

Interpreter and Transpiler for Simple Expressions on Nvidia GPUs using Julia

Daniel Roth



MASTERARBEIT

eingereicht am
Fachhochschul-Masterstudiengang

Software Engineering

in Hagenberg

im Januar 2025

Advisor:

DI Dr. Gabriel Kronberger

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Declaration

I hereby declare and confirm that this thesis is entirely the result of my own original work. Where other sources of information have been used, they have been indicated as such and properly acknowledged. I further declare that this or similar work has not been submitted for credit elsewhere. This printed copy is identical to the submitted electronic version.

Hagenberg, January 1, 2025

Daniel Roth

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Abstract

This should be a 1-page (maximum) summary of your work in English.

Kurzfassung

An dieser Stelle steht eine Zusammenfassung der Arbeit, Umfang max. 1 Seite. ...

Chapter 1

Introduction

This chapter provides an entry point for this thesis. First the motivation of exploring this topic is presented. In addition, the research questions of this thesis are outlined. Lastly the methodology on how to answer these questions will be explained. This master thesis is associated with the FFG COMET project ProMetHeus (#904919). The developed software is used and further developed for modelling in the ProMetHeus project.

1.1 Background and Motivation

Optimisation and acceleration of program code is a crucial part in many fields. For example video games need optimisation to lower the minimum hardware requirements which allows more people to run the game, increasing sales. Another example where optimisation is important are computer simulations. For those, optimisation is even more crucial, as this allows the scientists to run more detailed simulations or get the simulation results faster. Equation learning or symbolic regression is another field that can heavily benefit from optimisation. One part of equation learning, is to evaluate the expressions generated by a search algorithm which can make up a significant portion of the runtime. This thesis is concerned with optimising the evaluation part to increase the overall performance of equation learning algorithms.

The following expression $5 - \text{abs}(x_1) \sqrt{p_1}/10 + 2^{x_2}$ which contains simple mathematical operations as well as variables x_n and parameters p_n is one example that can be generated by the equation learning algorithm. Usually an equation learning algorithm generates multiple of such expressions per iteration. Out of these expressions all possibly relevant ones have to be evaluated. Additionally, multiple different values need to be inserted for all variables and parameters, drastically increasing the amount of evaluations that need to be performed.

In his blog, Sutter (2004) described how the free lunch is over in terms of the ever-increasing performance of hardware like the CPU. He states that to gain additional performance, developers need to start developing software for multiple cores and not just hope that on the next generation of CPUs the program magically runs faster. While this approach means more development overhead, a much greater speed-up can be achieved. However, in some cases the speed-up achieved by this is still not large enough and another approach is needed. One of these approaches is the utilisation

of Graphics Processing Units (GPUs) as an easy and affordable option as compared to compute clusters. Especially when talking about performance per dollar, GPUs are very inexpensive as found by Brodtkorb et al. (2013). Michalakes and Vachharajani (2008) have shown a noticeable speed-up when using GPUs for weather simulation. In addition to computer simulations, GPU acceleration also can be found in other places such as networking (S. Han et al., 2010) or structural analysis of buildings (Georgescu et al., 2013). These solutions were all developed using CUDA¹. However, it is also possible to develop assembly like code for GPUs using Parallel Thread Execution (PTX)² to gain more control.

1.2 Research Question

With these successful implementations of GPU acceleration, this thesis also attempts to improve the performance of evaluating mathematical equations, generated at runtime for symbolic regression using GPUs. Therefore, the following research questions are formulated:

- How can simple arithmetic expressions that are generated at runtime be efficiently evaluated on GPUs?
- Under what circumstances is the evaluation of simple arithmetic expressions faster on a GPU than on a CPU?
- Under which circumstances is the interpretation of the expressions on the GPU or the translation to the intermediate language Parallel Thread Execution (PTX) more efficient?

Answering the first question is necessary to ensure the approach of this thesis is actually feasible. If it is feasible, it is important to evaluate if evaluating the expressions on the GPU actually improves the performance over a parallelised CPU evaluator. To answer if the GPU evaluator is faster than the CPU evaluator, the last research question is important. As there are two major ways of implementing an evaluator on the GPU, they need to be implemented and evaluated to finally state if evaluating expressions on the GPU is faster and if so, which type of implementation results in the best performance.

1.3 Thesis Structure

In order to answer the research questions, this thesis is divided into the following chapters:

Chapter 2: Fundamentals and Related Work

In this chapter, the topic of this thesis is explored. It covers the fundamentals of equation learning and how this thesis fits into this field of research. In addition, the fundamentals of General Purpose GPU computing and how interpreters and transpilers work are explained. Previous research already done within this topic is also explored.

¹<https://developer.nvidia.com/cuda-toolkit>

²<https://docs.nvidia.com/cuda/parallel-thread-execution/>

Chapter 3: Concept and Design

Within this chapter, the concepts of implementing the GPU interpreter and transpiler are explained. How these two prototypes can be implemented disregarding concrete technologies is part of this chapter.

Chapter 4: Implementation

This chapter explains the implementation of the GPU interpreter and transpiler. The details of the implementation with the used technologies are covered, such as the interpretation process and the transpilation of the expressions into Parallel Thread Execution (PTX) code.

Chapter 5: Evaluation

The software and hardware requirements and the evaluation environment are introduced in this chapter. All three evaluators will be compared against each other and the form of the expressions used for the comparisons are outlined. The comparison will not only include the time taken for the pure evaluation, but it will also include the overhead, like PTX code generation. Finally, the results of the comparison of the GPU and CPU evaluators are presented to show which of these yields the best performance.

Chapter 6: Conclusion

In the final chapter, the entire work is summarised. A brief overview of the implementation as well as the evaluation results will be provided. Additionally, an outlook of possible future research is given.

With this structure the process of creating and evaluating a basic interpreter on the GPU as well as a transpiler for creating PTX code is outlined. Research is done to ensure the implementations are relevant and not outdated. Finally, the evaluation results will answer the research questions and determine if expressions generated at runtime can be evaluated more efficiently on the GPU than on the CPU.

Chapter 2

Fundamentals and Related Work

The goal of this chapter is to provide an overview of equation learning or symbolic regression to establish common knowledge of the topic and problem this thesis is trying to solve. First the field of equation learning is explored which helps to contextualise the topic of this thesis. The main part of this chapter is split into two sub-parts. The first part is exploring research that has been done in the field of general purpose computations on the GPU (GPGPU) as well as the fundamentals of it. Focus lies on exploring how graphics processing units (GPUs) are used to achieve substantial speed-ups and when and where they can be effectively employed. The second part describes the basics of how interpreters and compilers are built and how they can be adapted to the workflow of programming GPUs. When discussing GPU programming concepts, the terminology used is that of Nvidia and may differ from that used for AMD GPUs.

2.1 Equation learning

Equation learning is a field of research that can be used for understanding and discovering equations from a set of data from various fields like mathematics and physics. Data is usually much more abundant while models often are elusive which is demonstrated by Guillemot (2022) where they explain how validating the models against large amounts of data is a big part in creating such models. Because of this effort, generating equations with a computer can more easily lead to discovering equations that describe the observed data. In one instance Werner et al. (2021) described that they want to find an expression to predict the power loss of an electric machine based on known input values. They used four inputs, direct and quadratic current as well as temperature and motor speed, and they have an observed output which is the power loss. With the help of an equation learner, they were able to generate useful results.

A more literal interpretation of equation learning is demonstrated by Pfahler and Morik (2020). They use machine learning to learn the form of equations to simplify the discovery of relevant publications. Instead of searching for keywords which might differ from one field of research to another, they allow searching by the equations the publications use. This helps as the form of equations stay the same over different fields and are therefore not subject to specific terminology. However, this form of equation learning is not relevant for this thesis.

Symbolic regression is a subset of equation learning, that specialises more towards discovering mathematical equations. A lot of research is done in this field. Using the evolutionary algorithm genetic programming (GP) for different problems, including symbolic regression, was first popularised by Koza (1994). He described that finding a computer program to solve a problem for a given input and output, can be done by traversing the search space of relevant solutions. This fits well for the goal of symbolic regression, where a mathematical expression needs to be found to describe a problem with specific inputs and outputs. Later, Koza (2010) provided an overview of results that were generated with the help of GP and were competitive with human solutions, showing how symbolic regression is a useful tool. In their book *Symbolic Regression*, Kronberger et al. (2024) show how symbolic regression can be applied for real world scenarios. One of these scenarios is finding simpler but still accurate models for hydrodynamic simulations to speed up the design process of ship hulls. Another one is finding an expression to find the remaining capacity of a Lithium-ion battery by measuring its voltage. In total, they described ten scenarios from different domains to show the capabilities of symbolic regression.

Keijzer (2004), Gustafson et al. (2005), Korn (2011), Korn (2015), Brunton (2025) and many more presented ways of improving the quality of symbolic regression algorithms, making symbolic regression more feasible for problem-solving. Bartlett et al. (2024) describe an exhaustive approach for symbolic regression which can find the true optimum for perfectly optimised parameters while retaining simple and interpretable results.

Alternatives to GP for symbolic regression also exist with for example Bayesian Symbolic Regression as proposed by Jin et al. (2020). Their approach increased the quality of the results noticeably compared to GP alternatives by for example incorporating prior knowledge. In order to avoid overfitting, Bomarito et al. (2022) have proposed a way of using Bayesian model selection to combat overfitting and reduce the complexity of the generated expressions. This also helps with making the expressions more generalisable and therefore be applicable to unseen inputs.

Another alternative to meta-heuristics like GP is the usage of neural networks. One such alternative has been introduced by Martius and Lampert (2016) where they used a neural network for their equation learner with mixed results. Later, an extension has been provided by Sahoo et al. (2018). They introduced the division operator, which led to much better results. Further improvements have been described by Werner et al. (2021) with their informed equation learner. By incorporating domain expert knowledge they could limit the search space and find better solutions for particular domains. One drawback of these three implementations is the fact that their neural networks are fixed. An equation learner which can change the network at runtime and therefore evolve over time is proposed by Dong et al. (2024). Their approach further improved the results of neural network equation learners. In their work, Lemos et al. (2022) also used a neural network for symbolic regression. They were able to find an equivalent to Newton's law of gravitation and rediscovered Newton's second and third law only with trajectory data of bodies of our solar system. Although these laws were already known, this research has shown how neural networks and machine learning in general have great potential.

An implementation for an equation learner in the physics domain is proposed by Brunton et al. (2016). Their algorithm was specifically designed for nonlinear dynamics

often occurring in physical systems. An improvement to this approach was introduced by Sun et al. (2023) where they used Monte Carlo tree search. When compared to other implementations their equation learner was able to create better results but has the main drawback of high computational cost.

To generate an equation, first the operators need to be defined that make up the equation. It is also possible to define a maximum length for an expression as proposed by Koza (1994). Expressions also consist of constants as well as variables which represent the inputs. Assuming that a given problem has two variables and one parameter, the equation learner could generate an expression as seen in Equation 2.1 where x_n are the variables, p_1 is the parameter and O is the output which should correspond to the observed output for the given variables.

$$O = 5 - \text{abs}(x_1) + x_2 \sqrt{p_1}/10 \quad (2.1)$$

A typical equation learner generates multiple expressions at once. If for example the equation learner generates 300 expressions per GP generation, each of these expressions needs to be evaluated at least once to determine how well they can produce the desired output. Each expression lies in a different part of the search space and with only the variables, it would not easily be possible to explore the surrounding search space. To perform for example local search in this area, the parameter p_1 can be used. This local search phase helps to find the local or even global optimum. For example 50 local search steps can be used, meaning that each expression needs to be evaluated 50 times with the same variables, but different parameters. As a result, one GP generation consequently requires a total $300 * 50 = 15\,000$ evaluations of the expressions. However, typically more than one GP generation is needed to find a good local optimum. While the exact number of generations is problem specific, for this example a total of 100 generations can be assumed. Each generation again generates 300 expressions and needs to perform 50 local search steps. This results in a total of $300 * 50 * 100 = 1\,500\,000$ evaluations which need to be performed during the entire runtime of the GP algorithm. These values have been taken from the equation learner for predicting discharge voltage curves of batteries as described by Kronberger et al. (2024). Their equation learner converged after 54 generations, resulting in $300 * 50 * 54 \approx 800\,000$ evaluations. Depending on the complexity of the generated expressions, performing all of these evaluations takes up a lot of the runtime. Their results took over two days to compute on an eight core desktop CPU. While they did not provide runtime information for all problems they tested, the voltage curve prediction was the slowest. The other problems were in the range of a few seconds and up to a day. Especially the problems that took several hours to days to finish show, that there is still room for performance improvements. While a better CPU with more cores can be used, it is interesting to determine, if using GPUs can yield noticeable better performance.

2.2 General Purpose Computation on Graphics Processing Units

Graphics cards (GPUs) are commonly used to increase the performance of many different applications. Originally they were designed to improve performance and visual quality in games. Dokken et al. (2005) first described the usage of GPUs for general

purpose programming (GPGPU). They have shown how the graphics pipeline can be used for GPGPU programming. Because this approach also requires the programmer to understand the graphics terminology, this was not a great solution. Therefore, Nvidia released CUDA¹ in 2007 with the goal of allowing developers to program GPUs independent of the graphics pipeline and terminology. A study of the programmability of GPUs with CUDA and the resulting performance has been conducted by Huang et al. (2008). They found that GPGPU programming has potential, even for non-embarrassingly parallel problems.

Research is also done in making the low level CUDA development simpler. T. D. Han and Abdelrahman (2011) have described a directive-based language to make development simpler and less error-prone, while retaining the performance of handwritten code. To drastically simplify CUDA development, Besard et al. (2019b) showed that it is possible to develop with CUDA in the high level programming language Julia² with similar performance to CUDA written in C. In a subsequent study W.-C. Lin and McIntosh-Smith (2021) found, that high performance computing (HPC) on the CPU and GPU in Julia performs similar to HPC development in C. This means that Julia can be a viable alternative to Fortran, C and C++ in the HPC field. Additional Julia has the benefit of developer comfort since it is a high level language with modern features such as a garbage-collector. Besard et al. (2019a) have also shown how the combination of Julia and CUDA help in rapidly developing HPC software. While this thesis in general revolves around CUDA, there also exist alternatives by AMD called ROCm³ and a vendor independent alternative called OpenCL⁴.

