behavior of the program), we can improve performance.

As the behavior of `FORCES` changes, tag `N` is added to the tags set of this box. The new box and the new input port are annotated with predicate `Neighbors`, to denote that they are only part of the model when we want the neighbors feature. This transformation results in the architecture depicted in Figure 6.44.

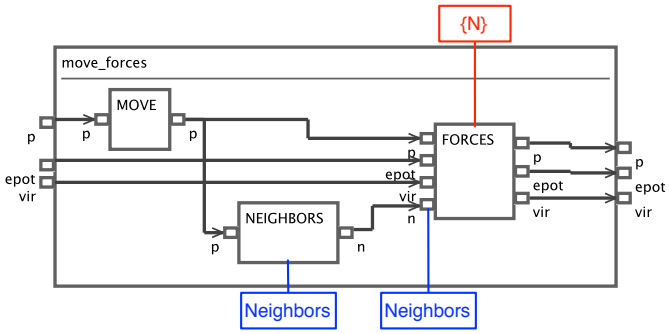


Figure 6.43: `move_forces` algorithm, with neighbors support.

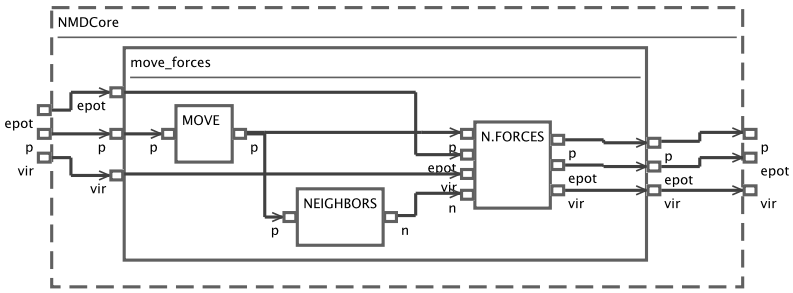


Figure 6.44: `NMDCore` after `move_forces` refinement.

We proceed with the transformations to parallelize the `FORCES` operation. First we add distributed memory parallelism, by using the `dm_forces` algorithm. As the `FORCES` operation was extended, we have to extend their implementations too. Figure 6.45 depicts the `Neighbors`-

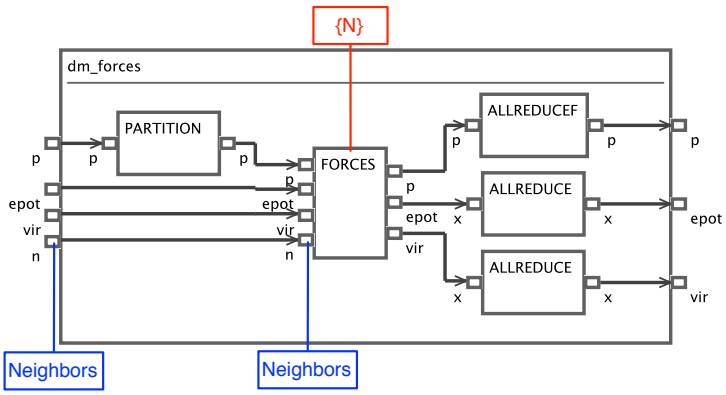


Figure 6.45: `dm_forces` algorithm, with neighbors support.

extended `dm_forces` algorithm. Essentially, we need to add the new input port `N` to the algorithm box and to the `FORCES` box, and a connector linking these two ports is added. The new input ports are annotated with predicate `Neighbors`. As we mentioned before, `N` is added to the tags set of `FORCES`. This transformation results in the architecture depicted in Figure 6.46.

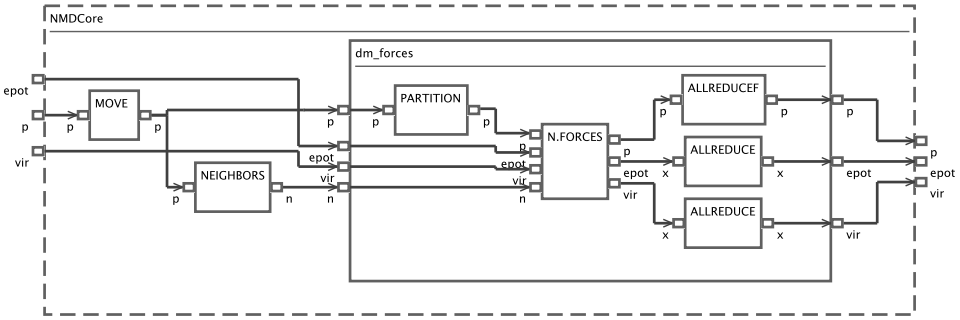


Figure 6.46: `NMDCore` after distributed memory refinement.

With the previous refinement, although we only apply the `FORCES` operation to a subset of the particles (the operation appears after the `PARTITION` operation), the same does not happens with the `NEIGHBORS` operation that is applied to the full set of particles, even though only a subset is need, and therefore this operation is not parallelized. However, a simple optimization can be used to swap the order of the `PARTITION` and the `NEIGHBORS` operations (when both operations appear immediately before a `FORCES` operation). This optimization is expressed by the templatized rewrite rules depicted in Figure 6.47. Boxes `_part` and `_forces` may either be `PARTITION` and `FORCES`, or `SMPARTITION` and `SMFORCES` (*i.e.*, this optimization can also be used to optimize an inefficient composition

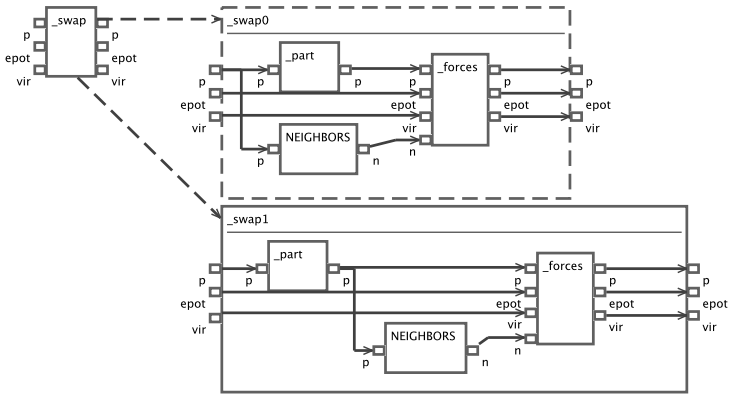


Figure 6.47: Swap optimization.

of boxes that results from the shared memory refinements, as we will see later). This optimization results in the architecture depicted in Figure 6.48.

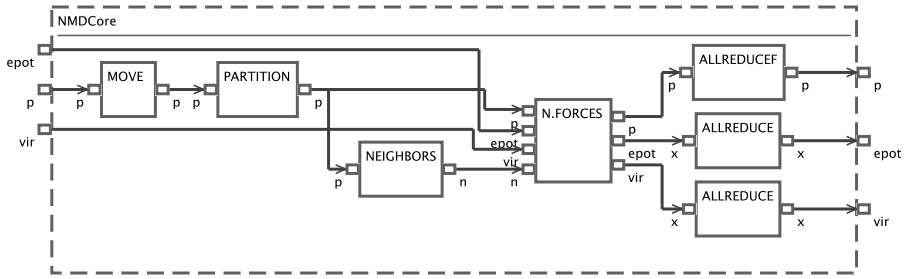


Figure 6.48: `NMDCore` after distributed memory swap optimization.

Next we apply the refinement for shared memory parallelization. The algorithm used in this refinement (`sm_forces`) needs to be extended in a similar way to `dm_forces`, so that it supports the `Neighbors` feature. It is depicted in Figure 6.49. This transformation results in the architecture depicted in Figure 6.50.

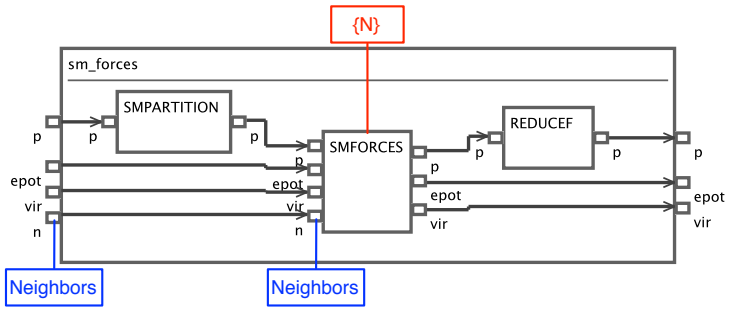


Figure 6.49: `sm_forces` algorithm, with neighbors support.

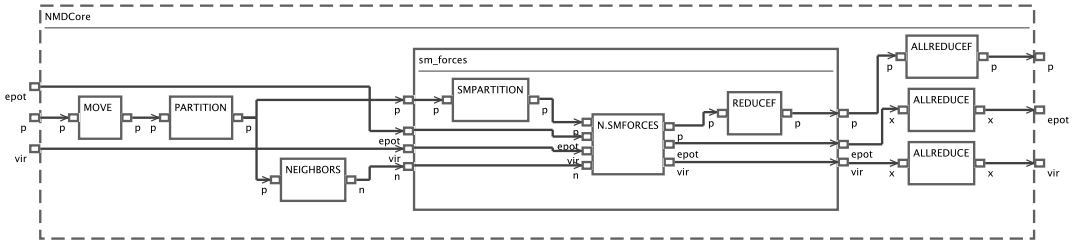


Figure 6.50: `NMDCore` after shared memory refinement.

We need again to use the swap optimization so that the neighbors are computed in parallel too. As we saw before, the optimization from Figure 6.47 can also be applied in the architecture from Figure 6.50 (after flattening it), yielding the architecture depicted in Figure 6.51.

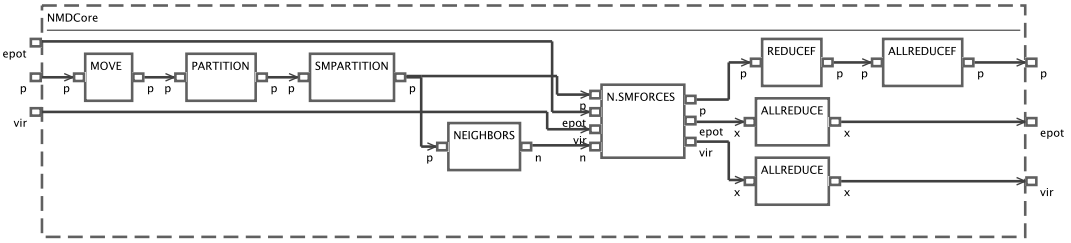


Figure 6.51: The `NMDCore` PSM.

