

České vysoké učení technické v Praze
Fakulta jaderná a fyzikálně inženýrská

Katedra softwarového inženýrství
Obor: Aplikace softwarového inženýrství



Paralelní LU rozklad pro GPU

Parallel LU Decomposition for the GPU

VÝZKUMNÝ ÚKOL

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Vedoucí práce: doc. Ing. Tomáš Oberhuber, Ph.D.
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Studijní program: Aplikace přírodních věd

Obor: Aplikace softwarového inženýrství

Název práce česky: Webová aplikace pro správu veřejné knihovny s pobočkami

Název práce anglicky: Web Application for Management of Public Library with Branch Offices

Pokyny pro vypracování:

1. Seznámit se s chodem veřejné knihovny z pohledu zaměstnance a čtenáře.
2. Prozkoumat existující řešení (nabízené funkce, výhody, nevýhody).
3. Na základě výše získaných informací identifikovat typy uživatelů a jim odpovídající funkce webové aplikace.
4. Navrhnout databázi (ERA model) a vybrat vhodný databázový systém, ve kterém bude reálnována.
5. Navrhnout vzhled webových stránek tak, aby obsahovaly vhodné funkce pro jednotlivé typy uživatelů, vybrat vhodný framework pro realizaci webové aplikace a implementovat ji s ohledem na známé bezpečnostní hrozby.
6. Vytvořit uživatelskou příručku pro jednotlivé typy uživatelů (včetně popisu instalace a požadovaného softwaru).

Doporučená literatura:

- [1] *Doctrine Project* [online]. Doctrine Team, 2006 [cit. 2016-10-19]. Dostupné z: <http://wwwdoctrine-project.org/>.
- [2] *PHP: Hypertext Preprocessor* [online]. Dánsko: The PHP Group, 2001 [cit. 2016-10-19]. Dostupné z: <http://php.net/>.
- [3] *Rychlý a pohodlný vývoj webových aplikací v PHP – Nette Framework* [online]. Praha: Nette framework, 2008 [cit. 2016-10-19]. Dostupné z: <https://nette.org/>.

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vedoucí práce

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Doba platnosti zadání je dva roky od data zadání.

s podpisem vedoucího katedry

Jan R
vedoucí katedry



**s podpisem
děkana fakulty**

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děkan

Prohlášení

Prohlašuji, že jsem svůj výzkumný úkol vypracoval samostatně a použil jsem pouze podklady (literaturu, projekty, SW atd.) uvedené v přiloženém seznamu.

Declaration

I declare that I have carried out my research project independently and I have used only the materials (literature, projects, software, etc.) listed in the bibliography.

V Praze dne

.....
Bc. Lukáš Čejka

Poděkování

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Paralelní LU rozklad pro GPU

Autor: Bc. Lukáš Čejka

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Obor: Aplikace softwarového inženýrství

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Introduction TODO

Put my introduction text here (1-3 pages, do not divide it into sub-pages).

Chapter 1

Theory

This chapter will present the core theory of areas used in this research assignment. Firstly, Graphical Processing Units (GPUs) will be introduced with an emphasis on the architecture of GPUs (only Nvidia GPUs as the Nvidia API, CUDA, was used to develop this project). Then, CUDA, will be described in greater detail. Finally, the theory behind Lower-Upper (LU) Decomposition will be presented.

1.1 GPUs

From an average consumer's perspective a Graphics Processing Unit (GPU) is a component of a computing system that performs graphical operations, for example, processing images. For the sake of the example, let image processing be simplified into the following: images are composed of pixels and each pixel needs to be processed. Since a GPU contains thousands of processing units it can perform a large number of operations in parallel, for example, processing a large number of pixels at once, thus making it highly efficient at image processing. While this has a wide range of uses, there is another field where the highly-parallel nature of the GPU can be utilized: General-Purpose Computing on Graphics Processing Units (GPGPU).

1.1.1 General-Purpose Computing on Graphics Processing Units (GPGPU)

As described in section 1.2 of the author's bachelor thesis *Formats for storage of sparse matrices on GPU* [42], GPUs started to evolve at the turn of the 21st century from purely graphics-processing units into devices capable of general-purpose computing, i.e. computation that is not necessarily related to graphics. The significance of this event lies in the use of graphics cards for seemingly any parallelizable computational task that would benefit from the abundance of slower processing units on a GPU rather than fewer faster processing units found on a CPU [40].

For reference, high-end desktop CPUs today usually have anywhere from 8 to 16 cores, while server CPUs can have upwards of 64 cores (not counting hyper-threading and similar technologies). In general, CPUs with more cores have a lower clock speed - see figure 1.1 for a selection of processors along with their core count and clock speeds [41].

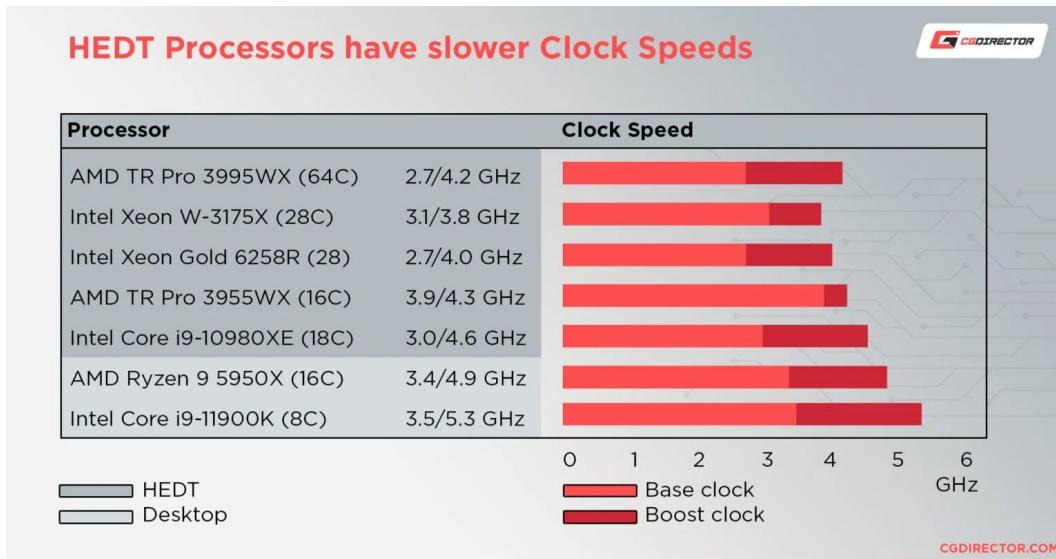


Figure 1.1: Selection of desktop and server CPUs - including number of cores and clock speed [41]. HEDT stands for High-End Desktop Processor - in this instance it also includes CPUs predominantly used in servers.

While CPUs are widely used for sequential tasks, they can also be used for tasks that can be described as parallelizable, for example, processing of requests to a server. They are not suitable for highly parallel tasks such as image processing, where GPUs excel due to their architecture. Figure 1.2 shows the comparison of a CPU and GPU architecture. The example CPU in the figure has - among other components - 4 cores each having its own L1 cache and controlling component. This configuration allows for executing a thread (series of operations) at a high speed and lower throughput (fewer number of threads running at once). Simply, the CPU is more suitable for rapid completion of serialized instructions.

Nvidia GPUs, on the other hand, are engineered to have many smaller controlling units called SMs (Stream Multiprocessors) that aim to schedule and task individual processing units found on the GPU. Furthermore, in figure 1.2 it can be seen that GPUs have a different cache structure. Specifically, GPUs only have two levels, whereas CPUs have three. In summary, the GPU has more transistors for processing data - namely operations that use floating-point computations. Moreover, the architecture of the GPU allows for it to compensate for memory access delays by performing computations simultaneously [40].

A prime example of where this characteristic gives a significant advantage to the GPU over the CPU is during matrix multiplication which will be described later in subsection 1.2.6.

For completion, see table 1.1 for a selection of GPUs along with their specifications.

The table shows specifications for two different categories of GPUs: consumer and professional (commercial). Consumer cards (in the table: GTX 1070, RTX 3060) can be found in regular desktop PCs and are intended more for video gaming, rather than raw computing power. However, these cards are mentioned as the optimization of this project's implementation was done on machines that included them. On the other hand, professional cards are intended mainly for GPGPU, or - in some specific cases - for machine learning.

Characteristics that can be used to compare GPUs are, for example, peak TFLOPS (TFLOPS - how many trillion floating-point operations can the processor perform per second), memory bandwidth, TDP. The value that clearly separates commercial cards from consumer cards is the peak FP64 (double precision)

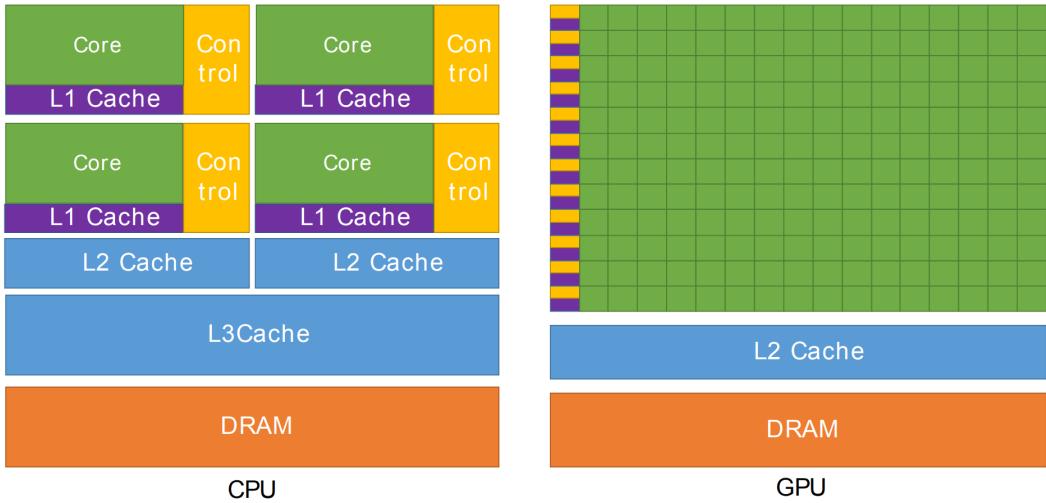


Figure 1.2: Comparison of the architecture of CPUs and GPUs. On one hand, CPUs have fewer cores, more complex controlling logic compared to GPUs and the cores of a CPU have a higher clock speed. On the other hand, GPUs have a much higher number of cores clocked at lower speeds. Taken from Nvidia's *CUDA C++ programming guide* [40].

TFLOPS, which is the highest for the A100 at 9.7 TFLOPS, with the V100 being slightly slower at 7.8 TFLOPS, whereas the consumer cards perform significantly worse at around 0.2 TFLOPS.

In summary, professional cards are heavily preferred when it comes to GPGPU, however, consumer cards can be and are used for development as they are more affordable.

1.2 Compute Unified Device Architecture (CUDA)

The Compute Unified Device Architecture (CUDA) is a programming model, sometimes referred to as a parallel computing platform, introduced by Nvidia in 2006 [39]. It is designed to give developers low-level access to GPU hardware, for example, fine-tuning assignment of processing units or memory allocation, thus, allowing them to utilize the full potential of GPUs and tailor their use for specific applications. CUDA supports a variety of programming languages, for example, C++ (used in this project) and Fortran, however, adaptations for other languages such as, Python, Perl, Java, Ruby, MATLAB, Julia, etc. have been created [28].

This section will first explain some basic terminology followed by the theory behind CUDA from the simplest concept - a thread - to how threads are managed. Then, memory will be introduced in a similar manner: from per-thread local memory to global memory. Subsequently, asynchronous concurrent execution will be described. Finally, basic CUDA extensions of the C++ language will be presented and their translation into the thread and memory management systems will be shown on a simple example program.

Nvidia	GTX 1070	RTX 3060	V100	A100
GPU	GP104 (Pascal)	GA106 (Ampere)	GV100 (Volta)	GA100 (Ampere)
SMs	15	28	80	108
TPCs	15	14	40	54
FP32 Cores / SM	NA	NA	64	64
FP32 Cores / GPU	NA	NA	5120	6912
FP64 Cores / SM	NA	NA	32	
FP64 Cores / GPU (excl. Tensor)	NA	NA	2560	3456
CUDA Cores / SM	128	128	NA	NA
CUDA Cores / GPU	1920	3584	NA	NA
Tensor Cores / SM	NA	4	8	16
Tensor Cores / GPU	NA	112	640	432
GPU Boost Clock	1683 MHz	1777 MHz	1530 MHz	1410 MHz
Peak FP32 TFLOPS	6.5	12.7	15.7	19.5
Peak FP64 TFLOPS	0.202	0.199	7.8	9.7
Peak Tensor TFLOPS	NA	51	125	312/624 ³
Memory Bandwidth	256 GB/s	360 GB/s	900 GB/s	1555 GB/s
Texture Units	120	112	320	432
Memory Interface	256-bit	192-bit	4096-bit HBM2	5120-bit HBM2
Memory Size	8 GB	12 GB	32 GB	80 GB
L2 Cache Size	2048 KB	3072 KB	6144 KB	40960 KB
Shared Memory Size / SM	96 KB	128 KB	Configurable up to 96 KB	Configurable up to 164 KB
Register File Size / SM	256 KB	256 KB	256 KB	256 KB
Register File Size / GPU	3840 KB	7168 KB	20480 KB	27648 KB
TDP	150 Watts	170 Watts	300 Watts	400 Watts
Transistors	7.1 billion	12 billion	21.1 billion	54.2 billion
GPU Die Size	314 mm ²	276 mm ²	815 mm ²	826 mm ²
Manufacturing Process	TSMC 16nm	Samsung 8N	12 nm FFN	7 nm N7

Table 1.1: Comparison of GPUs: GTX 1070 (Turing architecture), RTX 3060 (Ampere architecture), V100 (Volta architecture), A100 (Ampere architecture). The GPUs in this table assume the best possible configuration of their respective card, for example, the version with the most possible VRAM. Features that are important when it comes to card performance have been denoted in green. The data was obtained from various sources for the GTX 1070 [36, 37, 32, 33] the RTX 3060 [34, 35, 31, 30] and the A100 [38, 29].

1.2.1 Introductory terminology

CUDA introduces many unique concepts that come with their own naming scheme. This subsection will list and explain some basic terminology that will be used throughout the project [23]:

- **Host** - Central Processing Unit (CPU) and its memory. The host provides data to GPU and instructs it to execute various instructions.
- **Device** - Graphics Processing Unit (GPU) and its memory. The device executes specialized instructions provided by the host.

- **Kernel** - term used for a special type of function that, unlike regular functions, can only be called from the host and executed on the device. Furthermore, when a CUDA kernel is called it is executed in parallel across a number of threads.

1.2.2 Thread Management

This subsection will aim to describe how CUDA handles its basic execution units: threads. First, a thread itself will be defined and described followed by explanations of multiple encompassing thread structures.

CUDA thread The thread management system within CUDA begins, at the most basic level, with its smallest execution unit, a thread. According to *CUDA C++ Programming Guide* a thread is an executed sequence of operations [40]. Due to the highly-parallel nature of the GPU - spreading the workload across thousands of execution units - a CUDA thread is designed to be lightweight (unlike a typical CPU thread - assuming no hyper-threading is present). In this context, 'lightweight' signifies that the GPU is capable of easily switching between threads. An example showing how a set of instructions can be run on a set of 8 threads can be seen in figure 1.3.

In this project, the terms 'CUDA thread' and 'thread' will be used interchangeably. For a more detailed explanation of the difference between a CUDA thread and that of the CPU see *Format for storage of sparse matrices on GPU* [42].

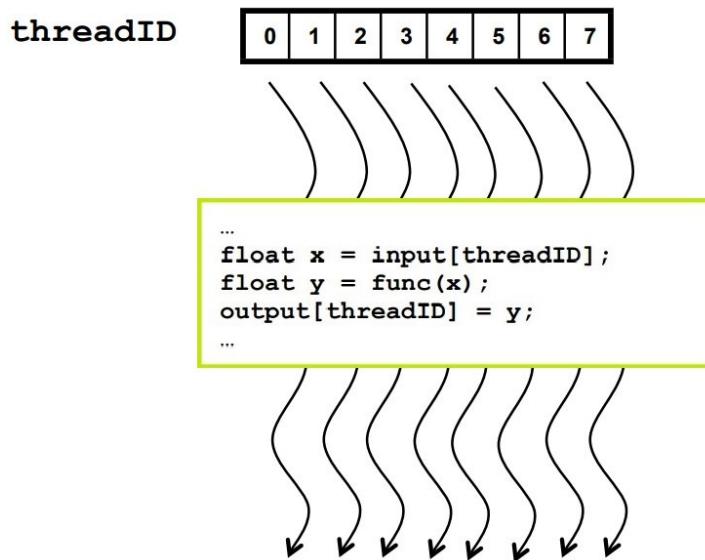


Figure 1.3: On an Nvidia GPU, eight threads with IDs from 0 to 7 execute the code in this example. A value from the array `input` with `threadID` as the index (i.e. each thread will read a value at a different index) is changed using the function `func(x)` and then stored in the same order as before into the array `output`. Taken from *Format for storage of sparse matrices on GPU* [42, 23].

Warp To execute thousands of threads simultaneously, SMs of an Nvidia GPU use the Single-Instruction Multiple-Thread (SIMT) execution model. The abbreviation SIMT comes from the amalgamation of

SIMD (Single-Instruction Multiple-Data) and multi-threading (executing multiple sequences of instructions simultaneously). Specifically, this approach comprises of multiple threads executing the same computations on different data items [27]. In terms of CUDA, the core of the SIMT architecture is a so-called 'warp' that is made up of 32 threads. In other words, the smallest number of threads that can be executed simultaneously is 32. If fewer threads are required, for example, only 1 thread, then CUDA will still allocate 32 threads with 31 being inactive. Similarly, if a subset of threads from a warp are to execute different instructions (e.g., as a result of a conditional statement) then the different sets of instructions are executed serially across their respective threads - this issue is known as 'thread divergence'. An example of thread divergence can be seen in figure 1.4; the warp in the example is simplified for the purpose of the explanation and as such contains only 8 threads.

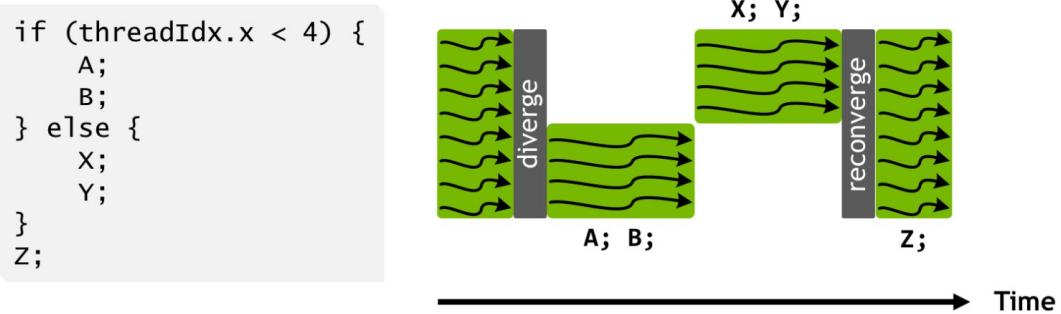


Figure 1.4: Conditional code execution by a warp of 8 threads; each thread is represented by one wavy line. Due to the condition, threads with an ID between 0 and 3 will only execute statements A and B. However, simultaneously, threads with IDs between 4 and 7 will be put on hold. Comparably, while threads with IDs between 4 and 7 will be executing statements X and Y, the remaining threads will be idle. Thus, thread divergence has occurred within the 8-thread warp. Taken from Nvidia's developer blog post: *Inside Volta: The World's Most Advanced Data Center GPU* [26].

Block It is not always necessary to use such granularity that warps are able to provide. Developers can choose to execute code on a group of up to 1024 threads (with CUDA Compute Capability greater than 3.5) - referred to as a block. Threads in a block can cooperate via shared memory (subsection 1.2.3 will explain more) and they can be synchronized - this is not possible for threads in different blocks. Threads in a block can be structured in 1, 2, or 3 dimensions (x, y, z); each thread has a unique ID in every dimension. The 1024 threads-per-block limit encompasses all 3 possible dimensions, in other words, the total number of threads must be at most 1024 across all dimensions (`num_threads_x_dim · num_threads_y_dim · num_threads_z_dim ≤ 1024`) [25, 40].

Grid In terms of CUDA a grid consists of multiple blocks of threads. Similarly to how threads can be structured within blocks, blocks can be structured within grids - up to 3 dimensions of blocks; each block has a unique ID in every dimension. The maximum number of blocks in every dimension is set to $2^{31} - 1$ (65 536). One of the main reasons for having another structure on top of blocks (apart from memory management - detailed explanation in subsection 1.2.3) stems from the fact that while the limit for threads per block is set to 1024, GPUs are capable of running a multitude more threads in parallel. This means that the grid structure allows for the same code to be executed simultaneously on a group of

⁰L. Durant, O. Giroux, M. Harris: *Inside Volta: The World's Most Advanced Data Center GPU*. URL: <https://devblogs.nvidia.com/inside-volta/>

thread blocks. However, it is important to note that there is a limit of how many threads can be active at once. When this limit is reached, blocks of threads are executed sequentially in such a way that allows for near-maximal concurrently active threads. Another noteworthy aspect is the difference between the terms 'number of allocated threads' and 'number of active threads'. The former means how many threads are allocated in total, i.e. both active (currently executing) and inactive (scheduled) threads, whereas the latter refers to threads that are actively being executed at a point in time.

A visualization of CUDA's thread structuring can be seen in figure 1.5.

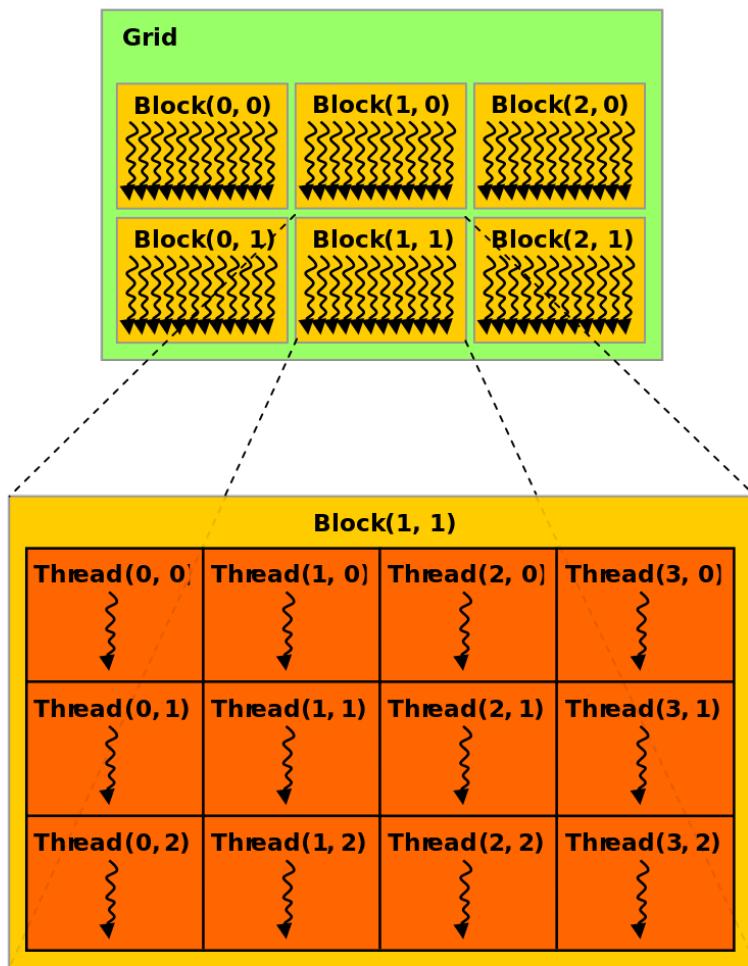


Figure 1.5: CUDA thread structuring of a 2D grid made up of 2D blocks of threads. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

1.2.3 Memory Management

The aim of this subsection is to present how memory management works in CUDA. Different types of memory available on the GPU will be presented, ranging from per-thread local to global memory.

Per-thread local memory When a kernel is executed on the GPU across a number of threads every thread has its own unique ID stored in a variable that is available within the kernel. This variable is stored in memory that is referred to as *per-thread local memory*. In other words, every thread has its own local memory where it can store variables. It is important to note that per-thread local memory consists of two different types - registers and local memory. Registers is on-chip memory (low latency and high bandwidth), however, it is limited in capacity at 255 32-bit registers per thread in CUDA Compute Capability 3.5 and higher, which does not allow for extensive kernels containing many variables. The compiler will store almost all variables allocated within the kernel into registers, with the exception of [40]:

- Arrays indexed with constant quantities
- Large structures or arrays that would use too much registers space
- Any variable if the kernel uses more registers than available - called *register spilling*

The variables and structures mentioned above that the compiler will not store in registers will instead be stored in purely local memory which resides in device memory. Device memory is also referred to as global memory which is off-chip and therefore, any accesses by threads into their purely local memory will be slower than accessing registers. Figure 1.6 shows available accesses of threads to different types of memory.

