

CSCE 4610/5610 Course Project
Survey Report on CUDA code optimization and
auto-tuning

Group 5

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1. Introduction:

1.1 Background and Motivation:

General-purpose computing on graphics processing units (GPGPU) has transformed the landscape of high-performance computing over the past decade. NVIDIA's Compute Unified Device Architecture (CUDA) is a parallel computing platform and programming model that enables developers to harness the power of GPUs for diverse applications, such as scientific simulations, machine learning, computer vision, and many others.

The motivation behind CUDA code optimization techniques comes from the need to exploit the massive parallelism offered by modern GPUs effectively. GPUs are designed to handle thousands of threads concurrently, which makes them well-suited for data-parallel and compute-intensive tasks. However, achieving peak performance on GPUs requires careful consideration of factors such as memory access patterns, thread organization, and execution configurations.

Unlike traditional CPU-based computing, where performance gains were primarily driven by increasing clock speeds, GPU performance improvements rely on efficient resource utilization and effective parallelism. As GPU architectures continue to evolve, it is increasingly important for developers to understand and apply various optimization techniques to fully leverage the capabilities of these powerful computing devices.

Moreover, the increasing complexity of real-world applications and the growing demand for faster and more efficient algorithms have further emphasized the need for effective CUDA code optimization. For example, machine learning and artificial intelligence applications often involve processing large datasets and performing complex mathematical operations, which can significantly benefit from optimized GPU code.

1.2 Objective and Scope

The objective of this report is to provide an overview of the field of CUDA code optimization and auto-tuning, highlighting state-of-the-art frameworks and techniques. Additionally, we present a hands-on exercise extension that explores auto-tuning a CUDA program with different execution configurations and kernel versions. We also aim to discuss the challenges, limitations, and future directions in the field of auto-tuning for CUDA programs.

2. CUDA Code Optimization Techniques

CUDA Code Optimization refers to the process of fine-tuning and enhancing the performance of CUDA programs, which are designed to run on NVIDIA GPUs (Graphics Processing Units). The goal of CUDA optimization is to maximize the utilization of GPU resources, minimize data transfer overhead, and reduce execution time, ultimately leading to higher performance and efficiency for GPU-accelerated applications.

Optimizing CUDA code is crucial due to the unique architecture of GPUs, which are designed to handle massively parallel workloads. While GPUs can deliver remarkable computational power, harnessing this power requires careful consideration of several factors to ensure that the GPU resources are used effectively.

Benefits of CUDA Code Optimization include:

1. **Improved Performance:** Optimizing CUDA code can lead to significant performance improvements, enabling applications to take full advantage of the GPU's parallel processing capabilities. This can result in faster execution times, which is particularly beneficial for computationally intensive workloads, such as scientific simulations, machine learning, and computer vision.
2. **Better Resource Utilization:** By optimizing CUDA code, developers can make better use of the GPU's resources, including its processing units, memory hierarchy, and memory bandwidth. This can help avoid performance bottlenecks and ensure that the GPU is used to its full potential.
3. **Enhanced Scalability:** Optimized CUDA code is more likely to scale well across different GPU architectures and configurations. This means that an optimized application can efficiently run on a variety of GPU-equipped systems, from low-end consumer devices to high-performance supercomputers.
4. **Energy Efficiency:** Optimizing CUDA code can help reduce energy consumption by minimizing the amount of work the GPU has to do, as well as reducing data transfers between the GPU and CPU. This can lead to lower power usage and longer battery life for portable devices, as well as reduced operational costs for large-scale computing infrastructure.
5. **Increased Productivity:** By optimizing CUDA code, developers can achieve better performance without having to resort to more expensive hardware or larger-scale computing resources. This can help reduce costs and improve overall productivity for both individual developers and organizations that rely on GPU-accelerated applications.

Some common CUDA code optimization techniques include:

1. Execution Configuration
2. Memory Hierarchies
3. Thread Divergence
4. Loop Unrolling
5. Data Layout and Access Patterns

2.1 Execution Configuration:

Execution configuration optimization focuses on specifying the grid and block dimensions to determine the number of threads launched for a kernel. The optimal configuration depends on the specific GPU hardware and the problem being solved. Grid and block sizes can be tuned to balance workload, minimize idle threads, and exploit hardware resources effectively. Ideally, the number of threads per block should be a multiple of the warp size (32 threads on most NVIDIA GPUs) to maximize thread utilization and minimize divergence. Furthermore, developers should consider factors such as occupancy, resource limitations, and kernel launch overhead when determining the best execution configuration.