6.2.4 Adding Blocks and Cells

When the set of particles is large enough to not fit in cache, there are additional optimizations that may be made to the program [YRP+07]. The use of a cache can be improved by using algorithms by B*locks*, which divide the set of particles in blocks that fit into the cache (similarly to the blocked algorithms used in DLA). This feature does not really change the structure of the algorithm; we simply need to use boxes that are prepared to deal with a list of blocks of particles, instead of a list of particles. Thus, the optimized architecture is obtained replaying the previous derivation, but now some boxes have an additional tag `B`. The final architecture is depicted in Figure 6.52.

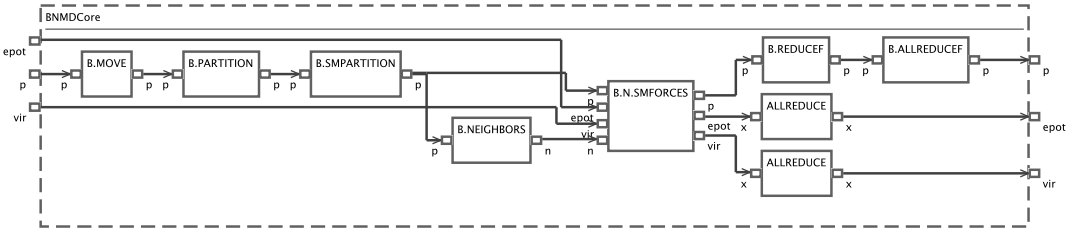


Figure 6.52: The `BNMDCore` PSM (`NMDCore` with blocks).

The blocks feature is important as it enables yet another optimization, which we call C*ells* [SS11]. Whereas the blocks feature just divides the list of particles in blocks randomly, the cells feature rearranges the blocks so that the particles in each block are spatially close, *i.e.*, the division in blocks is not random anymore. As particles interact with other particles that are spatially close to them, by rearranging the division of particles, for a given particle, we can reduce the list

of particles we have to check (to decide whether there will be interaction) to those particles that are in blocks spatially close to the block of the given particle. When we have the N*eighbors* feature, the same reasoning may be applied to optimize the computation of the neighbors list.

The starting point for this derivation is the PIM extended with features N*eighbors*, B*locks*, and C*ells* (called `CBNMDCore`), depicted in Figure 6.53, that uses the `UPDATEP` operation tagged with `C`, `B`, and `N`.

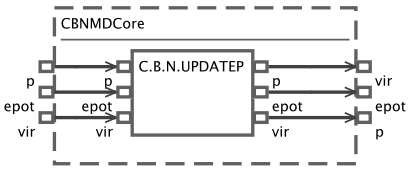


Figure 6.53: The `CBNMDCore` PIM.

From this PIM, we replay the previous derivation, using the `move_forces` algorithm. This algorithm is extended again, as shown in Figure 6.54. Box `PSORT` is added to rearrange the list of blocks of particles after moving the particles. These new rearranged list of blocks must then be used by boxes `NEIGHBORS` and `FORCES`. Thus, new connectors link the output of `PSORT` with `NEIGHBORS` and `FORCES`. Boxes `NEIGHBORS` and `FORCES` receive an additional tag `C`. The new `PSORT` box is annotated with predicate `Cells`. Additionally, the old connectors providing the list of blocks to boxes `NEIGHBORS` and `FORCES` shall not be used when this feature is enabled, therefore those connectors are annotated with predicate `not Cells`. This transformation produces the architecture depicted in Figure 6.55.

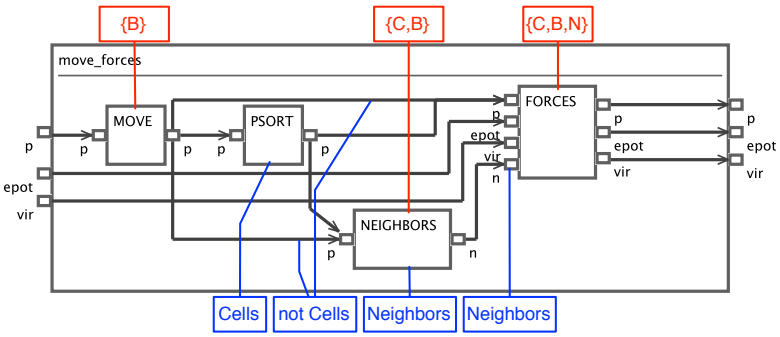


Figure 6.54: `move_forces` algorithm, with support for neighbors, blocks and cells.

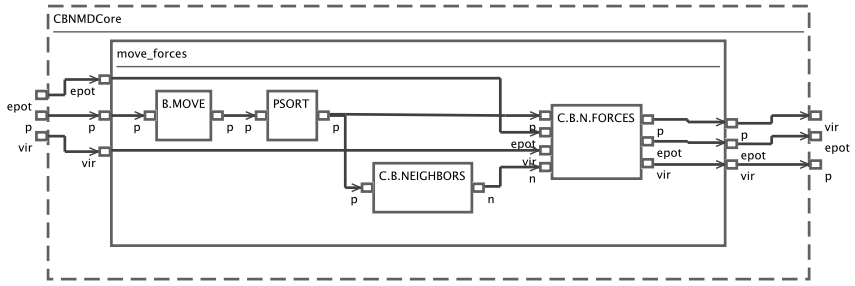


Figure 6.55: `CBNMDCore` after `move_forces` refinement.

We proceed with the transformations to parallelize the `FORCES` operation. First we add distributed memory parallelism, by using the `dm_forces` algorithm and swap optimization. Then we add shared memory parallelism, by using the `sm_forces` algorithm and the swap optimization again. Other than adding tag `C` to boxes `NEIGHBORS`, `FORCES`, `PARTITION`, and `SMPARTITION`, there is no other change to the (X)RDM. After we reapply the transformations we obtain the architecture depicted in Figure 6.56, which is the final PSM.

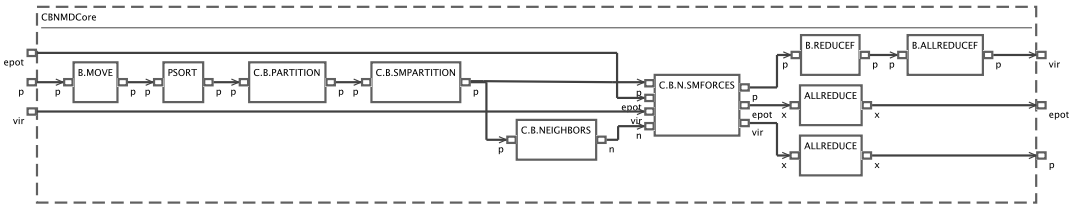


Figure 6.56: The `CBNMDCore` PSM.

Recap. We showed how we can encode the knowledge needed to obtain different MD simulations programs. We derived optimized implementations that use shared and distributed memory parallelism, and we showed how we can obtain four variants (with different optimizations) of the program for this target platform. Figure 6.57 illustrates the different derivations covered in this section.

Even though we only show derivations for one target platform, by removing some transformations from the derivation, we would be able to target shared memory platforms, and distributed memory platforms (individually). Moreover, besides the four combinations of features illustrated in this section, there are two other combinations of features we could use (as shown in Figure 6.32, we

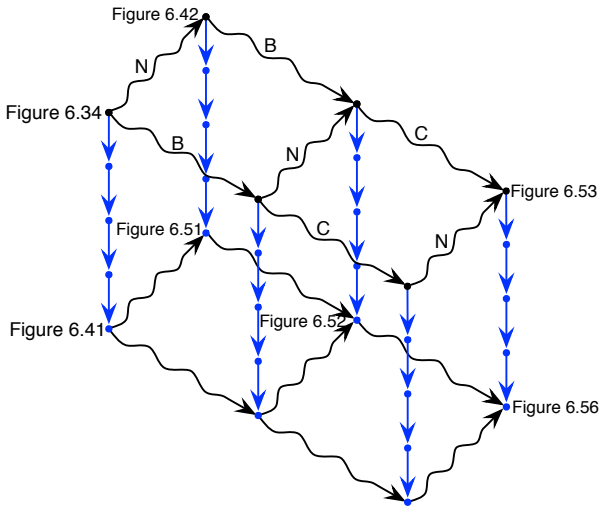


Figure 6.57: MD's extended derivations.

could also use combination of features `B.MDCore`, and `C.B.MDCore`). This means the knowledge encoded in the XRDM used for MD is enough to obtain a total of 18 optimized architectures (PSMs), targeting different platforms, and providing different features (optimizations), which users can enable according to their needs. That is, they can take advantage of a certain feature if the problem they have at hands benefits from using that feature, but they also avoid the downsides of the feature (overheads, load balancing problems, etc.) if the feature does not provide gains to compensate the downsides in a particular simulation.

The same set of PSMs could be obtained using refinements only. However, it would required multiple variants of algorithms to be modeled separately (for example, we would need the 6 different variants of `move_forces` algorithm to be modeled individually), leading to replicated information, which complicates development and maintenance.

Chapter 7

Evaluating Approaches with Software Metrics

We believe derivational explanations of dataflow designs are easier to understand and appreciate than a *big-bang* presentation of the final graph. Controlled experiments have been conducted to test this conjecture. The first experiments, which tried to measure (compare) the knowledge of the software acquired by users when exposed to the big-bang design and when exposed to the derivation, were inconclusive and did not show a significative advantage or disadvantage of using a derivational approach [FBR12]. Additional controlled experiments were conducted to determine the users perception of the derivational approach, to find out which method users (in this case, Computer Science students) prefer, and which method they think is better to implement, maintain, and comprehend programs. In this study, students showed a strong preference for the use of a derivational approach [BGMS13]. Despite some comments that the derivational approach has, in certain cases, too much overhead, and that such overhead is unjustifiable if the big-bang design is simple enough to be understood as a whole, the large majority of users comments were favorable to the derivational approach. Users pointed that the derivational approach allows them to divide the problem is smaller pieces, easier to understand, implement, and extend. Users also noted that the structure used to encode knowledge makes it easier to test the individual

components of the program, and detect bugs earlier.