As of CUDA Compute Capability 3.5, the amount of purely local memory available for every thread is only 512 KB [40]. In summary, per-thread local memory is often used sparingly to avoid register spilling and the accompanied slower memory access, however, if used efficiently, it can be helpful when complex indexing is required for some calculations.

Shared memory The next layer of memory is per-block memory referred to as *shared memory*. As the name suggests, this memory is shared by all threads belonging to a particular block. Similarly to registers, shared memory is on-chip and therefore it is fast, however, it is also limited in capacity depending on the CUDA Compute Capability version - see table 1.2 for specific values.

Compute Capability	3.5 - 6.2	7.0 - 7.2	7.5	8.0	8.6	8.7
Max. shared memory per block [KB]	48	96	64	163	99	163

Table 1.2: Maximum shared memory per thread block across different CUDA Compute Capabilities. Nvidia notes in their documentation that any value above 48 KB requires the use of dynamic shared memory. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

Shared memory can either be allocated statically or dynamically. The former needs the size of allotted memory to be known at compile time, for example, an array of constant size denoted within the kernel using a dedicated prefix that indicates it is meant to be stored in the shared memory of each thread's block. On the other hand, the latter - dynamic allocation of shared memory - allows for the size of required memory to be determined at runtime, however, this means that the developer must specify the size of the shared memory as one of the parameters when calling the kernel.

Shared memory of each block is divided into 32-bit (4-byte) memory modules called words. A single word can store a float, half a double, 32-bit int, etc. - anything that can be stored in 32 bits. Apart from

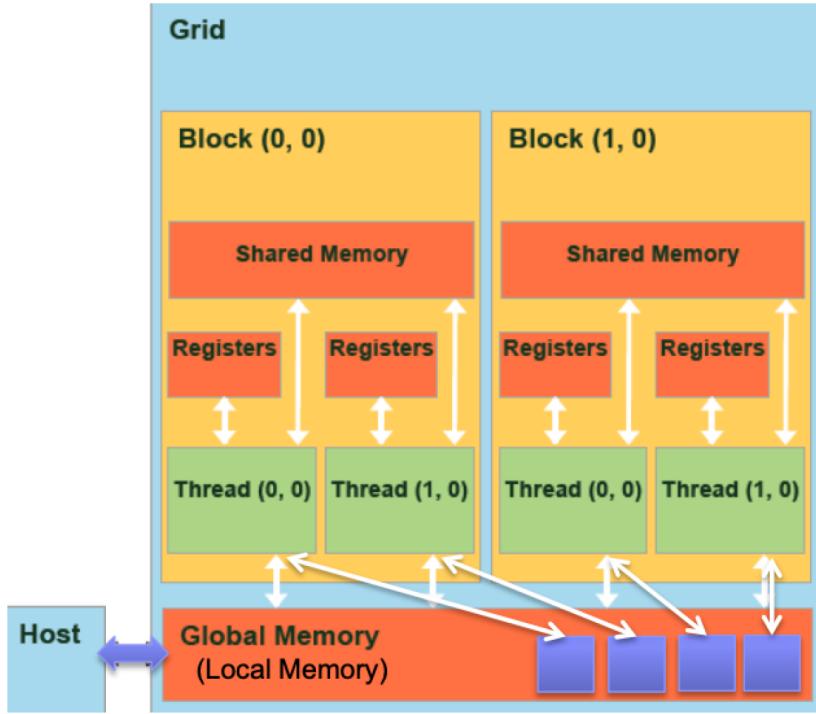


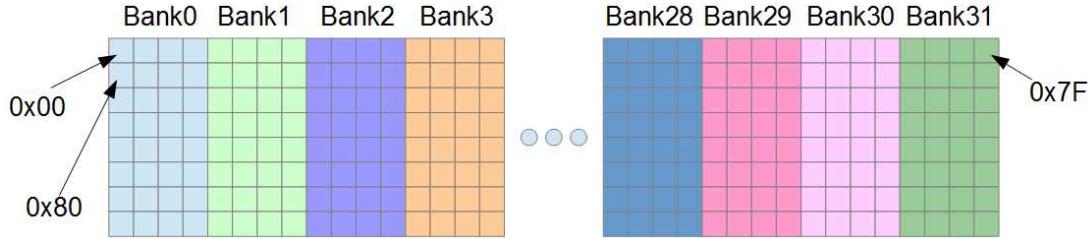
Figure 1.6: Different CUDA memory types visualized. Each thread has access to its local memory comprised of registers, local memory (blue squares in global memory), shared memory of its block, and global memory. Taken from Yao Hsiao's *GPU - CUDA introduction* [22].

words, there are 32 banks per block. Each bank contains a number of words depending on the size of shared memory allocated. Since the size of shared memory can be up to 48 KB or more - depending on the version of CUDA Compute Capability - then the number of words per bank can differ between versions. Figure 1.7 visualizes the division of shared memory into banks and words.

Manipulating memory in banks can be fast and efficient under certain conditions. Let us consider the following example: Figure 1.7b is the shared memory of a block that is used in a kernel. In this kernel, there is an array made up of 256 floats (32-bit) - each word in the figure is a single float. Furthermore, the IDs of words in the figure correspond to indices of floats in the array, thus, float values stored next to each other in memory belong to successive banks, for example, `arr[0]` belongs to `Bank0`, `arr[1]` belongs to `Bank1`, `arr[32]` belongs to `Bank0`, etc.

As mentioned by Chris Rose in *CUDA Succinctly* [21], this division of words into banks is salient as each bank can serve only 1 word to a warp at once. This means that if a single word is requested from each bank, then all 32 threads of a warp can be served by all 32 banks simultaneously and expeditiously. Data serving is also fast when the same word from shared memory is accessed by all threads of a warp; this is called a *broadcast* as shared memory is read once and the value is sent to all threads of the warp at once.

A concept similar to broadcasting is called a *multicast*, which is an operation that is used when the same word from any particular bank is accessed by more than 1 thread of a warp. In this case, the threads that accessed the word will all receive it simultaneously from its bank. Under good conditions, the multicast operation is as fast as a broadcast. It is important to note that multicast is only available for compute capability 2.0 and higher.



(a) Shared memory divided into banks (columns under each `Bank*`), words (4 same-color squares of a row) and bytes (individual squares). In the first row, the first 4 bytes under `Bank0` - beginning at address `0x00` - make up the `0th` word (as shown in Figure). The four bytes to the right of it (first row under `Bank1`) make up the `1st` word. Memory addresses of some bytes are shown hexadecimal.

Bank0	Bank1	Bank2	Bank3		Bank28	Bank29	Bank30	Bank31
0	1	2	3		28	29	30	31
32	33	34	35		60	61	62	63
64	65	66	67		92	93	94	95
96	97	98	99		124	125	126	127
128	129	130	131		156	157	158	159
160	161	162	163		188	189	190	191
192	193	194	195		220	221	222	223
224	225	226	227		252	253	254	255

Word indices

(b) Shared memory divided into banks (column under each `Bank*`) and words (individual rectangles with IDs inside).

Figure 1.7: Illustration of shared memory. In this example, there are 32 banks; each one has eight 4-byte (32-bit) words - in Figure 1.7a 1 byte is 1 square. Reading and writing into the `0th`, `32nd`, `64th`, etc. word is the responsibility of `Bank0`; reading and writing into the `1st`, `33rd`, `65th`, etc. word is the responsibility of `Bank1` and so on. Taken from *Chapter 6: Shared Memory of Cuda Succinctly* [21].

However, the operations above all assumed good conditions for reading and writing of data. The primary originator of bad conditions for accessing shared memory is called a *bank conflict*. Bank conflict describes an instance when threads of a warp request more than 1 word from any single bank. When this occurs, reading and writing of a word will be performed serially by the bank. For example - looking at Figure 1.7b - let thread `0` and thread `1` access words `0` and `32` respectively. Since both words belong to `Bank0`, then a bank conflict has occurred and the bank cannot distribute words' data in parallel. Instead, `Bank0` will firstly serve thread `0` with word `0` and then thread `1` with word `32`.

In order to facilitate further understanding, examples from *Cuda succinctly* [21] and *CUDA C++ Programming Guide* [40] are included below.

Firstly, Table 1.3 presents different shared memory access patterns - including notes on the speed of execution. Then, Figure 1.8 portrays shared memory access using random permutations, multicast and broadcast. Finally, Figure 1.9 shows examples of strided shared memory access with and without bank conflict - additionally, this figure also visualizes some examples from Table 1.3.

In summary, ensuring that bank conflicts do not occur is pivotal to achieving efficient use of shared memory and subsequently high bandwidth.

Access Pattern	Notes
<code>arr[0]</code>	Fast - broadcast to all threads of the grid
<code>arr[bID]</code>	Fast - broadcast to all threads of a block
<code>arr[tID]</code>	Fast - all threads request from different banks
<code>arr[tID/2]</code>	Fast - multicast; every 2 threads read from the same bank
<code>arr[tID*2]</code>	Slow - 2-way bank conflict
<code>arr[tID*3]</code>	Fast - all threads access different banks
<code>arr[tID*32]</code>	Egregiously slow - 32-way bank conflict

Table 1.3: Access patterns to shared memory. `arr` is an array stored in the shared memory of a thread block. `tID` is the ID of a thread and `bID` is the ID of a block. Taken from *Chapter 6: Shared Memory of Cuda Succinctly* [21].

Global memory The final, all-accessible memory layer is called *global memory*. Some sources also refer to it as *device memory* since global memory resides in the device's DRAM (Dynamic Random Access Memory) - not to be confused with the host's memory, often referred to as, RAM. The modifier 'global' represents the all-accessible aspect of this type of memory, as it can be accessed by the host and the device, thus, serving as a memory communication medium that can be used to transfer data between the two, and house input and output data for kernels [20]. Global memory is available for all threads on the device, regardless of what thread structure they belong to. In other words, all grids have access to the same global memory - shown in Figure 1.10.

Unlike shared memory, global memory functions similarly to RAM: it is initialized with the startup of the program, it will be available while the program is running, and it is terminated with the termination of the program. In order to use global memory, the developer must manually allocate memory on the device, then copy the data from the host to the device, and finally, de-allocate (free) the data from the device [20] once it is not required.

As mentioned above, in Paragraph *Per-thread local memory* in Subsection 1.2.3, for the purpose of this project global memory is assumed to be off-chip - for completion, an exception to this is mentioned by Mark Harris in *How to Access Global Memory Efficiently in CUDA C/C++ Kernels* [20]: "*Depending on the compute capability of the device, global memory may or may not be cached on the chip.*". Accessing (reading and writing) global memory is slower than accessing the aforementioned types of memory. In order to minimize this bottleneck, it is advised by Nvidia to keep the number of transactions that require accessing global memory to as few as possible [20]. One of the main concepts that achieves this is called *global memory coalesced access*. This methodology takes full advantage of the SIMD approach, specifically, instruction execution by threads in warps. In other words, it uses the fact that threads in a warp execute the same instruction simultaneously - in this instance: combine multiple memory accesses into a single transaction.

This means that upon the execution of a load instruction by all threads in a warp, the device will detect whether the threads are attempting to access successive global memory locations. If the accessed addresses are successive, then the accesses are coalesced (amalgamated) by the device into a consolidated access to consecutive DRAM locations [19].

More specifically, a single coalesced access into global memory - composed of a single access instruction

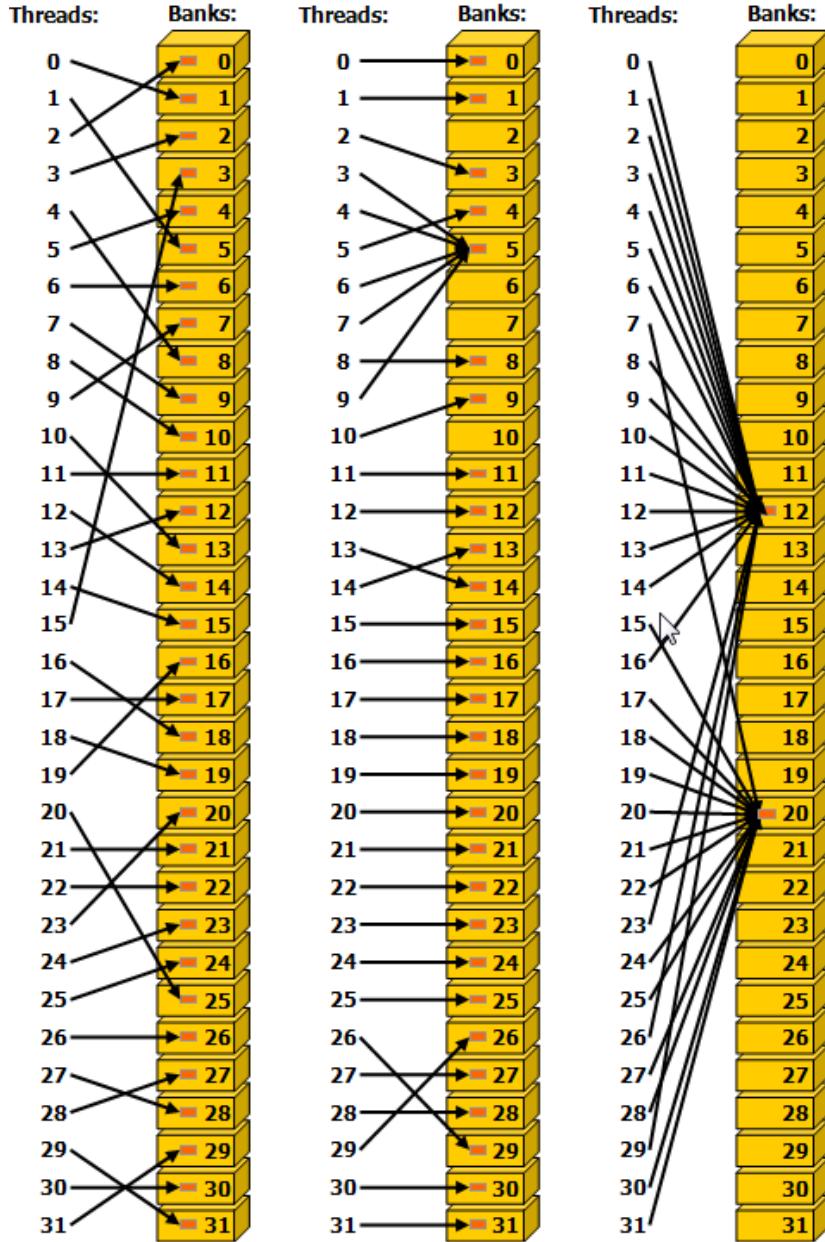


Figure 1.8: Irregular shared memory accesses on 3 separate examples; yellow rectangular cuboids are banks; small orange rectangles are words. The left sub-image shows threads of a warp accessing shared memory randomly, however, in such a way that does not cause bank conflicts. The middle sub-image shows shared memory accessed by threads using the multicast operation, specifically, threads 3, 4, 5, 6, 7 and 9 accessing the same word from bank 5; other threads all access one word any bank each - no bank conflict. The right sub-image shows threads accessing shared memory via 2 broadcast operations. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

performed by threads of a warp - occurs only if the following conditions are satisfied [17, 40]:

1. Each thread accesses a memory element of size 4, 8, or 16 bytes

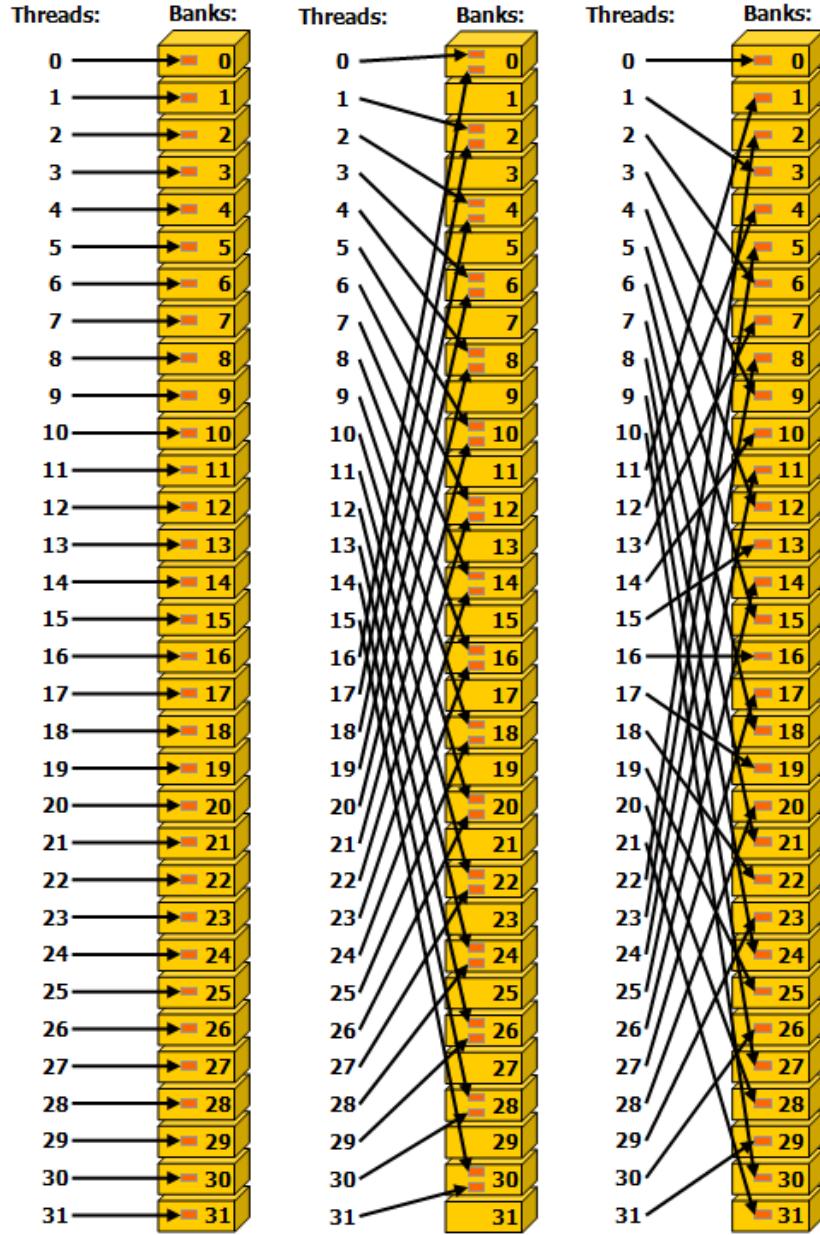


Figure 1.9: Shared memory access using striding on 3 separate examples; yellow rectangular cuboids are banks; small orange rectangles are words. The left sub-image shows threads of a warp accessing shared memory with a stride of 1 (no bank conflict). The middle sub-image shows shared memory accessed by threads with a stride of 2 (equivalent to `arr[tID*2]` from Table 1.3; 2-way bank conflict as threads access 2 different words from the same bank). The right sub-image shows threads accessing shared memory with a stride of 3 (equivalent to `arr[tID*3]` from Table 1.3; no bank conflict). Taken from Nvidia's *CUDA C++ Programming Guide* [40].

2. The device memory is accessed by memory transactions of 32, 64, or 128 bytes
3. Each segment must be aligned to its size - first address is a multiple of their size

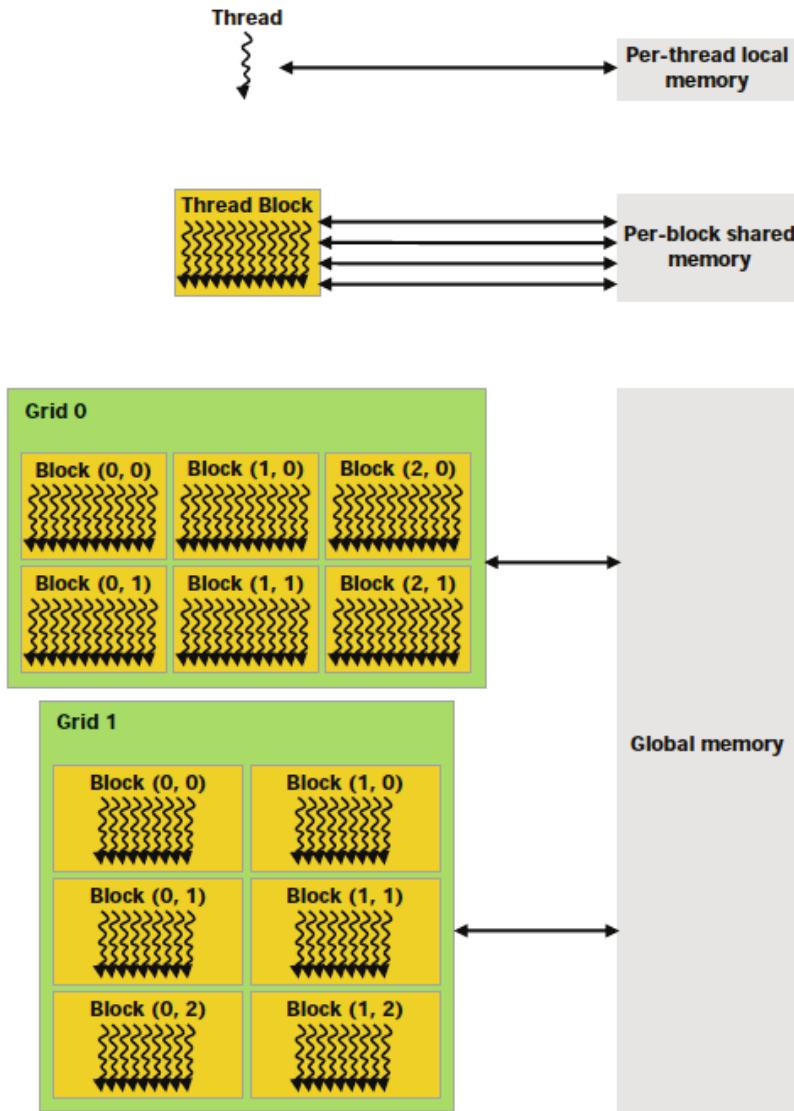


Figure 1.10: CUDA memory structuring. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

The alignment requirement signifies that accessing (reading and writing) words of size 1, 2, 4, 8, or 16 bytes within global memory instructions is supported. Moreover, if the size of data stored in global memory is 1, 2, 4, 8, or 16 bytes and it is aligned, then access to this data is joined into 1 memory transaction.

Ad point 2 of the conditions above: when threads of a warp access words larger than 4 bytes, then the memory request made by the warp is divided into separate 128-byte memory requests. These newly-formed requests are subsequently performed separately, based on the word size [40]:

- 8 bytes - 2 memory requests (1 for each half-warp)
- 6 bytes - 4 memory requests (1 for each quarter-warp)

Table 1.4 shows examples of built-in vector types that are aligned in global memory by default; the entire list can be found in Nvidia's *CUDA C++ Programming Guide* [40].

Type	Alignment
int1, int2, int3, int4	4, 8, 4, 16
long1, long2, long3, long4	8, 16, 8, 16
float1, float2, float3, float4	4, 8, 4, 16
double1, double2, double3, double4	8, 16, 8, 16

Table 1.4: Built-in vector types that are aligned by default. The suffix numbers specify the number of components the vector composes of, for example, a vector of type `int2` has 2 components: `(x, y)`. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

The size and alignment of other types, such as structures, must be approached manually: forcing the compiler to align them by using specifiers in code. For example, structures of 8 or 16 bytes that are to be aligned are declared using `__align__(8)` and `__align__(16)` respectively - shown in Listing 1.1.

```

1 struct __align__(8) {
2     float x;
3     float y;
4 };
5
6 struct __align__(16) {
7     float x;
8     float y;
9     float z;
10};

```

Listing 1.1: Declaration of to-be-aligned 8- and 16-byte structures. The lower example is aligned to 16 bytes as 12-byte alignment (3 4-byte floats) is not coalesced, therefore, 4 bytes are used for padding. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

On the other hand, if 8-byte or 16-byte words are not aligned, then reading them yields results offset by some words.

However, ultimately, if the size and alignment requirements are not adhered to, then the access to global memory is compiled into multiple instructions in such a way that they will not be fully coalesced, which leads to lower bandwidth and sub-optimal performance.

Examples of coalesced and non-coalesced memory accesses by a 16-thread warp are shown in Figures 1.11 and 1.12.

In summary, coalesced access (reading and writing) to global memory must be fulfilled in order to not lower bandwidth - especially when dealing with custom non-built-in vector types - as global memory is implicitly high-latency and low-bandwidth compared to other memory types mentioned above.