If not specified otherwise, the following section and its subsections use the information presented by Nvidia (2025b) in their CUDA programming guide. While in the early days of GPGPU programming a lot of research has been done to assess if this approach is feasible, it now seems obvious to use GPUs to accelerate algorithms. GPUs have been used early to speed up weather simulation models. Michalakes and Vachharajani (2008) proposed a method for simulating weather with the Weather Research and Forecast (WRF) model on a GPU. With their approach, they reached a speed-up of 5 to 2 for the most compute intensive task, with little GPU optimisation effort. They also found that the GPU usage was low, meaning there are resources and potential for more detailed simulations.

Generally, simulations are great candidates for using GPUs, as they can benefit heavily from a high degree of parallelism and data throughput. Köster et al. (2020b) have developed a way of using adaptive time steps on the GPU to considerably improve the performance of numerical and discrete simulations. In addition to the performance gains they were able to retain the precision and constraint correctness of the simulation. Black hole simulations are crucial for science and education for a better understanding of our world. Verbraeck and Eisemann (2021) have shown that simulating complex Kerr (rotating) black holes can be done on consumer hardware in a few seconds. Schwarzschild black hole simulations can be performed in real-time with GPUs as described by Hissbach et al. (2022) which is especially helpful for educational scenarios. While both approaches

¹<https://developer.nvidia.com/cuda-toolkit>

²<https://julialang.org/>

³<https://www.amd.com/de/products/software/rocm.html>

⁴<https://www.khronos.org/opencl/>

do not have the same accuracy as detailed simulations on supercomputers, they show how a single GPU can yield similar accuracy at a fraction of the cost.

Software network routing can also heavily benefit from GPU acceleration as shown by S. Han et al. (2010), where they achieved a significantly higher throughput than with a CPU only implementation.

Finite element structural analysis is an essential tool for many branches of engineering and can also heavily benefit from the usage of GPUs as demonstrated by Georgescu et al. (2013).

Generating test data for DeepQ learning can also significantly benefit from using the GPU (Köster et al., 2022).

However, it also needs to be noted, that GPUs are not always better performing than CPUs as illustrated by Lee et al. (2010), so it is important to consider if it is worth using GPUs for specific tasks.

2.2.1 Programming GPUs

The development process on a GPU is vastly different from a CPU. A CPU has tens or hundreds of complex cores with the AMD Epyc 9965⁵ having 192 cores and twice as many threads. To demonstrate how a modern CPU works Knuth (1999) introduced the MMIX architecture. It is a 64-bit CPU architecture containing many concepts and design decisions to compete with other CPUs on the market at that time. He provides the information in great detail and demonstrates the complexity of CPU architectures. Current CPUs are even more complex, and often contain features like sophisticated branch prediction among other things to achieve higher and higher performance. This makes a CPU perfect for handling complex control flows on a single program thread and even multiple threads simultaneously (Palacios & Triska, 2011). However, as seen in Section 2.2, this often is not enough. On the other hand, a GPU contains thousands or even tens of thousands of cores. For example, the GeForce RTX 5090⁶ contains a total of 21 760 CUDA cores. To achieve this enormous core count, a single GPU core has to be much simpler than a single CPU core. As described by Nvidia (2025b), a GPU designates much more transistors towards floating-point computations. This, however, results in less efficient integer arithmetic and control flow handling. There is also less Cache available per core and clock speeds are usually also much lower than those on a CPU. An overview of the differences of a CPU and a GPU architecture can be seen in Figure 2.1.

Despite these drawbacks, the sheer number of cores, makes a GPU a valid choice when considering improving the performance of an algorithm. Because of the high number of cores, GPUs are best suited for data parallel scenarios. This is due to the SIMD architecture of these cards. SIMD stands for Single-Instruction Multiple-Data and states that there is a single stream of instructions that is executed on a huge number of data streams. Franchetti et al. (2005) and Tian et al. (2012) describe ways of using SIMD instructions on the CPU. Their approaches lead to noticeable speed-ups of 3.3 and 4.7 respectively by using SIMD instructions instead of serial computations. Extending this to GPUs which are specifically built for SIMD/data parallel calculations shows why

⁵<https://www.amd.com/en/products/processors/server/epyc/9005-series/amd-epyc-9965.html>

⁶<https://www.nvidia.com/en-us/geforce/graphics-cards/50-series/rtx-5090/>

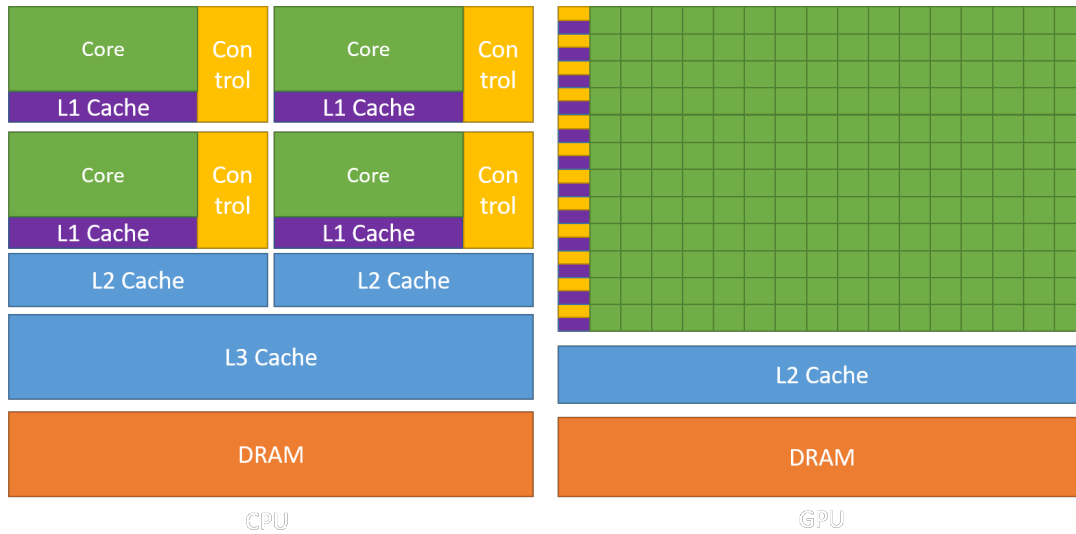


Figure 2.1: Overview of the architecture of a CPU (left) and a GPU (right). Note the higher number of simpler and smaller cores on the GPU (Nvidia, 2025b).

they are so powerful despite having less complex and slower cores than a CPU. It is also important to note, that a GPU also always needs a CPU, as the CPU is responsible for sending the data to the GPU and starting the GPU program. In GPGPU programming, the CPU is usually called the host, while the GPU is usually called the device.

Thread Hierarchy and Tuning

The thousands of cores on a GPU, as well as the threads created by the developer, are grouped together in several categories. This is the so-called thread hierarchy of GPUs. The developer can influence this grouping to a degree which allows them to tune their algorithm for optimal performance. In order to develop a well performing algorithm, it is necessary to know how this grouping works. Tuning the grouping is unique to each algorithm and also dependent on the GPU used, which means it is important to test a lot of different configurations to achieve the best possible result. This section aims at exploring the thread hierarchy and how it can be tuned to fit an algorithm.

At the lowest level of a GPU exists a Streaming Multiprocessor (SM), which is a hardware unit responsible for scheduling and executing threads and also contains the registers used by these threads. An SM is always executing a group of 32 threads simultaneously, and this group is called a warp. The number of threads that can be started is virtually unlimited. However, threads must be grouped in a block, with one block typically containing a maximum of 1024 threads but is often configured to be less. Therefore, if more than 1024 threads are required, more blocks must be created. Blocks can also be grouped into thread block clusters which is optional, but can be useful in certain scenarios. All thread blocks or thread block clusters are part of a grid, which manifests as a dispatch of the code run on the GPU, also called kernel (AMD, 2025b). All threads in one block have access to some shared memory, which can be used for L1 caching or communication between threads. It is important that the blocks can be

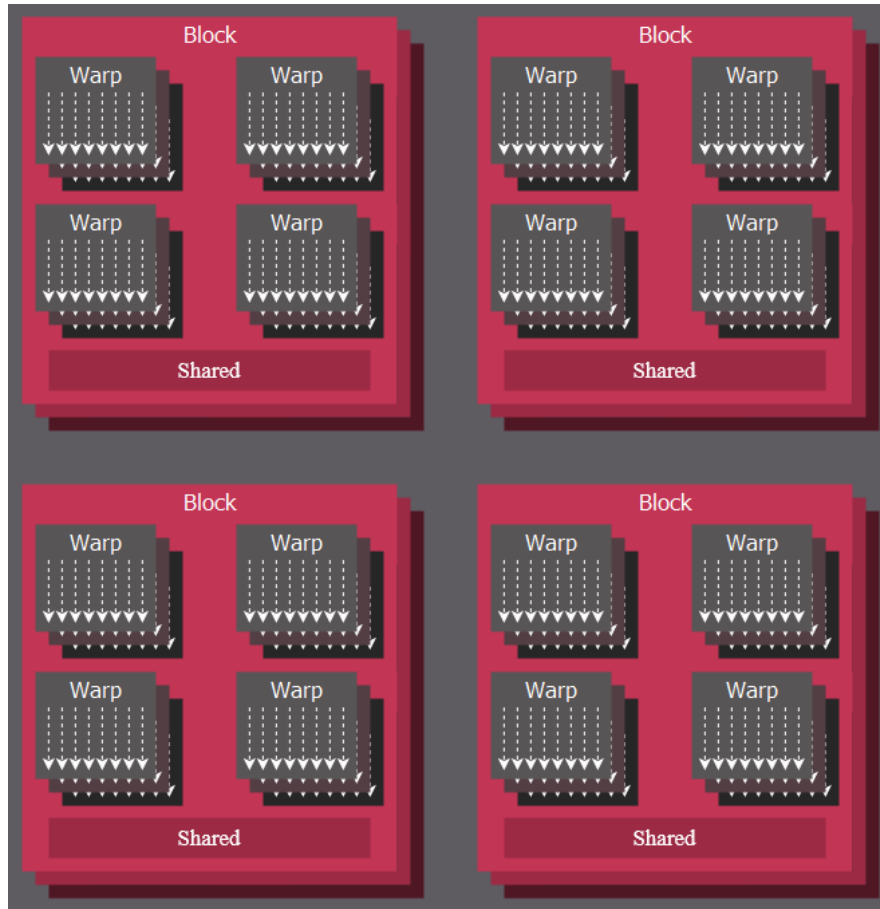


Figure 2.2: An overview of the thread hierarchy with blocks being split into multiple warps and their shared memory (AMD, 2025b).

scheduled independently, with no dependencies between them. This allows the scheduler to schedule blocks and threads as efficiently as possible. All threads within a warp are guaranteed to be part of the same block, and are therefore executed simultaneously and can access the same memory addresses. Figure 2.2 depicts how threads in a block are grouped into warps for execution and how they shared memory.

A piece of code that is executed on a GPU is written as a kernel which can be configured. The most important configuration is how threads are grouped into blocks. The GPU allows the kernel to allocate threads and blocks and block clusters in up to three dimensions. This is often useful because of the already mentioned shared memory, which will be explained in more detail in Section 2.2.1. Considering the case where an image needs to be blurred, it not only simplifies the development if threads are arranged in a 2D grid, it also helps with optimising memory access. As the threads in a block, need to access a lot of the same data, this data can be loaded in the shared memory of the block. This allows the data to be accessed much quicker compared to when threads are allocated in only one dimension. With one dimensional blocks it is possible that threads assigned to nearby pixels, are part of a different block, leading to a lot of duplicate

data transfer. The size in each dimension of a block can be almost arbitrary within the maximum allowed number of threads. However, blocks that are too large might lead to other problems which are described in more detail in Section 2.2.1.

Once a kernel is dispatched, all threads start at the same point in a program. However, because a thread may encounter instructions, such as branches, where it can take a different path to the other threads, or in other words diverge, each thread has a unique instruction pointer. This allows threads to work independently, even if they are part of the same warp. However, because of the SIMD architecture, all threads in a warp must execute the same instructions and if threads start to diverge, the SM must pause threads with different instructions and execute them later. Figure 2.3 shows how such divergences can impact performance. The situation described in the figure also shows, that the thread could re-converge after the divergence. On older hardware this does not happen and results in T2 being executed after T1 and T3 have finished. In situations where there is a lot of data dependent thread divergence, most of the benefits of using a GPU are likely to be lost. Threads not executing the same instruction is strictly speaking against the SIMD principle, but can happen in reality, due to data dependent branching. Consequently, this leads to poor resource utilisation, which in turn leads to poor performance. Another way in which threads can be paused (inactive threads) is the fact that sometimes, the number of threads started is not divisible by 32. In such cases, the last warp still contains 32 threads but only the threads with work are executed.

Modern GPUs implement what is known as the Single-Instruction Multiple-Thread (SIMT) architecture. In many cases a developer does not need to know the details of SIMT and can design fast, correct and accurate programs with just the SIMD architecture in mind. However, leveraging the power of SIMT can yield substantial performance gains by re-converging threads after data-dependent divergence has occurred. SIMT can also help with increasing the occupancy of the GPU. Occupancy and its importance to performance is discussed in detail in Section 2.2.1.