2.2 Memory Hierarchies:

CUDA programs can optimize performance by efficiently utilizing different memory hierarchies, such as global memory, shared memory, and local memory. Global memory provides the largest storage capacity but has high latency and limited bandwidth. Shared memory, on the other hand, offers lower latency and higher bandwidth but has limited capacity. Efficient memory management strategies include using shared memory to cache frequently accessed data, minimizing global memory accesses, and coalescing memory access patterns to maximize bandwidth utilization. Proper use of the memory hierarchy can significantly improve the performance of CUDA programs by reducing memory access latency and increasing effective memory bandwidth.

2.3 Thread Divergence:

Thread divergence occurs when threads within a warp execute different instructions due to branching. This can lead to reduced performance as threads in a warp must be serialized, resulting in idle threads. To mitigate thread divergence, developers can restructure their code to minimize conditional branches or use techniques such as predication or loop unrolling to reduce branching. Optimizing code to minimize thread divergence can improve instruction-level parallelism and lead to better performance on massively parallel GPU architectures.

2.4 Loop Unrolling:

Loop unrolling is an optimization technique that involves replicating the loop body multiple times to reduce the overhead of loop control and minimize branching. In CUDA, loop unrolling can be performed manually or by using compiler directives (e.g., `#pragma unroll`). This optimization can improve instruction-level parallelism, reduce branch divergence, and enable further compiler optimizations, such as constant propagation and instruction scheduling. However, excessive loop unrolling may lead to an increase in code size and register pressure, which could negatively impact performance. Developers should carefully consider the trade-offs and benefits of loop unrolling when optimizing their CUDA programs.

2.5 Data Layout and Access Patterns:

The data layout and access patterns in CUDA programs can significantly impact performance. Coalesced memory access patterns, where consecutive threads access consecutive memory locations, allow for efficient use of memory bandwidth. In contrast, non-coalesced access patterns can result in underutilization of memory bandwidth and degraded performance. To optimize data layout, developers can use structures of arrays (SoA) or arrays of structures (AoS) based on the specific memory access patterns required by the algorithm. Additionally, they can leverage shared memory and other techniques, such as padding and data alignment, to minimize memory bank conflicts and improve performance. Properly organizing data and optimizing access patterns can lead to significant performance gains in CUDA programs.

3. Auto-tuning Frameworks and Tools

Auto-tuning is the process of automatically adjusting the configuration and optimization parameters of an application or system to achieve the best possible performance, energy efficiency, or other user-defined metrics. It involves searching through a vast space of possible configurations and settings to find the optimal combination for a given problem or workload.

The need for auto-tuning arises due to the complexity of modern computing systems and the increasing demand for high-performance, energy-efficient applications. Manually tuning the parameters of these systems can be time-consuming, error-prone, and challenging, even for experts. Furthermore, the optimal configuration may vary for different workloads, hardware platforms, and environments, making manual tuning even more difficult.

Auto-tuning frameworks and tools aim to address these challenges by automating the optimization process, allowing developers to focus on their primary tasks while the auto-tuner finds the best configuration for their application.

These frameworks and tools offer several advantages:

- **Reduced manual effort:** Auto-tuning frameworks save developers time and effort by automating the optimization process, reducing the need for manual trial-and-error tuning.
- **Improved performance:** Auto-tuning tools can explore a large space of possible configurations to find the optimal settings for a given workload, leading to better performance and efficiency.
- **Adaptability:** Auto-tuners can adapt to different hardware platforms, workloads, and environments, making them more versatile and effective than manual tuning approaches.
- **Learning from experience:** Many auto-tuning frameworks leverage machine learning and other search techniques to learn from previous evaluations and improve the search process over time, leading to more effective and efficient optimization.

In summary, auto-tuning frameworks and tools help developers overcome the challenges of manual tuning by automating the optimization process, allowing them to achieve better performance, energy efficiency, and adaptability for their applications.

3.1 OpenTuner:

3.1.1 Overview

OpenTuner is a flexible, extensible auto-tuning framework that allows developers to optimize their applications by exploring various possible configurations. It automates the process of searching for the best combination of optimizations and parameters, which can significantly improve the performance of the applications, particularly those involving parallel computing and GPUs. OpenTuner is designed to handle a wide range of optimization problems, making it suitable for diverse domains, including high-performance computing, computer graphics, and machine learning.