Page-locked host memory This type of memory that can be utilized within CUDA is different from the previous types in that it is not located on the device. Page-locked host memory - sometimes referred to as pinned - resides in the memory of the host. The difference between it and the host's regular pageable memory is its permanent placement and other properties related to CUDA. Firstly, it can be allocated

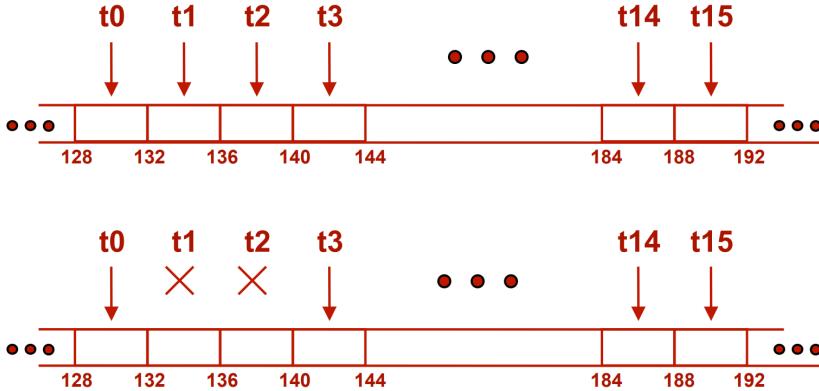


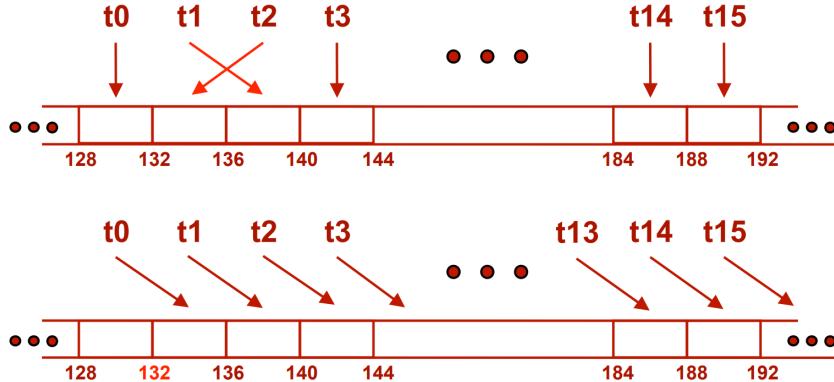
Figure 1.11: Coalesced access to global memory. Threads are denoted with `t<ID>` and the numbers below the rectangular memory locations are global memory addresses. In the upper image, all threads of the warp access successive memory addresses which house words of size 4 bytes (`float`), the size of the memory transaction is 64 bytes, and the segment is aligned to its size so that the first address is a multiple of its size: segment is 64 bytes and the starting address is 128: $128/64 = 2$. The lower image shows an example where 2 threads from the 16-thread warp do not access data. Thus, threads of the warp have 2 separate execution paths (thread/warp divergence) that are executed sequentially. However, from a memory standpoint, the access is still coalesced as all requirements are fulfilled. Taken from Martínez Manuel Ujaldón's *CUDA Optimizations, Debugging and Profiling* [17].

and de-allocated using functions that come with CUDA: `cudaHostAlloc()` and `cudaFreeHost()`, or, if the memory on the host has already been allocated using `malloc()` it can be registered - made available within cuda - using `cudaHostRegister()`. According to *CUDA C++ Programming Guide* [40] there are many advantages to using page-locked host memory:

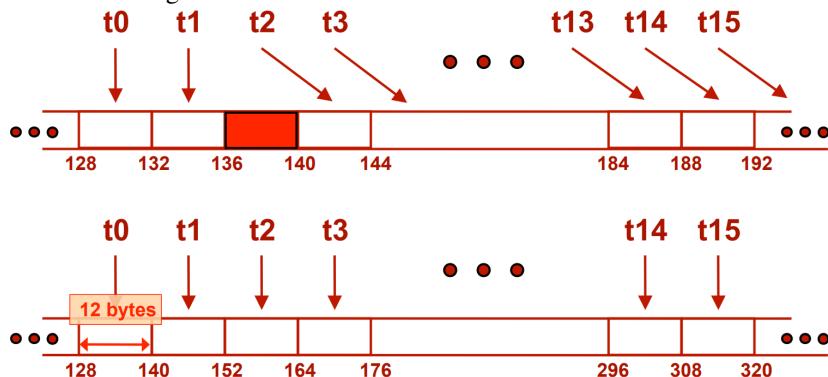
- Concurrent data transfer between page-locked host memory and device memory, and kernel execution - so-called *asynchronous concurrent execution* (detailed in Subsection 1.2.4).
- Elimination of data copying between the host and device by mapping page-locked host memory to the device's address space - so-called *mapped memory* (detailed below).
- Higher bandwidth when copying between page-locked host memory and device memory on systems with a front-side bus. Furthermore, if the page-locked host memory is allocated using the write-combining principle, then bandwidth can be even higher.

Along with the above-mentioned advantages there are drawbacks such as, the small size of page-locked host memory. Since it is often used by the operating system for paging (host stores data - to-be-used in main memory - in paged memory on a drive rather than in RAM) it is not an abundant resource. Therefore, incautious use can lead to allocation failures and reduced system performance [40].

Mapped memory As mentioned above one of the advantages of using page-locked host memory is the ability to map this type of memory to the device's address space which eliminates the need for copying data stored in this memory between the host and the device. Specifically, a block of page-locked host memory can be mapped to the device's address space by passing either the `cudaHostAllocMapped`



(a) In the upper image, 2 threads swap orders and thus do not access successive floats in global memory. However, according to *CUDA C++ Programming Guide* [40] this does not result in non-coalesced memory access. All other requirements are fulfilled. The lower image shows a scenario where the starting address is misaligned as the size of the memory segment is 64 bytes, but, the starting address is 132 which is not divisible by 64: $132/64 = 2.0625$. Therefore, access is misaligned and the memory segment is read in 2 sequential memory transactions: starting addresses 128 - 188 and starting addresses 192-252.



(b) In the upper image, threads $t_2 - t_{15}$ are misaligned with the original starting address. Thus, similarly to the lower image in Sub-figure 1.12a the memory transaction will be split into 2 sequential transactions. The lower image shows a situation where global memory houses 12-byte `struct` types. However, as Table 1.4 and Listing 1.1 show, 12-byte alignment is not supported and therefore global memory access is non-coalesced.

Figure 1.12: Examples of coalesced and non-coalesced access to global memory composed of 4-byte words (for example, `float`) with 1 exception being 12-byte structures. Taken from Martínez Manuel Ujaldón's *CUDA Optimizations, Debugging and Profiling* [17].

flag to `cudaHostAlloc()`, or, the `cudaHostRegisterMapped` flag to `cudaHostRegister()` [40]. Then, the block will have an address in host memory - given by `cudaHostAlloc()` (or `malloc()`) - and another in device memory. The address in device memory is accessible by using the function `cudaHostGetDevicePointer()`, which will provide a pointer that can be used in kernels. Even though this specific type of host memory is accessible from within a kernel, it is not stored on the device and, thus, accessing it is not as fast as accessing device memory.

Another advantage of using mapped memory is that copying the block of data between device memory and mapped host memory is done implicitly by kernels when needed, thus, the need to allocate a block in device memory is removed. However, a disadvantage of this characteristic is the potential read-after-write, write-after-read, or write-after-write complications that can arise when asynchronous concurrent execution (detailed in Subsection 1.2.4) is used [40]. These problems can be avoided by forcing memory

synchronizations, however, this can have an impact on performance.

Further caveats associated with the use of mapped memory can be found in *CUDA C++ Programming Guide* [40].

An overview of how the structure of hardware on a GPU and CUDA can be seen in Figure 1.13

1.2.4 Asynchronous concurrent execution

Within CUDA there are multiple operations that can be executed at the same time (concurrently) - namely [40]:

- Computation on the host
- Computation on the device
- Memory transfers from the host to the device and vice versa
- Memory transfers within the memory of a given device

However, it is important to note that there is a limit to concurrent load. According to *CUDA C++ Programming Guide* [40] the so-called *level of concurrency* is determined by the compute capability version of the device and its available feature set as detailed below.

This subsection will describe concurrent execution from different perspectives that are used in this project. Firstly, concurrent execution between the host and the device will be presented. Then, concurrent kernel execution will be introduced in greater detail and finally, the topic of streams will be described.

Concurrent execution between host and device Concurrent host execution means that once the host launches a kernel on the device, then it does not have to wait for the kernel to complete before moving on to the next instruction. CUDA has asynchronous library functions that make the host a controller which essentially sends computation jobs to the device. In other words, once a kernel is launched on the device, the host reclaims control immediately without waiting for the kernel to finish. This means that the host can go on to execute the next line of code.

Due to the asynchronous nature, this functionality is especially useful when it comes to queuing job for the device. The jobs are executed on the device by CUDA as soon as sufficient resources are available. Subsequently, the responsibility of managing the device is lifted from the host - allowing it to perform other tasks [40].

Host asynchrony is available for the following device operations [40]:

- Kernel launches
- Memory copies (only page-locked host memory):
 - Within a single device's memory
 - From host to device - memory block with a limited size of 64 KB
 - Performed by functions suffixed with `Async`
- Memory set function calls

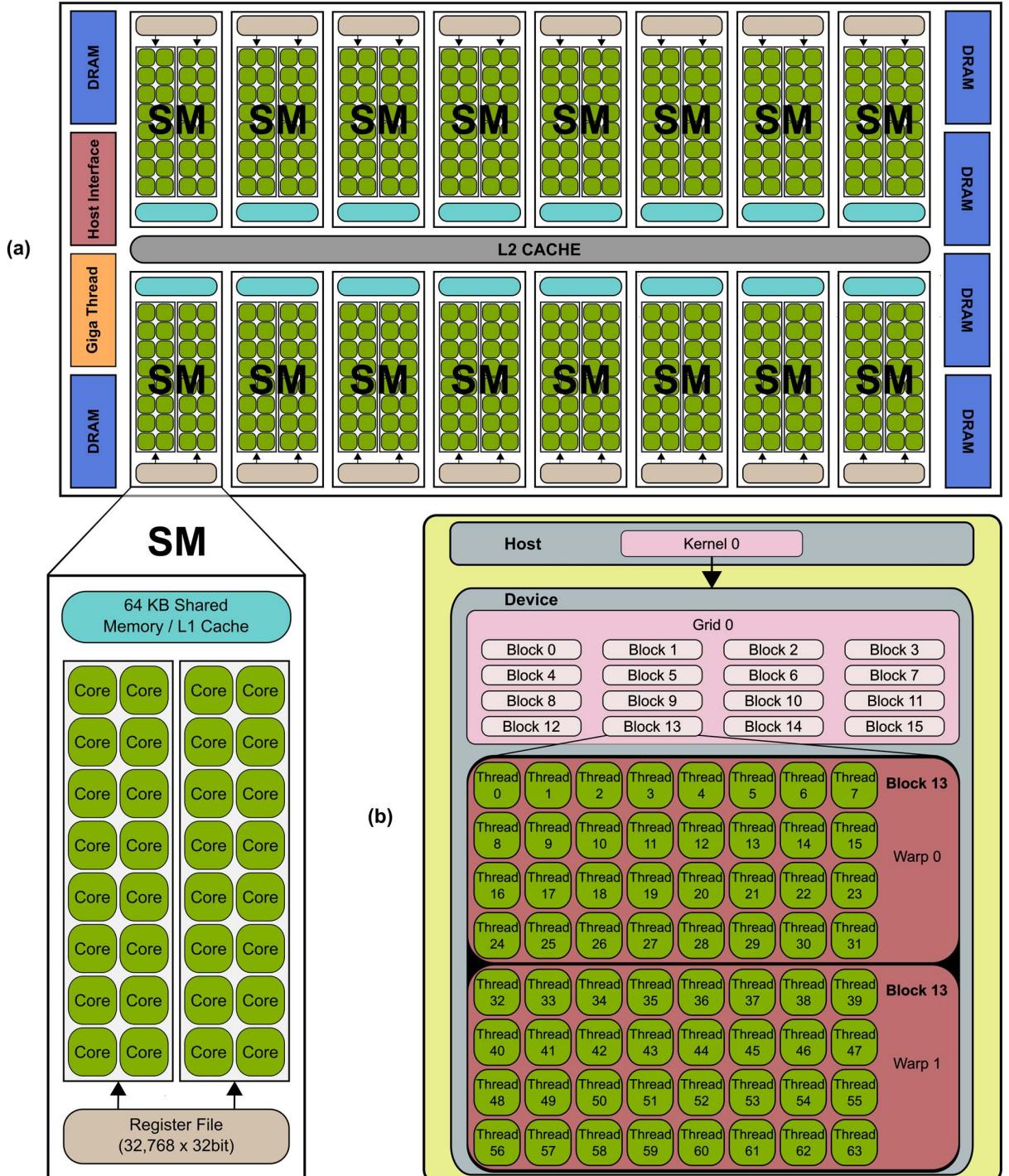


Figure 1.13: a) Usual architecture of an Nvidia Fermi GPU that comprises of SMs. Furthermore, each SM is made up of SP cores (Stream Processor cores) b) CUDA programming model controls the hardware of the GPU. Taken from *Accelerating Fibre Orientation Estimation from Diffusion Weighted Magnetic Resonance Imaging Using GPUs* [13].

Asynchronous concurrent execution between host and device can be disabled on a system for all CUDA

applications (kernel launches) by using the `CUDA_LAUNCH_BLOCKING` environment variable (set to `1`). However, Nvidia does not recommend using this feature in production - only during debugging.

Another noteworthy aspect is that kernel launches are implicitly synchronous when running a CUDA application via a profiler, for example, the Nvidia Visual Profiler. This behavior can be overridden in the profiler by explicitly enabling concurrent kernel profiling [40].

Concurrent kernel execution Similarly to the concept where the device can be running a kernel while the host is performing another task, kernels can be executed simultaneously on the device. Not all Nvidia devices support this functionality (only some devices with compute capability 2 and higher), therefore, it must be checked per-device using the `asyncEngineCount` device property (`0` if the device supports it). There are 3 main limitations when it comes to concurrent kernel execution: CUDA-defined maximum number of resident grids per device, no concurrent kernels from different CUDA contexts and resources available on the device. First, the CUDA-defined maximum resident grids per device will be explained. Since each kernel is launched on an individual grid of blocks of threads, then the maximum number of resident grids per device is effectively the maximum number of kernels that can be run concurrently on the device. The limit is a hard-set constant that depends on the compute capability version - Table 1.5.

Compute Capability	3.5 - 5.2	5.3	6.0	6.1	6.2	7.0	7.2	7.5 - 8.7
Max. resident grids per device	32	16	128	32	16	128	16	128

Table 1.5: Maximum number of resident grids per device depending on the CUDA compute capability version. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

The second limitation - CUDA context - signifies that if there are two CUDA applications running at the same time on a system, then two kernels - one from each context - will not be run in concurrently. Instead, the kernel that was launched second will be queued to execute until the first kernel has finished. The last limitation - device resources - is not as severe the previous 2 since kernels can still be launched concurrently, even if their cumulative required resources exceed the device's available resources. This is due to the fact that if more than 1 kernel is set to be launched concurrently, they are only run simultaneously if the available resources are sufficient for them all. If the resources available are not sufficient, then the kernels which would not get their requested resources are put aside until the resources are free. In this instance, resources represent memory and threads.

In terms of memory, an example of kernels that will often not run concurrently with other kernels are ones that require large amounts of local memory [40]. In terms of threads, the limiting factor is the maximum number of active threads - described at the end of the *Grid* paragraph in Subsection 1.2.2. For example, if 2 kernels are to be run concurrently, the total number of threads required by them at once must not exceed the maximum number of active threads on the device.

Therefore, whether kernels can be run concurrently is highly dependent on the resource requirements of each kernel and it is up to the device to manage all of these operations.

Streams

Streams can be used to effectively create and manage concurrency on the device, in other words, they are the means by which the above-mentioned operations are controlled. According to *CUDA C/C++ Streams and Concurrency* by Steve Rennich and Nvidia a CUDA *stream* can be defined as "A sequence

of operations that execute in issue-order on the GPU" [24]. To put it another way, a single stream is basically an open door through which instructions can be sent to the device - kernels.

While it is possible to have multiple streams active at once, the device has limited resource available (active threads and memory). Therefore, multiple active streams at once does not necessarily mean multiple kernels running simultaneously. Nevertheless, if multiple streams are active and each is given a different kernel, then these kernels can be executed concurrently if the device's limits are not overstepped - detailed above in paragraph *Concurrent kernel execution* in Section 1.2.4.

Unlike individual kernels, global memory is used by all streams without division, i.e. all streams have access to the same global memory and there is no part of global memory that would belong to a particular stream.

According to Nvidia's *CUDA C++ Programming Guide* [40], individual streams are not dependent on each other, meaning that they are able to execute commands separately or concurrently. However, this behavior does not have to be consistent, for example, communication between kernels is not defined. For this reason, Nvidia themselves recommend not relying on the accuracy of CUDA applications when attempting to make streams interact.

On the other hand, CUDA provides tools that can assist when synchronicity of streams is required.

This subsection will first present basic information on stream creation and destruction. Then, the topic of the default CUDA stream will follow and, finally, explicit and implicit synchronization will be detailed.

Creation and destruction A CUDA stream is created by initializing a stream object - type `cudaStream_t` in code - and then creating the stream itself using `cudaStreamCreate()`. The approach that is often used in examples by Nvidia is to create an array of streams as shown in Listing 1.2.

```

1 // Declare array of 2 stream objects
2 cudaStream_t streams[2];
3
4 // Create each stream
5 for (int i = 0; i < 2; ++i)
6     cudaStreamCreate(&streams[i]);

```

Listing 1.2: Creation of streams. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

In order to make a kernel run on a specific stream, the stream address must be specified as one of the launch parameters of the kernel - detailed in Subsection 1.2.5. Launching a kernel on a specific stream is shown in Listing 1.3.

```

1 // Launch MyKernelA using the 0th stream using 1 block made up of 1 thread and 0 ←
   bytes of dynamically allocated shared memory
2 MyKernelA<<<1, 1, 0, stream[0]>>>(inputVariableA)
3
4 // Launch MyKernelB using the 1st stream
5 MyKernelB<<<1, 1, 0, stream[1]>>>(inputVariableB)

```

Listing 1.3: Pseudo-code for launching 2 different kernels using 2 different streams. The instructions in this example would be executed from the host. Since each kernel is essentially an open door to the device for instructions, then, once `MyKernelA` is launched on `stream[0]`, the control is returned to the host without waiting for `MyKernelA` to finish. Subsequently, the host will immediately launch `MyKernelB` using `stream[1]`. In this example, each kernel is launched on a grid made up of 1 single-thread block with 0 bytes of dynamic shared memory allocated, thus, the device resources will not be exhausted and both kernels will run concurrently. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

When streams are no longer needed, they are to be destroyed using `cudaStreamDestroy()` - show below in Listing 1.4. If `cudaStreamDestroy()` is called while a stream is still performing tasks, then it will return without destroying the stream immediately - the destruction (release) of the stream's resources will be delayed until all work is completed on the stream.

```

1 // Destroy each stream
2 for (int i = 0; i < 2; ++i)
3     cudaStreamDestroy(stream[i]);

```

Listing 1.4: Destruction of streams. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

Default stream If a stream is not specified when launching a kernel, or when copying memory, then only the default stream - *Stream '0'* - is used and the instruction are executed in order with respect to the device (not concurrently as shown in the examples above) [40].

Nevertheless, it is possible to provide each host thread with its own default stream by setting the `-default-stream` compilation flag to `per-thread`, i.e. compiling using `nvcc ... -default-stream per-thread`.

The default option for the flag is `legacy`, which signifies that all host threads will use the special *NULL stream*. This stream is different from other streams as it uses implicit synchronization - detailed below in paragraph 1.2.4.

Explicit synchronization The first, and arguably the most used, type of synchronization when it comes to streams is explicit synchronization. In this instance, the 'explicit' modifier signifies that the synchronization is issued using one of the following functions from code [40, 16]:

- `cudaDeviceSynchronize()` - Synchronization of the entire device. This function servers as a checkpoint in code where streams will wait until they all get to this point in code.
- `cudaStreamSynchronize(cudaStream_t stream)` - Synchronization of a particular stream. This function takes a single `stream` as its input parameter and serves a checkpoint to wait for completion for all actions called before it.
- `cudaStreamWaitEvent(cudaStream_t stream, cudaEvent_t event)` - Execution delayed for commands added to the input `stream` until the input `event` completes.

Additionally, CUDA provides a function to check whether all commands of a stream that precede the current line of code have finished: `cudaStreamQuery()`. Further functions that can be used to manage streams can be found in section *6.4 Stream Management* in the *CUDA Runtime API* [16].

Implicit synchronization The opposing type of synchronization is called implicit, and, as mentioned in paragraph *Default stream* above, it is used by default under certain conditions - unless explicitly overridden by one of the functions above. Specifically, Nvidia states in *CUDA C++ Programming Guide* [40] that if there are 2 streams, then 2 commands - each from 1 stream - cannot be run simultaneously if the host thread issues any of the following operations:

- Page-locked host memory allocation
- Device memory allocation

- Device memory set
- Memory copy between 2 addresses to the same device memory
- Any CUDA command to the NULL stream
- Switch between the shared memory configurations

The hypothetical reasoning behind this is that if any of the operations above would be performed in parallel, it could create irresolvable conflicts. For example, if each stream tried to allocate memory on the device at the same location concurrently - impossible to be done in parallel without a conflict check. However, it can be argued that a conflict check is an unnecessary functionality as it is already present in some form when allocation happens sequentially.

Furthermore, there are certain operations that require a dependency check [40]:

- Any other commands within the same stream as the launch being checked
- Any call to `cudaStreamQuery()` on that stream

Thus, in order to improve application performance, Nvidia recommends developers issue all independent operations before dependent operations and delay any synchronization until necessary.

1.2.5 C++ CUDA Extensions

As previously mentioned at the beginning of Subsection 1.2, CUDA supports a variety of programming languages. Among them is C++, a widely-used, high-performance C-based language that implicitly allows low-level memory manipulation. CUDA provides many different extensions to C++, however, for the purpose of this project only the core basics that were used during its development along with some other important extensions will be detailed.

This subsection will divided into 2 main categories: outer-kernel and inner-kernel extensions. The former is made up of memory-related operations (allocating, copying and freeing data), kernel launch configurations, function extensions, streams, etc. - i.e. extensions not used within kernels. The latter consists of any operators, structures and declarations that are used in kernels.

Outer-kernel extensions

This category will first present a selection of important memory managing extensions along with those that were used during the development of this project. Then, kernel-specific extensions will be detailed. Finally, the last part will present function modifiers that state where a function can be executed. The extensions to C++ for streams were described above in the *Streams* part of Subsection 1.2.4.

Memory managing extensions CUDA offers many memory managing extensions to C++, however, there are a select few that are widely used for allocating, copying and freeing data [40, 16, 42]:

- `cudaMalloc(void** devPtr, size_t size)` - Function that allocates `size` bytes in device memory and stores the address in the `devPtr` pointer.

Note that since the pointer is to an address located in device memory, it is inaccessible from the host - access from the host would first require for the data to be copied using `cudaMemcpy()`.

This function is widely used when it comes to allocating anything from single variables to large arrays.

If the data was allocated successfully, then `cudaSuccess` is returned, otherwise one of `cudaErrorInvalidValue`, `cudaErrorMemoryAllocation` is returned - depending on the type of failure.

- `cudaMemcpy(void* dst, const void* src, size_t count, cudaMemcpyKind kind)` - Function that copies `count` bytes from the source memory address (`src`) to the destination memory address (`dst`). The `kind` parameter specifies the direction of copying; it has to be one of the following: `cudaMemcpyHostToHost`, `cudaMemcpyHostToDevice`, `cudaMemcpyDeviceToHost`, `cudaMemcpyDeviceToDevice`, or `cudaMemcpyDefault`.

Similarly to `cudaMalloc()`, if the data was copied successfully, then `cudaSuccess` is returned, otherwise one of `cudaErrorInvalidValue`, `cudaErrorInvalidMemcpyDirection` is returned - depending on the type of failure.

- `cudaFree(void* devPtr)` - Function that frees memory on the device that is pointed to by `devPtr`.

If the memory was successfully freed, then `cudaSuccess` is returned, otherwise `cudaErrorInvalidValue` is returned.

It is also worth noting that in order to be freed using `cudaFree()` the memory `devPtr` is pointing to must have been allocated by one of CUDA's memory allocation APIs, for example, `cudaMalloc()`, `cudaMallocAsync()`, etc. - the complete list can be found in Nvidia's *CUDA Runtime API: API Reference Manual* [16].