A stack-less re-convergence algorithm was proposed by Collange (2011) as an alternative to the default stack-based re-convergence algorithm. Their algorithm was able to achieve higher performance than the default one. Another approach for increasing occupancy using the SIMT architecture is proposed by Fung and Aamodt (2011). They introduced a technique for compacting thread blocks by moving divergent threads to new warps until they re-converge. This approach resulted in a noticeable speed-up between 17% and 22%. Another example where a SIMT aware algorithm can perform better was proposed by Köster et al. (2020a). While they did not implement techniques for thread re-convergence, they implemented a thread compaction algorithm. On data-dependent divergence it is possible for threads to end early, leaving a warp with only partial active threads. This means the inactive threads are still occupied and cannot be used for other work. Their thread compaction tackles this problem by moving active threads into a new thread block, releasing the inactive threads to perform other work. With this they were able to gain a speed-up of roughly 4 times compared to previous implementations. Adapting Multiple-Instruction Multiple-Data (MIMD) programs with synchronisation to run on SIMT architecture can be a difficult task, especially if the underlying architecture is not well understood. A static analysis tool and a transformer specifically designed to help avoid deadlocks with MIMD synchronisation is proposed by ElTantawy and Aamodt (2016). In addition, they proposed a hardware re-convergence

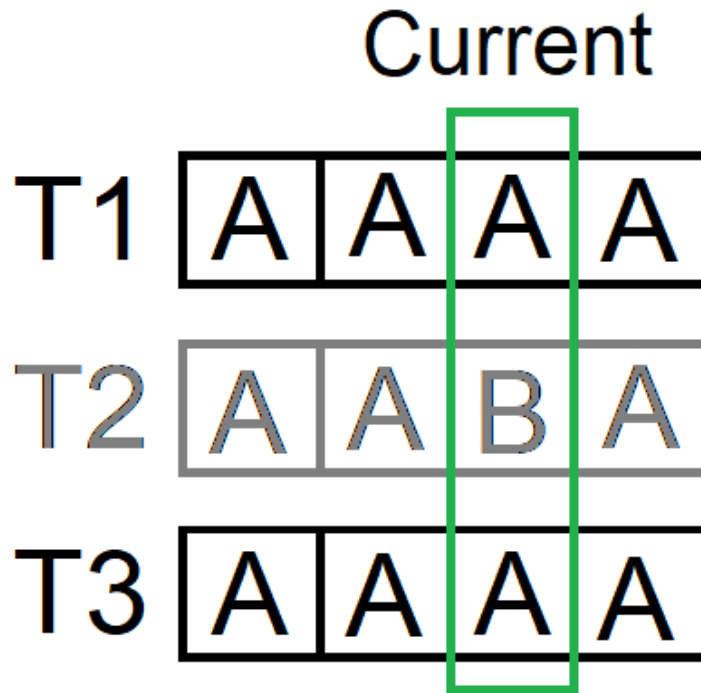


Figure 2.3: Thread T2 wants to execute instruction B while T1 and T3 want to execute instruction A. Therefore T2 will be an inactive thread this cycle and active once T1 and T3 are finished. This means that now the divergent threads are serialised.

mechanism that supports MIMD synchronisation. A survey by Khairy et al. (2019) explores different aspects of improving GPGPU performance architecturally. Specifically, they have compiled a list of different publications discussing algorithms for thread re-convergence, thread compaction and much more. Their main goal was to give a broad overview of many ways to improve the performance of GPGPU programming to help other developers.

Memory Model

On a GPU there are two parts that contribute to the performance of an algorithm. The one already looked at is the compute-portion of the GPU. This is necessary because if threads are serialised or run inefficiently, there is nothing that can make the algorithm execute faster. However, algorithms run on a GPU usually require huge amounts of data to be processed, as they are designed for exactly that purpose. The purpose of this section is to explain how the memory model of the GPU works and how it can influence the performance of an algorithm. In Figure 2.4 the memory layout and the kinds of memory available are depicted. The different parts will be explained in this section.

On a GPU there are multiple levels and kinds of memory available. All these levels and kinds have different purposes they are optimised for. This means that it is important to know what they are and how they can be best used for specific tasks. On the lowest

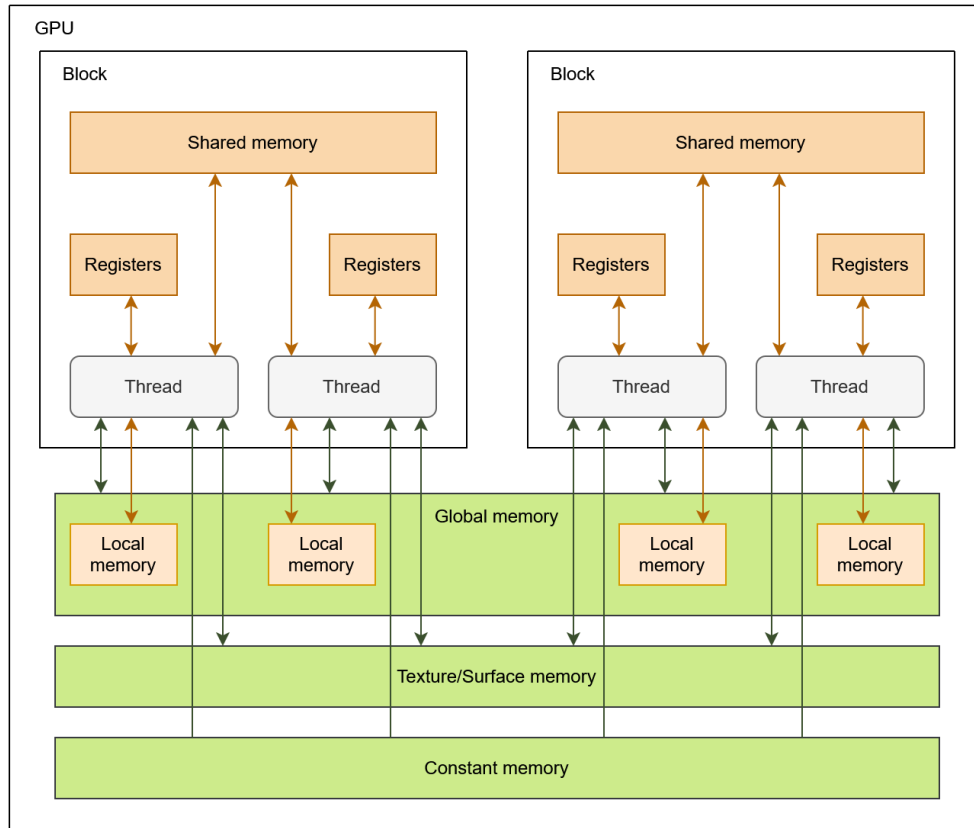


Figure 2.4: The layout of the memory in the GPU. The connections between the memory regions can be seen as well as the different kinds of memory available.

level, threads have registers and local memory available. Registers are the fastest way to access memory, but they are also the least abundant memory with up to a maximum of 255 32-Bit registers per thread on Nvidia GPUs and 256 on AMD GPUs (AMD, 2025a). However, using all registers of a thread can lead to other problems which are described in more detail in Section 2.2.1. In contrast to registers, local memory is significantly slower. This is due to the fact, that local memory is actually stored in global memory and therefore has the same limitations as explained later. This means that it is important to try and avoid local memory as much as possible. Local memory is usually only used when a thread is using too many registers. The compiler will then spill the remaining data into local memory and load it into registers once needed, slowing down the application drastically.

Shared memory is the next tier of memory on a GPU. Unlike local memory and registers, shared memory is shared between all threads inside a block. The amount of shared memory is depending on the GPU architecture but for Nvidia it hovers at around 100 Kilobyte (KB) per block. While this memory is slower than registers, its primary use-case is communicating and sharing data between threads in a block. If all threads in a block access a lot of overlapping data this data can be loaded from global memory into faster shared memory once. It can then be accessed multiple times, further increasing

performance. Loading data into shared memory and accessing that data has to be done manually. Because shared memory is part of the unified data cache, it can either be used as a cache or for manual use, meaning a developer can allocate more shared memory towards caching if needed. Another feature of shared memory are the so-called memory banks. Shared memory is always split into 32 equally sized memory modules also called memory banks. All available memory addresses lie in one of these banks. This means if two threads access two memory addresses which lie in different banks, the access can be performed simultaneously, increasing the throughput.

The most abundant and slowest memory is the global memory and resides in device memory. A key constraint of device memory and therefore global memory is, that can only be accessed in either 32, 64 or 128 byte chunks. This means if a thread wants to access 8 bytes from global memory, alongside the 8 bytes, the 24 bytes after the requested 8 bytes are also transferred. As a result, the throughput is only a fourth of the theoretical maximum. Therefore, it is important to follow optimal access patterns. What these optimal patterns are, are architecture dependent and are described in the according sections in the CUDA programming guide.

A small portion of device memory is allocated to constant memory. Constant memory is accessible by all threads and as the name implies, can not be written to by threads. It can be initialised by the CPU when starting a kernel if needed. As constant memory has a separate cache, it can be used to speed-up data access for constant and frequently accessed data.

Another special kind of memory is the texture and surface memory. According to AMD (2025b) texture memory is read-only memory, while surface memory can also be written to, which is the only difference between these two kinds of memory. Nvidia does not explicitly state this behaviour, but due to the fact that accessing textures is only performed via caches, it is implied that on Nvidia GPUs, texture memory is also read-only. As the name implies, this kind of memory is optimised for accessing textures. This means that threads of the same warp, accessing data which is spatially close together, will result in increased performance. As already mentioned, surface memory works the same way, with the difference, that it can be written to. It is therefore well suited for manipulating two- or three-dimensional data.

Occupancy

Occupancy describes the utilisation of a GPU. A high occupancy means, that there are Warps executing, or in other words, the cores are occupied with work. This is important, as a low occupancy means that the GPU is waiting for work to be scheduled and is therefore idle. As a result, it is desired to achieve high occupancy in order to increase the performance of an algorithm. It needs to be noted, that occupancy is not the only option for improving performance. As it is possible for the GPU to have a high occupancy while performing a lot of unnecessary or redundant work or utilising compute-resources that are slower. An example for the latter would be developing an algorithm that uses 64-bit floating point (FP64) numbers while 32-bit floating point (FP32) numbers would have sufficient accuracy. Because GPUs tend to have fewer FP64 compute-resources than they have FP32 compute-resources, performing FP64 operations will take longer. However, despite these drawbacks, having low occupancy will very likely result in per-

Compute Capability	8.9	10.x
Max. number of threads per block	1 024	
Warp size	32 threads	
Max. number of warps per SM	48	64
Max. number of blocks per SM	24	32
Max. number of threads per SM	1 536	2 048
Number of 32-bit registers per SM	64 000	
Max. number of 32-bit registers per block	64 000	
Max. number of 32-bit registers per thread	255	
Max. amount of shared memory per SM	100 Kilobytes	228 Kilobytes
Max. amount of shared memory per block	99 Kilobytes	227 Kilobytes

Table 2.1: A simplified version of the technical specifications for the Compute Capabilities 8.9 and 10.x (Nvidia, 2025b). These correspond to the Nvidia Ada Lovelace and Blackwell microarchitectures.

formance degradation while high occupancy will either improve performance or do no harm otherwise. Ways of achieving high occupancy will be outlined in this section as most other performance problems can be solved algorithmically.

When starting a kernel, the most important configuration is the number of threads and thread blocks that need to be started. This is important, as this has other effects on occupancy as well. In Table 2.1 the most notable limitations are presented that can affect occupancy. These limitations need to be considered when choosing a kernel configuration. It is important to note, that depending on the GPU and problem, the occupancy tuning might differ, and the same approach might perform well on one GPU but perform poorly on another GPU. Therefore, the things discussed here are only guidelines.

Tools like Nvidia Nsight Compute⁷ and Nsight Systems⁸ are essential for performance tuning. Nsight compute also contains an occupancy calculator which takes a kernel and computes how the configuration performs in terms of occupancy and also lets the developer try out different configurations (Nvidia, 2025c).

In general, it is important to have as many warps as possible ready for execution. While this means that a lot of warps could be executed but are not, this is actually desired. A key feature of GPUs is so-called latency hiding, meaning that while a warp waits for data to be retrieved for example, another warp ready for execution can now be run. With low occupancy, and therefore little to no warps waiting for execution, latency hiding does not work, as now the hardware is idle. As a result, the runtime increases which also explains why high occupancy is not guaranteed to result in performance improvements while low occupancy can and often will increase the runtime.

As seen in Table 2.1, there exist different limitations that can impact occupancy. The number of warps per SM is important, as this means this is the degree of parallelism achievable per SM. If due to other limitations, the number of warps per SM is below the maximum, there is idle hardware. One such limitation is the number of registers per

⁷<https://developer.nvidia.com/nsight-compute>

⁸<https://developer.nvidia.com/nsight-systems>

block and SM. In the case of compute capability 8.9, one SM can handle $32 * 48 = 1\,536$ threads. This leaves $64\,000 / 1\,536 \approx 41$ registers per thread, which is lower than the theoretical maximum of 255 registers per thread. Typically, one register is mapped to one variable in the kernel code, meaning a developer can use up to 41 variables in their code. However, if the variable needs 64 bits to store its value, the register usage doubles, as all registers on a GPU are 32-bit. On a GPU with compute capability 10.x a developer can use up to $64\,000 / 2\,048 \approx 31$ registers. Of course a developer can use more registers, but this results in less occupancy. However, depending on the algorithm using more registers might be more beneficial to performance than the lower occupancy, in which case occupancy is not as important. If a developer needs more than 255 registers for their variables the additional variables will spill into local memory which is, as described in Section 2.2.1, not desirable.

Additionally, shared memory consumption can also impact the occupancy. If for example a block needs all the available shared memory, which is almost the same as the amount of shared memory per SM, this SM can only serve this block. On compute capability 10.x, this would mean that occupancy would be at maximum 50% as a block can have up to 1 024 threads while an SM supports up to 2 048 threads. Again, in such cases it needs to be determined, if the performance gain of using this much shared memory is worth the lower occupancy.

Balancing these limitations and therefore the occupancy and performance often requires a lot of trial and error with help of the aforementioned tools. In cases where occupancy is already high and the amount of warps ready for execution is also high, other areas for performance improvements need to be explored. Algorithmic optimisation is always a good idea. Some performance improvements can be achieved by altering the computations to use different parts of the GPU. One of such optimisations is using FP32 operations wherever possible. Another well suited optimisation is to rewrite the algorithm to use as many Fused Multiply-Add (FMA) instructions. FMA is a special floating point instruction, that multiplies two values and adds a third, all in a single clock cycle (Nvidia, 2025a). However, the result might slightly deviate compared to performing these two operations separately, which means in accuracy sensitive scenarios, this instruction should be avoided. If the compiler detects a floating point operation with the FMA structure, it will automatically be compiled to an FMA instruction. To prevent this, in C++ the developer can call the functions `__fadd__` and `__fmul__` for addition and multiplication respectively.