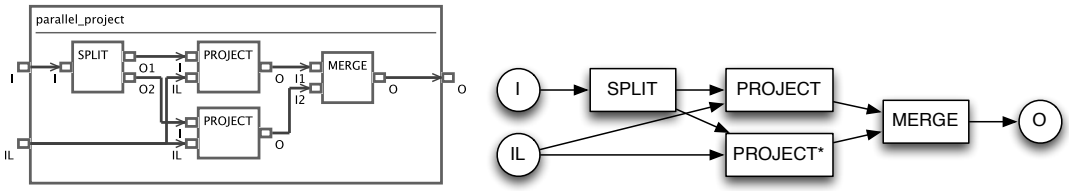
In this chapter we report an alternative (and supportive) study based on standard metrics (of McCabe and Halstead) to estimate the complexity of source code [Hal72, Hal77, McC76]. We adapt these metrics to estimate the complexity of dataflow graphs and to understand the benefits of DxT derivations of dataflow designs w.r.t. big-bang designs—where the final graph is presented without encoding/documenting its underlying design decisions.

7.1 Modified McCabe's Metric (MM)

McCabe's *cyclomatic complexity* is a common metric of program complexity [McC76]. It counts the linearly independent paths of a graph that represent the control flow of a program. This metric is important in software testing as it provides the minimum number of test cases to guarantee complete coverage.

We adapted this metric to measure the complexity and effort to understand dataflow graphs. Our metric measures the length (number of boxes) of a maximal set of linearly independent paths of a dataflow graph. Cyclomatic complexity captures the structure of the graph by considering all linearly independent paths (which basically increases as more outgoing edges are added to boxes). Our intuition goes beyond this to say that the number of boxes in a path also impacts the effort needed to understand it. Hence, our metric additionally includes the path length information.

We abstract DxT graphs to simple multigraphs by ignoring ports. For example, the dataflow graph of Figure 7.1a is abstracted to the graph of Figure 7.1b.



(a) (b)

Figure 7.1: A dataflow graph and its abstraction.

The graph from Figure 7.1b has 4 linearly independent paths:

- I → SPLIT → PROJECT → MERGE → O
- I → SPLIT → PROJECT* → MERGE → O
- IL → PROJECT → MERGE → O
- IL → PROJECT* → MERGE → O

The sum of the lengths of (number of interface nodes in) each path is 3+3+2+2 = 10. This is our measure of the complexity of the dataflow graph of Figure 7.1a.

The complexity of a set of graphs is the sum of the complexity of each graph present in the set. The complexity of a derivation is the complexity of a set of graphs that comprise (i) the initial dataflow graph of the program being derived, and (ii) the RHS of the rewrite rules used in the derivation. If the same rewrite rule is used more than once in a derivation, it is counted only once (as the rewrite rule is defined once, regardless of the number of times it is used).[1]

As an example, consider the derivation in Figure 7.2, previously discussed in Section 3.1. Figure 7.2e shows the final graph, which can be obtained incrementally transforming the initial graph shown in Figure 7.2a. From Figure 7.2a to Figure 7.2b, algorithms `parallel_project` and `parallel_sort` are used to refine PROJECT and SORT, respectively. From Figure 7.2b to Figure 7.2c we remove the modular boundaries of the algorithms previously introduced. From Figure 7.2c to Figure 7.2d we replace the subgraph identified by the dashed red lines, using the optimization specified by the rewrite rules previously depicted in Figure 3.13. After flattening Figure 7.2d, the final graph is obtained.

We measure the complexity of this derivation to be: 2 (initial graph) + 3 + 3 (`parallel_project`) + 3 + 3 (`parallel_sort`) + 2 + 2 + 2 + 0 + 0 (optimization[2]) = 20. The complexity of the final or big-bang graph is 4 + 4 =

[1] This is also the typical procedure when measuring the complexity of a program's source code. We take into account the complexity of a function/module, regardless of the number of times the function/module is used in the program.

[2] `ms_mergesplit` has three linearly independent paths of size 2. `ms_identity` has two linearly independent paths of size 0.

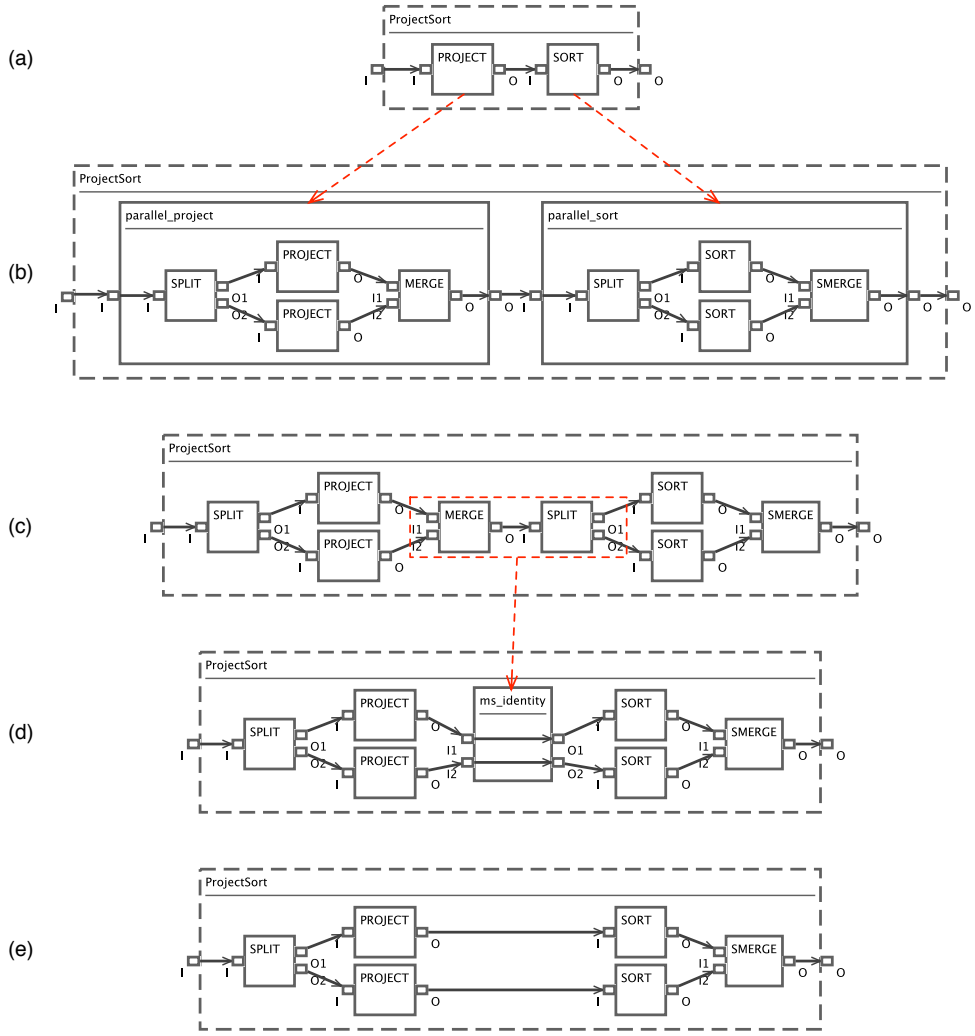


Figure 7.2: A program derivation.

8. In this case, we would say that the derivation is more than twice ($\frac{20}{8} = 2.5$) as complex as the big-bang.

We attach no particular significance to actual numbers for our *Modified McCabe (MM)* metric; rather what we do consider useful is the ratio of MM numbers: $\frac{\texttt{MM}_{\texttt{bigbang}}}{\texttt{MM}_{\texttt{DxT}}}$. In this study, we consider that a ratio bigger 1.5 is *significant*; a ratio between 1.25 and 1.5 is *noticeable*, and a ratio less than 1.25 is *small*. In the results presented we also use the signs "–" and "+" to specify whether the big-bang or the derivation is the best approach, respectively.

In the next sections we provide results for different case studies using MM

where we compare the big-bang and derivational approaches.

7.1.1 Gamma's Hash Joins

Table 7.1 shows the MM complexity of Gamma's Hash Joins and Gamma's Cascading Hash Joins.

	Big Bang	Derivation	Difference
HJoin (short)	26	21	**+small**
HJoin (long)	26	57	**−significant**
Casc. HJoin (long)	92	68	**+noticeable**
HJoin + Casc. HJoin (long)	118	74	**+significant**

Table 7.1: Gamma graphs' MM complexity.

HJoin (short) presents the MM number obtained for Gamma's Hash Join big-bang graph and its 2-step DxT derivation [GBS14]. The complexity of the big-bang graph is `26` and the complexity of the derivation is `21`. The reason why the derivation has lower complexity is because it reuses one of the rewrite rules twice. Still, the difference is **small**.

HJoin (long) lists complexity for the "standard" 7-step derivation of Gamma (presented in Section 4.1.1). It is `57`, well over twice that of the big-bang (`26`). The reason is that it exposes considerably more information (refinements and optimizations) in Gamma's design. The difference in this case is **significant**.

Reuse makes the complexity of the derivation lower than the complexity of the final graph. This is visible in the values for *Casc. HJoin (long)*, which shows complexity numbers for Cascading Hash Join (described in Section 4.1.2). In the derivation of this program all rules needed for Hash Join are used twice, and an additional optimization is also needed. This makes the big-bang approach **noticeably** more complex than the derivational approach.

In the last row (*HJoin + Casc. HJoin (long)*) we consider both programs at the same time. That is, for the final graphs column we count the complexity of the final graph for Hash Joins and the complexity of the final graph for Cascading Hash Joins. For the derivation column, we count the complexity of the initial graph for each program, and the complexity of the rewrite rules' graphs used in

each derivation. Reuse is further increased, which makes the big-bang approach **significantly** more complex ($\frac{118}{74} = 1.58$) than the derivational approach.

7.1.2 Dense Linear Algebra

Table 7.2 shows the results of measuring the complexity in DLA domain considering the two different programs described in Section 4.2, Cholesky factorization and LU factorization, each targeting three different hardware platforms. As usual, we provide complexity results for the final graphs and their derivations.