- `cudaMallocHost(void*** ptr, size_t size)` - Function that allocates `size` bytes of page-locked memory on the host and stores the address in the `ptr` pointer. The benefits and caveats of using page-locked memory are detailed in paragraph *Page-locked host memory* in Sub-section 1.2.3.

Expanding on the memory operations mentioned above, CUDA provides memory space specifiers that can be used to denote in what memory a variable ought to be stored. Among such often-used specifiers are [40]:

- `__device__` - Memory space specifier declaring that a variable is stored in global memory on the device. Since it resides in global memory, it is accessible by all threads from the grid and it is present for the lifetime of the CUDA application. It is noteworthy that if multiple CUDA devices are present in the system, then a variable with this specifier is a unique object for each device.
- `__shared__` - Memory space specifier declaring that a variable is stored in shared memory of a thread block. Since it resides in shared memory, it is only accessible by threads of a block as each block has its own unique object of this variable.

Listing 1.5 shows an example of how memory managing functions can be used in a host-device code that copies arrays.

```

1 int main(void)
2 {
3     float *a_h, *b_h; // data that will be allocated on host
4     float *a_d, *b_d; // data that will be allocated on device
5     int N = 14, nBytes, i;
6
7     nBytes = N * sizeof( float ); // required allocation size
8     a_h = (float *) malloc( nBytes ); // allocating host data
9     b_h = (float *) malloc( nBytes );
10    cudaMalloc( (void **) &a_d, nBytes ); // allocating device data
11    cudaMalloc( (void **) &b_d, nBytes );
12
13    // filling up host data
14    for( i = 0, i < N; i++ ) a_h[ i ] = 100.f + i;
15
16    // copying data from host -> device -> device -> host
17    cudaMemcpy( a_d, a_h, nBytes, cudaMemcpyHostToDevice );
18    cudaMemcpy( b_d, a_d, nBytes, cudaMemcpyDeviceToDevice );
19    cudaMemcpy( b_h, b_d, nBytes, cudaMemcpyDeviceToHost );
20
21    // checking that all data is equal
22    for( i = 0; i < N; i++ ) assert( a_h[ i ] == b_h[ i ] );
23
24    free( a_h ); free( b_h ); // freeing data on host
25    cudaFree( a_d ); cudaFree( b_d ); // freeing data on device
26    return 0;
27 }

```

Listing 1.5: Example of code that utilizes CUDA memory managing extensions of C++. Taken from *Formats for storage of sparse matrices on GPU* [42] and Nvidia’s *Getting Started with CUDA* presentation [23].

Kernels While the term *kernel* was introduced earlier in Subsection 1.2.1, the technical details will be covered in this part. In order to differentiate a kernel from a function, the `__global__` modifier must be used. Another distinction that kernels have compared to regular functions is the kernel launch configuration which has the following specific syntax: `<<< numBlocks, threadsPerBlock, sharedMemSize, stream >>>` where [40, 42]:

- `numBlocks` specifies the number of blocks in the grid and their structure;
- `threadsPerBlock` specifies the number of threads per block and their structure;
- `sharedMemSize` specifies the number of bytes that are to be dynamically allocated in shared memory for each block (on top of any statically allocated shared memory). This argument is not mandatory and its default value is 0;
- `stream` specifies stream to which the kernel should be sent for execution. This argument is also not mandatory and defaults to 0 - the default stream.

The `sharedMemSize` parameter is of type `size_t`, `stream` is of type `cudaStream_t`, and parameters `numBlocks` and `threadsPerBlock` can be either of type `int` or `dim3`. The `dim3` type

is a 3-dimensional `unsigned int` vector used to specify dimensions. It can be defined with up to 3 variables (1 for each dimension) with an implicit dimension value of 1, i.e., if a vector component (dimension) is not specified when declaring a `dim3` variable, it is by default initialized to 1.

For example, if `numBlocks` is of type `int`, then the grid is one-dimensional and composed of `numBlocks` blocks. Concordantly, if `threadsPerBlock` is type `int`, then all blocks in the grid will be one-dimensional with `threadsPerBlock` threads.

On the other hand if `threadsPerBlock` is a `dim3` variable, then the thread structure of all blocks can be up to three-dimensional. An example of a kernel being called with the properties above can be seen in Listing 1.6.

```

1 // Kernel definition
2 __global__ void MyKernel(float a, float b, float c)
3 {
4     // Kernel code here
5 }
6
7 int main()
8 {
9     ...
10    // Kernel invocation on a grid with 1 block of 8 * 1 * 1 threads
11    int numBlocks = 1;
12    dim3 threadsPerBlock(8); // Defaults to (8, 1, 1)
13    MyKernel<<<numBlocks, threadsPerBlock>>>(a, b, c);
14    ...
15 }
```

Listing 1.6: Example of C++ pseudocode of a Kernel launch on a grid consisting of 1 one-dimensional block that is made up of 8 threads. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

Function extensions In the part above, the `__global__` modifier was introduced as a specifier for functions that are to be considered kernels. Along with it, CUDA brings other function modifiers, or, as Nvidia calls them: *execution space specifiers* [40]:

- `__global__` - Modifier declaring that a function can be called from both the host and the device (as of compute capability 3.2 or higher). However, it can only be executed on the device. Additionally, a function denoted with this modifier must not belong to any class and it can only have a void return type. Furthermore, the launch configuration mentioned above in the *Kernels* paragraph must be specified for each call.
- `__device__` - Modifier declaring that a function can only be called from and executed on the device. This means that it can only be called from within kernels.
- `__host__` - Modifier declaring that a functions can only be called from and executed on the host. This means that it can only be called from regular functions, not kernels.

If no modifier is included for a function, it is compiled for the host only. However, if both `__device__` and `__host__` are specified for a function, then it is compiled both for the host and for the device. The complete list of modifiers can be found in *CUDA C++ Programming Guide* [40].

Inter-kernel extensions

This category comprises of variables, structures and operations etc. that are most often used within a kernel. First, the means by which developers are able to identify individual threads will be detailed. Then, different memory-type identifiers will be briefly presented along with established operations used to avoid erroneous behaviors in kernels.

Thread identification Once a kernel is launched on the device, it can be run concurrently on thousands of threads. This presents a scenario where the developer must distinguish what each thread will perform within the kernel. For this purpose, the following variables - among others - are available within every kernel for each thread [40]:

- `threadIdx` - ID of a thread within a block stored in a 3-component vector (1 component for each of 3 dimensions). For example, if the thread block is 2-dimensional, then `threadIdx.x` stores the thread's ID in the first dimension and `threadIdx.y` stores the thread's ID in the second dimension - the pair of IDs is unique only within the thread's block.
- `blockIdx` - ID of a block within a grid stored in a 3-component vector (1 component for each of 3 dimensions). Similarly to `threadIdx`, the block's ID in the first dimension is retrieved using `blockIdx.x`, the second using `blockIdx.y` and the third using `blockIdx.z`. Within a kernel, the block ID refers to the block of threads that the executing thread belongs to.
- `blockDimx` - Dimensions of a thread's block stored in a 3-component vector (1 component for each of 3 dimensions). For example, for a block made up of `32x16x2` threads: `blockDimx.x = 32`, `blockDimx.y = 16` and `blockDimx.z = 2`.

The variables above can be combined to calculate the global ID of a thread, i.e. the thread's ID within a grid:

$$\text{globalID} = \text{blockIdx.x} * \text{blockDimx.x} + \text{threadIdx.x}$$

The `globalID` is useful when working with matrices, for example, adding 2 matrices. In such an example, each thread would take 2 elements (1 from each matrix), add them and then store the result into a new matrix - as shown in Listing 1.7.

```
1 // Kernel definition
2 __global__ void MatAdd(float A[N][N], float B[N][N], float C[N][N])
3 {
4     // Get thread ID for each dimension -> use as matrix indices
5     int i = blockIdx.x * blockDim.x + threadIdx.x;
6     int j = blockIdx.y * blockDim.y + threadIdx.y;
7
8     // Check if the IDs are within the dimensions of the matrices
9     if (i < N && j < N)
10         C[i][j] = A[i][j] + B[i][j];
11 }
12
13 int main()
14 {
15     ...
16     // Number of threads per each 2-dimensional block is 16x16 = 256
17     dim3 threadsPerBlock(16, 16);
```

```

18
19 // Number of blocks in the grid depends on the matrix dimension (NxN)
20 dim3 numBlocks(N / threadsPerBlock.x, N / threadsPerBlock.y);
21
22 // Kernel launch: A + B = C
23 MatAdd<<<numBlocks, threadsPerBlock>>>(A, B, C);
24 ...
25 }

```

Listing 1.7: Example of C++ pseudocode of a kernel that adds 2 matrices using 2-dimensional thread blocks. Since each thread has a unique `globalID` for each of 2 dimensions, then those IDs can be used as indices for adding matrix elements. This simple example does not take into account allocation and copying data from host to device. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

Accompanying the code in Listing 1.7, Figure 1.14 visualizes how elements of a matrix can be divided into a grid comprising of 2-dimensional thread blocks.

Finally, as mentioned in paragraph *Global memory* in Subsection 1.2.3, the coalesced access of threads effectively means that neighboring threads access global memory. To add to this, it is important to mention that threads are considered neighboring in the first dimension. In other words, neighbors according to `threadIdx.x` values.

Memory specifiers and other operations Some memory space specifiers described in above in paragraph *Memory managing extensions* in Subsection 1.2.5 can be used within kernels, specifically the `__shared__` specifier. Its use within kernels is mostly related to statically allocated shared memory where the size of the variable or array is known during compilation [40]. An example showing this use of the specifier can be seen in Listing 1.11.

In paragraph *Shared memory* in Subsection 1.2.3, it was mentioned that threads of a block are able to share data purely among each other. However, this advantage can also bring problems, such as, some threads overwriting data that other threads have not finished using, or, some threads reading data that other threads have not yet written - known as a *race condition* [14]. CUDA addresses this issue by enabling the synchronization of threads in a block which can be done by calling the built-in function: `__syncthreads()`. This function can be seen as a meeting checkpoint for all threads of a particular block, i.e., threads of a block will wait at this point until every single thread in their block has finished their work until this point. To put it more clearly: threads of a block are halted on the line in code that contains `__syncthreads()` until all threads of the block arrive to it [40].

1.2.6 Matrix multiplication

In order to consolidate how CUDA can be used to accelerate the execution of a simple task, such as matrix multiplication, this subsection will present solutions to this task from Nvidia's *CUDA C++ Programming Guide* [40]. Furthermore, for the purpose of showcasing and stressing the importance of abiding by Nvidia's recommendations when it comes to best practices and optimal performance, 2 examples will be presented. The first example will only use global memory to read the input matrix and write the resulting matrix, i.e. without shared memory. On the other hand, the second example will use shared memory to minimize accessing global memory.

It is important to note that neither example is fully functional as the logic of some functions has been omitted due to unnecessary complexity and irrelevance to showcasing the capabilities of CUDA. In other

CUDA Grid

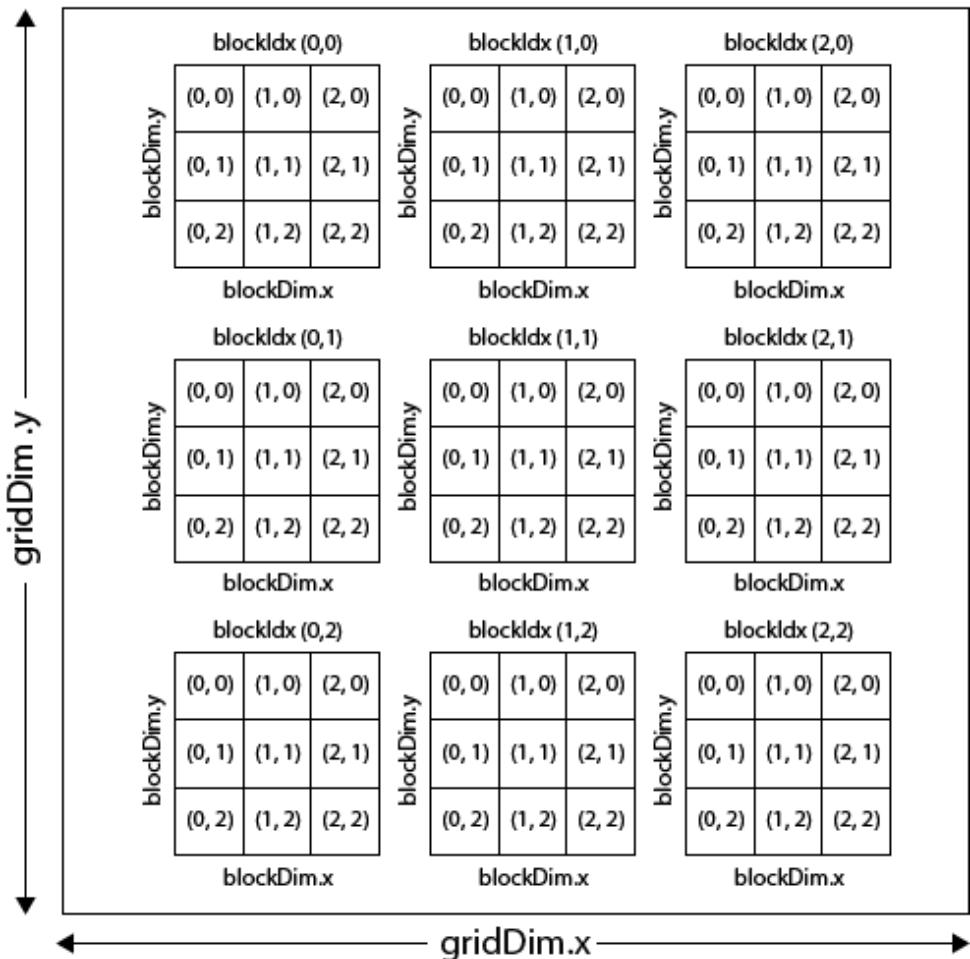


Figure 1.14: Grid made up of 2-dimensional thread blocks. Each square represents a thread with its IDs within its block (`threadIdx.x`, `threadIdx.y`). It can be imagined that each block is a sub-matrix and together all sub-matrices make up the full matrix. Taken from *CUDA Parallel Thread Management* [15].

words, the code shown will not compile, nor will it run - the full code can be found in Nvidia's *CUDA C++ Programming Guide* [40]. The full working example (`matrixMul.cu`) encompassed by the build automation tool `make` can be unpacked during the installation of a CUDA toolkit.

Before introducing the specifics of each example, their similarities will be presented.

First, the task that will be performed is matrix multiplication:

$$\mathbb{C} = \mathbb{A} \cdot \mathbb{B} \quad (1.1)$$

In the context of this operation all matrix dimensions are assumed such that it is a legal operation. Additionally, for simplicity, the dimensions of the matrices are assumed to be multiples of the thread block size. This limitation can be avoided by allocating an extra row and column of blocks in the grid

and setting a boundary condition in the kernel - each of the 2 examples (global vs shared memory) require slightly different approaches which will be described later.

Let each matrix be represented by a structure `Matrix`:

```

1 // Matrices are stored in row-major order:
2 // M(row, col) = *(M.values + row * M.width + col)
3 typedef struct {
4     int width;
5     int height;
6     float* values;
7 } Matrix;
```

Listing 1.8: Definition of the structure that will represent a matrix. The `width` variable stores the number of columns and `height` stores the number of rows the matrix has. The elements of the matrix are stored in row-major order in the single-precision (float) array: `values`. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

Furthermore, let there be a host function `MatMul` that will:

1. Take matrices $\mathbb{A}, \mathbb{B}, \mathbb{C}$ from Equation 1.1 as input structures: `A`, `B`, `C`.
2. Allocate memory for the matrix structures on the device.
3. Copy the matrix structures from host to device memory.
4. Invoke the matrix multiplication kernel with a constant thread block size set at compile time.
5. Copy the resulting matrix from device to host memory.
6. Free previously allocated memory from the device.

Listing 1.9 shows the implementation of the points mentioned above.

```

1 // Thread block size - 16x16 = 256 threads
2 #define BLOCK_SIZE 16
3
4 // Matrix multiplication - Host code
5 // Matrix dimensions are assumed to be multiples of BLOCK_SIZE
6 void MatMul( const Matrix A, const Matrix B, Matrix C )
7 {
8     // Allocate and copy A to device memory
9     Matrix d_A;
10    d_A.width = A.width; d_A.height = A.height;
11    size_t size = A.width * A.height * sizeof(float);
12    cudaMalloc( &d_A.values, size );
13    cudaMemcpy( d_A.values, A.values, size, cudaMemcpyHostToDevice );
14
15    // Allocate and copy B to device memory
16    Matrix d_B;
17    d_B.width = B.width; d_B.height = B.height;
18    size = B.width * B.height * sizeof(float);
19    cudaMalloc( &d_B.values, size );
20    cudaMemcpy( d_B.values, B.values, size, cudaMemcpyHostToDevice );
21
22    // Allocate C in device memory
```

```

23 Matrix d_C;
24 d_C.width = C.width; d_C.height = C.height;
25 size = C.width * C.height * sizeof(float);
26 cudaMalloc( &d_C.values, size );
27
28 // Invoke kernel
29 dim3 threadPerBlock( BLOCK_SIZE, BLOCK_SIZE );
30 dim3 numBlocks( B.width / threadPerBlock.x, A.height / threadPerBlock.y );
31 MatMulKernel<<< numBlocks, threadPerBlock >>>( d_A, d_B, d_C );
32
33 // Read C from device memory
34 cudaMemcpy( C.values, d_C.values, size, cudaMemcpyDeviceToHost );
35
36 // Free device memory
37 cudaFree( d_A.values );
38 cudaFree( d_B.values );
39 cudaFree( d_C.values );
40 }
```

Listing 1.9: Definition of the function that will allocate and copy all matrices to the device, invoke the kernel and then free the device memory. The size of the thread block is constant and set during compile time using the `#define` macro. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

The `Matrix` structure and `MatMul` function conclude the equivalent part of the examples.

Example without shared memory

The first example uses only global memory access, i.e. without shared memory. This means that the kernel - invoked on line 31 in Listing 1.9 - receives the `Matrix` structures stored in global memory and each thread reads from and writes to the same global memory whenever they need to.

The kernel is launched on a grid of thread such that each thread is responsible for calculating exactly 1 element of the resulting `C` matrix. For example, let there be a thread with indices `row_id` and `col_id`. This thread will perform element-wise multiplication of row `row_id` from matrix `A` and column `col_id` from matrix `B`. Then, it will store the sum of these elements as the resulting value `C(row_id, col_id)` into matrix `C`.

The visualization of this approach is shown in Figure 1.15 and the kernel is presented in Listing 1.10.

```

1 // Matrix multiplication kernel called by MatMul()
2 __global__ void MatMulKernel( Matrix A, Matrix B, Matrix C )
3 {
4     // Each thread computes one element of C by accumulating results into Cvalue
5     float Cvalue = 0;
6     int row = blockIdx.y * blockDim.y + threadIdx.y;
7     int col = blockIdx.x * blockDim.x + threadIdx.x;
8     for( int i = 0; i < A.width; ++i )
9         Cvalue += A.values[row * A.width + i] * B.values[i * B.width + col];
10
11    C.values[row * C.width + col] = Cvalue;
12 }
```

Listing 1.10: Definition of the matrix multiplication kernel that uses global memory without shared memory. Each thread has a variable `Cvalue` stored in registers into which it calculates its specific `C(row, col)` matrix element. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

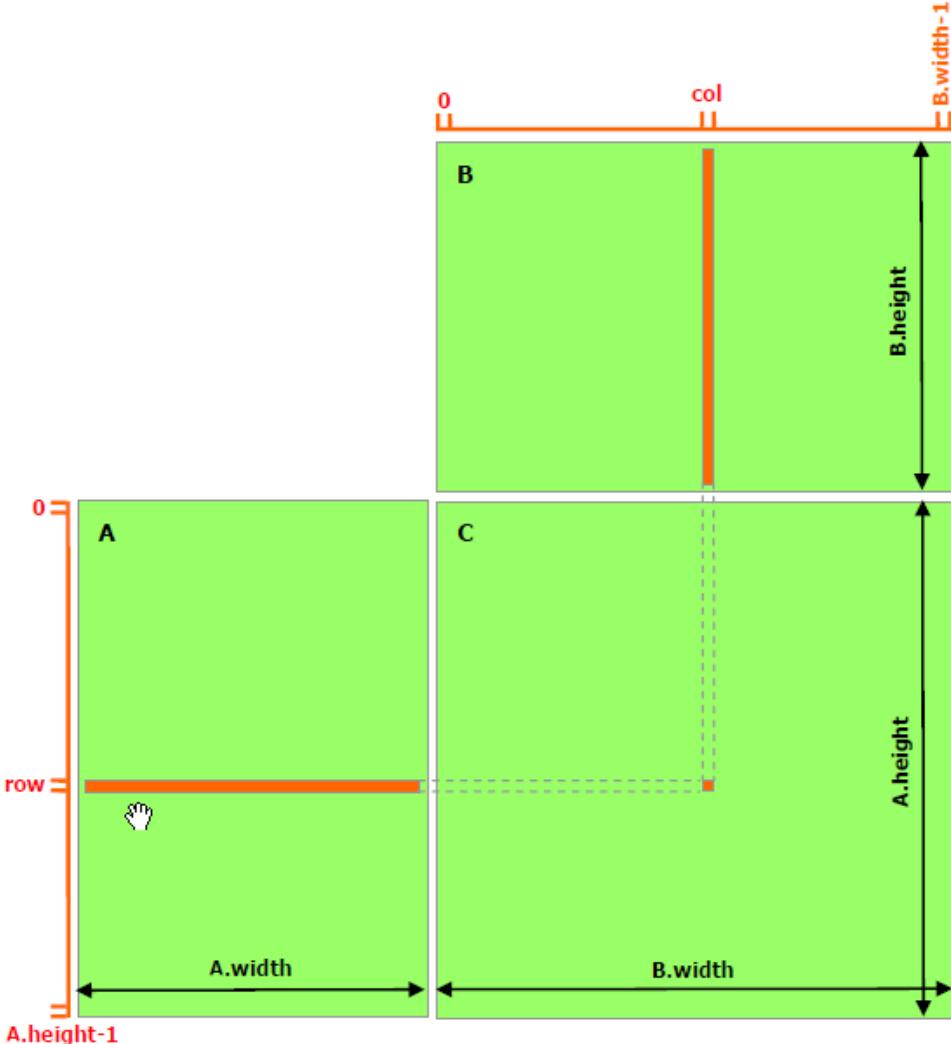


Figure 1.15: Visualization of the execution of the kernel that does not use shared memory - shown in Listing 1.10. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

As can be seen in Listing 1.10, each thread performs `A.width + B.height` reads from global memory when calculating its `Cvalue`. Since CUDA threads are executed simultaneously in a warp of 32 threads, the memory access to global memory should be coalesced for the threads within each warp. Nevertheless, this kernel is sub-optimal as accessing global memory is considered sub-optimal when avoidable.

At the end of the introduction to Subsection 1.2.6, it was mentioned that in order to eliminate the "matrix dimensions being multiples of `BLOCK_SIZE`" requirement, the kernel would need to include a boundary condition. In this example, the condition would be simply to allocate an extra column and row of thread blocks to the grid. This would mean that the last row and column of blocks would overlap the dimensions of the matrix. Then, the kernel would be terminated for threads that are outside the matrix dimensions, i.e. if either `row` is greater than `A.height` or `col` is greater than `B.width`. However, it is noteworthy that this will result in thread divergence, even though in this instance it will not have a large impact on overall performance as one of the execution paths would be a simple `return` statement.

Example with shared memory

The second example uses both global and shared memory. Similarly to the approach without using shared memory, each thread is responsible for calculating a single element of the resulting `C` matrix. However, in this example, each thread is also responsible for loading elements of matrices `A` and `B` from global memory into shared memory. Thus, shared memory is the primary means of obtaining elements for calculations. Overall, the calculation is changed from each thread calculating its individual element to a block of threads iterating over sub-matrices of `A` and `B`.

In order to make use of shared memory, matrix `C` is divided into sub-matrices of `BLOCK_SIZE x BLOCK_SIZE` elements (\mathbb{C}_{sub}). Then, each sub-matrix \mathbb{C}_{sub} is computed by a single thread block; each thread within a thread block is responsible for the computation of an element in \mathbb{C}_{sub} . In the previous approach, each thread performed element-wise multiplication of a row and a column to form a resulting element of matrix `C` - effectively a multiplication of an `1xn` and `nx1` matrix. The approach with shared memory expands this concept to blocks. In other words, the sub-matrix \mathbb{C}_{sub} is a result of multiplying 2 rectangular sub-matrices of `A` and `B` (illustrated in Figure 1.16) - denoted \mathbb{A}_{rect} and \mathbb{B}_{rect} for the purpose of this explanation:

1. \mathbb{A}_{rect} is a `BLOCK_SIZE x A.width` sub-matrix of `A` that has the same row indices as \mathbb{C}_{sub} .
2. \mathbb{B}_{rect} is a `B.height x BLOCK_SIZE` sub-matrix of `B` that has the same column indices as \mathbb{C}_{sub} .