2.2.2 Parallel Thread Execution

While in most cases a GPU can be programmed in a higher level language like C++ or even Julia⁹, it is also possible to program GPUs with the low level language Parallel Thread Execution (PTX) developed by Nvidia. A brief overview of what PTX is and how it can be used to program GPUs is given in this section. Information in this section is taken from the PTX documentation (Nvidia, 2025d) if not stated otherwise.

PTX defines a virtual machine with an own instruction set architecture (ISA) and is designed for data-parallel processing on a GPU. It is an abstraction of the underlying hardware instruction set, allowing PTX code to be portable across Nvidia GPUs. In

⁹<https://juliagpu.org/>


```

1 .func loop(.param .u32 N)
2 {
3   .reg .u32 %n;
4   .reg .pred %p;
5
6   ld.param.u32 %n, [N];
7 Loop:
8   setp.eq.u32 %p, %n, 0;
9   @%p bra     Done;
10  sub.u32     %n, %n, 1;
11  bra        Loop;
12 Done:
13 }

```

Program 2.1: A PTX program fragment depicting how loops can be implemented.

order for PTX code to be usable for the GPU, the driver is responsible for compiling the code to the hardware instruction set of the GPU it is run on. A developer typically writes a kernel in CUDA using C++, for example, and the Nvidia compiler generates the PTX code for that kernel. This PTX code is then compiled by the driver once it is executed. The concepts for programming the GPU with PTX and CUDA are the same, apart from the terminology which is slightly different. For consistency, the CUDA terminology will continue to be used.

Syntactically, PTX is similar to assembler style code. Every PTX code must have a `.version` directive which indicates the PTX version and an optional `.target` directive which indicates the compute capability. If the program works in 64 bit addresses, the optional `.address_size` directive can be used to indicate that, which simplifies the code for such applications. After these directives, the actual code is written. As each PTX code needs an entry point (the kernel) the `.entry` directive indicates the name of the kernel and the parameters needed. It is also possible to write helper functions with the `.func` directive. Inside the kernel or a helper function, normal PTX code can be written. Because PTX is very low level, it assumes an underlying register machine, therefore a developer needs to think about register management. This includes loading data from global or shared memory into registers if needed. Code for manipulating data like addition and subtraction generally follow the structure `operation.datatype` followed by up to four parameters for that operation. For adding two FP32 values together and storing them in the register `%n`, the code looks like the following:

```
add.f32    %n, 0.1, 0.2;
```

Loops in the classical sense do not exist in PTX. Instead, a developer needs to define jump targets for the beginning and end of the loop. The Program in 2.1 shows how a function with simple loop can be implemented. The loop counts down to zero from the passed parameter `N` which is loaded into the register `%n` in line 6. If the value in the register `%n` reached zero the loop branches at line 9 to the jump target at line 12 and the loop has finished. All other used directives and further information on writing PTX code can be taken from the PTX documentation (Nvidia, 2025d).

2.3 Compilers

Compilers are a necessary tool for many developers. If a developer wants to run their program it is very likely they need one. As best described by Aho et al. (2006) in their dragon book, a compiler takes code written by a human in some source language and translates it into a destination language readable by a computer. This section briefly explores what compilers are and research done in this old field of computer science. Furthermore, the topics of transpilers and interpreters are explored, as their use-cases are very similar.

Aho et al. (2006) and Cooper and Torczon (2022) describe how a compiler can be developed, with the latter focusing on more modern approaches. They describe how a compiler consists of two parts, the analyser, also called frontend, and the synthesiser also called backend. The frontend is responsible for ensuring syntactic and semantic correctness and converts the source code into an intermediate representation, an abstract syntax tree (AST), for the backend. Generating code in the target language, from the intermediate representation is the job of the backend. This target code can be assembly or anything else that is needed for a specific use-case. This intermediate representation also makes it simple to swap out frontends or backends. The Gnu Compiler Collection GCC (2025) takes advantage of using different frontends to provide support for many languages including C, C++, Ada and more. Instead of compiling source code for specific machines directly, many languages compile code for virtual machines instead. Notable examples are the Java Virtual Machine (JVM) (Lindholm et al., 2025) and the low level virtual machine (LLVM) (Lattner & Adev, 2004). Such virtual machines provide a bytecode which can be used as a target language for compilers. A huge benefit of such virtual machines is the ability for one program to be run on all physical machines the virtual machine exists for, without the developer needing to change that program (Lindholm et al., 2025). Programs written for virtual machines are compiled into their respective bytecode. This bytecode can then be interpreted or compiled to physical machine code and then be run. According to the JVM specification Lindholm et al. (2025) the Java bytecode is interpreted and also compiled with a just-in-time (JIT) compiler to increase the performance of code blocks that are often executed. On the other hand, the common language runtime (CLR)¹⁰, the virtual machine for languages like C#, never interprets the generated bytecode. As described by Microsoft (2023) the CLR always compiles the bytecode to physical machine code using a JIT compiler before it is executed.

2.3.1 Interpreters

Interpreters are a different kind of program for executing source code. Rather than compiling the code and executing the result, an interpreter executes the source code directly. Languages like Python and JavaScript are prominent examples of interpreted languages, but also Java, or more precise Java-Bytecode, is also interpreted before it gets compiled (Lindholm et al., 2025). However, interpreters can not only be used for interpreting programming languages. It is also possible for them to be used in GP. Langdon and Banzhaf (2008) have shown how a SIMD interpreter can be efficiently used for evaluating entire

¹⁰<https://learn.microsoft.com/en-us/dotnet/standard/clr>

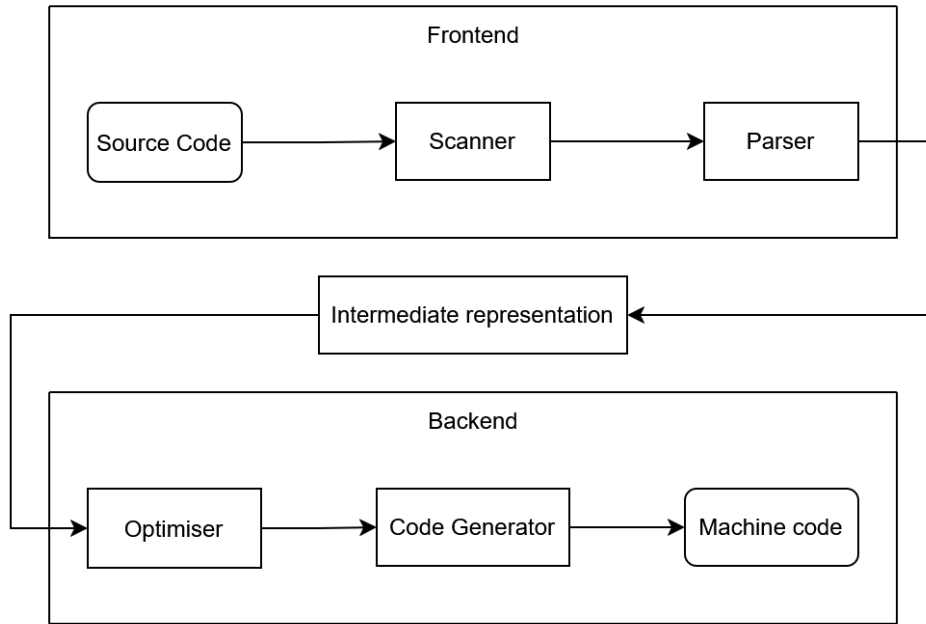


Figure 2.5: A simplified overview of how the architecture of a compiler looks, using Flex and Bison.

GP populations on the GPU directly. In a later work Cano and Ventura (2014) further improved this interpreter. They used the fact that a GP individual represents a tree which can be split into independent subtrees. These can be evaluated concurrently and with the help of communication via shared memory, they were able to evaluate the entire tree. With this they achieved a significant performance improvement over previous implementations. As shown by Dietz and Young (2010), it is even possible to develop an interpreter that can execute MIMD programs on a SIMD GPU. However, as noted by the authors, any kind of interpretation comes with an overhead. This means that with the additional challenges of executing MIMD programs on SIMD hardware, their interpreter, while achieving reasonable efficiency, still suffers from performance problems. Another field where interpreters can be useful are rule-based simulations. Köster et al. (2020a) has shown how they implemented a GPU interpreter for such simulations. In addition with other novel performance improvements in running programs on a GPU, they were able to gain a speed-up of 4 over non-interpreted implementations. While publications like Fua and Lis (2020) and Gherardi et al. (2012) have shown, interpreted languages often trail behind in terms of performance compared to compiled languages, interpreters per se are not slow. And while they come with performance overhead as demonstrated by Dietz and Young (2010) and Romer et al. (1996), they can still be a very fast, easy and powerful alternative for certain tasks.

2.3.2 Transpilers

With the concepts already mentioned, it is possible to generate executable code from code written in a programming language. However, sometimes it is desired to convert a program from one programming language to another and therefore the major difference between these use-cases is the backend. A popular transpiler example is the TypeScript transpiler, which transforms TypeScript source code into JavaScript source code (Microsoft, 2025). Other examples for transpilers are the C2Rust transpiler (Ling et al., 2022) that transpiles C code into Rust code as well as the PyJL transpiler (Marcelino & Leitão, 2022) which transpiles Python code into Julia code. Chaber and Ławryńczuk (2016) proposed a transpiler that takes MATLAB and C code and transforms it into pure and optimised C code for an STM32 microcontroller. An early example for a transpiler has been developed by Intel (1978) where they built a transpiler for transforming assembly code for their 8080 CPU to assembly code for their 8086 CPU. Transpilers can also be used in parallelisation environments, like OpenMP (C.-K. Wang & Chen, 2015). There also exists a transpiler that transforms CUDA code into highly parallel CPU code. Moses et al. (2023) described this transpiler, and they found that the generated code performs noticeably better than doing this transformation by hand. When designing complex processors and accelerators, Register-transfer level (RTL) simulations are essential (L.-T. Wang et al., 2009). In a later study Zhang et al. (2020) have shown how RTL simulations can be performed on GPUs with a speed-up of 20. This led to D.-L. Lin et al. (2023) developing a transpiler to transform RTL into CUDA kernels instead of handwriting them. They compared their results with a CPU implementation running on 80 CPUs, where they found that the transpiled CUDA version was 40 times faster. Using transpilers for software backend and business logic has been proposed by Bastidas Fuertes et al. (2023a). Their approach implemented a programming language that can be transpiled into different programming languages, for usage in a multi-programming-language environment that share some business logic. In another study, Bastidas Fuertes et al. (2023b) reviewed over 600 publications to map the use of transpilers alongside their implementations in different fields of research, demonstrating the versatility of transpiler use.

Chapter 3

Concept and Design

To be able to determine whether evaluating mathematical expressions on the GPU is better suited than on the CPU, a prototype needs to be implemented. More specifically, a prototype for interpreting these expressions on the GPU, as well as a prototype that transpiles expressions into code that can be executed by the GPU. The goal of this chapter, is to describe how these two prototypes can be implemented conceptually. First the requirements for the prototypes as well as the data they operate on are explained. This is followed by the design of the interpreter and the transpiler. The CPU interpreter will not be described, as it already exists.

3.1 Requirements and Data

The main goal of both prototypes or evaluators is to provide a speed-up compared to the CPU interpreter already in use. However, it is also important to determine which evaluator provides the most speed-up. This also means that if one of the evaluators is faster, it is intended to replace the CPU interpreter. Therefore, they must have similar capabilities, and therefore meet the following requirements:

- Multiple expressions as input.
- All input expressions have the same number of variables (x_n), but can have a different number of parameters (p_n).
- The variables are parametrised using a matrix of the form $k \times N$, where k is the number of variables in the expressions and N is the number of different parametrizations for the variables. This matrix is the same for all expressions.
- The parameters are parametrised using a vector of vectors. Each vector v_i corresponds to an expression e_i .
- The following operations must be supported: $x + y$, $x - y$, $x * y$, x / y , x^y , $|x|$, $\log(x)$, e^x and \sqrt{x} . Note that x and y can either stand for a value, a variable, or another operation.
- The results of the evaluations are returned in a matrix of the form $k \times N$. In this case, k is equal to the N of the variable matrix and N is equal to the number of input expressions.

With this, the required capabilities are outlined. However, for a better understand-

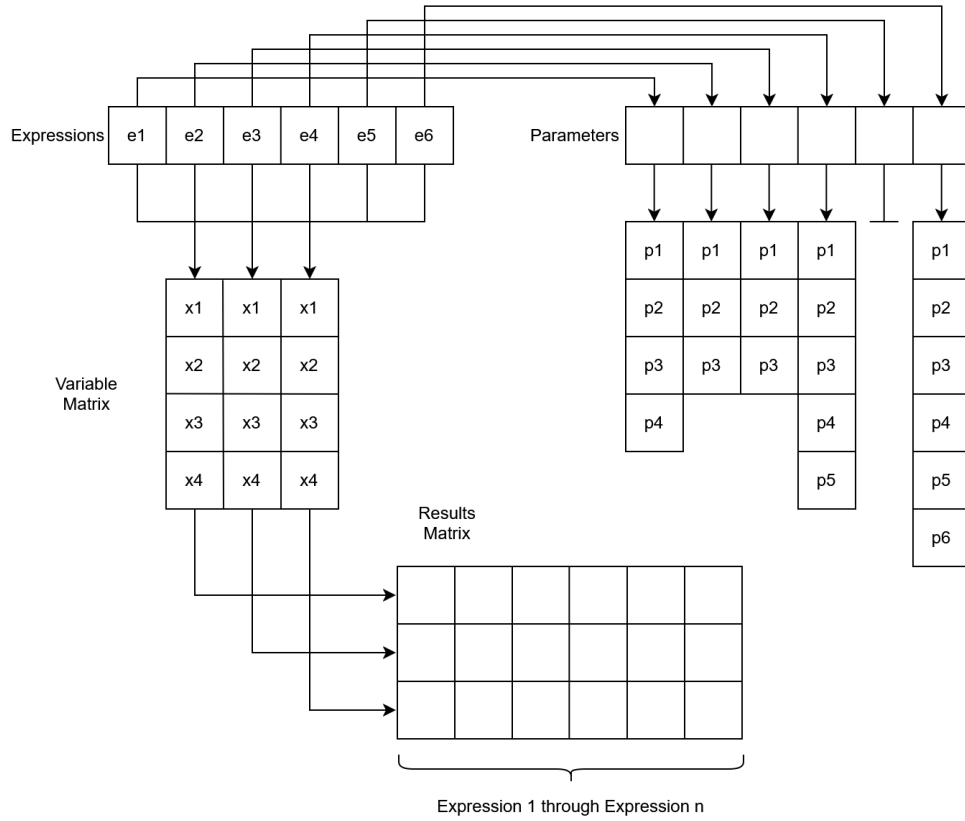


Figure 3.1: This diagram shows how the input and output looks like and how they interact with each other.

ing, the input and output data need to be explained further. The first input contains the expressions that need to be evaluated. These can be of any length and can contain constant values, variables and parameters, all of which are linked together with the supported operations. In the simplified example shown in Figure 3.1, there are six expressions e_1 to e_6 .