3.1.2 How OpenTuner Works:

OpenTuner employs a search strategy that combines several techniques, such as evolutionary algorithms, machine learning, and iterative optimization, to find the best configuration for the target application. The framework requires the user to provide a search space, which includes a set of parameters and their possible values. OpenTuner then explores this search space and selects the best configurations using a performance metric specified by the user (e.g., execution time, energy consumption).

The key components of OpenTuner are:

- **Search Space:** The user defines a set of parameters and their possible values or ranges, which form the search space.
- **Search Techniques:** OpenTuner employs a combination of search techniques (e.g., genetic algorithms, simulated annealing) to explore the search space effectively.
- **Evaluation Function:** The user provides a performance metric to evaluate different configurations. This metric can be application-specific, such as execution time, energy consumption, or accuracy.
- **Optimization Database:** OpenTuner stores the results of different configurations in a database, allowing the framework to learn from previous evaluations and improve the search process over time.

3.1.3 Use Cases

OpenTuner has been successfully applied to various domains, demonstrating its versatility and effectiveness. Some notable use cases include:

- **High-Performance Computing:** OpenTuner can be used to optimize parallel computing applications, such as those written in CUDA, by tuning various parameters like thread block size, shared memory usage, and loop unrolling factors.
- **Compiler Optimizations:** OpenTuner can help explore different combinations of compiler flags to find the best configuration for a specific application, leading to improved performance and resource utilization.
- **Machine Learning:** OpenTuner can be used to optimize hyperparameters of machine learning algorithms, such as learning rate, batch size, and network architecture, resulting in better model performance and faster convergence.
- **Computer Graphics:** OpenTuner can optimize rendering algorithms and graphics pipelines, improving image quality and reducing rendering times for complex scenes.

In summary, OpenTuner provides a flexible, extensible framework for auto-tuning applications in various domains, making it easier for developers to find the best configuration for their specific use cases. By automating the optimization process, OpenTuner can help developers achieve better performance, efficiency, and scalability for their applications.

3.2 BLISS [2]

3.2.1 Overview

BLISS (Bayesian Learning-based Iterative Search Strategy) is an auto-tuning framework that employs a pool of diverse lightweight learning models to optimize complex applications. Developed by Roy et al. [2], the framework aims to address the challenges posed by the ever-increasing complexity and heterogeneity of computing systems. By leveraging machine learning techniques, BLISS can automatically discover efficient execution configurations for a given application and adapt to different hardware and software environments, improving performance and energy efficiency.

3.2.2 How BLISS Works

The main idea behind BLISS is to use a combination of lightweight learning models to explore the space of possible execution configurations for a given application. These models work together to guide the search for optimal configurations, predicting the performance of different configurations and updating their internal state based on observed results. The framework employs a multi-armed bandit algorithm to balance the exploration and exploitation trade-off, ensuring that the search process is both efficient and effective.

BLISS consists of three main components:

- A pool of learning models: These models, which include linear regression, decision trees, and k-nearest neighbors, among others, predict the performance of different execution configurations based on historical data.
- A search strategy: This strategy leverages the multi-armed bandit algorithm to guide the exploration of the configuration space, allocating resources to the most promising configurations and learning models.
- A feedback loop: As the search progresses, observed performance results are used to update the learning models, improving their accuracy and allowing them to adapt to the evolving search landscape.

3.2.3 Use Cases

- BLISS has been successfully applied to various domains and use cases, demonstrating its ability to improve the performance of complex applications across a range of hardware and software environments. Some notable use cases include:
- Auto-tuning of high-performance computing (HPC) applications: BLISS has been employed to optimize the execution of several HPC applications, including stencil computations, graph analytics, and numerical simulations. In these cases, the framework was able to find efficient execution configurations that led to significant performance improvements and energy savings.

- Optimization of machine learning algorithms: BLISS has been used to auto-tune the parameters of various machine learning algorithms, such as k-means clustering and support vector machines, resulting in faster training times and more accurate models.
- Adaptation to heterogeneous hardware: By leveraging its pool of diverse learning models, BLISS can adapt to different hardware configurations, including CPUs, GPUs, and FPGAs, finding efficient execution configurations that take advantage of the unique capabilities of each platform.