The rectangular sub-matrices \mathbb{A}_{rect} and \mathbb{B}_{rect} are split into `BLOCK_SIZE x BLOCK_SIZE` sub-matrices \mathbb{A}_{sub} and \mathbb{B}_{sub} . A thread block will begin its computation by multiplying the leftmost \mathbb{A}_{sub} with the uppermost \mathbb{B}_{sub} , then it will move to the next \mathbb{A}_{sub} on the right and to the next \mathbb{B}_{sub} below. After every iteration, each thread appends its partial sum to the `Cvalue` variable that it is responsible for in the \mathbb{C}_{sub} sub-matrix. The computation of \mathbb{C}_{sub} is finished once the thread block reaches and multiplies the rightmost \mathbb{A}_{sub} and the lowermost \mathbb{B}_{sub} sub-matrix.

The reasoning behind splitting \mathbb{A}_{rect} and \mathbb{B}_{rect} into multiple \mathbb{A}_{sub} and \mathbb{B}_{sub} respectively stems from the use of shared memory in every iteration for a particular block:

1. All threads of the block load \mathbb{A}_{sub} and \mathbb{B}_{sub} from global memory to a two-dimensional array residing in the block's shared memory.
2. Each thread of the block performs its computation, i.e. it multiplies row `row_id` from \mathbb{A}_{sub} with column `col_id` from \mathbb{B}_{sub} and sums the resulting values (`row_id` and `col_id` are the thread's IDs).
3. Each thread stores the temporary result to its local variable `Cvalue` stored in its registers.
4. If there still is a \mathbb{A}_{sub} to the right and a \mathbb{B}_{sub} below, then, all threads of the block move to them and continue to step 1.
5. Otherwise, the computation is finished and all threads store their local variable `Cvalue` to the element that they're responsible in \mathbb{C}_{sub} that resides in global memory.

The visualization of this approach is shown in Figure 1.16 and the kernel is presented in Listing 1.11.

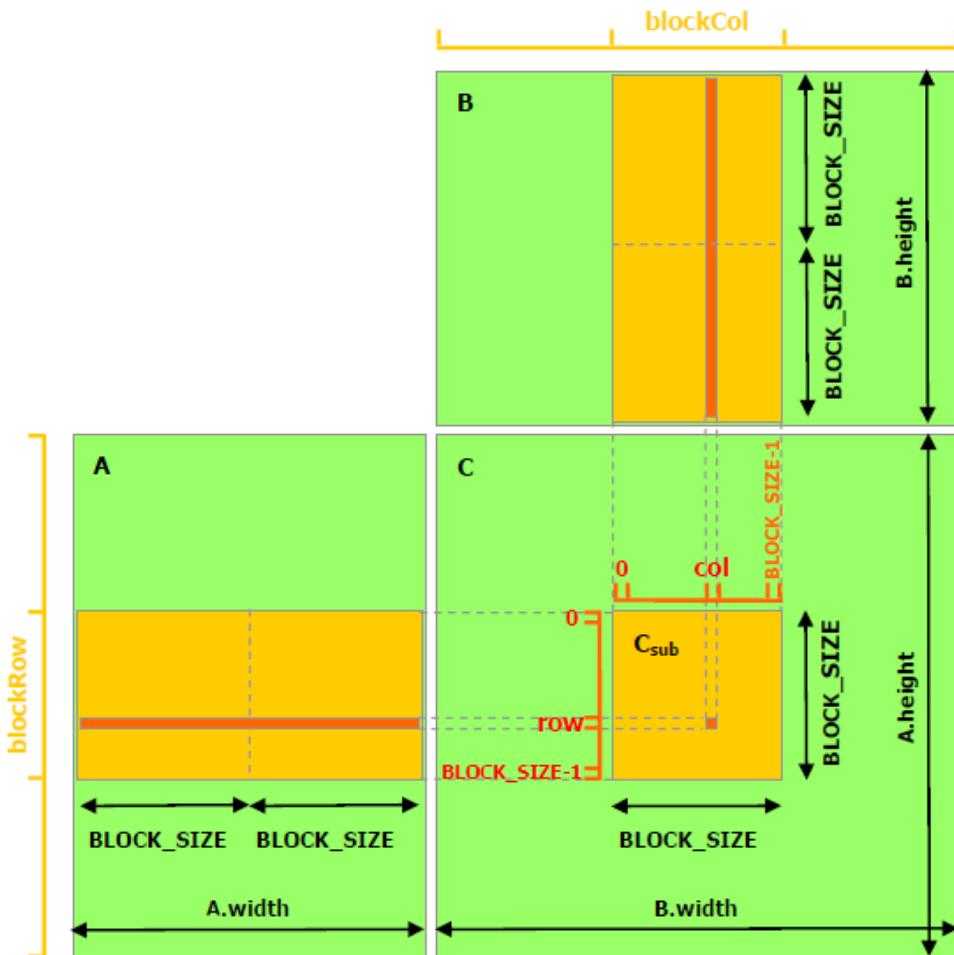


Figure 1.16: Visualization of the execution of the kernel that uses shared memory - shown in Listing 1.11. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

```

1 // Matrix multiplication kernel called by MatMul()
2 __global__ void MatMulKernel( Matrix A, Matrix B, Matrix C )
3 {
4     // Block row and column - indices of the sub-matrices within A and B ←
5     // respectively
6     int blockRow = blockIdx.y;
7     int blockCol = blockIdx.x;
8
9     // Each thread block computes one sub-matrix Csub of C
10    Matrix Csub = GetSubMatrix( C, blockRow, blockCol );
11
12    // Each thread computes one element of Csub by accumulating results into Cvalue
13    float Cvalue = 0;
14
15    // Thread row and column within Csub
16    int row = threadIdx.y;
17    int col = threadIdx.x;

```

```

18 // Loop over all the sub-matrices of A and B that are required to compute Csub ←
19 // by multiplying each pair of sub-matrices together and accumulate the results
20 for( int i = 0; i < (A.width / BLOCK_SIZE); ++i ) {
21
22     // Get sub-matrix Asub of A
23     Matrix Asub = GetSubMatrix( A, blockRow, i );
24
25     // Get sub-matrix Bsub of B
26     Matrix Bsub = GetSubMatrix( B, i, blockCol );
27
28     // Shared memory used to store Asub and Bsub respectively
29     __shared__ float As[BLOCK_SIZE][BLOCK_SIZE];
30     __shared__ float Bs[BLOCK_SIZE][BLOCK_SIZE];
31
32     // Load Asub and Bsub from device memory to shared memory
33     // Each thread loads one element of each sub-matrix
34     As[row][col] = GetElement( Asub, row, col );
35     Bs[row][col] = GetElement( Bsub, row, col );
36
37     // Synchronize to make sure the sub-matrices are loaded before starting the ←
38     // computation
39     __syncthreads();
40     // Multiply Asub and Bsub together
41     for( int k = 0; k < BLOCK_SIZE; ++k )
42         Cvalue += As[row][k] * Bs[k][col];
43
44     // Synchronize to make sure that the preceding computation is done before ←
45     // loading two new sub-matrices of A and B in the next iteration
46     __syncthreads();
47 }
48
49 // Write Csub to device memory – each thread writes one element
50 SetElement( Csub, row, col, Cvalue );
51 }
```

Listing 1.11: Definition of the matrix multiplication kernel that uses both global memory with shared memory.

The `GetSubMatrix(mtx, row, col)` is a function returns a `BLOCK_SIZE x BLOCK_SIZE` sub-matrix of a matrix that is located `col` sub-matrices to the right and `row` sub-matrices down from the upper-left corner of a the specified `Matrix`. The `GetElement(sub_mtx, row, col, val)` function returns the element found at a matrices `row` and `col` indices. Taken from Nvidia's *CUDA C++ Programming Guide* [40].

Unlike the previous example, the code shown in Listing 1.11 has less accesses to global memory which leads to an performance improvement as detailed later in the *Comparison of examples* part of Subsection 1.2.6. Concretely, in the kernel above, each thread performs only `A.width/BLOCK_SIZE + B.height/BLOCK_SIZE` reads from global memory when loading sub-matrices `Asub` and `Bsub` into shared memory. This means that all threads will perform `BLOCK_SIZE` times less accesses to global memory and `A.width + B.height` accesses to shared memory instead. Equivalently to the example before, the access to global memory is coalesced. Thus, by Nvidia's recommendations, this kernel can be considered being close to optimal.

In order to eliminate the "matrix dimensions being multiples of `BLOCK_SIZE`" requirement, the kernel would need to include a boundary condition. In the earlier approach it was a matter of allocating extra blocks and terminating the kernel for threads that would reach out of matrix bounds. However, for this approach - with shared memory - that method would result in incorrect results as the threads that would

reach out of bounds for one matrix read elements into shared memory from the other matrix. Thus, the boundary condition is split into:

1. If the thread would reach out of bounds of a particular matrix, load the edge element, i.e. the last element of the row/col before the thread would reach out of bounds. This condition would be used when the elements are being loaded from global into shared memory.
2. Then let the computation continue as normal - to avoid thread divergence of threads.
3. Once the computation si done, terminate the threads that would reach out of bounds of matrix \mathbb{C} before they write their results to global memory.

This solution ensures correct results and avoids a case of thread divergence in the main loop which would occur multiple times during the computation. However, the thread divergence will still occur when deciding which value to load from global memory and when terminating the kernel for some threads. Nevertheless, similarly to the previous approach, in this instance thread divergence will not have a large impact on overall performance as one of the execution paths would be a simple assignment operation in the first condition and a `return` statement in the second condition.

Comparison of both examples

In order to show the performance difference, benchmarks for both examples using single precision were run on a set of matrices with varying dimensions - from 160 by 160 to 16000 by 16000. The hardware and software specifications of the machine used for the benchmarks can be found in Table 1.6. Furthermore, the full code can be found in Attachment A.

CPU	Ryzen 9 5900x @ 3.7 GHz (12 cores, 24 threads)
RAM	32GB RAM
GPU	Nvidia GeForce GTX 1070 8GB GDDR5 (256.3 GByte/s)
Operating System	Ubuntu 20.04.4 LTS (Focal Fossa)
Compiler	GCC 8.4.0
CUDA	CUDA 11.5

Table 1.6: Specifications of the platform that the matrix multiplication benchmarks were run on.

The operation measured during the benchmark was only the multiplication of matrices

$$\mathbb{C} = \mathbb{A} \cdot \mathbb{B}$$

In other words, allocation and copying of the matrices was not included in the measurement. Furthermore, the operation was looped 10 times - the measured FLOPS and run times were averaged from the 10 recorded loops. The values in Matrix \mathbb{A} were all set to 1 and to 0.1 in matrix \mathbb{B} . The benchmark results in FLOPS can be found in Figure 1.17 and Table 1.7 shows the results in milliseconds.

As can be seen in Figure 1.17 and Table 1.7, the approach that utilizes shared memory achieved between 2-4 times the number of GFLOPs per second and similarly faster execution times compared to the approach that does not use shared memory and instead relies only on global memory. Additionally, the difference seems to be increasing with growing matrix dimensions, however, this statement has not been verified for dimensions greater than 16000 by 16000.

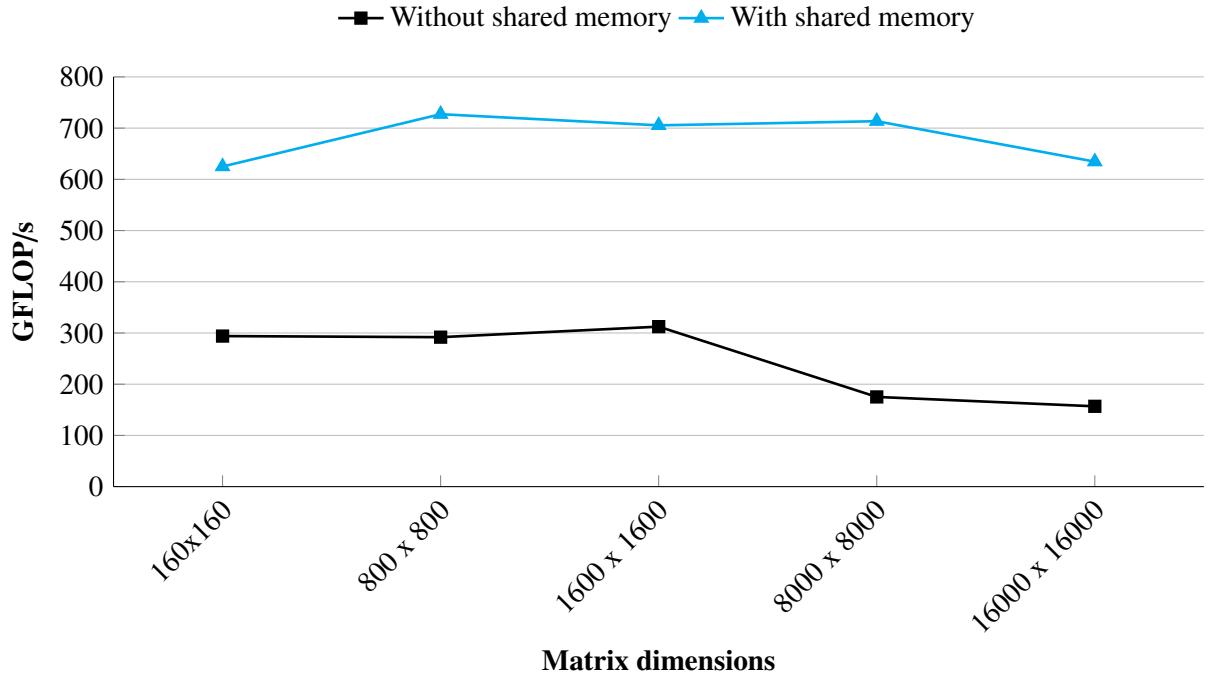


Figure 1.17: Matrix multiplication results of matrices with varying dimensions; matrices are filled with 1 element. The values - presented in GFlop/s - are averages from 10 loops of the operation.

Matrix dimensions	Results [msec]	
	Without shared memory	With shared memory
160 x 160	0.028	0.013
800 x 800	3.509	1.408
1600 x 1600	26.224	11.613
8000 x 8000	5846.247	1435.221
16000 x 16000	52226.867	12910.967

Table 1.7: Matrix multiplication results of matrices with varying dimensions; matrices are filled with 1 element. The values - presented in milliseconds - are averages from 10 loops of the operation.

1.3 LU Decomposition

It can be argued that, in recent years, computational systems and software layers allowing developers to use them to their full potential have developed significantly - Nvidia GPUs and CUDA. Subsequently, many novel uses have been found for such powerful computing systems, especially in areas that require results to be available quickly on demand. An example of such an area is solving systems of linear equations. Being one of the fundamental parts of numerical linear algebra, the requirement for their solution arises not only in computer science, but also in physics, engineering, chemistry, etc.

While there are many different methods capable of solving a system comprising of more than one linear

equation, in this project, Lower-Upper (LU) decomposition will be detailed.

In order to show how LU decomposition can be used to solve a simple system of linear equations an example will be presented.

First, it is necessary to introduce the system. For the purpose of the explanation, let the coefficients of the following system of linear equations:

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 &= b_1, \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 &= b_2, \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 &= b_3, \end{aligned} \quad (1.2)$$

be re-written into the matrix form

$$\mathbb{A}\mathbf{x} = \mathbf{b}, \quad (1.3)$$

where

$$\mathbb{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}. \quad (1.4)$$

In order to be able to use LU decomposition, matrix \mathbb{A} must be a square matrix ($n \times n$) that is also strongly regular. This requirement can be relaxed to only requiring regularity by properly ordering the rows and columns of the matrix using a permutation matrix \mathbb{P} , however, such a procedure will not be present in this project, and therefore all coefficient matrices are required to be strongly regular.

Second, using a *decomposition algorithm* the coefficient matrix \mathbb{A} is decomposed into the product of a lower triangular matrix \mathbb{L} and a upper triangular matrix \mathbb{U} :

$$\mathbb{A} = \mathbb{L}\mathbb{U}, \quad (1.5)$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}. \quad (1.6)$$

Then, substituting Equation 1.3 into Equation 1.3 yields:

$$\mathbb{L}\mathbb{U}\mathbf{x} = \mathbf{b}. \quad (1.7)$$

Third, the matrix form from Equation 1.7 is used to obtain the solution to the system of linear equations using forward and backward substitution:

1. Solve the equation $\mathbb{L}\mathbf{y} = \mathbf{b}$ (where only \mathbf{y} is not known):

$$\begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}. \quad (1.8)$$

2. Solve the equation $\mathbb{U}\mathbf{x} = \mathbf{y}$ (where only \mathbf{x} is not known):

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}. \quad (1.9)$$

It is noteworthy that since the values on the right-hand side (vector \mathbf{b}) are only required in step 3 (equations 1.8 and 1.9), they are not required for the process of decomposition itself. Thus, if there is more than 1 right side in the system of linear equations, matrix \mathbb{A} needs to be decomposed into matrices \mathbb{L} and \mathbb{U} only once; the same principle is valid even if the right side is not known ahead of time. In other words, \mathbb{L} and \mathbb{U} can be used to solve the system for different right-hand sides without the need for repeated decomposition. Additionally, this concept can be seen as an advantage for LU decomposition compared to Gaussian elimination as the latter requires the right-hand side to obtain the system's upper triangular matrix and subsequently use it for backward substitution. This concept is described, for example, by George Lindfield and John Penny in *Numerical Methods: Linear Equations and Eigensystems* [8].

In summary, from the steps above, it can be argued that the *decomposition algorithm* mentioned in step 2 is one of the key components of the procedure and as such it will be the main topic of this project.

1.3.1 Crout method

This subsection aims to explain in greater detail the decomposition algorithm mentioned above in step 2. There are many different procedures to decompose matrix \mathbb{A} into matrices \mathbb{L} and \mathbb{U} such that $\mathbb{A} = \mathbb{L}\mathbb{U}$. One such procedure, developed by Prescott Durand Croutis, is the *Crout method* - sometimes also referred to as *Crout matrix decomposition* or *Crout factorization* [12].

This method differs from similar procedures in that the resulting \mathbb{U} matrix is a unit upper triangular matrix, while \mathbb{L} remains to be a lower triangular matrix. A unit triangular matrix differs from a regular triangular matrix in that its main diagonal is comprised solely of ones. In other words, all elements on the main diagonal of \mathbb{U} are equal to 1 ($u_{11} = u_{22} = u_{33} = 1$):

$$\begin{bmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{bmatrix}. \quad (1.10)$$

Algorithm The Crout matrix decomposition algorithm is based on sequentially filling in matrices $\mathbb{L}_{n \times n}$ and $\mathbb{U}_{n \times n}$ using elements from matrix $\mathbb{A}_{n \times n}$. At the core of this filling-in are the following formulas and their conditions for l_{ij} and u_{ij} :

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj} \quad i \geq j, \quad (1.11)$$

$$u_{ij} = \frac{1}{l_{ii}} \left(a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj} \right), \quad i < j, \quad (1.12)$$

$$\begin{aligned} u_{ij} &= 1 & i = j, \\ i, j &\in \widehat{n}. \end{aligned} \quad (1.13)$$

Specifically, the algorithm first computes a column j in \mathbb{L} and then row j in \mathbb{U} . This process repeats itself for j from 1 to n . The pseudo-code implementing the algorithm can be seen in Listing 1.12 and the visualization of the algorithm's advance is shown in Figure 1.18.

```

1 void crout_method(A, L, U) {
2     int i, j, k;
3     double sum = 0;
4
5     // Fill main diagonal of U with 1s
6     for (i = 0; i < n; i++) {
7         U[i][i] = 1;
8     }
9
10    // Loop through the main diagonal
11    for (j = 0; j < n; j++) {
12
13        // Compute column j in L
14        for (i = j; i < n; i++) {
15            sum = 0;
16            for (k = 0; k < j; k++) {
17                sum += L[i][k] * U[k][j];
18            }
19            L[i][j] = A[i][j] - sum;
20        }
21
22        // Compute row j in U
23        for (i = j; i < n; i++) {
24            sum = 0;
25            for (k = 0; k < j; k++) {
26                sum = sum + L[j][k] * U[k][i];
27            }
28            if (L[j][j] == 0) {
29                printf("det(L) close to 0!\n Can't divide by 0...\\n");
30                exit(EXIT_FAILURE);
31            }
32            U[j][i] = (A[j][i] - sum) / L[j][j];
33        }
34    }
35 }
```

Listing 1.12: C++ Pseudo-code implementing Crout's matrix decomposition algorithm. It assumes that $A[n][n]$ is a two-dimensional array that represents the invertible square coefficient matrix A ; $L[n][n]$ and $U[n][n]$ are also two-dimensional arrays representing matrices L and U respectively. Furthermore, it is assumed that L and U are populated with zeros. Derived from *Crout's LU Factorization* [11], *Numerical recipes: the art of scientific computing* [12] and *Crout matrix decomposition* [10].

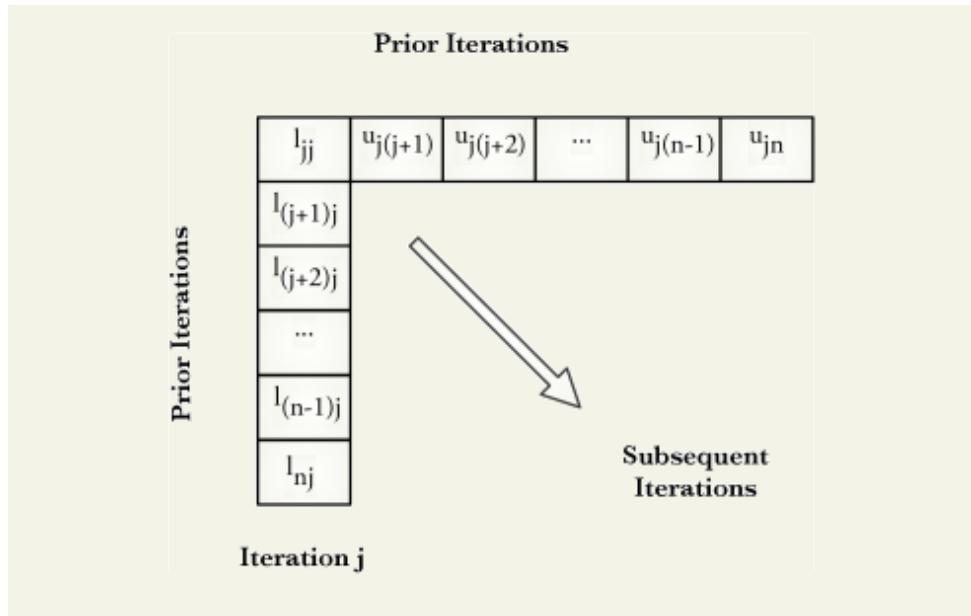


Figure 1.18: Sequence of computations of the Crout method. First, column j in \mathbb{L} is computed and then row j of \mathbb{U} . Taken from Vismor's *Crout's LU Factorization* [11].

1.3.2 Numerical method

When solving systems of linear equations there are 2 main groups of methods:

1. Direct methods - theoretically, the exact solution will be obtained after a finite amount of steps (e.g. Crout method).
2. Iterative methods - theoretically, these methods converge to the solution, however, the exact solution is not guaranteed to be found (numerical methods).

The Crout method as described in Subsection 1.3.1 is a direct method, meaning that it provides an exact solution. Furthermore, it is strictly sequential, meaning that there is seemingly no room for parallelization.

However, Hartwig Anzt et al. in their paper *ParILUT - A Parallel Threshold ILU for GPUs* [43] describe different approaches to generating incomplete factorizations. An example of such a group of approaches is referred to as *ParILU algorithms* which are distinct in the fact that they abandon the methodology akin

to Gaussian elimination. Rather, these methods use "*fixed-point iterations to approximate the incomplete factors on a pre-defined sparsity pattern*" - iterative methods. The authors in the paper explain method belonging to this group as algorithms that do not take every non-zero into account.

However, for the purpose of this paper, it was decided to derail from this principle - exclude any sparsity pattern conditions - and focus purely on the iterative aspect of the methodology. In other words, use the fixed-point iterating algorithm that - according to the authors - converges to a sufficiently approximate solution of $\mathbb{A} = \mathbb{L}\mathbb{U}$ without taking into account sparsity patterns.