Next is the variable matrix. An entry in this matrix corresponds to one variable in every expression. The row indicates which variable it holds the value for. For example the values in row three, are used to parameterise the variable x_3 . Each column holds a different set of variables. Each expression must be evaluated using each set of variables. In the provided example, there are three variable sets, each containing the values for four variables x_1 to x_4 .

After all expressions have been evaluated using all variable sets, the results of these evaluations must be stored in the result matrix. Each entry in this matrix holds the result of the evaluation of one expression parameterised with one variable set. The row indicates the variable set and the column indicates the expression.

The prototypes developed in this thesis, are part of a GP algorithm for symbolic regression. This means that the expressions that are evaluated, represent parts of the

search space of all expressions being made up of any combination of allowed operators, the set of input variables, a set of parameters and constants. This means that the size of the search space grows exponentially. Exploring this search space by simply generating expressions, evaluating them once and then generating the next set of expressions leaves much of the search space unexplored. To combat this, parameters are introduced. These allow the algorithm to perform some kind of local search. To enable this, the prototypes must support not only variables, but also parameters.

The parameters themselves are unique to each expression, meaning they have a one-to-one mapping to an expression. Furthermore, as can be seen in Figure 3.1, each expression can have a different number of parameters, or even no parameters at all. However, with no parameters, it wouldn't be possible to perform parameter optimisation. This is in contrast to variables, where each expression must have the same number of variables. Because parameters are unique to each expression and can vary in size, they are not structured as a matrix, but as a vector of vectors.

An important thing to consider, is the volume and volatility of the data itself. The example used above has been drastically simplified. It is expected, that there are hundreds of expressions evaluate per GP generation. Each of these expressions may contain between ten and 50 tokens. A token is equivalent to either a variable, a parameter, a constant value or an operator.

Usually, the number of variables per expression is around ten. However, the number of variable sets can increase drastically. It can be considered, that 1 000 variable sets is the lower limit. On the other hand, 100 000 can be considered as the upper limit. Considering that one variable takes up 4 bytes of space and 10 variables are needed per expression, at least $4 * 10 * 1\,000 = 40\,000$ bytes and at most $4 * 10 * 100\,000 = 400\,000$ bytes need to be transferred to the GPU for the variables.

These variables do not change during the runtime of the symbolic regression algorithm. As a result the data only needs to be sent to the GPU once. This means that the impact of this data transfer is minimal. On the other hand, the data for the parameters is much more volatile. As explained above, they are used for parameter optimisation and therefore vary from evaluation to evaluation and need to be sent to the GPU very frequently. However, the amount of data that needs to be sent is also much smaller. TODO: ONCE I GET THE DATA SEE HOW MANY BYTES PARAMETERS TAKE ON AVERAGE

3.2 Architecture

Based on the requirements and data structure above, the architecture of both prototypes can be designed. While the requirements only specify the input and output, the components and workflow also need to be specified. This section aims at giving an architectural overview of both prototypes, alongside their design decisions.

A design decision that has been made for both prototypes is to split the evaluation of each expression into a separate kernel or kernel dispatch as seen in Figure 3.2. As explained in Section 2.2.1, it is desirable to reduce the occurrence of thread divergence as much as possible. Although the SIMT programming model tries to mitigate the negative effects of thread divergence, it is still a good idea to avoid it when possible. For this use-case, thread divergence can easily be avoided by not evaluating all expressions in

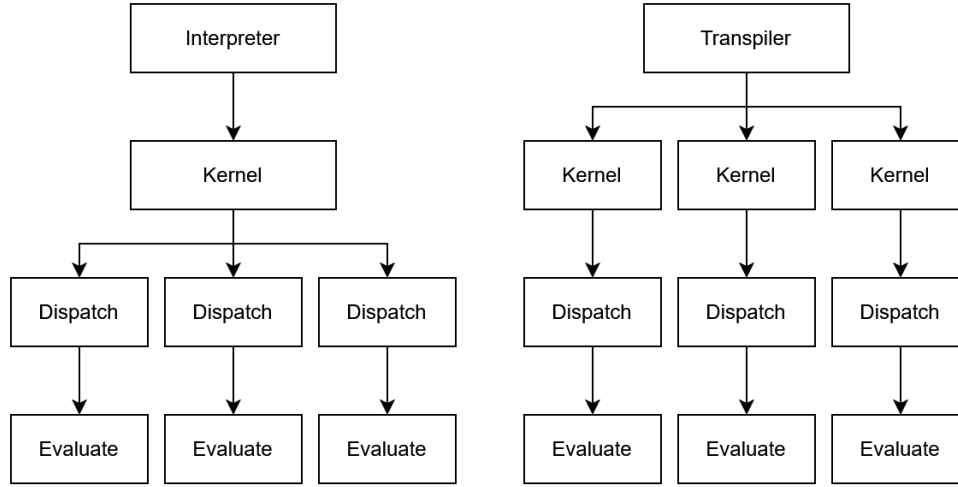


Figure 3.2: The interpreter has one kernel that is dispatched multiple times, while the transpiler, has multiple kernels that are dispatched once. This helps to eliminate thread divergence.

a single kernel or kernel dispatch. GPUs are able to have multiple resident grids, with modern GPUs being able to accommodate 128 grids concurrently (Nvidia, 2025b). One grid corresponds to one kernel dispatch, and therefore allows up-to 128 kernels to be run concurrently. Therefore, dispatching a kernel for each expression, further increases GPU utilisation. In the case of the interpreter, having only one kernel that can be dispatched for each expression, also simplifies the kernel itself. This is because the kernel can focus on evaluating one expression and does not require additional code to handle multiple expressions at once. Similarly, the transpiler can also be simplified, as it can generate many smaller kernels rather than one big kernel. Additionally, the smaller kernels do not need any branching, because the generated code only needs to perform the operations as they occur in the expression itself. This also reduces the overhead on the GPU.

3.2.1 Pre-Processing

The first step in both prototypes is the pre-processing step. It is needed, as it simplifies working with the expressions in the later steps. One of the responsibilities of the pre-processor is to verify that only allowed operators and symbols are present in the given expressions. This is comparable to the work a scanner like Flex¹ performs. Secondly, this step also converts the expression into an intermediate representation. In essence, the pre-processing step can be compared to the frontend of a compiler as described in Section 2.3. If new operators are required, the pre-processor must be extended as well. Otherwise, expressions containing these operators would be treated as invalid and never reach the evaluator.

The conversion into the intermediate representation transforms the expressions from infix-notation into postfix notation. This further allows the later parts to more easily

¹<https://github.com/westes/flex>

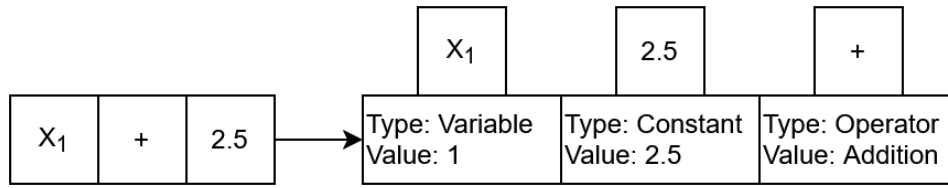


Figure 3.3: This diagram shows how an expression will be transformed in the pre-processing step.

evaluate the expressions. One of the major benefits of this notation is the implicit operator precedence. It allows the evaluators to evaluate the expressions token by token from left to right, without needing to worry about the correct order of operations. One token represents either an operator, a constant value, a variable or a parameter. Apart from the intermediate representation containing the expression in postfix notation, it also contains information about the types of the tokens themselves. This is all that is needed for the interpretation and transpilation steps. A simple expression like $x + 2$ would look like depicted in figure 3.3 after the pre-processing step.

It would have also been possible to perform the pre-processing step on the GPU. However, pre-processing only one expression can not easily be split into multiple threads, which means one GPU thread would need to process one expression. As described in Section 2.2 a single GPU thread is slower than a single CPU thread and as a result means the processing will also be slower. Furthermore, it wouldn't make sense to process all expressions in a single kernel. This would lead to a lot of thread divergence, which essentially means processing one expression after the other. The SIMT programming model might help with parallelising at least some parts of the processing work. However, the generated expressions can differ a lot from each other and restricting them to be similar and therefore SIMT friendly, would likely reduce the overall quality of the symbolic regression algorithm. Therefore, it does not make sense to perform the processing step on the GPU.

The already mentioned concept of processing one expression per thread can also be used on the CPU, which is better designed for this type of work. Concepts such as caching processed expressions, or caching parts of the processed expressions can also be employed on the CPU to speed up pre-processing. This would not be possible on the GPU, because a GPU can not save state between two kernel dispatches. This is a typical example of code that is better run on the CPU and shows how the CPU and GPU need to work together and exploit their respective strengths to achieve the best performance.

3.2.2 Interpreter

The interpreter consists of two parts. The CPU side is the part of the program, that interacts with both the GPU and the caller. An overview of the components and the workflow of the interpreter is shown in Figure 3.4. Once the interpreter has received the expressions, they are pre-processed. This ensures that the expressions are valid,

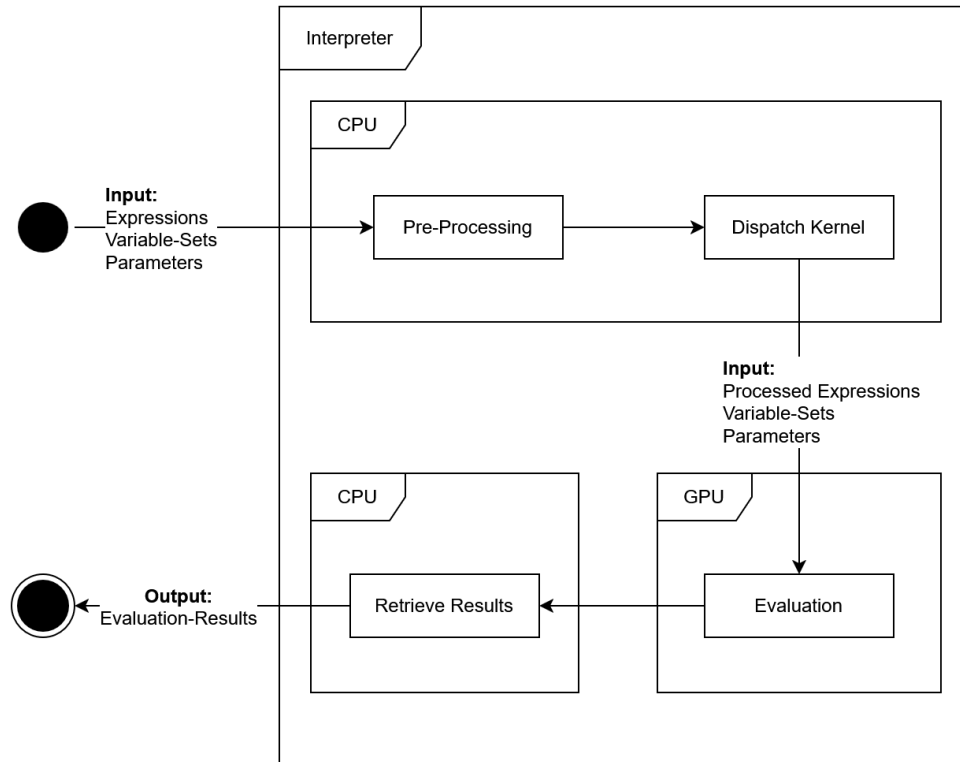


Figure 3.4: This diagram depicts the coarse-grained workflow of the interpreter. It shows how the parts interact with each other and with the system it will operate in.

and that they are transformed into the intermediate representation needed to evaluate them. The result of this pre-processing step is then sent to the GPU, which performs the actual interpretation of the expressions. In addition to the expressions, the data for the variables and parameters must also be sent to the GPU.

Once all the data is present on the GPU, the interpreter kernel can be dispatched. As already described, the kernel will be dispatched for each expression to reduce thread divergence. In fact, dispatching the same kernel multiple times with different expressions, means, there will not occur any thread divergence which will be explained later.

After the GPU has finished evaluating all expressions with all variable sets, the result is stored in a matrix on the GPU. The CPU then retrieves the results and returns them to the caller in the format specified by the requirements.

Evaluating the expressions is relatively straight forward. Because the expressions are in postfix notation, the actual interpreter just needs to iterate over all the tokens and perform the appropriate tasks. If the interpreter encounters a binary operator, it simply needs to read the previous two values and perform the operation specified by the operator. For unary operators, only the previous value needs to be read. As already mentioned, expressions in postfix notation implicitly contain the operator precedence, therefore no look-ahead or other strategies need to be used to ensure correct evaluation. This also means that each token is visited exactly once and no unnecessary or overhead

work needs to be done. The Algorithm 3.1 shows how the interpreter works. Note that this is a simplified version, that only works with additions, multiplications, constants and variables.