	Big Bang	Derivation	Difference
Chol (blk)	15	21	–**noticeable**
Chol (unblk)	6	23	–**significant**
Chol (dm)	28	43	–**significant**
LU (blk)	8	13	–**significant**
LU (unblk)	8	15	–**significant**
LU (dm)	24	40	–**significant**
Chol + LU	89	94	–**small**

Table 7.2: DLA graphs' MM complexity.

The first three rows show complexity values for blocked, unblocked and distributed memory implementations of Cholesky factorization. The big-bang approach is always the best, and the difference is **noticeable** in one case, and **significant** in the other two.

The next three rows show complexity values for implementations of LU factorization for the three target hardware platforms mentioned before. The big-bang approach is again the best, and the differences are **significant** in all cases.

Row *Chol + LU* shows the results for the case where we consider all implementations (blocked, unblocked and distributed memory) for both programs at the same time. The complexity of the derivations is still higher than the final graphs, but now the difference is **small**.

We can see that as more programs are added to the domain, the disadvantage of the derivational approach gets smaller. This can be easily explained by the reuse of knowledge in the same domain. That is, as new programs are added, less and less new rules are needed, as they are likely to have been added before

for the derivation of a previous program. Therefore, the complexity grow of supporting new programs is smaller in the derivational approach than in the big-bang graphs.

7.1.3 UpRight

Table 7.3 lists the complexity of variations of UpRight, supporting different sets of functional or non-functional properties.

	Big Bang	Derivation	Difference
SCFT	88	76	**+small**
ACFT	164	164	**none**
ASCFT	150	101	**+noticeable**
AACFT	242	183	**+noticeable**
UpRight All	644	390	**+significant**

Table 7.3: SCFT graphs' MM complexity.

Row *SCFT* refers to the SCFT server derivation (presented in Section 6.1.2). The derivation is simpler than the big-bang, but the difference is **small**. Row *ACFT* refers to the ACFT server derivation, which adds recovery capabilities to SCFT (as described in Section 6.1.3). In this case, both approaches have basically the same complexity. Row *ASCFT* refers to the SCFT server with authentication, which adds authentication to SCFT (as described in Section 6.1.5). The derivation is simpler than the big-bang, and the difference is **noticeable**. Row *AACFT* refers to the ACFT server with authentication, that is, SCFT with recovery and authentication capabilities (as described in Section 6.1.4). The derivation is simpler than the big-bang, and the difference is again **noticeable**.

Finally, row *UpRight All* shows the results for the case where all variations are considered together. The complexity of the big-bang approach is equal to the sum of the complexity of each individual variant. For derivations, rewrite rules are reused, which contributes for a lower grow in complexity. As a result, the big-bang approach is now **significantly** more complex ($\frac{644}{390} = 1.65$) than the derivational approach.

7.1.3.1 Extensions

We considered four different variants of UpRight. Those variants can be modeled independently, but as we saw earlier (Section 6.1), due to the similarities between some of the rewrite rules used, we can use extensions to simplify the definition of the RDM. This further increases reuse of rewrite rules, and reduces the complexity associated with the graphs used in the derivational approach. In Table 7.4 we report the impact of using extensions in graphs' complexity.

	Big Bang	Derivation	Difference
UpRight (ext.)	644	183	**+significant**
UpRight (ext. all)	302	183	**+significant**

Table 7.4: UpRight variations' complexity.

For *UpRight (ext.)* we used extensions to model the rewrite rules used in the derivations, which reduces the complexity of the derivation, as expected (several rewrite rules are superimposed in a single rewrite rule). Therefore, the derivational approach becomes even better than the big-bang approach.

For *UpRight (ext. all)* we use extensions not only for rewrite rules, but also for the initial and final graphs, that is, the different initial/final graphs are also superimposed (*i.e.*, extensions are useful not only to model rewrite rules, but may also be used to model programs). Even though the complexity of the final graphs is reduced to less than a half, it is still **significantly** more complex ($\frac{302}{183} = 1.65$) than the derivational approach. This is consistent with the idea presented in [RGMB12], that extensions are essential to handle complex software architectures.

7.1.4 Impact of Replication

ReFlO provides a compact notation to express ports, boxes and connectors that may appear a variable number of times in the same position (see Section 3.2.1.3). Replication reduces the number of boxes and connectors, simplifying repetitive graphs, which results in simpler graphs/models. In Table 7.5 we provide results

for complexity for three of the case studies previously analysed, where we applied replication.

	Big Bang	Derivation	Difference
HJoin (long)	13	31	**−significant**
HJoin + Casc. HJoin (long)	51	40	**+noticeable**
SCFT	11	28	**−significant**

Table 7.5: MM complexity using replication.

The use of simpler graphs for initial graphs, final graphs, and rewrite rules results in lower MM complexities for both the big-bang and derivational approaches. However, comparing these values with the ones previously presented, we can observe different levels of reduction of complexity for each approach. That is, the reduction of complexity resulting from the use of replication is typically higher in the big-bang approach, which sometimes changes the relation between the approaches (*e.g.*, for SCFT, the big-bang approach is now significantly less complex than the derivational approach).

Replication simplifies complex dataflow graphs, so these observations are in line with those we presented previously. However, we cannot evaluate the impact of the additional annotations required by replication, to fully understand whether replication is really beneficial or not, and to be able to properly compare the big-bang and derivational approaches.

7.2 Halstead's Metric (HM)

Halstead proposed metrics to relate the syntactic representation of a program with the effort to develop or understand it [Hal72, Hal77]. The metrics are based on the number of operators and operands present in a program. The following properties are measured:

- the number of distinct operators used in the program (η_1);
- the number of distinct operands used in the program (η_2);
- the total number of operators used in a program ($\mathtt{N}_1$); and

- the total number of operands used in a program ($\mathtt{N}_2$).

Given values for the above, other metrics are computed, namely the program's *volume* (V), *difficulty* (D), and *effort* (E) to implement. Let $\eta = \eta_1 + \eta_2$, and $\mathtt{N} = \mathtt{N}_1 + \mathtt{N}_2$, the following equations are used to compute the properties:

- $\mathtt{V} = \mathtt{N} \times \log_2(\eta)$
- $\mathtt{D} = \eta_1/2 \times \mathtt{N}_2/\eta_2$
- $\mathtt{E} = \mathtt{V} \times \mathtt{D}$

Volume captures the amount of space needed to encode the program. It is also related to the number of mental comparisons we have to make to search for an item in the vocabulary (operands and operators). *Difficulty* increases as more operators are used ($\eta_1/2$). It also increases when operands are reused multiple times. This metric tries to capture the difficulty of writing or understanding the program.[3] Finally, *effort* captures the effort needed to implement the program, and it is given by the volume and the difficulty of a program.

Nickerson [Nic94] adapted this metric to visual languages, like that of ReFlO. In this case, graph nodes (boxes) are operators, and edges (connectors) are operands. We consider edges with the same origin (source port) as reuse of the same operand.

As an example, consider the dataflow program from Figure 7.1a. We have unique boxes parallel_project, SPLIT, PROJECT, and MERGE, therefore $\eta_1 = 4$. PROJECT is used twice, therefore $\mathtt{N}_1 = 5$. We have 8 edges, two of them

[3]The difficulty value is supposed to be in the interval $[1, +\infty)$, where a program with difficulty 1 would be obtained in a language that already provides a function that implements the desired behavior. In this case, we would need 2 (distinct) operators, the function itself, and an assignment operator (or some sort of operator to store the result). The number of operands would be equal to the number of inputs and outputs (say $\mathtt{n} = \mathtt{n}_\mathtt{i} + \mathtt{n}_\mathtt{o}$), which would also be the number of distinct operands. Therefore, the difficulty would be given by $\mathtt{D} = 2/2 \times \mathtt{n}/\mathtt{n} = 1$. Our adaptation of the metric is consistent with this rule, as any program directly implemented by a box has $\mathtt{D} = 1$. Note, however, that an identity program (that simply outputs its inputs), can be implemented simply using the assignment operator and therefore it has $\mathtt{D} = 1/2 \times \mathtt{n}/\mathtt{n} = 1/2$. The same happens for a dataflow program that simply outputs its input.

with source `parallel_project.IL`, therefore $\eta_2 = 7$, and $\mathtt{N}_2 = 8$. Given these measures, we can now compute the remaining metrics:

- $\eta = \eta_1 + \eta_2 = 4 + 7 = 11$
- $\mathtt{N} = \mathtt{N}_1 + \mathtt{N}_2 = 5 + 8 = 13$
- $\mathtt{V} = \mathtt{N} \times \log_2(\eta) = 13 \times \log_2(11) \approx 44.97$
- $\mathtt{D} = \eta_1/2 \times \mathtt{N}_2/\eta_2 = 4/2 \times 8/7 \approx 2.28$
- $\mathtt{E} = \mathtt{V} \times \mathtt{D} = (13 \times \log_2(11)) \times (4/2 \times 8/7) \approx 102.79$

For a set of dataflow graphs, the volume and effort is given by the sum of the volume and the effort of each graph present in the set. The difficulty of the set is computed dividing its effort by its volume.

We now present the values obtained applying this metric to the same case studies used in Section 7.1. In HM, effort is the property that takes into account the volume/size and structure of the graphs, thus we believe the effort is the property computed by HM comparable to the complexity given by the MM.[4] For this reason, in this section we relate the values for effort with the complexity values previously obtained.

7.2.1 Gamma's Hash Joins

Table 7.6 shows the results obtained using HM for Gamma's Hash Joins and Gamma's Cascading Hash Joins dataflow graphs, and some of its derivations. The case studies used are the same used as in Table 7.1.

If we compare the columns `E` for the big-bang and derivational approaches with the values for complexity obtained with MM (previously shown in Table 7.1), we notice that the results can be explained in a similar way, even though the *Difference*s are not exactly the same. As for MM, in *HJoin (short)*,

[4] In Section 7.4 we show that the values obtained for complexity (MM) and effort (HM) are strongly correlated.