Specifically, the algorithm is as follows:

1. Provide an initial guess (estimate) of matrices \mathbb{L}^0 and \mathbb{U}^0 . For example, using \mathbb{A} :

$$\begin{aligned} l_{ij}^0 &= a_{ij} & i < j, \\ u_{ij}^0 &= a_{ij} & i > j, \\ u_{ii}^0 &= 1 & i = j. \end{aligned}$$

2. Using the formulas in Equations 1.11 and 1.11 calculate the next iteration of \mathbb{L}^t and \mathbb{U}^t (where $t \in \widehat{\mathbb{N}}_0$ denotes the iteration): \mathbb{L}^{t+1} and \mathbb{U}^{t+1}

$$\begin{aligned} l_{ij}^{t+1} &= a_{ij} - \sum_{k=1}^{j-1} l_{ik}^t u_{kj}^t & i \geq j, \\ u_{ij}^{t+1} &= \frac{1}{l_{ii}^t} \left(a_{ij} - \sum_{k=1}^{i-1} l_{ik}^t u_{kj}^t \right) & i < j \end{aligned} \quad (1.14)$$

3. If either $|\mathbb{L}^{t+1} - \mathbb{L}^t|$ or $|\mathbb{U}^{t+1} - \mathbb{U}^t|$ is greater than some tolerance, e.g. 0.001, then go back to step 2.
4. If both differences are smaller than the tolerance, then the algorithm has iteratively converged to an approximate solution of $\mathbb{A} = \mathbb{L}\mathbb{U}$.

On one hand, the number of iterations it takes the algorithm to converge to a solution is not possible to accurately predict and therefore could lead to poor performance if performed sequentially. On the other hand, since \mathbb{L}^{t+1} and \mathbb{U}^{t+1} are calculated independently, the operation can be run in parallel.

Another noteworthy, but unverified, aspect of this method's convergent nature is related to rounding errors. Specifically, since Crout's method is direct, it can be theorized that rounding errors may result in it providing less accurate results compared to its numerical modification. This thought stems from the fact that the numerical method converges and thus - under specific convergence rules - may arrive at a more accurate solution. However, this is purely a hypothesis and remains to be verified.

Joining together the highly parallel nature of CUDA-enabled Nvidia GPUs and such a heavily parallelizable algorithm is the main focus of this project and will be detailed further in the following chapters.

Chapter 2

Implementation TO

This chapter will present the implementation of the *Decomposition* project that was built around the algorithms described in Sections 1.3.1 and 1.3.2. First, the *TNL* library¹ will be introduced briefly as it contains a structure that was paramount to the implementation of this project. Then, the description of the *Decomposition* project itself will follow. Finally, the last section will present how the iterative algorithm, mentioned in Section 1.3.2, was fine-tuned for optimal performance using CUDA.

2.1 TNL Library TO

The Template Numerical Library (TNL) is a collaborative, open-source project licensed under the MIT license. It aims to use modern programming paradigms combined with the computational power of parallel architectures to provide highly performant numerical solvers and simulations. In terms of parallel architectures, TNL supports both multi-core CPUs (using OpenMP²) and GPUs (as of July 2022 only CUDA-enabled Nvidia GPUs with compute capability 9.0 or higher [6]). As TNL is written in C++ (with the exception of some helping Python/Bash scripts) it is designed to benefit from C++ templates and the advantages they bring. For example, the use of template specializations allows for minimal run-time overhead which makes execution of architecture-dependent code simple and fast [7]. Further up-to-date information regarding TNL can be found on the project's website³.

While TNL contains, among others, many different data structures. For the purpose of this project only the one used during development will be introduced.

Dense Matrix As mentioned at the end of Section 1.3.2, the goal of this project is to combine the parallel nature of CUDA-enabled Nvidia GPUs and the heavily parallelizable algorithm described in the same section (labeled as *Iterative Crout method* for the purpose of this project).

Therefore, in order to store all matrices involved in the computation, an efficient, robust and intuitive data structure was required. While in terms of matrices TNL mainly revolves around sparse implementations (i.e. efficiently storing and performing operations with matrices that have more zero than non-zero elements), it also possesses the opposite: *dense matrices*. As the name suggest, dense matrices are matrix

¹TNL Library GitLab repository URL: <https://gitlab.com/twl-project/twl>

²OpenMP website URL: <https://www.openmp.org/>

³TNL project website URL: <https://tnl-project.org/>

structures densely populated with elements. In other words, a dense matrix stores every single element, regardless of its value (zeros and non-zeros are stored). In TNL, the class representing the dense matrix data structure is called `DenseMatrix` and it is located in the `TNL::Matrices` namespace. Similarly to the majority of classes representing matrices in TNL, it inherits from the `Matrix` class; the visualization of inheritance can be found in Figure 2.1.

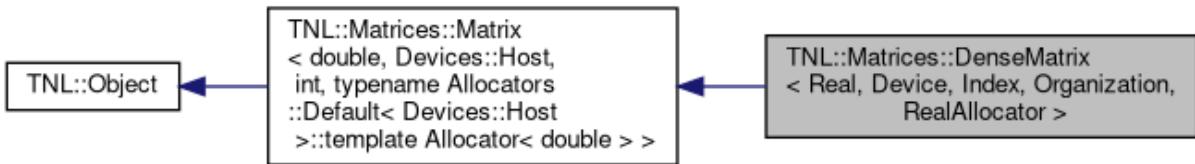


Figure 2.1: Inheritance diagram for the `TNL::Matrices::DenseMatrix` class. Taken from the *Template Numerical Library Documentation* [6].

In the diagram shown in Figure 2.1 the `DenseMatrix` class contains the following template parameters [6]:

- `Real` - Datatype of the matrix's elements, for example, `float` or `double` (default).
- `Device` - Type of device that the matrix structure is stored on. Its value can be either `TNL::Devices::Host` (default) or `TNL::Devices::Cuda`. The former indicates that the structure is stored in host memory, whereas the latter indicates that the data is stored in device memory. Furthermore, this parameter dictates which of the class's methods can be called and what device-dependent code should be executed.
- `Index` - Datatype of the matrix's index, for example, `short`, `int` (default), or `long`.
- `Organization` - Type of matrix element ordering. It can be either `RowMajorOrder` or `ColumnMajorOrder`. The former indicates that the elements of the matrix are stored in row-major order in a `DenseMatrix` instance's 1D array `values`, whereas the latter dictates that the elements are stored in the array in a column-major order. Implicitly, row-major order is used when the structure is allocated on the host and column-major order if it is allocated on the device.
- `RealAllocator` - Allocator for the matrix elements.

The `DenseMatrix` class contains an assortment of methods with varying functionalities - from the initialization of an entire matrix via arrays to per-element lambda functions and CUDA-tailored algorithms. In terms of this project, the most used methods were those that set and get elements, which can be done by using `setElement()` and `getElement()` respectively. Alternatively, for setting and getting elements, `DenseMatrix` possesses the overloaded operator: `operator()`, which allows the developer to write cleaner code that conveys its purpose more clearly. From the perspective of performance, both approaches are congruous as they take the same arguments and compute the index of the element in the instance's 1D array. Nonetheless, there is a difference between the two approaches: `operator()` has the `__cuda_callable__` prefix, which specifies that it can be called from both host functions and CUDA kernels. However, this prefix comes with certain caveats:

- Data allocated on the host can only be accessed by `operator()` from host functions.

- Data allocated on the device can only be accessed by `operator()` from the device, specifically, from CUDA kernels. For example, if an instance of `DenseMatrix` has `Device` set to `TNL::Devices::Cuda` and `operator()` would be used to access data from a host function, then the program would fail.

The limitations above are not present for the other approach (`setElement()` and `getElement()`). In other words, both `setElement()` and `getElement()` can be used from host functions and CUDA kernels, irrespective of where the `DenseMatrix` instance is allocated. However, this convenience has a pitfall: accessing data stored on the other device type. For example, let an instance of `DenseMatrix` be stored in device memory. Then, if it is accessed from a host function using `getElement()`, the procedure will be slow and only the value of the element will be returned. Listing 2.1 shows an example of both approaches - including the caveats and pitfalls.

```

1 #include <iostream>
2 #include <TNL/Matrices/DenseMatrix.h>
3 #include <TNL/Devices/Host.h>
4
5 template< typename Device >
6 void setElements()
7 {
8     // Create an instance of 5x5 DenseMatrix
9     TNL::Matrices::DenseMatrix< double , Device > matrix( 5 , 5 );
10
11    // Set elements of the main diagonal using setElement()
12    for( int i = 0; i < 5; i++ )
13        matrix.setElement( i, i, i );
14
15    // Increment elements of the main diagonal using operator()
16    for( int i = 0; i < 5; i++ )
17        matrix( i, i ) += i;
18 }
19
20 int main( int argc, char* argv[] )
21 {
22     // This example will run without any problems
23     std::cout << "Set elements on host:" << std::endl;
24     setElements< TNL::Devices::Host >();
25
26 #ifdef HAVE_CUDA
27     // This example will fail on the second setting of elements
28     std::cout << "Set elements on CUDA device:" << std::endl;
29     setElements< TNL::Devices::Cuda >();
30 #endif
31 }
```

Listing 2.1: Code example showing the use of `setElement()`, and `operator(); getElement()` and getting a matrix element using `operator()` would be done similarly. The example requires the TNL library to already be installed. As mentioned in the code, the `setElements()` function will run correctly when evoked using the `TNL::Devices::Host` template parameter. However, if the `DenseMatrix` instance is allocated on the device, then the first setting of elements (using `setElement()`) will be slow due to the data transfer between the host and the device - each call will mean a unique data transfer. Furthermore, the second setting of elements (using `operator()`) will fail as `operator()` will be called from a host function on a `DenseMatrix` instance allocated on the device. For the second setter to work, it would need to be called from within a kernel. Taken from section `Tutorials/Matrices/DenseMatrices` in the *Template Numerical Library Documentation* [6].

More detailed information on the structure's implementation can be found under `Namespaces/TNL/Matrices/DenseMatrices` in *Template Numerical Library Documentation* [6] and further examples of usage can be found under `Tutorials/Matrices/DenseMatrices`.

2.2 Decomposition project TO

Even though the `DenseMatrix` class from TNL is used in the Decomposition project - and a select few solvers are already implemented in TNL - it was decided to create a separate repository⁴ in GitLab solely for this rendition of decomposition. Since the project is continually under development it is only available internally, i.e. to users belonging to the TNL group on the Mathematical Modelling Group's⁵ GitLab page⁶.

Although development was done outside of TNL, its structuring and building processes were adopted with minor changes to allow for easier familiarization and to keep the option of incorporating the Decomposition project into TNL open for the future. The compilation/installation of the project is done using the `install` Bash script that was adopted from TNL. The script itself serves as a wrapper for the `build` script that takes several building arguments, for example, the mandatory target parameter allows the user to choose to build one of the following:

- `all` - compile the entire project including all other targets and the algorithm implementations.
- `benchmark` - compile the benchmark only.
- `tests` - compile the unit tests only.

Additionally, the `build` script provides optional parameters that can aid in compilation, for example:

- `-install` - enables installation of the Decomposition project files into `$HOME/.local/include`.
- `-cmake` - allows the user to supply the path to the CMake that is to be used for compilation.

⁴Decomposition GitLab repository URL: <https://mmg-gitlab.fjfi.cvut.cz/gitlab/tnl/lu-decomposition>

⁵MMG main page URL: <https://geraldine.fjfi.cvut.cz/mmg/index.php>

⁶TNL GitLab group URL: <https://mmg-gitlab.fjfi.cvut.cz/gitlab/tnl>

- `-with-cuda-arch` - allows the user to specify the CUDA compute capability version to compile the project with. While there is an auto-detect feature for this parameter, the manual setting can be indispensable in some situations, for example, when running the benchmark on a computational cluster the compilation is usually done beforehand on a node that is not guaranteed to have a CUDA-enabled GPU.

The full list of compilation options (`build` script usage) can be found in Attachment B.

The `build` script then calls CMake⁷ which subsequently takes care of the build process using instructions from `CMakeLists.txt` files interspersed throughout the project.

The Decomposition project was written in *C++* which was extended by *CUDA* (GPU programming) and *GoogleTest*⁸ (unit testing - approach adopted from TNL's matrix unit tests). Additionally, *Python*⁹ and *Bash*¹⁰ were used when adopting scripts from TNL, for example, a python script that creates tables and graphs in HTML from json files generated by the benchmark.

In this section, each part of the project's structure will be briefly described. First, unit tests will be detailed followed by the implementation of the Crout method (introduced in Section 1.3.1), along with the Iterative Crout method (introduced in Section 1.3.2). Finally, the last part focuses on the benchmark implementation that aims to put into perspective the performance differences between the direct and iterative approach.

The ordering of topics follows the development process which was inspired by Test-driven development¹¹ (TDD). Specifically, the unit tests were written first; they were purposefully failing. Then, the implementation of the Crout method, along with the Iterative Crout method followed; this saw the unit tests passing. Finally, the benchmark was added as a feature at the end - without unit tests.

2.2.1 Unit Tests TO

Despite the simplicity of this project - implementation of two short algorithms - quality assurance is still a key factor that aims to minimize erring development. Not counting manual verification of functionalities, unit tests are the most basic form of quality assurance. They allow for continual development with near-instant feedback on any changes in the implementation.

As mentioned before, GoogleTest⁸ was chosen as the testing framework. The main reasons behind this choice were:

- GoogleTest was used successfully to implemented unit tests in TNL.
- GoogleTest has the ability to run tests of a test suite across class instances with different hard-set template parameter values.
- GoogleTest is simple to use and can be easily integrated with the Decomposition project.
- GoogleTest fully supports *C++* and is still actively being developed (roughly at least one merged pull request a week as of July 2022).

⁷CMake website URL: <https://cmake.org/>

⁸GoogleTest GitHub repository URL: <https://github.com/google/googletest>

⁹Python website URL: <https://www.python.org/>

¹⁰Bash website URL: <https://www.gnu.org/software/bash/>

¹¹Test-driven development Wikipedia page URL: https://en.wikipedia.org/wiki/Test-driven_development

As the testing infrastructure was mostly adopted from TNL (detailed in Section 3.1 of the author's bachelor thesis *Formats for storage of sparse matrices on GPU* [42]) it will only be described briefly.

For each algorithm (Crout method and Iterative Crout method) a suite of unit tests was written. The aim of the tests was to verify that a matrix was decomposed within some reasonable error range which was obtained by comparing the decomposition result to either existing solutions or solutions computed by programs, such as MATLAB¹². Examples of tests are:

- `test_CroutMethod2x2MatrixDecompose< MatrixType >()` - Test that the algorithm will decompose a 2x2 matrix correctly. The decomposition of a small matrix is likely to produce its exact solution, thus, tests where a such a matrix is decomposed can have zero tolerance when it comes to checking for errors in computation.
- `test_CroutMethod38x38MatrixDecompose< MatrixType >()` - Test that the algorithm will decompose a 38x38 matrix correctly with some tolerance. The tolerance for solutions is required as the larger the dimensions, the more prone to differences the solutions are. This erring behavior is due to the limited accuracy of double and single precision when compared to, for example, MATLAB.
- `test_CroutMethod10x10DecomposeSingularMatrixShouldFail< MatrixType >()` - Test that the algorithm will fail to decompose a 10x10 singular matrix. The execution of the program will fail as such a matrix cannot be decomposed without a permutation matrix which is not in the scope of this project.

In the examples of tests above, the `MatrixType` template parameter represents an instance of the `DenseMatrix` class from the set of instances which can be seen in Listing 2.2. Additionally, Listing 2.3 shows the implementation of the 2x2 matrix test mentioned above in the list of examples and also in Listing 2.2.

```

1 template< typename Matrix >
2 class ILUCroutMethodTest : public ::testing::Test
3 {
4     protected:
5         using MatrixType = Matrix;
6     };
7
8 using MatrixTypes = ::testing::Types<
9 TNL::Matrices::DenseMatrix< float , TNL::Devices::Host , short >,
10 TNL::Matrices::DenseMatrix< double , TNL::Devices::Host , short >,
11 TNL::Matrices::DenseMatrix< float , TNL::Devices::Host , int >,
12 TNL::Matrices::DenseMatrix< double , TNL::Devices::Host , int >,
13 TNL::Matrices::DenseMatrix< float , TNL::Devices::Host , long >,
14 TNL::Matrices::DenseMatrix< double , TNL::Devices::Host , long >
15 #ifdef HAVE_CUDA
16 ,TNL::Matrices::DenseMatrix< float , TNL::Devices::Cuda , short , TNL::Algorithms::←
17     Segments::RowMajorOrder >,
18 TNL::Matrices::DenseMatrix< double , TNL::Devices::Cuda , short , TNL::Algorithms::←
19     Segments::RowMajorOrder >,
20 TNL::Matrices::DenseMatrix< float , TNL::Devices::Cuda , int , TNL::Algorithms::←
21     Segments::RowMajorOrder >,
22 TNL::Matrices::DenseMatrix< double , TNL::Devices::Cuda , int , TNL::Algorithms::←
23     Segments::RowMajorOrder >,
```

¹²MATLAB website URL: <https://www.mathworks.com/products/matlab.html>

```

20 TNL::Matrices::DenseMatrix< float , TNL::Devices::Cuda , long , TNL::Algorithms::←
    Segments::RowMajorOrder >,
21 TNL::Matrices::DenseMatrix< double , TNL::Devices::Cuda , long , TNL::Algorithms::←
    Segments::RowMajorOrder >
22 #endif
23 >;
24
25 TYPED_TEST_SUITE( ILUCroutMethodTest , MatrixTypes );
26
27 TYPED_TEST( ILUCroutMethodTest , croutMethod2x2MatrixDecomposeTest )
28 {
29     using MatrixType = typename TestFixture::MatrixType;
30     test_CroutMethod2x2MatrixDecompose< MatrixType >();
31 }

```

Listing 2.2: Implementation of the set of `DenseMatrix` instances and one test using GoogleTest. The unit tests are all run for each instance. The test suite is tied to the set of instances using `TYPED_TEST_SUITE` and each test is added to the test suite using the declaration `TYPED_TEST`. Taken from the Decomposition project repository on GitLab⁴.

```

1 template< typename Matrix >
2 void test_CroutMethod2x2MatrixDecompose()
3 {
4     const Matrix A( {
5         { 4, 24 },
6         { 2, 15 }
7     } );
8
9     Matrix L, U;
10    L.setLike( A );
11    U.setLike( A );
12
13    Decomposition::LU::CroutMethodIterative::decompose( A, L, U );
14
15    EXPECT_EQ( L.getElement( 0, 0 ), 4.0 );
16    EXPECT_EQ( L.getElement( 0, 1 ), 0.0 );
17    EXPECT_EQ( L.getElement( 1, 0 ), 2.0 );
18    EXPECT_EQ( L.getElement( 1, 1 ), 3.0 );
19
20    EXPECT_EQ( U.getElement( 0, 0 ), 1.0 );
21    EXPECT_EQ( U.getElement( 0, 1 ), 6.0 );
22    EXPECT_EQ( U.getElement( 1, 0 ), 0.0 );
23    EXPECT_EQ( U.getElement( 1, 1 ), 1.0 );
24 }

```

Listing 2.3: Implementation of the test where a 2x2 `DenseMatrix` instance is decomposed. As mentioned before, the matrix decomposed in this test is small and therefore the decomposed \mathbb{L} and \mathbb{U} matrices are expected to be exact solutions rather than within some range of the exact solution. Taken from the Decomposition project repository on GitLab⁴.

Since the unit tests are run with every compilation of the algorithms they had to be lightweight. Thus, matrix dimensions of tested matrices ranged from 2x2 to only 38x38 and included the following: 2x2, 3x3, 4x4, 10x10, 19x19 and 38x38. The larger dimensions - from 10x10 - were chosen to test a specific part of the Iterative Crout method's implementation on the GPU: matrix convergence by sections (detailed in Section 2.2.2).

2.2.2 LU Decomposition TO

The core of the Decomposition project is made up of the Crout method and the Iterative Crout method, detailed in Section 1.3.1 and Section 1.3.2 respectively. This part contains a description of their implementations. First, it is necessary to introduce a memory-saving concept used in this project. Then, the requirements for the implementations will be presented and, finally, the description of the implementations of the individual algorithms will follow.

Memory-saving concept Whenever LU decomposition was mentioned in the previous chapters and sections, it was presented as decomposing matrix \mathbb{A} into matrices \mathbb{L} and \mathbb{U} . However, since `DenseMatrix` stores every element of a matrix and the upper triangle of \mathbb{L} and the lower triangle of \mathbb{U} are zeros, then only half of the elements stored in the two matrices are used during decomposition. Therefore, to avoid using memory unnecessarily, another approach was used in alongside the original: store \mathbb{L} and \mathbb{U} into a single matrix \mathbb{Z} . The lower triangle of matrix \mathbb{Z} (including the main diagonal) would house the elements of \mathbb{L} and the upper triangle (excluding the 1s on the main diagonal) would be made up of elements from \mathbb{U} .

While this approach uses less memory, it has some drawbacks:

- it is not aligned with the convention of LU decomposition to return two matrices; and
- it does not store the 1s found on the main diagonal of \mathbb{U} .

Thus, in order for the decomposed solution to be used it may be required to extract matrices \mathbb{L} and \mathbb{U} from matrix \mathbb{Z} - this step is not implemented in the Decomposition project currently and is up to the user to handle it for now.

Nevertheless, to save memory, in this project every decomposing method is written in two variants:

1. Decompose matrix \mathbb{A} into matrices \mathbb{L} and \mathbb{U} .
2. Decompose matrix \mathbb{A} into matrix \mathbb{Z} which contains elements of \mathbb{L} and \mathbb{U} - except for their zero-filled triangles and the main diagonal of \mathbb{U} .

Implementation requirements To put the algorithms mentioned earlier into context of the project's tasks, the tasks requiring some sort of implementation were the following:

1. Implement a parallel version of LU decomposition in CUDA for GPUs.
2. Measure the acceleration of the GPU version of the LU decomposition against the CPU version.

In other words, this means implementing the following:

1. Crout method for the CPU detailed in Section 1.3.1.
2. Iterative Crout method for the GPU detailed in Section 1.3.2.

As mentioned at the beginning of this Section, the process of development was inspired by TDD. Thus, once unit tests were implemented and successfully failing, the implementation of the algorithms began.

Crout method The Crout method - as described in Section 1.3.1 - was implemented only for the CPU as implementing it on the GPU would not bring any interesting results since it is a sequential algorithm. Since the implementation of the Crout method in the Decomposition project differs slightly from the pseudo-code shown in Listing 1.12, the code is shown only in Attachment C.

One of the noticeable differences between the pseudo-code from Listing 1.12 and the implementations is that the lines where the elements on the main diagonal of \mathbb{U} are all set to 1s are not present in the latter. They were removed as it was observed that they were not needed since the algorithm would compute them regardless.

Iterative Crout method According to the requirements mentioned above, the Iterative Crout method was to be implemented only on the GPU, however, in order to verify the correctness of the results its first version was also implemented on the CPU.

The CPU version served purely as a means to verify that the GPU version did not exhibit unexpected behaviors due to parallelism, for example, race conditions. In this instance, a race condition refers to a scenario where one thread would overwrite a value before another thread would read the old value. After a brief comparison of results produced by the CPU and GPU versions on a set of matrices no differences were found. Thus, even though originally it was planned for the CPU version to mirror the GPU version and have it continually verify the results, this approach was abandoned due to the large computational time required for the CPU version to complete. In summary, the CPU version only mirrors the initial GPU version and was not developed further.

The GPU version of the Iterative Crout method went through various optimizations during development - the different concepts are detailed in Section 2.3. This section will only present the latest - and for now final - GPU version that uses matrix \mathbb{Z} .

The GPU implementation can be split into two parts:

1. Convergence by sections.
2. Convergence of a single section using the Iterative Crout method detailed in Section 1.3.2.

Convergence by sections This part leverages advantages from both the sequential and parallel versions of the Crout method in order to optimize the entire procedure.

Similarly to the Iterative algorithm detailed in Section 1.3.2, the *convergence by sections* concept begins by providing an initial estimate of matrix \mathbb{Z} , for example, $\mathbb{Z} = \mathbb{A}$. Then, \mathbb{Z} is divided into equally-sized sub-matrices (in this project, the sub-matrices are called *sections* and are labeled with $_{sub}$, for example, \mathbb{Z}_{sub}). Then, beginning in the top-left corner, the sections are sequentially converged (equivalent to a sub-matrix being decomposed) using the Iterative Crout method algorithm described in Section 1.3.2. The order in which sections are converged is crucial to achieving near-optimal execution times; it is shown in Figure 2.2.