Algorithm 3.1: Interpreting an equation in postfix notation

```

1: procedure Evaluate(expr: PostfixExpression)
2:   stack  $\leftarrow$  []
3:   while HasTokenLeft(expr) do
4:     token  $\leftarrow$  GetNextToken(expr)
5:     if token.Type = Constant then
6:       Push(stack, token.Value)
7:     else if token.Type = Variable then
8:       Push(stack, GetVariable(token.Value))
9:     else if token.Type = Operator then
10:      if token.Value = Addition then
11:        right  $\leftarrow$  Pop(stack)
12:        left  $\leftarrow$  Pop(stack)
13:        Push(stack, left + right)
14:      else if token.Value = Multiplication then
15:        right  $\leftarrow$  Pop(stack)
16:        left  $\leftarrow$  Pop(stack)
17:        Push(stack, left * right)
18:      StoreResult(Pop(stack))

```

The handling of constants and variables is very simple. Constants only need to be stored on the stack for later use. Variables also only need to be stored on the stack. However, their value must first be loaded from the variable matrix according to the token value of the variable. Since the entire variable matrix is sent to the GPU, the index of the variable set is also needed to load the variable value. However, for the sake of simplicity, it has been omitted from the algorithm.

When an operator token is encountered, the handling becomes more complex. The value of the token indicates the type of operation to be applied. For binary operators, the top two values on the stack need to be used as input to the operator. For unary operators, only the top value of the stack needs to be used as an input. Once the result has been computed, it must be stored at the top of the stack to be used as an input for the next operation.

At the end of the algorithm, the stack contains one last entry. This entry is the value computed by the expression with the designated variable set and parameters. In order to send this value back to the CPU, it must be stored in the result matrix. The last statement performs this action. It again has been simplified to omit the index of the expression and variable set needed to store the result at the correct location.

The Algorithm 3.1 in this case resembles the kernel. This kernel will be dispatched for each expression that needs to be evaluated, to prevent thread divergence. Thread divergence can only occur on data-dependent branches. In this case, the while loop and every if and else-if statement contains a data-dependent branch. Depending on the expression passed to the kernel, the while loop may run longer than for another

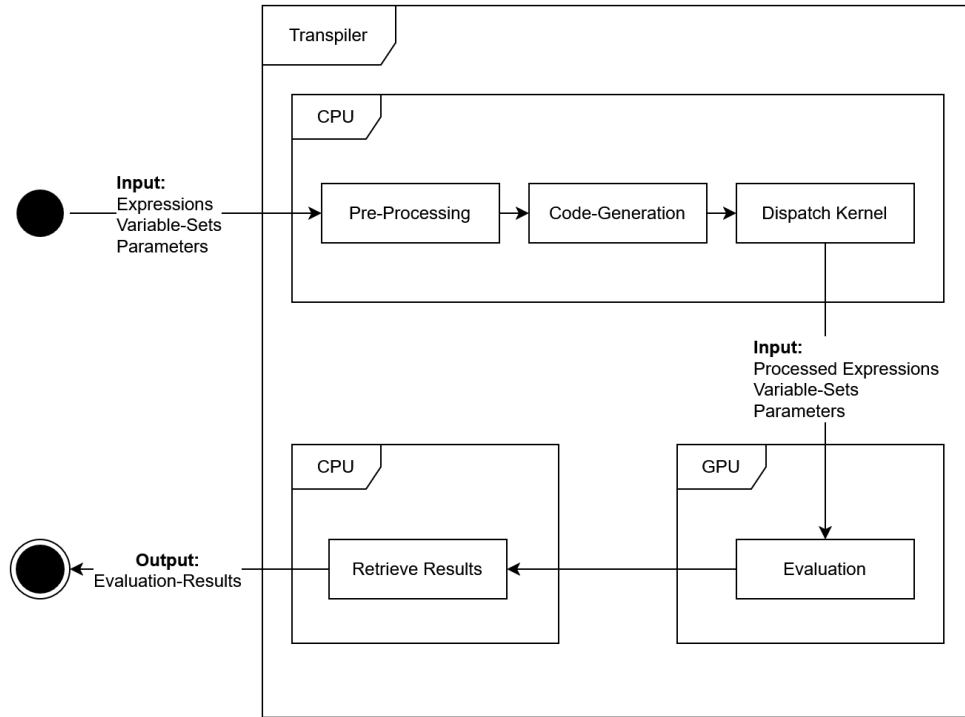


Figure 3.5: This diagram depicts the coarse-grained workflow of the transpiler. It shows how the parts interact with each other and with the system it will operate in.

expression. Similarly, not all expressions have the same constants, operators or variables in the same order, and would therefore cause each thread to take a different path. However, one expression always has the same constants, operators and variables in the same locations, meaning that all threads will take the same path. This also means that although the interpreter contains many data-dependent branches, these branches only depend on the expression itself. Because of this, all threads will follow the same path and will therefore never diverge from one another as long as they are executing the same expression.

3.2.3 Transpiler

Similar to the interpreter, the transpiler also consists of a part that runs on the CPU and a part that runs on the GPU. Looking at the components and workflow of the transpiler, as shown in Figure 3.5, it is almost identical to the interpreter. However, the key difference between the two, is the additional code generation, or transpilation step. Apart from that, the transpiler also needs the same pre-processing step and also the GPU to evaluate the expressions. However, the GPU evaluator generated by the transpiler works very differently to the GPU evaluator for the interpreter. The difference between these evaluators will be explained later.

Before the expressions can be transpiled into PTX code, they have to be pre-processed. As already described, this step ensures the validity of the expressions and

transforms them into the intermediate representation described above. As with the interpreter, this also simplifies the code generation step. By transforming the expressions into postfix notation, the code generation follows a similar pattern to the interpretation already described.

Algorithm 3.2 shows how the transpiler takes an expression, transpiles it and then returns the finished code. It can be seen that the while loop is largely the same as the while loop of the interpreter. The main difference is in the operator branches, because now code needs to be generated instead of the result of computing the expression. Therefore, the branches themselves call their designated code generation function, such as *GetAddition*. This function returns the PTX code responsible for the addition. However, this function must return more than just the code that performs the addition. When executed, this addition also returns a value which will be needed as an input by other operators. Therefore, not only the code fragment must be returned, but also the reference to the result.

This reference can then be put on the stack for later use, just as the interpreter stores the value for later use. The code fragment must also be added to the already generated code so that it can be returned to the caller. As with the interpreter, there is a final value on the stack when the loop has finished. Once the code has been executed, this value is the reference to the result of the expression. This value then needs to be stored in the result matrix, so that it can be retrieved by the CPU after all expressions have been executed on the GPU. Therefore, a final code fragment must be generated to handle the storage of this value in the result matrix. This fragment must then be added to the code already generated, and the transpilation process is complete.

The code generated by the transpiler is the kernel for the transpiled expressions. This means that a new kernel must be generated for each expression that needs to be evaluated. This is in contrast to the interpreter, which has one kernel and dispatches it once for each expression. However, generating one kernel per expression results in a much simpler kernel. This allows the kernel to focus on evaluating the postfix expression from left to right. There is no overhead work such as branching or managing a stack. However, this overhead is now shifted to the transpilation step on the CPU which can be seen in Algorithm 3.2. There is also a noticeable overhead in that a kernel has to be generated for each expression. In cases like parameter optimisation, many of the expressions will be transpiled multiple times as the transpiler is called multiple times with the same expressions.

Both the transpiler and the interpreter have their respective advantages and disadvantages. While the interpreter puts less load on the CPU, the GPU has to perform more work. Much of this work involves branching or managing a stack, and therefore involves many instructions that are not used to evaluate the expression itself. However, this overhead can be mitigated by the fact, that all this work is performed in parallel rather than sequentially.

On the other hand, the transpiler performs more work on the CPU. The kernels are much simpler, and most of the instructions are used to evaluate the expressions themselves. Furthermore, as explained in Section 2.2.2, any program running on the GPU, must be transpiled into PTX code before the driver can compile it into machine code. Therefore, the kernel written for the interpreter, must also be transpiled into PTX. This overhead is in addition to the branch instruction overhead. The self-written

Algorithm 3.2: Transpiling an equation in postfix notation

```

1: procedure Transpile(expr: PostfixExpression): String
2:   stack  $\leftarrow$  []
3:   code  $\leftarrow$  ""
4:   while HasTokenLeft(expr) do
5:     token  $\leftarrow$  GetNextToken(expr)
6:     if token.Type = Constant then
7:       Push(stack, token.Value)
8:     else if token.Type = Variable then
9:       (codeFragment, referenceTo Value)  $\leftarrow$  GetVariable(token.Value)
10:      Push(stack, referenceTo Value)
11:      Append(code, codeFragment)
12:     else if token.Type = Operator then
13:       if token.Value = Addition then
14:         right  $\leftarrow$  Pop(stack)
15:         left  $\leftarrow$  Pop(stack)
16:         (referenceTo Value, codeFragment)  $\leftarrow$  GetAddition(left, right)
17:         Push(stack, referenceTo Value)
18:         Append(code, codeFragment)
19:       else if token.Value = Multiplication then
20:         right  $\leftarrow$  Pop(stack)
21:         left  $\leftarrow$  Pop(stack)
22:         (referenceTo Value, codeFragment)  $\leftarrow$  GetMultiplication(left, right)
23:         Push(stack, referenceTo Value)
24:         Append(code, codeFragment)
25:   codeFragment  $\leftarrow$  GenerateResultStoring(Pop(stack))
26:   Append(code, codeFragment)
   return code

```

transpiler removes this intermediate step by transpiling directly into PTX. In addition, the generated code is tailored to evaluate expressions and does not need to generate generic PTX code, which can reduce transpilation time.

Unlike the GPU, the CPU can manage state across multiple kernel dispatches. Concepts such as caches can be employed by the transpiler to reduce the overhead on the CPU. In cases such as parameter optimisation, where expressions remain the same across multiple calls, the resulting PTX code can be cached. As a result, the same expression doesn't need to be transpiled multiple times which drastically reducing the transpilation time. This is an important optimisation as this can improve the overall performance of the transpiler.

Chapter 4

Implementation

This chapter focuses on the implementation phase of the project, building upon the concepts and designs previously discussed. It begins with an overview of the technologies employed for both the CPU and GPU parts of the application. This is followed by a description of the pre-processing or frontend phase. The chapter concludes with a detailed overview of the core components, the interpreter and the transpiler.

4.1 Technologies

This section describes the technologies used for both the CPU side of the prototypes and the GPU side. The rationale behind these choices, including consideration of their performance implications, is presented. In addition, the hardware limitations imposed by the choice of GPU technology are outlined.

4.1.1 CPU side

Both prototypes were implemented using the Julia programming language. It was chosen mainly, because the current symbolic regression algorithm is also implemented in Julia. Being a high-level programming language, with modern features such as a garbage collector, support for meta-programming and dynamic typing, it also offers great convenience to the developer.

More interestingly however, is the high performance that can be achieved with this language. It is possible to achieve high performance despite the supported modern features, which are often deemed to be harmful to performance. Bezanson et al. (2017) have shown how Julia can provide C-like performance while supporting the developer with modern quality of life features. The ability of Julia to be used in high performance computing scenarios and to be competitive with C has been demonstrated by W.-C. Lin and McIntosh-Smith (2021). This shows how Julia is a good and valid choice for scenarios where developer comfort and C-like performance are needed.

4.1.2 GPU side

In addition to a programming language for the CPU, a method for programming the GPU is also required. For this purpose, the CUDA API was chosen. While CUDA offers

robust capabilities, it is important to note that it is exclusively compatible with Nvidia GPUs. An alternative would have been OpenCL, which provides broader compatibility by supporting GPUs from Nvidia, AMD and Intel. However, considering Nvidia’s significant market share and the widespread adoption of CUDA in the industry, the decision was made to use CUDA.

A typical CUDA program is primarily written C++ and Nvidia also provides their CUDA compiler `nvcc`¹ for C and C++ and their official CUDA programming guide (Nvidia, 2025b) also uses C++ for code examples. It is also possible to call C++ code from within Julia. This would allow for writing the kernel and interacting with the GPU in C++, leveraging the knowledge built up over several years.

CUDA and Julia

Instead of writing the kernel in C++ and calling it from Julia, a much simpler and effective alternative can be used. The Julia package `CUDA.jl`² enables a developer to write a kernel in Julia similar to how a kernel is written in C++ with CUDA. One drawback of using `CUDA.jl` however, is the fact that it is much newer compared to CUDA and therefore does not have years of testing and bug fixing in its history, which might be a concern for some applications. Apart from writing kernels with `CUDA.jl`, it also offers a method for interacting with the driver, to compile PTX code into machine code. This is a must-have feature as otherwise, it wouldn’t have been possible to fully develop the transpiler in Julia.

Additionally, the JuliaGPU initiative³ offers a collection of additional packages to enable GPU development for AMD, Intel and Apple and not just for Nvidia. However, `CUDA.jl` is also the most mature of the available implementations, which is also a reason why CUDA has been chosen instead of for example OpenCL.

Again, the question arises if the performance of `CUDA.jl` is sufficient to be used as an alternative to C++ and CUDA. Performance studies by Besard et al. (2019a), W.-C. Lin and McIntosh-Smith (2021) and Faingnaert et al. (2022) have demonstrated, that `CUDA.jl` provides sufficient performance. They found that in some cases `CUDA.jl` was able to perform better than the same algorithm implemented in C and C++. This provides the confidence, that Julia alongside `CUDA.jl` is a good choice for leveraging the performance of GPUs to speed-up expression evaluation.

4.2 Pre-Processing

The pre-processing or frontend step is very important. As already explained in Chapter 3, it is responsible for ensuring that the given expressions are valid and that they are transformed into an intermediate representation. This section aims to explain how the intermediate representation is implemented, as well as how it is generated from a mathematical expression.

¹<https://docs.nvidia.com/cuda/cuda-compiler-driver-nvcc/>

²<https://cuda.juliagpu.org/>

³<https://juliagpu.org/>

4.2.1 Intermediate Representation

The intermediate representation is mainly designed to be lightweight and easily transferrable to the GPU. Since the interpreter runs on the GPU, this was a very important consideration. Because the transpilation process is done on the CPU, and is therefore very flexible in terms of the intermediate representation, the focus was mainly on being efficient for the interpreter.

The intermediate representation cannot take any form. While it has already been defined that expressions are converted to postfix notation, there are several ways to store the data. The first logical choice is to create an array where each entry represents a token. On the CPU it would be possible to define each entry as a pointer to the token object. Each of these objects could be of a different type, for example one object that holds a constant value while another object holds an operator. In addition, each of these objects could contain its own logic about what to do when it is encountered during the evaluation process. However, on the GPU, this is not possible, as an array entry must hold a value and not a pointer to another memory location. Furthermore, even if it were possible, it would be a bad idea. As explained in Section 2.2.1, when loading data from global memory, larger chunks are retrieved at once. If the data is scattered across the GPU's global memory, a lot of unwanted data will be transferred. This can be seen in Figure 4.1, where if the data is stored sequentially, far fewer data operations and far less data in general needs to be transferred.