	Big Bang			Derivation			Difference
	V	D	E	V	D	E	E
HJoin (short)	97.5	3	292.6	97.0	1.88	182.4	**+significant**
HJoin (long)	97.5	3	292.6	262.5	2.02	529.9	**–significant**
Casc. HJoin (long)	217.7	3	653.0	312.6	1.92	600.3	**+small**
HJoin + Casc. HJoin (long)	315.2	3	945.5	324.2	1.89	611.9	**+significant**

Table 7.6: Gamma graphs' volume, difficulty and effort.

we have a lower value for the derivational approach (although now the difference is significant). The benefits of using the derivational approach (in terms of effort according to HM) disappear if we choose the long derivation (*HJoin (long)*). As for MM, in *Casc. HJoin (long)* and *HJoin + Casc. HJoin (long)*, the benefits of the derivational approach, even using the long derivation, become present again. Thus, HM also indicates that the derivational approach, when the reusability of rewrite rules is low and/or when optimizations are needed, is likely to be more complex/require additional effort. Moreover, as reuse increases, the benefits of the derivational approach increase.

We have, however, new metrics provided by HM. It is important to note that even though the derivational approach may require more effort when we have few opportunities for reuse and optimizations, the difficulty of the derivational approach is still typically lower than the difficulty of the big-bang approach. That is, even in those cases, the derivational approach contributes to make the representation of the program simpler (the additional effort results from the volume of the derivational approach, which is bigger than in the big-bang approach).

7.2.2 Dense Linear Algebra

Table 7.7 shows the results obtained using HM in the DLA programs.

In these case studies the results obtained using MM and HM are different. Whereas with MM the big-bang approach was always better than the derivational approach, with HM we conclude the derivational approach is sometimes better. Still, we can see a similar trend with both metrics: when we add more programs to be derived, the increase in complexity/effort is higher in the big-bang approach

	Big Bang			Derivation			Difference
	V	D	E	V	D	E	E
Chol (blk)	49.0	3	147.1	110.3	2.08	229.9	**–significant**
Chol (unblk)	32.3	2.25	72.6	146.3	1.95	285.8	**–significant**
Chol (dm)	118.9	5.7	677.7	256.4	2.21	567.0	**+small**
LU (blk)	35.8	2.67	95.6	67.1	1.89	126.8	**–noticeable**
LU (unblk)	35.8	2.67	95.6	85.15	1.92	163.6	**–significant**
LU (dm)	109.4	6.15	673.0	253.3	2.15	544.4	**+small**
Chol + LU	381.3	4.62	1761.7	557.4	1.95	1088.6	**+significant**

Table 7.7: DLA graphs' volume, difficulty and effort.

than in the derivational approach. That is, for the individual implementations we have four cases where the big-bang approach is better (with **noticeable** and **significant** differences), and two cases where the derivational approach is better (but with a **small** difference). When we group all implementations of both programs, the derivational approach becomes the best, and the difference becomes **significant**.

Moreover, as for Gamma's Hash Joins, we can also observe that the use of the derivational approach results in a bigger volume, but also in lower difficulty.

7.2.3 UpRight

Table 7.8 shows the results obtained using the HM for the variants of UpRight. As before, the case studies used are the same used to obtain the values presented in Table 7.3.

	Big Bang			Derivation			Difference
	V	D	E	V	D	E	E
SCFT	229.1	5	1145.6	378.0	2.02	762.5	**+significant**
ACFT	311.5	5.5	1713.4	590.8	2.13	1255.9	**+noticeable**
ASCFT	325.9	6.5	2118.6	550.5	1.96	1076.3	**+significant**
AACFT	405.9	6.5	2638.4	763.3	2.06	1572.6	**+significant**
UpRight All	1272.5	5.99	7616.0	1169.6	2.20	2573.8	**+significant**

Table 7.8: SCFT graphs' volume, difficulty and effort.

Again, the analysis of these results for effort is similar to the analysis we made for the results obtained using MM (Table 7.3). The derivational approach

provides the best results. We see an increase in the benefits of the derivational approach when we consider all programs together. As for the domains analysed previously in this section, we can observe that the use of the derivational approach results in a bigger volume (except when all programs are considered together), but lower difficulty.

7.2.3.1 Extensions

Table 7.9 shows the results obtained for the HM when using extensions.

	Big Bang			Derivation			Difference
	V	D	E	V	D	E	E
UpRight (ext.)	1272.5	5.99	7616.0	838.5	2.20	1476.8	**+significant**
UpRight (ext. all)	410.0	7.02	2878.1	690.0	2.14	1476.8	**+significant**

Table 7.9: UpRight variations' volume, difficulty and effort.

When we use extensions to model the variations of the rewrite rules used in the derivations, we can further increase the reuse of rewrite rules, reducing the effort associated with the derivations, as shown in the row *UpRight (ext.)*.

When the same approach is used for the initial and final graphs, the effort associated with the final graphs is reduced to less than a half, but the effort associated with the derivations is still **significantly** lower (row *UpRight (ext. all)*).

As for the MM, these numbers support the observation made in [RGMB12] that extensions are essential to handle complex software architectures.

7.2.4 Impact of Replication

In Table 7.10 we provide the values obtained with the HM for the case studies where replication was used.

The use of replication results in lower values for volume and effort. The difficulty is not affected significantly. As for MM, we verify that the reduction of effort is typically bigger in the big-bang approach than in the derivational approach.

	Big Bang			Derivation			Difference
	V	D	E	V	D	E	E
HJoin (long)	60	3	180	190.6	2.03	386.0	**–significant**
HJoin + Casc. HJoin (long)	170.6	3	511.7	242.6	1.87	453.6	**+small**
SCFT	100.9	5	504.3	225.2	2.05	461.5	**+small**

Table 7.10: Graphs' volume, difficulty and effort when using replication.

7.3 Graph Annotations

In the previous sections we presented the results of evaluating the complexity of graphs resulting from using the big-bang or the derivational approach when building programs. The metrics used only take the graph into account. There is, however, additional information contained in some graphs (*a.k.a.* annotations), which is used to express the knowledge needed to derive the programs. We are referring to the templates instantiation specification, the replication info, and the annotations used to specify extensions. Although this info is not represented by a graph, and therefore cannot be measured by MM, when using the HM we can take the additional info into account. To do so, we simply count the operators and operands present in the annotations, as usual for the HM when applied to source code.

> We caution readers that the following results put together numbers for concepts at different levels of abstraction, which probably should have a different "weight" in the metrics. However, we are not able to justify a complete separation and simply present the results with this warning.

7.3.1 Gamma's Hash Joins

In Table 7.10 we showed results for Gamma case studies when using replication. Replication reduces the complexity of the graphs. However, annotations on boxes and ports are needed to express how they are replicated. Table 7.11 adds the impact of these annotations to the values previously shown.

	Big Bang			Derivation			Difference
	V	D	E	V	D	E	E
HJoin (long)	81.7	5.25	429.1	282.3	2.96	835.5	**−significant**
HJoin + Casc. HJoin (long)	232.7	5.55	1291.3	355.8	2.57	915.3	**+noticeable**

Table 7.11: Gamma graphs' volume, difficulty and effort (including annotations) when using replication.

We previously mentioned that the use of replication results in higher reductions of complexity for the big-bang approach than for the derivational approach, making the ratios more favorable to the big-bang approach. However, when we add the impact of the replication annotations, we notice that (i) replication increases difficulty and effort (when compared to the results from Table 7.6),[5] and (ii) the positive impact on ratios for the big-bang approach becomes lower. For example, whereas in Table 7.10 the difference between the big-bang and derivational approaches for *HJoin + Casc. HJoin (long)* was **small**, the same difference is now **noticeable**.

7.3.2 Dense Linear Algebra

In DLA domain we make use of templates to reduce the number of rewrite rules we need to specify. Table 7.12 adds the impact of the annotations needed to specify the valid templates instantiations to the values previously presented in Table 7.7.[6]

	Big Bang			Derivation			Difference
	V	D	E	V	D	E	E
LU (dm)	118.9	5.7	677.7	280.4	2.11	591.0	**+small**
Chol + LU	381.3	4.62	1761.7	592.0	1.90	1123.2	**+significant**

Table 7.12: DLA graphs' volume, difficulty and effort (including annotations).

[5] It is worth mentioning, however, that the models using replication are more expressive than the models that do not use replication. In models using replication an element (box, port, connector) may be replicated any number of times, whereas in the models considered for Table 7.6 boxes are replicated a predefined number of times.

[6] Templates are only useful in the distributed memory version of LU factorization and when we put all implementations together, even though in Section 4.2 we have used templatized rewrite rules in other derivations. In this study, in the cases templates did not provide benefits, they were not used. Therefore only two rows of the table are shown.

In this case the annotations affect the derivational approach only. Still, the impact is minimal and the differences between both approaches are not affected significantly, which means the derivational approach has better results, although the differences are slightly lower.

7.3.3 UpRight

In the different UpRight scenarios considered before, we used annotations for replication, templates, and extensions. Table 7.13 adds the impact of these annotations to the values previously presented in Tables 7.8, 7.9, and 7.10.

	Big Bang			Derivation			Difference
	V	D	E	V	D	E	E
SCFT	229.1	5	1145.6	537.9	1.73	932.5	**+small**
UpRight All	1272.5	5.99	7616.0	1329.5	2.06	2743.8	**+significant**
UpRight (ext.)	1272.5	5.99	7616.0	961.6	2.43	2333.7	**+significant**
SCFT (replication)	154.8	11.37	1759.7	565.0	3.02	1703.7	**+small**

Table 7.13: SCFT graphs' volume, difficulty and effort.

In rows *SCFT* and *UpRight All* we are taking into account the impact of the template annotations on the numbers presented in Table 7.8. The numbers for the derivational approaches become higher, *i.e.*, the benefits of the derivational approach are now smaller. Still, in both cases the derivational approach has lower effort, and when considering all program, the difference is **significant**.

Row *UpRight (ext.)* adds the impact of template and extension annotations to the numbers presented in Table 7.9. There is an increase in volume, difficulty and effort. However, the big-bang approach still requires **significantly** more effort than the derivational approach.

Finally, row *SCFT (replication)* adds the impact of template and replication annotations to the numbers presented in Table 7.10. On one hand, we have template annotations that penalize the derivational approach. On the other hand, we have replication annotations that penalize more the big-bang approach. Thus, the derivational approach is still better than the big-bang approach, and the difference remains small.