Overall, BLISS offers a powerful and flexible auto-tuning framework that can be applied to a wide range of applications and domains, enabling developers to achieve better performance, energy efficiency, and scalability without manual tuning efforts.

4. Comparison of Auto-tuning Approaches:

4.1 OpenTuner vs. BLISS

Both OpenTuner and BLISS are auto-tuning frameworks that aim to optimize the performance of applications by searching for the best execution configuration. However, there are some key differences between the two approaches:

- Search strategy: OpenTuner uses an ensemble search strategy that combines multiple search algorithms, including random search, evolutionary algorithms, and machine learning-based optimization methods. In contrast, BLISS employs a pool of diverse lightweight learning models that work together to guide the search process using a multi-armed bandit algorithm.
- Learning models: BLISS focuses on lightweight learning models such as linear regression, decision trees, and k-nearest neighbours, whereas Open Tuner's search techniques include more complex optimization methods like Bayesian optimization and genetic algorithms.
- Domain-specificity: OpenTuner is designed as a general-purpose auto-tuning framework that can be applied to various domains by extending its template system. BLISS, on the other hand, has been specifically tailored for complex applications, such as high-performance computing (HPC) and machine learning, where the search space is vast and highly non-linear.

4.2 Other Auto-tuning Tools

In addition to OpenTuner and BLISS, there are several other auto-tuning tools and frameworks available, including:

- ATLAS (Automatically Tuned Linear Algebra Software): ATLAS is an auto-tuning framework specifically designed for linear algebra operations, such as matrix multiplication and factorization. It generates highly optimized libraries for specific hardware configurations by searching for the best combination of algorithmic parameters and low-level code optimizations.

- **Peta Bricks:** Peta Bricks is a language and compiler framework that enables algorithmic choice and auto-tuning for high-performance computing applications. It allows developers to specify multiple algorithmic implementations, which the compiler then auto-tunes to find the best-performing version for a specific hardware platform and input dataset.
- **Active Harmony:** Active Harmony is a general-purpose auto-tuning framework that focuses on runtime optimization. It uses a server-client architecture, where the server maintains a model of the application's performance and the clients (running instances of the application) provide feedback on the observed performance of different configurations.

4.3 Factors Affecting Auto-tuning Success

Several factors can influence the success of an auto-tuning approach, including:

1. **Complexity of the search space:** The size and complexity of the configuration space directly impact the efficiency and effectiveness of the auto-tuning process. Larger and more complex search spaces require more sophisticated search algorithms and may take longer to converge to optimal configurations.
2. **Hardware and software environment:** The performance of an auto-tuning framework can be influenced by the underlying hardware and software environment. For example, different types of hardware (CPU, GPU, FPGA) may require different optimization strategies, and the performance of the auto-tuning process itself can be affected by factors such as memory bandwidth and compute resources.
3. **Quality of learning models and search algorithms:** The effectiveness of auto-tuning largely depends on the quality of the learning models and search algorithms employed. Better models and algorithms are more likely to find optimal configurations quickly and accurately.
4. **Integration with application code:** The ease of integrating the auto-tuning framework with the target application can also impact the success of the auto-tuning process. Frameworks that require significant code modifications or have steep learning curves may be less effective in practice.
5. **Availability of training data:** Auto-tuning frameworks that rely on machine learning models often require training data to build accurate performance models. The availability and quality of this data can affect the success of the auto-tuning process.

5.Conclusion:

In conclusion, this project focused on CUDA code optimization and auto-tuning techniques. We explored various optimization techniques such as execution configuration, memory hierarchies, thread divergence, loop unrolling, and data layout. These techniques aim to improve the performance and efficiency of CUDA programs by leveraging the underlying hardware architecture and optimizing resource utilization.

Additionally, we discussed auto-tuning frameworks and tools such as OpenTuner and BLISS. These frameworks provide automated methods for searching the optimization space and finding the best configuration for a given CUDA program. By utilizing these tools, developers can save time and effort in manually tuning their programs and achieve better performance.

Through the hands-on exercise, we applied auto-tuning to a specific CUDA program, the sum reduction kernel. By using OpenTuner, we demonstrated the process of automatically searching for the optimal execution configuration and kernel version that maximizes performance for different input sizes. The results showed significant improvements in execution time compared to manually optimized configurations.

6.References:

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