Because of this and because the GPU does not allow pointers, another solution is required. Instead of storing pointers to objects of different types in an array, it is possible to store one object with meta information. The object thus contains the type of the stored value, and the value itself, as described in Section 3.2.1. The four types that need to be stored in this object, differ significantly in the value they represent.

Variables and parameters are very simple to store. Because they represent indices to the variable matrix or the parameter vector, this (integer) index can be stored as is in the value property of the object. The type can then be used to determine whether it is an index to a variable or a parameter access.

Constants are also very simple, as they represent a single 32-bit floating point value. However, because of the variables and parameters, the value property is already defined as an integer and not as a floating point number. Unlike languages like Python, where every number is a floating point number, in Julia they are different and therefore cannot be stored in the same property. Creating a second property for constants only is not feasible, as this would introduce 4 bytes per object that need to be sent to the GPU which most of the time does not contain a defined value.

To avoid sending unnecessary bytes, a mechanism provided by Julia called reinterpret can be used. This allows the bits of a variable of one type, to be treated as the bits of another type. The bits used to represent a floating point number are then interpreted as an integer and can be stored in the same property. On the GPU, the same concept can be applied to reinterpret the integer value as a floating point value for further calculations. This is also the reason why the original type of the value needs to be stored alongside the value in order for the stored to be interpreted correctly and the expressions to be evaluated correctly.

Operators are very different from variables, parameters and constants. Because they

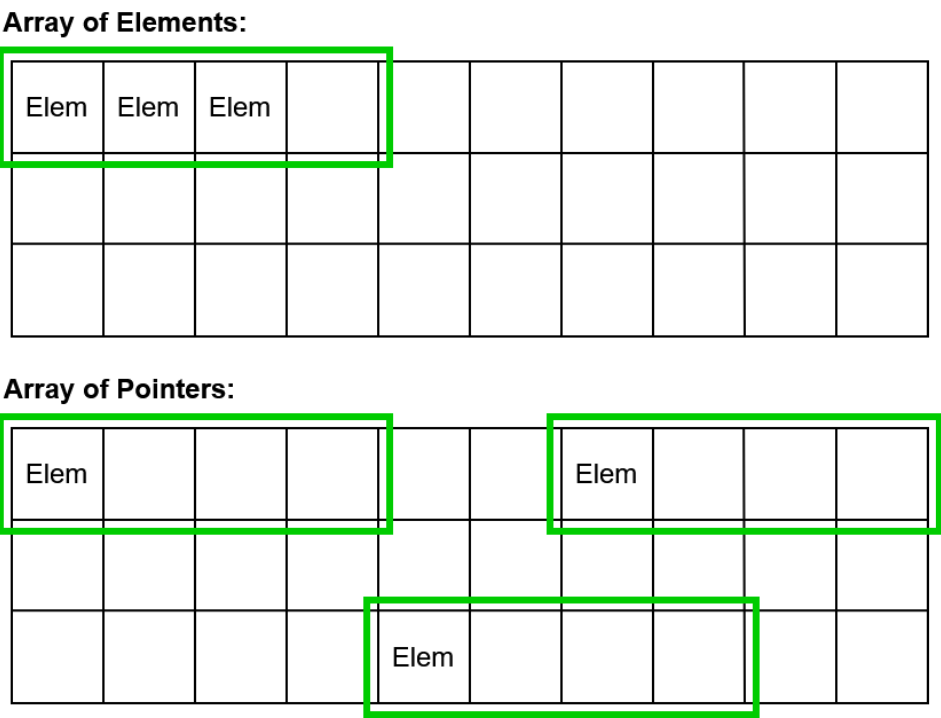


Figure 4.1: Loading data from global memory on the GPU always loads 32, 64 or 128 bytes (see Section 2.2.1). If pointers were supported and data would be scattered around global memory, many more data load operations would be required. Additionally, much more unwanted data would be loaded.

represent an operation rather than a value, a different way of storing them is required. An operator can be mapped to a number to identify the operation. For example, if the addition operator is mapped to the integer 1, then when the evaluator encounters an object of type operator and a value of 1, it will know which operation to perform. This can be done for all operators which means it is possible to store them in the same object with the same property. and only the type needs to be specified. The mapping of an operator to a value is often called an operation code, or opcode, and each operator is represented as one opcode.

With this, the intermediate representation is defined. Figure 4.2 shows how a simple expression would look after the pre-processing step. Note that the vluae 2.5 has been reinterpreted as an integer, resulting in the seemingly random value.

4.2.2 Processing

Now that the intermediate representation has been defined, the processing step can be implemented. This section describes the structure of the expressions and how they are processed. It also explains the process of parsing the expressions to ensure their validity and converting them into the intermediate representation.

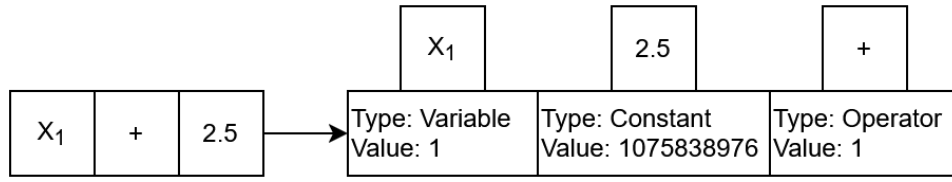


Figure 4.2: The expression $x_1 + 2.5$ after it has been converted to the intermediate representation. Note that the constant value 2.5 stores a seemingly random value due to it being reinterpreted as an integer.

Expressions

With the pre-processing step, the first modern feature of Julia has been used. As already mentioned, Julia provides extensive support for meta-programming, which is important for this step. Julia represents its own code as a data structure, which allows a developer to manipulate the code at runtime. The code is stored in the so-called Expr object as an Abstract Syntax Tree (AST), which is the most minimal tree representation of a given expression. As a result, mathematical expressions can also be represented as such an Expr object instead of a simple string. Which is a major benefit, because these expressions can then be easily manipulated by the symbolic regression algorithm. This is the main reason why the pre-processing step requires the expressions to be provided as an Expr object instead of a string.

Another major benefit of the expressions being stored in the Expr object and therefore as an AST, is the included operator precedence. Because it is a tree where the leaves are the constants, variables or parameters (also called terminal symbols) and the nodes are the operators, the correct result will be calculated when evaluating the tree from bottom to top. As can be seen in Figure 4.3, the expression $1 + x_1 \log(p_1)$, when parsed as an AST, contains the correct operator precedence. First the bottom most subtree $\log(p_1)$ must be evaluated before the multiplication, and after that, the addition can be evaluated.

It should be noted however, that Julia stores the tree as a list of arrays to allow a node to have as many children as necessary. For example the expression $1 + 2 + \dots + n$ contains only additions, which is a commutative operation, meaning that the order of operations is irrelevant. The AST for this expression would contain the operator at the first position in the array and the values at the following positions. This ensures that the AST is as minimal as possible.

Parsing

To convert the AST of an expression into the intermediate representation, a top-down traversal of the tree is required. The steps for this are as follows:

1. Extract the operator and convert it to its opcode for later use.
2. Convert all constants, variables and parameters and operators to the object (expression element) described in Section 4.2.1.
3. Append the expression elements to the postfix expression.

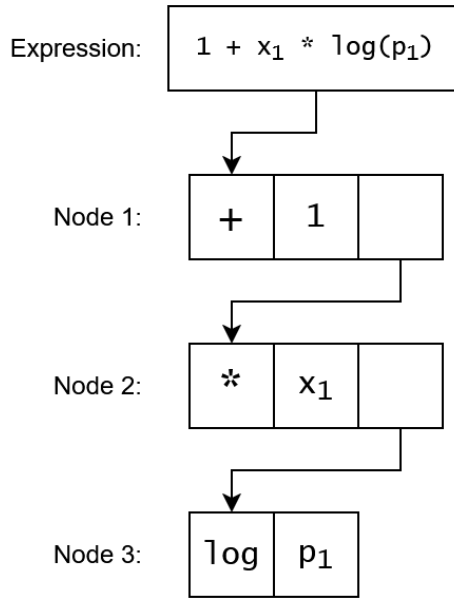


Figure 4.3: The AST for the expression $1 + x_1 \log(p_1)$ as generated by Julia. Some additional details Julia includes in its AST have been omitted as they are not relevant.

4. If the operator is a binary operator and there are more than two expression elements, append the operator after the first two elements and then after each element.
5. If a subtree exists, apply all previous steps and append it to the existing postfix expression.
6. Append the operator
7. Return the generated postfix expression/intermediate representation.

The validation of the expression is performed throughout the parsing process. Validating that only correct operators are used is performed in step 1. To be able to convert the operator to its corresponding opcode, it must be validated that an opcode exists for it, and therefore whether it is valid or not. Similarly, converting the tokens into an expression element object ensures that only valid variables and parameters are present in the expression. This is handled in step 2.

As explained above, a node of a binary operator can have n children. In these cases, additional handling is required to ensure correct conversion. This handling is summarised in step 4. Essentially, the operator must be added after the first two elements, and for each subsequent element, the operator must also be added. The expression $1 + 2 + 3 + 4$ is converted to the AST $+ 1 2 3 4$ and without step 4 the postfix expression would be $1 2 3 4 +$. If the operator is added after the first two elements and then after each subsequent element, the correct postfix expression $1 2 + 3 + 4 +$ will be generated.

Each subtree of the AST is its own separate AST, which can be converted to postfix notation in the same way the whole AST can be converted. This means that the algorithm only needs to be able to handle leaf nodes, and when it encounters a subtree,

it recursively calls itself to parse the remaining AST. Step 5 indicates this recursive behaviour.

While the same expression usually occurs only once, sub-expressions can occur multiple times. In the example in Figure 4.3, the whole expression $1 + x_1 \log(p_1)$ is unlikely to be generated more than once by the symbolic regression algorithm. However, the sub-expression $\log(p_1)$ is much more likely to be generated multiple times. This means that the generation of the intermediate representation for this subtree only needs to be done once and can be reused later. Therefore, a cache can be used to store the intermediate representation for this sub-expression and access it again later to eliminate the parsing overhead.

Caching can be applied to both individual sub-expressions as well as the entire expression. While it is unlikely for the whole expression to recur frequently, either as a whole or as part of a larger expression, implementing a cache will not degrade performance and will, in fact, enhance it if repetitions do occur. In the context of parameter optimisation, where the evaluators are employed, expressions will recur, making full-expression caching advantageous. The primary drawback of caching is the increased use of RAM. However, given that RAM is plentiful in modern systems, this should not pose a significant issue.

4.3 Interpreter

The implementation is divided into two main components, the CPU-based control logic and the GPU-based interpreter as outlined in the Concept and Design chapter. This section aims to describe the technical details of these components. First the CPU-based control logic will be discussed. This component handles the communication with the GPU and is the entry point which is called by the symbolic regression algorithm. Following this, the GPU-based interpreter will be explored, highlighting the specifics of developing an interpreter on the GPU.

An overview of how these components interact with each other is outlined in Figure 4.4. The parts of this figure are explained in detail in the following sections.

4.3.1 CPU Side

The interpreter is given all the expressions it needs to interpret as an input. Additionally, it needs the variable matrix as well as the parameters for each expression. All expressions are passed to the interpreter as an array of Expr objects, as they are needed for the pre-processing step or the frontend. The first loop as shown in Figure 4.4, is responsible for sending the expressions to the frontend to be converted into the intermediate representation. After this step, the expressions are in the correct format to be sent to the GPU and the interpretation process can continue.

Before the GPU can start with the interpretation, the data needs to be sent to the GPU. Because the variables are already in matrix form, transferring the data is fairly straightforward. Memory must be allocated in the global memory of the GPU and then be copied from RAM into the allocated memory. Allocating memory and transferring the data to the GPU is handled implicitly by the CuArray type provided by CUDA.jl.

As the interpreter needs to be optimised for parameter optimisation workloads, this

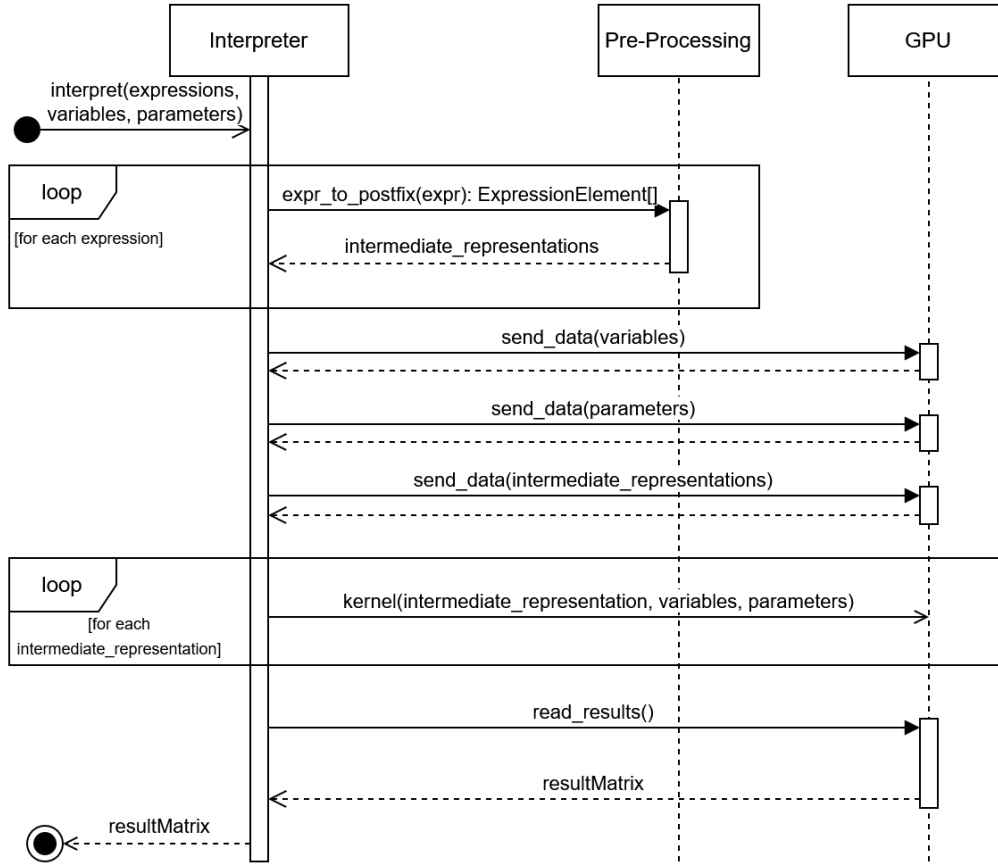


Figure 4.4: The sequence diagram of the interpreter.

step is actually performed before the interpreter is called. The variables never change, as they represent the observed inputs of a system that needs to be modelled by the symbolic regression algorithm. Therefore, it would be wasteful to re-transmit the variables for each step of the parameter optimisation part. If they are transmitted once and then reused throughout the duration of the parameter optimisation part, a lot of time can be saved. It would even be possible to transfer the data to the GPU before the symbolic regression algorithm starts, saving even more time. However, as this would require a change to the symbolic regression algorithm, the decision has been made to neglect this optimisation. It is still possible to modify the implementation at a later stage with minimal effort, if required.