7.4 Discussion

We believe that our proposed metrics provide reasonable measures for the complexity/effort associated with the use of each approach. The HM captures more information about the graphs, which make us believe it is more accurate. Moreover, HM provides values for different aspects of the graphs, whereas MM only provides an estimate for complexity (that we consider similar to the effort in HM). However, we notice that both metrics provided comparable results, which are typically explained in similar ways.[7]

The numbers provide insights about which approach is better. Even though it is difficult to define a criteria to determine what differences are significant, the numbers in general show a common trend: as more programs are considered (for a certain domain) the complexity/effort of the derivational approach has lower increase than the complexity of the big-bang approach, and eventually the derivational approach becomes better. This is consistent with the benefits we can expect from modularizing a program's source code, where we are likely to increase the amount of code needed if there are no opportunities for reuse. However, when we have to implement several programs in the same domain, we can expect to be able to reuse the modules created. Even when this is not case, modularized program may require more code, but we expect to benefit from modularizing a program by dividing the problem in smaller parts, easier to understand and maintain than the whole [Par72].

Besides the trend observed when the number of programs in a domain increases, we also note that the type of transformations used in each domain influences the benefits of using a derivational approach. For example, in domains such as databases or DLA we have refinements/optimizations that remove boxes, which reduce the complexity of the resulting architecture, favouring the big-bang approach. On the other hand, almost all optimizations used in UpRight (rotations) increase the complexity of the resulting architecture, therefore we are likely

[7] The Pearson correlation coefficient for the complexity/effort of the 39 distinct pairs is 0.9579 ($p < 0.00001$), which denotes a strong positive linear correlation between complexity (MM) and effort (HM).

to obtain results more favorable to the derivational approach earlier (*i.e.*, with less programs being derived) in this domain.

In the more complex scenario we have (UpRight without extensions), the complexity of the big bang approach is `1.7` times greater than the complexity of the derivational approach, and the effort for the big-bang approach is `2.8` times greater than for the derivational approach (when we consider annotations), which we believe it is a significant difference to justify the use of the derivational approach.

Not all knowledge of a graph or rewrite rules is captured in the graph structure and size. Therefore, for the HM we also presented numbers that take into account different types of graph annotations supported by `ReFlO`. These results still show benefits for the derivational approach.

Metrics and controlled experiments: perspective. Before we started looking for metrics to compare the big-bang with the derivational approach, controlled experiments have been conducted to answer questions such as *which approach is better to understand a program?*, or *which approach is better to modify a program?*. The Gamma's Hash Joins (long derivation) and SCFT programs were used in these studies. Our work on the derivational approach was originally motivated by the difficulties in understanding a program developed using the big-bang approach. The use of the derivational approach allowed us to tackle these difficulties, and understand the program design. Thus, we assumed from the beginning that the use of a derivational approach would be beneficial. However, the experimental results did not support this hypothesis, as no significant difference was noted regarding ability to understand or modify the programs using the different approaches, which surprised us. The results obtained with these metrics help us to understand those results. Considering the result of Table 7.11 (row *HJoin (long)*) and Table 7.13 (row *SCFT (replication)*), where we have numbers for the forms of the case studies used closer to the ones used in the controlled experiments, we can see that, for Gamma's Hash Joins, the derivational approach requires more effort (according to HM) than the big bang approach,

and for SCFT both approaches require similar amounts of effort. This is consistent with the results obtained in the first controlled experiments [FBR12]. On the other hand, the derivational approach has lower difficulty. That is, the lower difficulty should make it easier for users to understand the program when using the derivational approach, which is likely to make users to prefer this kind of approach. This match the results obtained for the second series of controlled experiments [BGMS13]. Considering the additional volume required by the derivational approach, it is expected that the derivational approach does not provide better results in the case studies considered (particularly in terms of time spent when using a particular approach).

Chapter 8

Related Work

8.1 Models and Model Transformations

The methodology we propose, as previously mentioned, is built upon ideas promoted by KBSE. Unfortunately, the reliance on sophisticated tools and specification languages compromised its success [Bax93], and few examples of successful KBSE systems exist. AMPHION [LPPU94] is one of them. It uses a DSL to write abstract specifications (theorems) of problems to solve, and term rewriting to convert the abstract specification in a program. The AMPHION knowledge base captures relations between abstract concepts and their concrete implementation in component libraries, allowing it to find a way of composing library components that is equivalent to the specification. Their focus was on the conversion between different abstraction levels (*i.e.*, given a specification AMPHION would try to synthesize an implementation for it), not the optimization of architectures to achieve properties such as efficiency or availability.

Rule-based query optimization (RBQO) structured and reduced the complexity of query optimizers by using query rewrite rules, and it was essential in the building of extensible database systems [Fre87, GD87, HFLP89]. Given a query, a query optimizer has to find a good *query evaluation plan (QEP)* that provides an efficient strategy to obtain the results from the database system. In RBQO the possible optimizations are described by transformation rules, provid-

ing a high-level implementation independent, notation for this knowledge. In this way, the rules are separated from the optimization algorithms, increasing modularity and allowing incremental development of query optimizers, as new rules can be added, either to support more sophisticated optimizations or optimization for new features of the database, without changing the algorithms that apply the rules. The transformation rules specify equivalence between queries, *i.e.*, they say that a query which matches a pattern (and possibly some additional conditions), may be replaced by other query.[1]

Rules also specify the valid implementations for query operators. Based on the knowledge stored in these rules, a rewrite engine produces many equivalent QEPs. Different approaches can be used to choose the rules to apply at each moment, and to reduce the number of generated QEPs, such as priorities attributed by the user [HFLP89], or the gains obtained in previous applications of the rules [GD87]. Later, cost functions are used to estimate the cost of each QEP, and the most efficient is chosen. This is probably the most successful example of the use of domain-specific knowledge, encoded as transformations, to map high-level program specifications to efficient implementations.

It is well-known that the absence of information of the design process that explains how an implementation is obtained from a specification complicates software maintenance [Bax92]. This led Baxter to propose a structure for a design maintenance system [Bax92].

We use a dataflow notation in our work. This kind of graphical notation has been used by several other tools such as LabVIEW [Lab], Simulink [Sim], Weaves [GR91], Fractal [BCL+06], or StreamIt [Thi08]. However, they focus on component specification and construction of systems composing those components. We realized that transformations (in particular optimizations) play an essential role when building efficient architectures using components. LabVIEW does support optimizations, but only when mapping a LabVIEW model to an

[1] In effect, this is basic mathematics. (Conditionally-satisfied) equals are replaced by equals. In doing so, the semantics of the original query is never changed by each rewrite. However, the performance of the resulting plan may be different. Finding the cheapest plan that has the same semantics of the original query is the goal of RBQO.

executable. Users can *not* define refinements and optimizations, but LabVIEW compiler technicians can. More than using a dataflow notation for the specification of systems, we explore it to encode domain-specific knowledge as dataflow graph transformations.

In the approach we propose, transformations are specified declaratively, providing examples of the graph "shapes" that can be transformed (instead of defining a sequence instructions that result in the desired transformation), which has two main benefits. First, it makes easier for domain experts (the ones with the knowledge about the valid domain transformations) to specify the transformations [Var06, BW06, WSKK07, SWG09, SDH+12]. Other approaches have been proposed to address this challenge. Baar and Whittle [BW06] explain how a metamodel (*e.g.*, for dataflow graphs) can be extended to also support the specification of transformations over models. In this way, a concrete syntax, similar to the syntax used to define models, is used to define model transformations, making those transformations easier to read and understand by humans. We also propose the use of the concrete syntax to specify the transformations. *Model transformation by example (MTBE)* [Var06, WSKK07] proposes to (semi-)automatically derive transformation rules based on set of key examples of mappings between source and target models. The approach was improved with the use of Inductive Logic Programming to derive the rules [VB07]. The rules may later be manually refined. Our rules provide examples in minimal context, and unlike in MTBE, we do not need to relate the objects of the source and target model (ports of interfaces are implicitly related to the ports of their implementations). Additionally, MTBE is more suited for exogenous transformations, whereas we use endogenous transformations [EMM00, HT04]. More recently, a similar approach, *model transformation by demonstration* [SWG09] was proposed, where users show how source models are edited in order to be mapped to the target models. A tool [SGW11] captures the user actions and derives the transformations conditions and the operations needed to perform the transformations. However, in our approach it is enough to provide the original element and its possible replacements.

The other benefit of our approach to specify transformations is that it makes domain knowledge (that we encode as transformations) more accessible to non-experts, as this knowledge is encoded in a graphical and abstract way, relating alternative ways of implementing a particular behavior. Capturing algebraic identities is on the base of algebraic specifications and term rewriting systems. RBQO [Loh88, SAC+79] is also a successful example of the application of these ideas, where, as in our case, the goal is to optimize programs. Program verification tools, such as CafeOBJ [DFI99] or Maude [CDE+02], are another common application. As our transformations are often bidirectional, our system is in fact closer to a *Thue system* [Boo82] than an abstract rewriting system [BN98].

Graph grammars [Roz97] are a well-known method to specify graph transformations. They also provide a declarative way to define model/graph transformations using examples. In particular, our rules are specified in a similar way to productions in the *double-pushout approach* for hypergraphs [Hab92]. Our transformations are better captured by hypergraph rewrite rules, due to the role of ports in the transformations (that specify the gluing points in the transformation). Despite the similarities, we did not find useful results in the theory of graphs grammars to apply in our work. In particular, we explored the use of critical pair analysis [Tae04] to determine when patterns would not need to be tested, thus improving the process of detecting opportunities for optimization.[2]

Our methodology provides a framework for model simulation/animation, which allows developers to predict properties of the system being modeled without having to actually build it. LabVIEW and Simulink are typical examples of tools to simulate dataflow program architectures. Ptolemy II [EJL+03] provides modeling and animation support for heterogeneous models. Other tools exist for different types of models, such as UML [CCG+08, DK07], or Colored Petri Nets [RWL+03].

Our work has similarities with *model-driven performance engineering*

[2]The results obtained were not useful in practice, as (i) there were too many overlaps in the rules we use, meaning that pattern would have to be tested almost always, and (ii) even with smaller models the computation of critical pairs (using the Agg tool) would take hours, and often fail due to lack of hardware resources.