The order of convergence of sections is derived from the fact that a single element in \mathbb{Z} , for example, z_{ij} (where $i, j \in \widehat{n}$), is computed using only some elements above and to the left of it. Specifically, only $2x$ (where $x = \min(i, j)$) elements will be used, i.e. in row i only columns $[0, x]$ and in column j only rows $[0, x]$. This means that the quality of an element's value greatly depends on the quality of the elements used to compute it (quality refers to how close an element is to its final (converged) value in a given iteration). The visualization of what elements are used to compute a single element z_{ij} is shown in Figure 2.3.

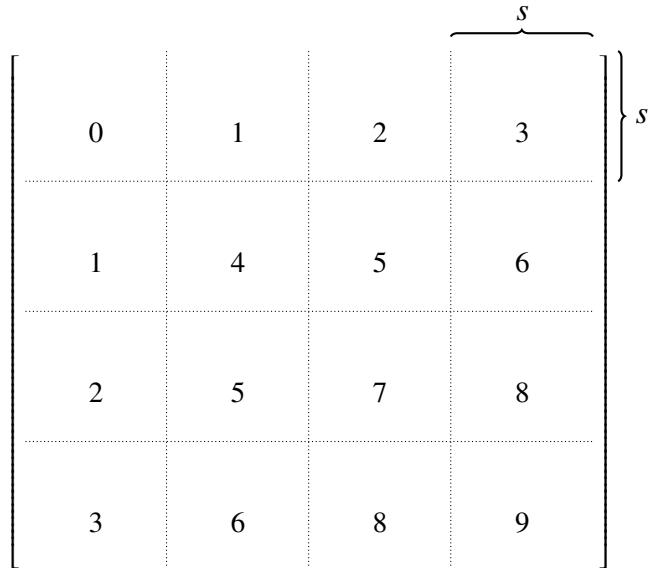


Figure 2.2: Visualization of matrix \mathbb{Z} divided into sections of size $s \times s$. The order in which sections are converged is denoted by the number in each section. First, the upper-left-most section (section '0') is converged, then, the sections below and to the right of it (sections labeled with a '1') are converged in parallel. Then, certain sections to the right and below of each section '1' (sections labeled with '2') are converged in parallel etc.

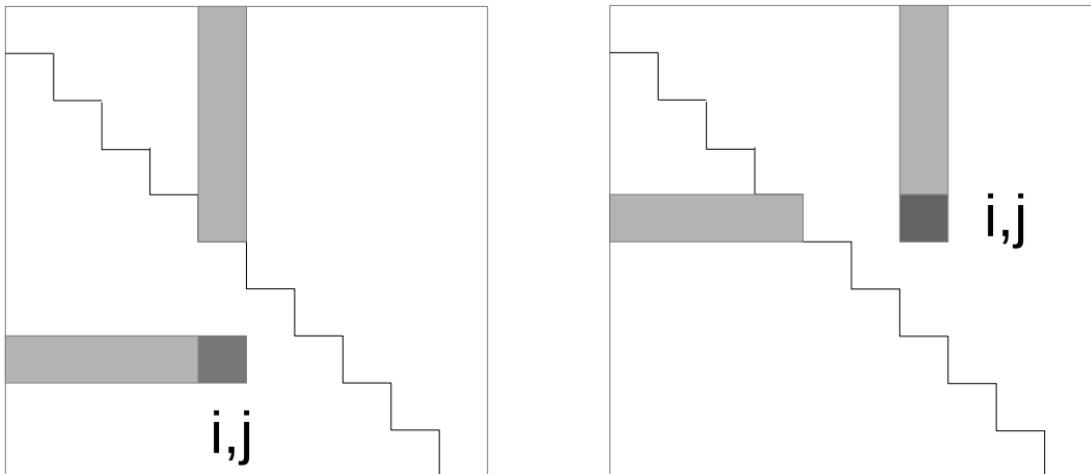


Figure 2.3: Examples showing the elements used (shaded regions) to calculate an element at row i and column j (dark square). As described earlier, only elements with indices in the interval $[0, \min(i, j)]$ are used in the element's row and column. Taken from E. Chow's and A. Patel's *Fine-Grained Parallel Incomplete LU Factorization* [5].

The implementation of the Iterative Crout method for the GPU using matrix \mathbb{Z} is shown in Listing 2.4. The listing does not contain the decomposition kernel itself as it is shown later in Listing 2.5 in *Convergence of a single section*.

```

1 template< typename Matrix1, typename Matrix2 >
2 void CroutMethodIterative::decompose( Matrix1& A, Matrix2& Z )

```

```

3 {
4     using Real    = typename Matrix1::RealType;
5     using Device  = typename Matrix1::DeviceType;
6     using Index   = typename Matrix1::IndexType;
7
8     Index num_rows = A.getRows();
9     Index num_cols = A.getColumns();
10
11    Matrix2 Znew;
12    Znew.setLike( Z );
13    Z = A;
14    bool converged = true;
15    Real tolerance = 0;
16
17    // Compute the size of a section
18    Index sectionSize = min( max( num_cols / 10, (Index)256 ), (Index)1024 );
19    sectionSize = ( sectionSize + BLOCK_SIZE - 1 ) / BLOCK_SIZE * BLOCK_SIZE;
20
21    // Determine the number of blocks based on the section size
22    Index blocks = sectionSize / BLOCK_SIZE;
23    dim3 threadsPerBlock( BLOCK_SIZE, BLOCK_SIZE );
24    dim3 blocksPerGrid( blocks, blocks );
25
26    // Copy required data to the GPU
27    Matrix1* matrixA_kernel      = TNL::Cuda::passToDevice( A );
28    Matrix2* matrixZ_kernel      = TNL::Cuda::passToDevice( Z );
29    Matrix2* matrixZnew_kernel   = TNL::Cuda::passToDevice( Znew );
30    bool*   converged_kernel     = TNL::Cuda::passToDevice( converged );
31    Real*   tolerance_kernel    = TNL::Cuda::passToDevice( tolerance );
32
33    // Initialize the converged switch to page-locked host memory
34    bool* converged_host = NULL;
35    cudaMallocHost( (void **) &converged_host, sizeof(bool) );
36
37    // Allocate and initialize an array of 2 stream handles
38    int nstreams = 2;
39    cudaStream_t *streams = (cudaStream_t *)malloc(nstreams * sizeof(cudaStream_t));
40    for (int i = 0; i < nstreams; i++) {
41        cudaStreamCreate(&(streams[i]));
42    }
43
44    // Initialize variables for keeping track of where the main diagonal section ←
45    // begins and ends
46    Index diag_start, diag_end, sStart, sEnd;
47
48    // Converge by sections
49    for( diag_start = 0, diag_end = min( num_cols, sectionSize ); diag_start < ←
50        diag_end; diag_start += sectionSize, diag_end = min( num_cols, diag_end + ←
51        sectionSize ) ) {
52        // Converge the diagonal section first using the Default stream
53        do {
54            *converged_host = true;
55            cudaMemcpy( converged_kernel, converged_host, sizeof(bool), ←
56                      cudaMemcpyHostToDevice );
57
58            DecomposeKernel< Real, Index ><<< blocksPerGrid, threadsPerBlock >>>( ←
59                matrixA_kernel, matrixZ_kernel, matrixZnew_kernel, diag_start, diag_end, ←
60                diag_start, diag_end, tolerance_kernel, converged_kernel );

```

```

55 // Synchronize after execution of kernel before copying value of converged
56 cudaDeviceSynchronize();
57 cudaMemcpy( converged_host, converged_kernel, sizeof(bool), ←
58     cudaMemcpyDeviceToHost );
59 } while( !*converged_host );

60
61 // Converge sections below and to the right of the main diagonal section using←
62 // the two streams
63 for( sStart = diag_end, sEnd = min( num_cols, diag_end + sectionSize ); sStart<←
64     < sEnd; sStart += sectionSize, sEnd = min( num_cols, sEnd + sectionSize ←
65 ) ) {
66 do {
67     *converged_host = true;
68     cudaMemcpy( converged_kernel, converged_host, sizeof(bool), ←
69         cudaMemcpyHostToDevice );
70
71     // Run Stream 1: iterate columns - rows should stay the same
72     DecomposeKernel< Real, Index ><<< blocksPerGrid, threadsPerBlock, 0, ←
73         streams[0] >>>( matrixA_kernel, matrixZ_kernel, matrixZnew_kernel, ←
74             sStart, sEnd, diag_start, diag_end, tolerance_kernel, converged_kernel←
75         );
76
77     // Run Stream 2: iterate rows - columns should stay the same
78     DecomposeKernel< Real, Index ><<< blocksPerGrid, threadsPerBlock, 0, ←
79         streams[1] >>>( matrixA_kernel, matrixZ_kernel, matrixZnew_kernel, ←
80             diag_start, diag_end, sStart, sEnd, tolerance_kernel, converged_kernel←
81         );
82
83     // Synchronize after execution of kernels before copying value of ←
84     // converged
85     cudaDeviceSynchronize();
86     cudaMemcpy( converged_host, converged_kernel, sizeof(bool), ←
87         cudaMemcpyDeviceToHost );
88 } while( !*converged_host );
89 }
90

```

Listing 2.4: GPU implementation of the Iterative Crout method. Some code has been omitted as it is not important for the description, for example, checking if the input matrix is square. Overall, the code performs the following: initialization of variables (including CUDA grid specifications, page-locked host memory, streams, etc.), then the entire matrix \mathbb{A} is decomposed using the *Convergence by sections* concept. The constant `BLOCK_SIZE` dictates how many threads are present in a single thread block. The `converged_host` variable is purposefully initialized using page-locked host memory as its value is copied between the host and device in every iteration of the do-while loop. Thus, as described in *Page-locked host memory* in Section 1.2.3, the higher bandwidth provided can help reduce the overall time spent copying during computation. Taken from the Decomposition project repository on GitLab⁴.

One of the first performance-determining aspects shown in Listing 2.4 is the size of a section (`sectionSize` or s). It affects both the speed of computation and the accuracy of results (detailed further in Chapter 3). Specifically, the phrase "*accuracy of results*" refers to how much the matrix resulting from $\mathbb{L} \cdot \mathbb{U}$ differs from the original input matrix \mathbb{A} . How the size of a section is calculated changed many times throughout development. Initially, the size of a section is set to 1/10 of the dimensions of \mathbb{Z} , however, this value must be within the interval [256, 1024]. If it is outside of this interval, then the size is set to the interval's

closest endpoint (256 or 1024). Then, its value is rounded to the nearest multiple of `BLOCK_SIZE` (8, 16, or 32) that is larger than the original `sectionSize` due to CUDA-related reasons described later in *Convergence of a single section*.

In Figure 2.2 it can be seen that some sections are converged in parallel. In general, a section can be converged optimally only if specific sections above and to the left of it are already converged. The specific sections that the to-be-converged section depends are the same as the elements required to converge a specific element quickly. In order to imagine this better, the dark square in Figure 2.3 can be considered as the to-be-converged section and the shaded regions can be considered as the sections that must be converged before it. It is noteworthy that the general concept - how a section can be converged optimally - allows for more than 2 sections can be converging simultaneously. This and any other potential performance improvements are detailed in Section 2.3.

As can be seen in Listing 2.4 each section is converged using a decomposition kernel. Since each kernel is launched on a grid of blocks that are made up of threads, then each section is converged using a grid. Thus, in order to facilitate parallel convergence of sections, CUDA streams (detailed in Section 1.2.4) were used. Specifically, sections that encompass the main diagonal (main diagonal sections) are converged using the default stream and sections converged in parallel were each given a separate stream, i.e. two streams are created and each is used to converge one of the parallel sections. For example - using the numbering of sections from Figure 2.2 - first, section '0' is converged using the default stream. Then, sections labeled with a '1' are converged - each using a different stream. Following that, sections labeled with a '2' are converged - each using a different stream - and so on until sections labeled with a '3'. Then section '4' is converged, again using the default stream.

In summary, converging the input matrix by sections is faster than converging all of it at once since its elements - especially those in the lower-right corner - will have higher quality elements available for the computation of their value. For example, let z_{ij} (located in the lower-right corner of \mathbb{Z}) be the currently computed element. If the entire matrix \mathbb{Z} is being converged at once and if it is a large matrix, then, since elements in the first few rows and columns (excluding the 1st row and column as their values are taken directly from \mathbb{A} and not altered further) are highly inaccurate they will cooperatively produce even less accurate elements in the later rows and columns - a snowball effect of low quality elements. Thus, during the first few iterations z_{ij} will be calculated using low quality elements and it will be far from its final converged value. Slowly, through multiple iterations the quality of elements will increase row-by-row and column-by-column which will in turn slowly converge z_{ij} . Thus, when converging the entire matrix simultaneously, computing elements found further in the matrix (elements near and in the lower-right corner of the matrix) is a waste of resources and time. Ultimately, this makes convergence by sections more optimal.

Convergence of a single section While the previous part detailed how an entire matrix is converged by sections, this part describes how a single section is converged. A single section denotes a $s \times s$ sub-matrix of matrix \mathbb{Z} that is labeled \mathbb{Z}_{sub} . Since the sub-matrix (section) is not being decomposed itself as a matrix, rather this part of matrix \mathbb{Z} is being decomposed, then, the phrase "*single section is converged*" is befitting. In technical terms this means providing a series of inputs (sub-matrices, indexes, tolerance values, etc.) to a kernel that is executed on the device. First, for the explanation of the decomposition kernel, it is necessary to slightly alter the algorithm from Section 1.3.2 - using matrix \mathbb{Z} instead of \mathbb{L} and \mathbb{U} - to the perspective of a section:

- Given input matrices \mathbb{A} and \mathbb{Z}^t calculate the next iteration of a specific sub-matrix: \mathbb{Z}_{sub}^{t+1} :

$$\begin{aligned} z_{ij}^{t+1} &= a_{ij} - \sum_{k=1}^{j-1} z_{ik}^t z_{kj}^t & i \geq j, \\ z_{ij}^{t+1} &= \frac{1}{z_{ii}^t} \left(z_{ij} - \sum_{k=1}^{i-1} z_{ik}^t z_{kj}^t \right) & i < j. \end{aligned} \tag{2.1}$$

- Check if the section has converged according to the tolerance rule: $|\mathbb{Z}_{sub}^{t+1} - \mathbb{Z}_{sub}^t| > tol$ (where tol is some hard-set value, for example, 0.0001). If the tolerance rule has not passed, then go back to step 2.
- If the tolerance rule has passed, then the algorithm has arrived to an approximate solution of a sub-matrix in LU (stored in \mathbb{Z}).

Note that the value of the tol parameter is another important factor that determines the performance (speed of execution and accuracy of results). If the value of the parameter is too high, for example, 1.5 then the algorithm will converge faster, however, the matrix resulting from LU will differ more significantly from \mathbb{A} , i.e. the decomposition will be inaccurate. On the other hand, the closer the tolerance value is to zero, the more accurate the results will be, however, it will take longer for the algorithm to converge. This parameter went through many changes, before finally settling to 0.0. The reasons behind this decision were the following:

- *Convergence by sections* allows for greater granularity as the quality of each $s \times s$ section depends on the quality of specific sections that were converged before it. Thus, setting the tolerance parameter to zero means that the elements of a section are computed using elements that are as accurate as possible.
- Testing the solution on a set of matrices that comprised of 61 sparse, dense, small and large matrices revealed that the difference in performance when setting the tolerance value near zero (for example, 0.0001) and just zero was negligible. However, the accuracy of results when $tol = 0.0$ was significantly higher - detailed further in Section 2.3 and Chapter 3.
- The testing further revealed that the accuracy of results can decrease if the dimensions of the input matrix increase. Thus, it was decided that even though speed of convergence is important, it loses meaning if the produced results are unusable.

The implementation of the decomposition kernel using matrix \mathbb{Z} is shown in Listing 2.5.

```

1 template< typename Real, typename Index, typename Matrix1, typename Matrix2 >
2 __global__ void DecomposeKernel( const Matrix1* _A, Matrix2* _Z, Matrix2* _Znew, ←
3   const Index col_sStart, const Index col_sEnd, const Index row_sStart, const ←
4   Index row_sEnd, const Real* tolerance, bool* converged )
5 {
6   auto& A = *_A; auto& Z = *_Z; auto& Znew = *_Znew;
7   // Get a thread's sub-matrix ID that is offset to become a global ID of Z
8   Index row = blockIdx.y * blockDim.y + threadIdx.y + row_sStart;

```

```

8 Index col = blockIdx.x * blockDim.x + threadIdx.x + col_sStart;
9
10 Index tx = threadIdx.x;
11 Index ty = threadIdx.y;
12 Real sum = 0;
13
14 // Set overreaching thread ID to the closest edge of the matrix's dimensions
15 Index max_col = col_sEnd - 1;
16 Index max_row = row_sEnd - 1;
17 Index new_row = min( row, max_row );
18 Index new_col = min( col, max_col );
19
20 // Get the smallest index of the thread's element and offset it by BLOCK_SIZE ←
21 // preparation for the use of shared memory
22 Index min_row_col = min( new_row, new_col ) - BLOCK_SIZE;
23
24 // Initialize shared memory
25 __shared__ Real ZsLower[BLOCK_SIZE][BLOCK_SIZE];
26 __shared__ Real ZsUpper[BLOCK_SIZE][BLOCK_SIZE];
27
28 Index i, k;
29
30 // Compute the sum needed for element (row, col) by loading blocks of elements ←
31 // from global to shared memory and multiplying them
32 for ( i = 0; i <= min_row_col; i += BLOCK_SIZE ) {
33     ZsLower[ty][tx] = Z( new_row, i + tx );
34     ZsUpper[ty][tx] = Z( i + ty, new_col );
35
36     __syncthreads();
37
38 #pragma unroll
39     for( k = 0; k < BLOCK_SIZE; ++k ) {
40         sum += ZsLower[ty][k] * ZsUpper[k][tx];
41     }
42     __syncthreads();
43 }
44
45 // Loop unrolling means looping by multiples of BLOCK_SIZE
46 // If the number of remaining elements is less than BLOCK_SIZE, then compute ←
47 // them separately
48 ZsLower[ty][tx] = Z( new_row, min( i + tx, max_col ) );
49 ZsUpper[ty][tx] = Z( min( i + ty, max_row ), new_col );
50 __syncthreads();
51 Index t_to_use = row >= col ? tx : ty;
52 for( k = 0; k < t_to_use; ++k ) {
53     sum += ZsLower[ty][k] * ZsUpper[k][tx];
54 }
55
56 // Terminate threads whose ID reaches out of matrix dimensions
57 if( row >= row_sEnd || col >= col_sEnd ) {
58     return;
59 }
60
61 // Compute the value of element (row, col) in the new iteration
62 if( row >= col ) {
63     Znew( row, col ) = A( row, col ) - sum;
64 } else {
65     if( Z( row, row ) == 0 ) {

```

```

63     printf( "Key element: %f\t(row:%d, col:%d)\n", Z( row, row ), (int)row, (int)col );
64     assert( Z( row, row ) != 0 );
65 }
66 Znew( row, col ) = ( A( row, col ) - sum ) / Z( row, row );
67 }
68
69 // Check if the element (row, col) has converged
70 if( abs( Znew( row, col ) - Z( row, col ) ) > *tolerance ) {
71     *converged = false;
72 }
73
74 // Assign element for this iteration
75 Z( row, col ) = Znew( row, col );
76 }

```

Listing 2.5: The constant `BLOCK_SIZE` is by default hard-coded to be equal to 8 in the `CroutMethodIterative` header file using the `#define` macro. The kernel takes matrices \mathbb{A} , \mathbb{Z} (iteration t of \mathbb{Z}), and \mathbb{Z}_{new} (iteration $t + 1$ of \mathbb{Z}) as input parameters, and uses other input variables to offset the threads in the grid so that only a specific section of \mathbb{Z} is computed. Note that the kernel is not part of the `CroutMethodIterative` class since kernels cannot be members of a class - as mentioned in *Function extensions* in Section 1.2.5 - however, it is located in the same file that it is called from. Taken from the Decomposition project repository on GitLab⁴.

The kernel presented in Listing 2.5 has the following input parameters:

- `col_sStart` - Starting column index of the section in matrix \mathbb{Z} .
- `col_sEnd` - Ending column index of the section in matrix \mathbb{Z} .
- `row_sStart` - Starting row index of the section in matrix \mathbb{Z} .
- `row_sEnd` - Ending row index of the section in matrix \mathbb{Z} .
- `tolerance` - Tolerance parameter stored in global memory of the device. All threads only need to read it in order to check the tolerance rule for their element.
- `converged` - Boolean switch stored in global memory of the device that determined whether element `(row, col)` has converged. At the end of the kernel, each thread evaluates whether its element has converged according to the convergence rule described above. While it is generally considered bad practice for multiple threads to write to a single address in memory, in this instance, it is befitting. The reasoning is that for the algorithm to perform another iteration, only one thread needs to set `converged = false`. As long as the value of `converged` is copied from the device to the host after all threads have finished executing the kernel, then the intended behavior occurs. This is assured using the `cudaDeviceSynchronize()` function used in lines 57 and 74 in Listing 2.4 as explained in *Explicit synchronization* in Section 1.2.4.

From the parameters listed above, the first four are used to determine where in matrix \mathbb{Z} the thread's element is located. Together, the threads then converge the elements of the intended section. The remaining input parameters are specifically prefixed with a `_` as they are not used, instead, pointers to their memory address are initialized in such a way that allows for clean use of the overloaded `operator()` which

is detailed *Dense Matrix* in Section 2.1.

Furthermore, other than the input parameters and CUDA-related extensions detailed *Inter-kernel extensions* in Section 1.2.5 the kernel also has access to the macro-defined `BLOCK_SIZE` variable. The `BLOCK_SIZE` constant is set using the `#define` macro to make the compiler unroll the `for` loop during compile time using `#pragma unroll`. Loop unrolling is a compiler optimization that reduces the work done by the processing thread. Specifically, it removes the need for the processing thread to initialize the loop variable, evaluate the condition and increment the variable [4]. However, if the number of loops in a `for` loop is now known during compile time, then the loop cannot be unrolled. An example showing loop unrolling is shown in Listing 2.6.

```

1 // Hard-set constant - value is known by the compiler at compile time
2 #define BLOCK_SIZE 8
3
4 // Original for loop
5 for( k = 0; k < BLOCK_SIZE; ++k ) {
6     sum += ZsLower[ty][k] * ZsUpper[k][tx];
7 }
8
9 // For loop transformed using loop unrolling during compilation
10 sum += ZsLower[ty][0] * ZsUpper[0][tx];
11 sum += ZsLower[ty][1] * ZsUpper[1][tx];
12 sum += ZsLower[ty][2] * ZsUpper[2][tx];
13 sum += ZsLower[ty][3] * ZsUpper[3][tx];
14 sum += ZsLower[ty][4] * ZsUpper[4][tx];
15 sum += ZsLower[ty][5] * ZsUpper[5][tx];
16 sum += ZsLower[ty][6] * ZsUpper[6][tx];
17 sum += ZsLower[ty][7] * ZsUpper[7][tx];

```

Listing 2.6: Example demonstrating loop unrolling. In this specific case, if loop unrolling is used, then the processor will not have to: initialize `k`, evaluate `k < BLOCK_SIZE` nine times and increment `k` eight times. If `BLOCK_SIZE` would be obtained as an input parameter, then the loop would not be unrolled as the input parameter is not known during compile time. Taken from *Embedded Computing for High Performance* [4].

Another important aspect of the implementation lies at the core of the kernel: use of shared memory. Since each section is assigned a grid made up of blocks, then each block has limited shared memory available to it as described in *Shared memory* in Section 1.2.3. Overall, shared memory is used exactly as described in the matrix multiplication *Example with shared memory* in Section 1.2.6 with an exception. In the example - depicted in Figure 1.16 - the blocks loop through the entire matrix. As explained earlier in *Convergence by sections* in Section 2.2.2 and shown in Figure 2.3 using all elements in the row and column of an element is not required. Thus, in this implementation, the thread block finishes looping once the last required block of elements is used for the computation. However, this presented an obstacle if loop unrolling is used as it was on line 105 in the example code attached in Listing A.1 of Attachment A. The obstacle is that once the thread block arrives to the last block of elements required for the computation, it must stop at specific elements, i.e. each thread needed to stop at a different element. In other words, the number of loops required for each thread in the last block of elements is not known at compile time. This means that loop unrolling is not possible for the last block of required elements and it can only be performed for the blocks before. For this purpose the variable `min_row_col` is offset by `BLOCK_SIZE` to make the loop using loop unrolling end sooner. The remaining elements are then computed using a regular `for` loop (lines 43 - 51 in Listing 2.5).