Once the variables are transmitted, the parameters also must be transferred to the GPU. Unlike the variables, the parameters are stored as a vector of vectors. In order to transmit the parameters efficiently, they also need to be put in a matrix form. The matrix needs to be of the form $k \times N$, where k is equal to the length of the longest inner vector and N is equal to the length of the outer vector. This ensures that all values can be stored in the matrix. It also means that if the inner vectors are of different lengths, some extra unnecessary values will be transmitted, but the overall benefit of treating

```

1 function convert_to_matrix(vecs::Vector{Vector{T}}, invalidElement::T)::Matrix{T}
    where T
2     maxLength = get_max_inner_length(vecs)
3
4     # Pad the shorter vectors with the invalidElement to make all equal length
5     paddedVecs = [vcat(vec, fill(invalidElement, maxLength - length(vec))) for vec in
        vecs]
6     vecMat = hcat(paddedVecs...) # transform vector of vectors into column-major
        matrix
7
8     return vecMat
9 end
10
11 function get_max_inner_length(vecs::Vector{Vector{T}})::Int where T
12     return maximum(length.(vecs))
13 end
14

```

Program 4.1: A Julia program fragment depicting the conversion from a vector of vectors into a matrix of the form $k \times N$.

them as a matrix outweighs this drawback. The Program 4.1 shows how this conversion can be implemented. Note that it is required to provide an invalid element. This ensures defined behaviour and helps with finding errors in the code. After the parameters have been brought into matrix form, they can be transferred to the GPU the same way the variables are transferred.

Similar to the parameters, the expressions are also stored as a vector of vectors. The outer vector contains each expression, while the inner vectors hold the expressions in their intermediate representation. Therefore, this vector of vectors also needs to be brought into matrix form the same way the parameters are brought into matrix form. To simplify development, the special opcode *stop* has been introduced, which is used for the invalidElement in Program 4.1. As seen in Section 4.3.2, this element is used to determine if the end of an expression has been reached during the interpretation process. This removes the need for additional data to be sent which stores the length of each expression to determine if the entire expression has been interpreted or not. Therefore, a lot of overhead can be reduced.

Once the conversion into matrix form has been performed, the expressions are transferred to the GPU. Just like with the variables, the expressions remain the same over the course of the parameter optimisation part. Therefore, they are transferred to the GPU before the interpreter is called, to reduce the amount of unnecessary data transfer.

In addition to the already described data that needs to be sent, two more steps are required that have not been included in the Sequence Diagram 4.4. The first one is the allocation of global memory for the result matrix. Without this, the kernel would not know where to store the interpretation results. Therefore, enough global memory needs to be allocated so that the results can be stored and retrieved after all kernel executions have finished.

Only raw data can be sent to the GPU, which means that information about the data is missing. The matrices are represented as flat arrays, which means they have lost

expr elem	expr elem	expr elem	expr elem	expr elem		expr elem	expr elem	expr elem
var	var	var	var	var	var	var	var	var
param	param			param	param			

Figure 4.5: The expressions, variables and parameters as they are stored in the GPU's global memory. Note that while on the CPU they are stored as matrices, on the GPU, they are only three arrays of data. The thick lines represent, where a new column and therefore a new set of data begins.

their column and row information. This information must be sent separately to let the kernel know the dimensions of the expressions, variables and parameters. Otherwise, the kernel does not know at which memory location the second variable set is stored for example. Figure 4.5 shows how the data is stored without any information about the rows or columns of the matrices. The thick lines help to identify where a new column, and therefore a new set of data begins. However, the GPU has no knowledge of this and therefore the additional information must be transferred to ensure that the data is accessed correctly.

Once all the data is present on the GPU, the CPU can dispatch the kernel for each expression. This dispatch requires parameters that specify the number of threads and their organisation into thread blocks. In total, one thread is required for each variable set and therefore the grouping into thread blocks is the primary variable. Taking into account the constraints explained in Section 2.2.1, this grouping needs to be tuned for optimal performance. The specific values alongside the methodology for determining these values will be explained in Chapter 5.

In addition, the dispatch parameters also include the pointers to the location of the data allocated and transferred above, as well as the index of the expression to be interpreted. Since all expressions and parameters are sent to the GPU at once, this index ensures that the kernel knows where in memory to find the expression it needs to interpret and which parameter set it needs to use. After the kernel has finished, the result matrix needs to be read from the GPU and passed back to the symbolic regression algorithm.

Crucially, dispatching a kernel is an asynchronous operation, which means that the CPU does not wait for the kernel to finish before continuing. This allows the CPU to dispatch all kernels at once, rather than one at a time. As explained in Section 3.2, a GPU can have multiple resident grids, meaning that the dispatched kernels can run concurrently, drastically reducing evaluation times. Only once the result matrix is read from the GPU does the CPU have to wait for all kernels to finish execution.

4.3.2 GPU Side

With the GPU's global memory now containing all the necessary data and the kernel being dispatched, the interpretation process can begin. Before interpreting an expression, the global thread ID must be calculated. This step is crucial because each variable set is assigned to a unique thread. Therefore, the global thread ID determines which variable set should be used for the current interpretation instance.

Moreover, the global thread ID ensures that excess threads do not perform any work. As otherwise these threads would try to access a variable set that does not exist and therefore would lead to an illegal memory access. This is necessary because the number of required threads often does not align perfectly with the number of threads per block multiplied by the number of blocks. If for example 1031 threads are required, then at least two thread blocks are needed, as one thread block can hold at most 1024 threads. Because 1031 is a prime number, it can not be divided by any practical number of thread blocks. If two thread blocks are allocated, each holding 1024 threads, a total of 2048 threads is started. Therefore, the excess $2048 - 1031 = 1017$ threads must be prevented from executing. By using the global thread ID and the number of available variable sets, these excess threads can be easily identified and terminated early in the kernel execution.

Afterwards the stack for the interpretation can be created. It is possible to dynamically allocate memory on the GPU, which enables a similar programming model as on the CPU. Winter et al. (2021) have even compared many dynamic memory managers and found, that the performance impact of them is rather small. However, if it is easily possible to use static allocations, it still offers better performance. In the case of this thesis, it is easily possible which is the reason why the stack has been chosen to have a static size. Because it is known that expressions do not exceed 50 tokens, including the operators, the stack size has been set to 25, which should be more than enough to hold the values and partial results, even in the worst case.

Main Loop

After everything has been initialised, the main interpreter loop starts interpreting the expression. Because of the intermediate representation, the loop simply traverses the expression from left to right. On each iteration the type of the current token is checked, to decide which operation to perform.

If the current token type corresponds to the *stop* opcode, the interpreter knows that it has finished. This simplicity is the reason why as explained above, this opcode has been introduced.

More interestingly is the case, where the current token corresponds to an index to either the variable matrix, or the parameter matrix. If that is the case, then the value of the token is important. To access one of these matrices first, the correct starting index needs to be calculated. As already explained, all information about the layout of the data is lost during transfer. At this stage, the kernel only knows the index of the first element of either of the matrices, the index of the variable set and parameter set, as well as the index of the value inside the current variable set or parameter set. However, it is not known where the boundaries of the sets are and therefore the additionally transferred data about the layout is used in this step to calculate the index of the first

element per set. With this calculated index and the index stored in the token, the correct value can be loaded. After the value has been loaded, it is stored at the top of the stack for later use.

Constants work very similar, as the token value is read and added to the top of the stack. However, since constants have been reinterpreted as integers for easy transfer to the GPU, this must be reversed before adding the value to the stack.

Evaluating the expression is happening if the current token is an operator. The value of the token is the opcode, which determines the operation that needs to be performed. If the opcode corresponds to a unary operator, only the top value of the stack needs to be popped for the operation. The operation is then performed on this value and the result is added back to the stack. On the other hand, if the operator corresponds to a binary operator, the top two values need to be popped. These are then used for the operation and the result is again added back to the stack.

With this it would also be possible to add support for ternary operators. An example would be a Fused Multiply-Add (FMA) operator. While this operator does not exist in Julia, the frontend can generate it, if it encounters a sub-expression that follows the form $x * y + z$. As this expression performs the multiplication and addition in a single clock cycle instead of two, it would be a feasible optimisation. However, detecting such sub-expressions is more complicated, which is the reason it is not supported in the current implementation.

Once the interpreter loop is finished, the result of the evaluation needs to be stored in the result matrix. By using the index of the current expression, as well as the index of the current variable set, the index where the result must be stored can be calculated. The last value on the stack is the result, which will be stored in the result matrix at the calculated location.

4.4 Transpiler

Talk about how the transpiler has been developed (probably largest section, because it just has more interesting parts); CPU-side part will be much larger than GPU side

- UML-Ablaufdiagram

- Front-End and Back-End Caching of back-end results

- PTX code generated and compiled using CUDA.jl (so basically using the driver) and then executed

- Memory access (global memory and register management especially register management)

Chapter 5

Evaluation

The aim of this thesis is to determine whether at least one of the GPU evaluators is faster than the current CPU evaluator. This chapter describes the performance evaluation. First, the environment in which the performance tests are performed is explained. Then the individual results for the GPU interpreter and the transpiler are presented. In addition, this part also includes the performance tuning steps taken to achieve these results. Finally, the results of the GPU evaluators are compared to the CPU evaluator in order to answer the research questions of this thesis.

5.1 Test environment

Explain the hardware used, as well as the actual data (how many expressions, variables etc.)

three scenarios -> few, normal and many variable sets;; expr repetitions to simulate parameter optimisation Benchmarktools.jl -> 1000 samples per scenario

5.2 Results

talk about what we will see now (results only for interpreter, then transpiler and then compared with each other and a CPU interpreter)

5.2.1 Interpreter

Results only for Interpreter (also contains final kernel configuration and probably quick overview/recap of the implementation used and described in Implementation section)

5.2.2 Performance tuning

Document the process of performance tuning

Initial: CPU-Side single-threaded; up to 1024 threads per block; bounds-checking enabled (especially in kernel)

1.) Blocksize reduced to a maximum of 256 -> moderate improvement in medium and large 2.) Using @inbounds -> noticeable improvement in 2 out of 3 3.) Tuned

blocksize with NSight compute -> slight improvement 4.) used int32 everywhere to reduce register usage -> significant performance drop (probably because a lot more waiting time “latency hiding not working basically”, or more type conversions happening on GPU? look at generated PTX code and use that as an argument to describe why it is slower) 5.) reverted previous; used fastmath instead -> improvement (large var set is now faster than on transpiler)

5.2.3 Transpiler

Results only for Transpiler (also contains final kernel configuration and probably quick overview/recap of the implementation used and described in Implementation section)

5.2.4 Performance tuning

Document the process of performance tuning

Initial: CPU-Side single-threaded; up to 1024 threads per block; bounds-checking enabled

1.) Blocksize reduced to a maximum of 256 -> moderate improvement in medium and large 2.) Using @inbounds -> small improvement only on CPU side code 3.) Tuned blocksize with NSight compute -> slight improvement 4.) Only changed things on interpreter side 5.) Only changed things on interpreter side

5.2.5 Comparison

Comparison of Interpreter and Transpiler as well as Comparing the two with CPU interpreter

talk about that compute portion is just too little. Only more complex expressions with higher var set count benefit well (make one or two performance evaluations, with 10 larger expressions and at least 1k var sets and present that here as point for that statement)

Chapter 6

Conclusion and Future Work

Summarise the results talk again how a typical input is often not complex enough (basically repeat that statement from comparison section in evaluation)

6.1 Future Work

talk about what can be improved

Frontend: 1.) extend frontend to support ternary operators (basically if the frontend sees a multiplication and an addition it should collapse them to an FMA instruction)

Transpiler: 1.) transpile expression directly from Julia AST -> would save time because no intermediate representation needs to be created (looses step and gains performance, but also makes transpiler itself more complex) 2.) Better register management strategy might be helpful -> look into register pressure etc.

CPU Interpreter: Probably more worth to dive into parallelising cpu interpreter itself (not really future work, as you wouldn't write a paper about that)

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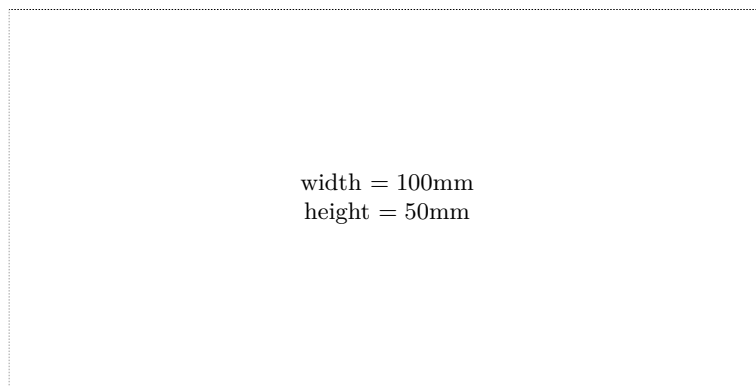
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