(MDPE) [FJ08]. However, we focus on endogenous transformations, and how those transformations improve architecture's quality attributes, not exogenous transformations, as it is common in MDPE. Our solution for cost estimation can be compared with the *coupled model transformations* proposed by Becker [Bec08]. However, the cost estimates (as well as other interpretations) are transformed in parallel with the program architecture graphs, not during $\mathcal{M}2\mathcal{T}$ transformations. Other solutions have been proposed for component based systems [Koz10]. KLAPER [GMS05] provides a language to automate the creation of performance models from component models. Kounev [Kou06] shows how *queueing Petri nets* can be used to model systems, allowing prediction of its performance characteristics. The *Palladio component model* [BKR09] provides a powerful metamodel to support performance prediction, adapted to the different developer roles. We do not provide a specific framework for cost/performance estimates. Instead, we provide a framework to associate properties with models, which can be used to attain different goals.

Properties are similar to attributes in an *attributed graph* [Bun82] which are used to specify pre- and postconditions. Allowing implementations to have stronger preconditions than their interfaces, we may say that the rewrite rules may have *applicability predicates* [Bun82] or *attribute conditions* [Tae04], which specify a predicate over the attributes of a graph when a match/morphism is not enough to specify whether a transformation can be applied. Pre- and postconditions were used in other component systems, such as Inscape [Per87], with the goal of validating component compositions. In our case, the main purpose of pre- and postconditions is to decide when transformations can be applied. Nevertheless, they may also be used to validate component compositions.

Abstract interpretations [CC77, NNH99] define properties about a program's state and specify how instructions affect those properties. The properties are correct, but often imprecise. Still, they provide useful information for compilers to perform certain transformations. In our approach, postconditions play a similar role. They compute properties about operation outputs based on properties of their inputs, and the properties may be used to decide whether a transformation

can be applied or not. As for abstract interpretations, the properties computed by postconditions have to describe output values correctly. In contrast, properties used to compute costs, for example, are often just estimates, and therefore may not be correct, but in this case approximations are usually enough. The Broadway compiler [GL05] used the same idea of propagating properties about values, to allow the compiler to transform the program. Broadway separated the compiler infrastructure from domain expertise, and like in our approach, the goal was to allow users to specify domain-specific optimizations. However, Broadway had limitations handling optimizations that replace complex compositions of operations. Specifying pre- and postconditions as properties that are propagated is also not new. This was the approach used in the Inscape environment [Per89a, Per89b], and later by Batory and Geraci [BG97], and Feiler and Li [FL98]. Interpretations provide alternative views of a dataflow graph that are synchronized as it is incrementally changed [RVV09].

8.2 Software Product Lines

We use extensions to support optional features in dataflow graphs, effectively modeling an SPL of dataflow graphs. There are several techniques in which features of SPLs can be implemented. Some are compositional, including AHEAD [Bat04], FeatureHouse [AKL09], and AOP [KLM+97], all of which work mainly at code level. Other solutions have been proposed to handle SPLs of higher-level models [MS03, Pre04].

We use an annotative approach, where a single set of artifacts, containing all features/variants superimposed, is used. Artifacts (*e.g.*, code, model elements) are annotated with feature predicates to determine when these artifacts are visible in a particular combination of features. Preprocessors are a primitive example [LAL+10] of a similar technique. Code with preprocessor directives can be made more understandable by tools that color code [FPK+11] or that extract views from it [SGC07]. More sophisticated solutions exist, such as XVCL [JBZZ03], Spoon [Paw06], Spotlight [CPR07], or CIDE [KAK08]. How-

ever, our solution works at a model level, not code.

Other annotative approaches also work at the model level. In [ZHJ04] an UML profile is proposed to specify model variability in UML class diagrams and sequence diagrams. Czarnecki and Antkiewicz [CA05] proposed a template approach, where model elements are annotated with presence conditions (similar to our feature predicates) and meta-expressions. FeatureMapper [HKW08] allows the association of model elements (*e.g.*, classes and associations in a UML class diagram) to features. Instead of annotating final program architectures directly (usually too complex), we annotate model transformations (simpler) that are used to derive program implementations. This reduces the complexity of the annotated models, and it also makes the extensions available when deriving other implementations, making extensions more reusable.

We provide an approach to extract an SPL from legacy programs. REPLACE [BGW+99] is an alternative to reengineer existing systems into SPLs. FeatureCommander [FPK+11] aids users visualizing and understanding the different features encoded in preprocessor-based software. Other approaches have been proposed with similar intent, employing refactoring techniques [KMPY05, LBL06, TBD06].

Extracting variants from an XRDM is similar to program slicing [Wei81]. Slicing has been generalized to be used with models [KMS05, BLC08], in order to reduce its complexity and make easier for developers to analyse models. These approaches are focused on the understandability of the artifacts, whereas in our work the focus is on rule variability. Nevertheless, `ReFlO` projections remove elements from rewrite rules that are not needed for a certain combination of features, which we believe also contribute to improve rewrite rules understandability. In [Was04] Wasowski proposes a slice-based solution where SPLs are specified using restrictions that remove features from a model, so that a variant can be obtained.

`ReFlO` supports analyses to verify whether all variants of an XRDM that can be produced meet the metamodel constrains. The analysis method used is based on solutions previously proposed by Czarnecki and Pietroszek [CP06] and

Thaker *et al.* [TBKC07].

8.3 Program Optimization

Peephole optimization [McK65] is an optimization technique that looks at a sequence of low-level instructions (this sequence is called the *peephole*, and its size is usually small), and tries to find an alternative set of instructions, which produces the same result, but that is more efficient. There are several optimizations this technique enables. For example, it can be use to compute expressions involving only constants in compile time, or to remove unnecessary operations, which sometimes result from the composition of high-level operations. Compilers also use loop transformations in order to get more efficient code, namely improving data locality or exposing parallelism [PW86, WL91, WFW+94, AAL95, BDE+96]. Data layout transformations [AAL95, CL95] is another strategy that can be used to improve locality and parallelism. The success of these kind of techniques is limited for two reasons: the compiler only has access to the code, where most of the information about the algorithm was lost, and sometimes the algorithm used in the sequential code is not the best option for a parallel version of the program.

When using compilers or when using libraries, sometimes there are parameters that we can vary to improve performance. PHiPAC [BACD97] and ATLAS [WD98] address this question with parameterized code generators that produce the different functions with different parameters, and time them in order to find out which parameters should be chosen for a specific platform. Yotov *et al.* [YLR+05] proposed an alternative approach, where although they still use code generators, they try to predict the best parameters using a model-driven approach, instead of timing the functions with different parameters. Several algorithms were proposed to estimate the optimal parameters [DS90, CM95, KCS+99].

Spiral [PMS+04] and Build to Order BLAS [BJKS09] are examples of domain specific tools to support the generation of efficient low-level kernel func-

tions, where empirical search is employed to choose the best implementation. In this work the focus is not the automation of the synthesis process, but the methodology used to encode the domain. Tools such as Spiral or Build to Order BLAS are useful when we have a complete model of a domain, whereas the tools we propose are to be used both by domain experts in the process of building those domain models, and later by other developers to optimize their programs. Nevertheless, this research work is part of a larger project that also aims to automate the derivation of efficient implementations. Therefore, we provide the ability to export our models to code that can be used with DxTer [MPBvdG12, MBS12] a tool that, like Spiral and Build to Order BLAS, automates the design search for the optimized implementation. The strategy we support to search the design space is based on cost functions, and not on empirical search.

Program transformations have been used to implement several optimizations in functional programming languages, such as function call inline, conditionals optimizations, reordering of instructions, function specialization, or removal of intermediate data structures [JS98, Sve02, Voi02, Jon07]. Although this method is applied at higher levels of abstraction than loop transformations or peephole optimization, this approach offers limited support for developers to extend the compiler with domain-specific optimizations.

In general, our main focus is on supporting higher-level domain-specific design decisions, by providing an extensible framework to encode expert knowledge. However, our approach is complemented by several other techniques that may be used to optimize the lower-level code implementations we rely on when generating code.

8.4 Parallel Programming

Several techniques have been proposed to overcome the challenges presented by parallel programming. One of the approaches that has been used is the development of languages with explicit support to parallelism. Co-array Fortran [NR98], Unified Parallel C (UPC) [CYZEG04], and Titanium [YSP+98] are extensions

to Fortran, C and Java, respectively, which provide constructors for parallel programming. They follow the *partitioned global address space (PGAS)* model, which presents to the developer a single global address space, although it is logically divided among several processors, hiding communications from developers. Nevertheless, the developer still has to explicitly distribute the data, and assign work to each process. Mixing the parallel constructors with the domain-specific code, programs become difficult to maintain and evolve.

Z-level Programming Language (ZPL) [Sny99] is an array programming language. It supports the distribution of arrays among distributed memory machines, and provides implicit parallelism on the operations over distributed arrays. The operations that may require communications are, however, explicit, which allows the developer to reason about performance easily (WYSIWYG performance model [CLC+98]). However, this language can only explore data parallelism and when we use array based data structures. Chapel [CCZ07] is a new parallel programming languages, developed with the goal of improving productivity in the development of parallel programs. It provides high-level abstractions to support data-parallelism, task-parallelism, concurrency, and nested parallelism, as well as the ability to specify how data should be distributed. It tries to achieve a better portability avoiding assumptions about the architecture. Chapel is more general than ZPL, as it is not limited to data parallelism in arrays. However, the developer has to use language constructors to express more complex forms of parallelism or data distributions, mixing parallel constructors and domain-specific code, and making programs difficult to maintain and evolve.

Intel Threading Building Blocks (TBB) [Rei07] is a library and framework that uses C++ templates to support parallelism. It provides high-level abstractions to encode common patterns of task parallelism, allowing the programmer to abstract the platform details. OpenMP [Boa08] is a standard for shared memory parallel programming in C, C++ and Fortran. It provides a set of compiler directives, library routines and variables to support parallel programming and allows incremental development, as we can add parallelism to a program adding annotations to the source code, in some cases without need to change the original

code. It provides high-level mechanisms to deal with scheduling, synchronization, or data sharing. These approaches are particularly suited for some well-known patterns of parallelism (*e.g.*, the parallelization of a loop), but they offer limited support for more complex patterns, which requires considerable effort from the developer to explore them. Additionally, these technologies are limited to shared memory parallelism.

These approaches raise the level of abstraction at which developers work, hiding low-level details with more abstract language concepts or libraries. Nevertheless, the developer still has to work at code level. Moreover, none of the approaches allow the developer to easily change the algorithms, or provide high-level notations to specify domain-specific optimizations.

Some frameworks take advantage of algorithmic skeletons [Col91], which can express the structure of common patterns used in parallel programming [DFH+93]. To obtain a program, this structure is parameterized by the developer with code that implements the domain functionality. A survey on the use of algorithmic skeletons for parallel programming is presented in [GVL10]. These methodologies/frameworks raise the level of abstraction, and remove parallelization concerns from domain code. However, developers have to write the code according to rules imposed by frameworks, and using the abstractions provided by them. Skeletons may support optimization rewrite rules to improve performance on compositions of skeletons [BCD+97, AD99, DT02]. However, they are limited to general (predefined) rules, and do not support domain-specific optimizations.

One of the problems of parallel programming is the lack of modularity. In traditional approaches the domain code is usually mixed with parallelization concerns, and these concerns are spread among several modules (tangling and scattering in aspect-oriented terminology) [HG04]. Several works have used *aspect-oriented programming (AOP)* [KLM+97] to address this problem. Some of them tried to provide general mechanisms for parallel programming, for shared memory environments [CSM06], distributed memory environments [GS09], or grid environments [SGNS08]. Other works focused on solutions for particular soft-

ware applications [PRS10]. AOP can be used to map sequential code to parallel code without forcing the developer to write its code in a particular way. However, starting with a sequential implementation, the developer is not able to change the algorithm used. In our approach, we leverage from the fact we start with an abstract program specification, where we have the flexibility to choose the algorithms to be used during the derivation process. Finally, AOP is limited regarding the transformations that it can make to code/programs. For example, it is difficult to use AOP to apply optimizations that break encapsulation boundaries.

Chapter 9

Conclusion

The growing complexity of hardware architectures has moved the burden of improving performance of programs from hardware manufacturers to software developers, forcing them to create more sophisticated software solutions to make full use of hardware capabilities.

Domain experts created (reusable) optimized libraries. We argue that those libraries offer limited reusability. More important (and useful) than being able to reuse operations provided by libraries, is to be able to reuse the knowledge that was used to build those libraries, as knowledge offers additional opportunities for reuse. Therefore, we proposed an MDE approach to shift the focus from optimized programs/libraries to the knowledge used to build them.

In summary, the main contributions of this thesis are:

Conceptual framework to encode domain knowledge. We defined a framework to encode and systematize domain knowledge that experts use to build optimized libraries and program implementations. The models used to encode knowledge relate the domain operations with their implementation, capturing the fundamental equivalences of the domain. The encoded knowledge defines the transformations—refinements and optimizations—that we can use to incrementally map high-level specifications to optimized program implementations. In this way, the approach we propose contributes to make domain knowledge and optimized pro-

grams/libraries more understandable to non-experts. The transformations can be mechanically applied by tools, thus enabling non-experts to reuse expert knowledge. Our framework also uses extension transformations, where we can incrementally produce derivations with more and more features (functionality), until a derivation with all desired features is obtained. Moreover, extensions provide a practical mechanism to encode product lines of domain models, and to reduce the amount of work required to specify knowledge in certain application domains.

Interpretations framework. We designed an interpretations mechanism to associate different kinds of behavior to models, allowing users to animate them and predict properties about the programs they are designing. Among the applications of interpretations is the estimation of different performance costs, as well as code generation.

`ReFlO` tool. We developed `ReFlO` to validate our approach and show that we can mechanize the development process with the knowledge we encoded. The development of `ReFlO` was essential to understand the limitations of preliminary versions of the proposed approach, and improve it, in order to support the different case studies defined.

Our work is built upon simple ideas (refinement, optimization, and extension transformations). Nevertheless, more sophisticated details are required to apply it in a broad range of case studies (*e.g.*, pre- and postconditions, supported by alternative representations), to make the approach more expressive in representing knowledge (*e.g.*, replication), or to reduce the amount of work required to encode knowledge (*e.g.*, templates). Besides optimizations, we realized that the ability to use nonrobust algorithms is also essential to allow the derivation of efficient program implementations in certain application domains.

We rely on a DSML to specify transformations and program architectures. We believe that providing a graphical notation and tools (along with the declarative nature of rewrite rules) is important to the success of the approach. However, the use of graphical modeling notations also has limitations. For example,

tools to work with graphical model representations are typically significantly less mature and stable than tools to work with textual representations.

We use a dataflow notation but we do not impose a particular model of computational or strategy to explore parallelism. Different domains may use different ways to define how programs execute when mapped to code (*i.e.*, when is each operation/box executed, how data is communicated, etc.), or how parallelism is obtained (*e.g.*, by using the implicit parallelism exposed by a dataflow graph, or using an SPMD approach).

We showed how `ReFlO` could be used in different domains, where existing programs were reverse engineered, to expose the development process as a sequence of incremental transformations, and contributing to make the process systematic. Not all domains may be well suited for this approach, though (because algorithms and programs are not easily modeled using dataflow models, or because the most relevant optimizations are decided at runtime—as it often happens in irregular applications—, for example). The same applies to the types of parallelism explored (low-level parallelism, such as ILP, would require to expose too many low-level details in models, erasing the advantages of models in handling the complexity of programs). We focused on regular domains, and loop- and procedure-level parallelism.

We provide the ability to export knowledge encoded in `ReFlO` to an external tool, DxTer, which automates the search for the best implementation of a program. However, we note that there are different ways to model equivalent knowledge, and the best way to model it for interactive (mechanical) development and for automated development may not be the same. For interactive development we try to use small/simple rules, which are typically easier to understand, and better to expose domain knowledge. DxTer often requires several simple rules to be joined together (and replaced) to form a more complex rule, in order to reduce the size of the design space generated by those rules. As an automated system, unlike humans, DxTer can easily deal with complex rewrite rules, and benefit from the reduced design space obtained in this way.

We believe that our approach is an important step to make the process of

developing optimized software more systematic, and therefore more understandable and reusable. The knowledge systematization contributes to bring software development closer to a science, and it is the first step to enable the automation of the development process.

9.1 Future Work

In order to improve the DxT approach and `ReFlO` tool different lines of research can be explored in future work. We describe some below:

Loop transformations. Support for lower-level optimization techniques, such as loops transformations, is an important improvement for this work. It would allow us to leverage from domain-specific knowledge to overcome compiler limitations in determining when and how loop transformations can be applied, namely when the loop bodies involve calls to complex operations or even to external libraries (which complicates the computation of the information necessary to decide whether the loop transformation can be applied) [LMvdG12]. This would require us to add support for loops in our notation, which we believe is feasible. However, the development of a mechanism to support loop transformations in multiple domains may be challenging. This topic was explored for the DLA domain [LMvdG12, Mar14], but its solution is not easily applicable to other domains.

Irregular Domains. During our research we applied our approach and tools to different domains. We have worked mainly with regular domains, however we believe the approach may also be useful when dealing with irregular application domains. (In fact, we recently started working with an irregular domain—*phylogenetic reconstruction* [YR12]—that showed promising results, although it also required more sophisticated dataflow graphs and components to deal with the highly dynamic nature of the operations used [NG15].)

Additional hardware platforms. In the case studies analysed we deal with general purpose shared and distributed memory systems. However, GPUs (and other types of hardware accelerators) are also an important target hardware platform that is worth exploring. Basic support for GPUs may be obtained choosing primitive implementations optimized for GPUs, but DxT/`ReFlO` may also be useful to optimize compositions of operations, avoiding (expensive) memory copies (in the same way we optimize compositions of redistributions in DLA to avoid communications).

Connection with algorithmic skeletons. Algorithmic skeletons have been used to define well-known parallel patterns, some of them capturing the structure of parallel implementations we used when encoding domains with DxT/`ReFlO`. We believe it is worth exploring the complementarity of DxT/`ReFlO` and algorithmic skeletons, namely to determine whether it can be used as a skeletons framework (such framework should overcome a typical limitation of skeletons frameworks regarding the specification of domain-specific optimizations).

DSL for interpretations. Probably the most important topic to explore is a DSL for interpretations (currently specified using Java code), in order to raise the level of abstraction at which they are specified, and to make easier to export the knowledge they encode to other formats and tools. In particular, this would allow to export (certain) interpretations to DxTer, improving the integration between this tool and `ReFlO`. Moreover, specific features targeting common uses for interpretations (*e.g.*, pre- and post-conditions, cost estimates, code generation) could be considered. In order to determine the expressiveness and features required by such a DSL, we believe, however, it would be necessary to explore additional domains.

Workflow specification language. Workflow systems are becoming more and more popular to model scientific workflows [DGST09]. Even though it was not developed as a workflow system, `ReFlO` provides some useful features for this purpose, namely its graphical capabilities, its flexible model of

computation, its interpretations framework, and the ability to encode possible refinements and optimizations for abstract workflows, which would allow scientists to customize the workflow for their use cases. Therefore, we believe it would be worth exploring the use of `ReFlO` as a workflow system.

`ReFlO` usability and performance improvements. When dealing with graphical models, usability is often a problem. Unfortunately, and despite significant improvements in the recent past, libraries and frameworks to support the development of graphical modeling tools have limitations, which compromises their adoption. In particular, `ReFlO` would greatly benefit from a better automatic graph layout engine, specialized for the notation we use. Several other improvements can be applied to enhance `ReFlO` usability, namely providing features that users typically have when using code (*e.g.*, better copy/paste, reliable undo/redo, search/replace). The use of lower-level frameworks would be necessary to provide these improvements. This would also allow the optimization of the transformation engine provided by `ReFlO`, in case performance becomes a concern.

Empirical studies. Empirical studies have been conducted to validate the DxT approach [FBR12, BGMS13]. Still, additional studies would be useful to better evaluate DxT/`ReFlO`, and determine how they can be further improved.

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