As detailed in *Shared memory* in Section 1.2.3 when using shared memory, it is important to avoid a

bank conflict. In the kernel shown in Listing 2.5 shared memory is read from only on lines 38 and 50. Specifically, in the multiplication operation `ZsLower[ty][k] * ZsUpper[k][tx]` shared memory is being read from in two different ways (also detailed in *Shared memory* in Section 1.2.3):

- `ZsLower[ty][k]` - All threads in a warp have the same `ty` id. This means that for a given `k` all threads of a warp access the same location in shared memory - known as a *Broadcast* - which is a fast data-serving strategy.
- `ZsUpper[k][tx]` - Each thread in a warp has a unique and linearly increasing `tx`. This means that for a given `k` each thread of a warp accesses one word in a different bank. In other words, a single word is requested from each bank by a unique thread, thus, all 32 threads of a warp are served by all 32 banks simultaneously and expeditiously.

In *Convergence by sections*, it was mentioned that the size of a section must be a multiple of `BLOCK_SIZE`. Although `sectionSize` is not used directly in the kernel, the use of shared memory needed to be explained in order to present the reasoning for this limitation. Lines 53 - 56 in Listing 2.5 show that any threads whose shifted global ID overreaches the matrix dimensions are terminated. In a typical CUDA kernel, this step would be performed near the beginning of the kernel. However, in this case, the threads that overreach are needed for loading data from global to shared memory. For example, looking at Figure 1.16, if the matrix dimensions were not a multiple of `BLOCK_SIZE` and the blocks computing the last columns were partly outside of matrix dimensions, then the of right-most threads of the upper block (matrix \mathbb{B}) would reach out of matrix dimensions and they should - under normal circumstances - be terminated to avoid erroneous behavior. However, the same threads are concurrently being used to load data from global to shared memory in the left block (matrix \mathbb{A}) - there the threads would not reach out of bounds. For this reason, the threads cannot be terminated when computing the sum and that is also the reason why their cut global ID is used during calculation. The threads mentioned compute sums identical to the threads whose global ID is on the edge of the matrix's dimensions. Then, the values computed by the cut threads is discarded once they are terminated. Thus, if `sectionSize` is not a multiple of `BLOCK_SIZE`, then loop unrolling would not be possible as the block of elements loaded into shared memory would not cover the entire section.

2.2.3 Benchmark TO

As mentioned in *Implementation requirements* in Section 2.2.2 one of the goals of this project was to measure the acceleration of the GPU version of the LU decomposition against the CPU version. For this purpose a benchmark system was implemented. In its majority, the structuring and code was adopted from the SpMV TNL Benchmark structure¹³ which was implemented by one of the main developers for TNL, Ph.D. student Jakub Klinkovský. However, some logic was reworked specifically for this project. The benchmarking procedure is initiated from a Bash script¹⁴ and it involves running the entire benchmark six times. Specifically, for each precision (single or double) it is run three times - each with a different number of threads per block: 8, 16, or 32; i.e. blocks of 8×8 , 16×16 , or 32×32 threads. More threads per block are not possible since the maximum numbers of threads per block is 1024 - detailed in

¹³TNL SpMV Benchmark GitLab repository URL: <https://gitlab.com/tnl-project/tnl/-/tree/main/src/Benchmarks/SpMV>

¹⁴Benchmark script URL in the Decomposition GitLab repository: <https://mmg-gitlab.fjfi.cvut.cz/gitlab/tnl/lu-decomposition/-/blob/master/src/Benchmark/scripts/run-decomposition-benchmark>

Block in Section 1.2.2. While the "threads-per-block" part of the benchmark was initially added to determine the optimal number of threads per block, it was never apparent from any benchmark run which value is optimal, therefore, it was kept for future development. Each run of the benchmark involves decomposing a set of matrices; each matrix is stored in an `.mtx` file. Specifically, the subroutine for benchmarking a matrix is as follows (assuming the `precision` and `threads-squared-per-block` arguments are set):

1. Load the matrix from its `.mtx` file using the `MatrixReader` class implemented in TNL¹⁵ to an instance of `DenseMatrix`.
2. Compute the decomposition using the CPU implementation of the Crout method described in *Crout method* in Section 2.2.2 and, if specified, compute the maximum difference of $|A - LU|$. Then, log statistics such as execution time, bandwidth achieved, maximum difference, etc. into the log file.
3. Compute the decomposition using the GPU implementation of the Iterative Crout method described in *Iterative Crout method* in Section 2.2.2 and, if specified, compute the maximum difference of $|A - LU|$. Then, log statistics such as execution time, bandwidth achieved, maximum difference, etc. into the log file.

Additionally, the log file can be transformed into an HTML table and data such as bandwidth and relative speedup can be plotted into graphs using a convenient Python script¹⁶ - originally adopted from TNL and later modified.

As mentioned in Section 3.2 of the author's bachelor thesis *Formats for storage of sparse matrices on GPU* [42], benchmarks can be used to identify issues missed by unit tests. This claim persisted during the development of this project as some matrices were too large to be stored using `DenseMatrix` on the GPU. Furthermore, the benchmark implementation played a crucial role when optimizing the solution.

2.3 Optimization TO

In the preceding sections, it was mentioned that the *Decomposition* project went through various optimizations during development. This section aims to summarize the evolution of the GPU LU decomposition implementation from its initial naive version to its present form. Additionally, a selection of concepts that were attempted, but ultimately ended up being sub-optimal will also be described. The performance of each change was measured by running the benchmark on a set of 50 sparse and dense matrices with varying dimensions between 27×27 and 10581×10581 . This section will not present specific results (execution time, bandwidth, etc.), nor will some of the matrices will be presented or described in greater detail; that will be shown in Chapter 3.

Initial naive implementation The initial naive implementation was designed in such a manner where the entire matrix was decomposed by a single CUDA grid. In other words, each thread would compute

¹⁵ `MatrixReader` class header file in the TNL GitLab repository URL: <https://gitlab.com/tnl-project/tnl/-/blob/main/src/TNL/Matrices/MatrixReader.h>

¹⁶ Transforming Python script GitLab repository URL: <https://mmg-gitlab.fjfi.cvut.cz/gitlab/tnl/lu-decomposition/-/blob/master/src/Benchmark/scripts/decomposition-benchmark-make-tables-json.py>

one element in each iteration, then, the tolerance rule would be imposed (with $tol = 0.001$). The kernel and how convergence was handled withing `CroutMethodIterative::decompose()` is shown in Listing 2.7.

```

1 template< typename Real, typename Index, typename Matrix1, typename Matrix2 >
2 __global__ void DecomposeKernel( const Matrix1* A, Matrix2* Z, Matrix2* Znew, ←
3     Index row_size )
4 {
5     int row = blockIdx.y * blockDim.y + threadIdx.y;
6     int col = blockIdx.x * blockDim.x + threadIdx.x;
7
8     if( row < row_size && col < row_size ) {
9         Index k;
10        Real sum = 0;
11
12        if( row >= col ) {
13            sum = 0;
14            for( k = 0; k < col; k++ ) {
15                sum = sum + Z->getElement( row, k ) * Z->getElement( k, col );
16            }
17
18            Znew->setElement( row, col, A->getElement( row, col ) - sum );
19        }
20        else {
21            TNL_ASSERT( Z->getElement( row, row ) != 0, std::cerr << "Z( " << row << ", ←
22                " << row << " ) = 0. Cannot divide by 0!" << std::endl );
23            sum = 0;
24            for( k = 0; k < row; k++ ) {
25                sum = sum + Z->getElement( row, k ) * Z->getElement( k, col );
26            }
27
28            Znew->setElement( row, col, ( A->getElement( row, col ) - sum ) / Z->←
29                getElement( row, row ) );
30        }
31    }
32 }
33
34 template< typename Matrix1, typename Matrix2 >
35 void CroutMethodIterative::decompose( Matrix1& A, Matrix2& Z )
36 {
37     // ...
38     do {
39         DecomposeKernel< RealType, IndexType, Matrix1, Matrix2 ><<< blocksPerGrid, ←
40             threadsPerBlock >>>( matrix1_kernel, matrix2_kernel, matrix2new_kernel, ←
41                 num_rows );
42
43         // Determine if Z has converged by computing the maximum absolute difference ←
44         // between Z and Znew, and comparing it with a hard-set tolerance
45         converged = matrixDifferenceTolerable( Znew, Z );
46
47         Z = Znew;
48     } while( !converged );
49     // ...
50 }
```

Listing 2.7: Initial naive implementation of the GPU version of the Iterative Crout method. Taken from the Decomposition project repository on GitLab⁴.

As can be seen in Listing 2.7, the implementation had several drawbacks:

- The condition on line 7 caused divergence of threads (described in *Warp* in Section 1.2.2). However, this affected only the warps whose threads would overreach the matrix dimensions.
- The condition on line 11 also caused divergence of threads. However, in this instance the majority of warps were affected.
- All operations with elements of the input matrices are done in the device's global memory. Reading from global memory is sub-optimal compared to reading from shared memory, however, global memory bandwidth is even lower if the access to memory is not coalesced. Since the number of loops each thread performed in its `for` differed, then further thread divergence and non-coalesced memory access occurred as a consequence.
- The inefficient convergence described at the end of *Convergence by sections* in Section 2.2.2 is precisely the means of convergence used in this naive implementation.

In summary, this implementation was sub-optimal, however, it served as a foundation for future development.

Dynamic parallelism Following the initial naive implementation, it was theorized that the sub-optimal performance stemmed from repeatedly copying between device and host. The reasoning behind this thought came from the fact that the tolerance rule was checked on the host (line 39 in Listing 2.7). Practically, this meant that matrices `Z` and `Znew` were copied between the host and device in every iteration. Dynamic parallelism¹⁷ was found as a potentially suitable solution. The solution involved having one main kernel, that would then house the tolerance-checking `do-while` cycle which would launch another kernel from within itself. However, this solution ultimately proved sub-optimal and as such, it was abandoned in favor of a multiple kernel setup.

Multiple kernels The multiple kernel setup involved splitting the logic done on the host (checking for convergence and assigning the newly-computed value of `Z` to `Znew`) into two kernels:

- `ConvergenceKernel` - Kernel that would check whether `Z` converged to an approximate solution.
- `MatrixAssignKernel` - Kernel that would assign `Z` to `Znew`.

These three kernel would then be called in every iteration of the `do-while` cycle - shown in Listing 2.8.

```
1  do
2  {
3      *converged_host = true;
4      cudaMemcpy(converged_kernel, converged_host, sizeof(bool), __
5          cudaMemcpyHostToDevice);
```

¹⁷CUDA Dynamic Parallelism API and Principles URL: <https://developer.nvidia.com/blog/cuda-dynamic-parallelism-api-principles/>

```

6     DecomposeKernel< RealType ><<< blocksPerGrid, threadsPerBlock >>>( ←
7         matrixA_kernel, matrixZ_kernel, matrixZnew_kernel, num_rows );
8
9     ConvergenceKernel< RealType ><<< blocksPerGrid, threadsPerBlock >>>( ←
10        matrixZ_kernel, matrixZnew_kernel, num_rows, converged_kernel );
11
12    MatrixAssignKernel<<< blocksPerGrid, threadsPerBlock >>>( matrixZ_kernel, ←
13        matrixZnew_kernel, num_rows );
14
15    cudaMemcpy( converged_host, converged_kernel, sizeof(bool), ←
16        cudaMemcpyDeviceToHost );
17 } while( !*converged_host );

```

Listing 2.8: Solution that replaced the procedure presented on lines 31 - 44 in Listing 2.7. Taken from the Decomposition project repository on GitLab⁴.

Ultimately this solution improved the performance over both the *Initial naive implementation* and the failed solution involving *Dynamic parallelism*.

Calculation by tiles using shared memory The core of the decomposition kernel from the multiple kernel setup was still the same as in the *Initial naive implementation* (lines 7 - 28 in Listing 2.7). Thus, in order to improve performance the core logic was re-worked. Since the algorithm for computing LU decomposition is similar to matrix multiplication - with minor differences - the logic from CUDA's *Example with shared memory* shown in Listing 1.11 was adopted. Listing 2.9 shows the replacement for the lines mentioned earlier.

```

1 int tx = threadIdx.x;
2 int ty = threadIdx.y;
3
4 RealType sum = 0;
5
6 for (int i = 0; i <= num_rows; i += BLOCK_SIZE) {
7     __shared__ RealType ZsLower[BLOCK_SIZE][BLOCK_SIZE];
8     __shared__ RealType ZsUpper[BLOCK_SIZE][BLOCK_SIZE];
9
10    // Possible non-coalesced global memory access and thread divergence
11    ZsLower[ty][tx] = (row >= num_rows || i + tx >= num_rows) ? 0 : Z->getElement(←
12        row, i + tx );
13    ZsUpper[ty][tx] = (col >= num_rows || i + ty >= num_rows) ? 0 : Z->getElement(←
14        i + ty, col );
15
16    // Synchronize to make sure the matrices are loaded
17    __syncthreads();
18
19    // Get global ID of max current position
20    int glob_id = i + BLOCK_SIZE;
21
22    if( row >= col ) {
23        // If row < BLOCK_SIZE or col < BLOCK_SIZE, then use the for loop without ←
24        #pragma unroll
25        if( col >= glob_id ) {
26            #pragma unroll
27            for( int k = 0; k < BLOCK_SIZE; ++k ) {
28                sum += ZsLower[ty][k] * ZsUpper[k][tx];
29            }

```

```

27     } else {
28         for( int k = 0; k < tx; k++ ) {
29             sum += ZsLower[ty][k] * ZsUpper[k][tx];
30         }
31         break;
32     }
33 } else {
34     if( row >= glob_id ) {
35         #pragma unroll
36         for( int k = 0; k < BLOCK_SIZE; ++k ) {
37             sum += ZsLower[ty][k] * ZsUpper[k][tx];
38         }
39     } else {
40         for( int k = 0; k < ty; ++k ) {
41             sum += ZsLower[ty][k] * ZsUpper[k][tx];
42         }
43         break;
44     }
45 }
46 // Synchronize to make sure that the preceding computation is done before ←
47 // loading two new sub-matrices in the next iteration
48 __syncthreads();
49 }
50
51 // Terminate overreaching threads
52 if( row >= num_rows || col >= num_rows ) {
53     return;
54 }
55
56 // Compute the element (row, col)
57 if( row >= col ) {
58     Znew->setElement( row, col, A->getElement( row, col ) - sum );
59 } else {
60     if( Z->element( row, row ) == 0 ) {
61         printf( "Key element: %f\n", Z->element( row, row ) );
62         printf( "row:%d\ncol:%d\n", row, col );
63         assert( Z->element( row, row ) != 0 );
64     }
65     Znew->setElement( row, col, ( A->getElement( row, col ) - sum ) / Z->←
66         getElement( row, row ) );
67 }

```

Listing 2.9: Calculation of a single iteration of the GPU Iterative Crout method using logic from Listing 1.11. Taken from the Decomposition project repository on GitLab⁴.

While the procedure shown in Listing 2.9 removed some of the inefficiencies that the previous solution posed, it still contained some undesired behaviors. For example, the nested conditions that made sure each thread stopped its computation at the desired element. The conditions could cause thread divergence in almost any warp. Nevertheless, the re-worked part of the implementation performed better than its predecessor and it was accepted as an optimization.

Elimination of conditions As mentioned in *Calculation by tiles using shared memory*, one of the sub-optimal aspects of the decomposition kernel's core was the handling of conditions. To solve this issue,

another approach was devised that would almost entirely eliminate the need for conditions. Specifically, lines 6 - 49 in Listing 2.9 were replaced with the code shown in Listing 2.10.

```

1 int max_id = num_rows - 1;
2 int new_row = min( row, max_id );
3 int new_col = min( col, max_id );
4
5 // Each thread needs to end its calculation by its smallest dimension
6 // Offset by BLOCK_SIZE, so in the for loop it is not needed to check `i + ←
7 // BLOCK_SIZE <= min_row_col` in every iteration
8 int min_row_col = min( new_row, new_col ) - BLOCK_SIZE;
9
10 // Allocate Lower and Upper submatrices from matrix Z into which shared memory ←
11 // will be loaded.
12 __shared__ RealType ZsLower[BLOCK_SIZE][BLOCK_SIZE];
13 __shared__ RealType ZsUpper[BLOCK_SIZE][BLOCK_SIZE];
14
15 // Initialize loop variable outside of loop
16 int i;
17
18 // End the for loop early if this thread needs to end its calculation in the ←
19 // current loop's submatrix
20 // The original condition in the for loop was: `i + BLOCK_SIZE <= min_row_col` ←
21 // Since all threads in a block either need to end their calculations in a ←
22 // submatrix, or they all do not
23 // Submatrices are iterated until the loops gets to a submatrix where the ←
24 // threads would need to end their calculations
25 // This means that the threads would need to end their calculation before ←
26 // BLOCK_SIZE and the pragma loop could not be used. In that case, a loop ←
27 // specific is needed for that thread
28 for ( i = 0; i <= min_row_col; i += BLOCK_SIZE ) {
29     ZsLower[ty][tx] = Z( new_row, i + tx );
30     ZsUpper[ty][tx] = Z( i + ty, new_col );
31
32     // Synchronize to make sure the matrices are loaded
33     __syncthreads();
34
35     #pragma unroll
36     for( int k = 0; k < BLOCK_SIZE; ++k ) {
37         sum += ZsLower[ty][k] * ZsUpper[k][tx];
38     }
39
40     // Synchronize after computation before loading new submatrices
41     __syncthreads();
42 }
43
44 // Perform calculations remaining for each thread
45 // Check that threads would not reach out of range when loading data using min
46 ZsLower[ty][tx] = Z( new_row, min( i + tx, max_id ) );
47 ZsUpper[ty][tx] = Z( min( i + ty, max_id ), new_col );
48
49 // Synchronize the threads before working with data loaded from global memory
50 __syncthreads();
51
52 int t_to_use = row >= col ? tx : ty;
53 for( int k = 0; k < t_to_use; ++k ) {
54     sum += ZsLower[ty][k] * ZsUpper[k][tx];
55 }
```

Listing 2.10: Core of the decomposition kernel with the inefficient conditions replaced by a combination of the `min()` function and helpful variables. Taken from the Decomposition project repository on GitLab⁴.

This approach further improved the performance and thus it was accepted as an optimization. Ultimately, except for combining all three kernels into one, this was the final change before the final implementation - *Convergence by sections* - was introduced.

Note that up until this point the tolerance value was set to 0.001, however, with the introduction of *Convergence by sections* the accuracy of results was inadequate. Thus, through testing it was observed that 0.0 was the optimal value as it greatly improved the accuracy of results while only slightly reducing the speed of execution.

Additionally, the interval for the size of the section in the first version of *Convergence by sections* was [512, 1024]. While discovering the optimal interval range, it was observed that even with the tolerance value set to zero, if the section size was decreased to less than 256×256 then the results produced were less accurate; this behavior remains unexplained. Theoretically, since the zero-tolerance rule leaves no room for errors, it should not matter whether what the section size is. On the other hand, it is possible that there was an error somewhere in the implementation, however, it has not been found yet.

Other explored improvements After arriving at the final implementation, two potential improvements were explored:

1. Section size set to 1/2 of the maximum number of active threads permitted by the GPU.
2. Convergence by anti-diagonal sections.

Section size dependent on maximum active threads The first explored improvement aimed to tailor the solution to the capabilities of the GPU used for the computation. The concept of the maximum number of active threads was explained in *Grid* in Section 1.2.2 and in *Concurrent kernel execution* in Section 1.2.4. The maximum number of active threads for a specific GPU can be obtained using the following formula:

$$\text{maxActiveThreads} = \text{SMcount} \cdot \text{maxThreadsPerSM},$$

which can be implemented using the CUDA `cudaDeviceProp`¹⁸ structure as shown in Listing 2.11.

```
1 int cuda_device = 0;
2 cudaDeviceProp deviceProp;
3 cudaGetDevice(&cuda_device);
4 cudaGetDeviceProperties(&deviceProp, cuda_device);
5
6 int maxActiveThreads = deviceProp.multiProcessorCount * ←
7     deviceProp.maxThreadsPerMultiProcessor;
8
9 // Two (sectionSize x sectionSize) sections will be running in parallel at most
10 int sectionSize = sqrt(maxActiveThreads/2);
11 // Round sectionSize to a multiple of BLOCK_SIZE
```

¹⁸ `cudaDeviceProp` Struct Reference URL: <https://docs.nvidia.com/cuda/cuda-runtime-api/structcudaDeviceProp.html>

```

11 sectionSize = (sectionSize/BLOCK_SIZE)*BLOCK_SIZE; // WHY IS THIS DIFFERENT FROM ←
THE PREVIOUS WAY TO CALCULATE sectionSize

```

Listing 2.11: Code detailing the calculation of the size of a section based on the maximum number of active threads for a given GPU. The structure `cudaDeviceProp` contains properties and information about the given CUDA device. Taken from the Decomposition project repository on GitLab⁴.

While this change significantly improved the speed of execution, the results it produced were less accurate than that of the final implementation. It seems that the same behavior as when `sectionSize` was set below 256 - described at the end of *Elimination of conditions* - occurred. Since a solution to the problem of inaccuracy was not found, this change was not accepted.

Convergence by anti-diagonal sections At the end of *Convergence by sections* in Section 2.2.2 it was mentioned that more than two sections can be converged simultaneously. Furthermore, this can be done while still adhering to the general rule of optimal convergence that states: "certain sections above and to the left of a section must be converged in order for the section to converge optimally". In this instance "optimally" means quickly and accurately. Following the rule of optimal convergence, Figure 2.4 shows an alternative order of convergence: *Convergence by anti-diagonal sections*.

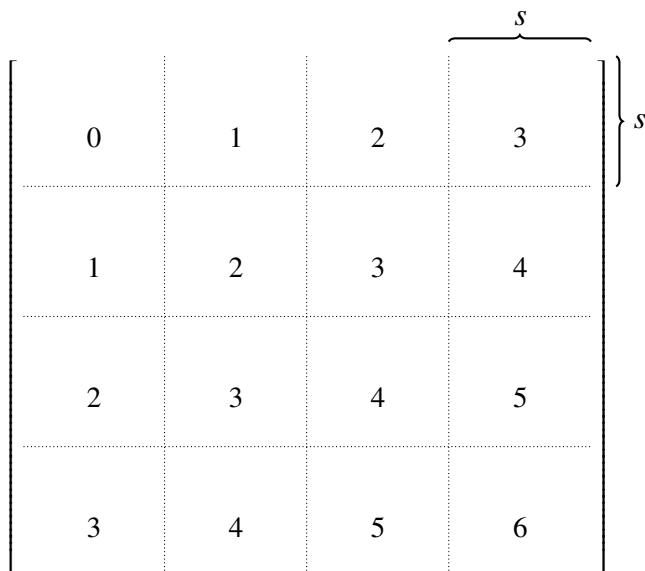


Figure 2.4: Visualization of matrix \mathbb{Z} divided into sections of size $s \times s$. The order in which sections are converged is denoted by the number in each section. First, the upper-left-most section (section '0') is converged, then, the sections below and to the right of it (sections labeled with a '1') are converged in parallel. Then, all sections below and to the right of each section labeled with a '1' are converged (sections labeled with a '2') in parallel, and so on.

Theoretically, this order of convergence allows for more parallelization than the final implementation as more independent elements are converged at once. However, practically, the implementation was not as performant as the final implementation (detailed in *Iterative Crout method* in Section 2.2.2). The reason for this was that the indexing system was too complex and required more overhead computation. Further attempts at lowering the overhead computations were not successful and as such, the solution was put

aside. Note that in the attempted implementation all sections in an anti-diagonal were iterated until all of them converged. This means that even if one section converged, it was still being computed over and over if another section in the same anti-diagonal was not yet converged. Furthermore, the order of execution pictured in Figure 2.4 does not take into account all possible orders of execution. For example, the left-most section labeled with a '4' can be converged before the section above it, since the elements in the former only use the elements from sections '1' and '2' in the same column and section '3' in the same row.

The solution to this problem would be to implement a more complex order execution system, which would keep track of which sections can be converged based on whether the sections it depends on are already converged. In other words, as soon as all sections a section depends would be converged, then the convergence of this section would be immediately scheduled on the GPU.

Another advantage of such a system would be its future-proof nature. In the final implementation `sectionSize` is restricted to the interval [256, 1024]. The number of threads allocated by the final implementation is more than most modern GPUs are capable of actively running. However, if future GPUs are capable of running more threads at once than required by the final implementation, then the GPU's resources would be under-utilized since sections that can be converged would be waiting until they are scheduled for execution. On the other hand, a solution involving the order execution system would allocate as many threads as possible without compromising on the quality of converged elements. While such a system has neither been designed, nor implemented, it is a possible feature to consider for future development.

Chapter 3

Comparing Decomposition Implementations TO

In Section 2.2.3 the benchmark structure implemented in order to compare the performance of the GPU version of the LU decomposition and the CPU version was presented. During the development of the project the benchmark was run on many different platforms, such as, smaller compute servers, or the HELIOS cluster¹ belonging to the Department of Mathematics; both are found in the Faculty of Nuclear Sciences and Physical Engineering of the Czech Technical University in Prague. This chapter will present and analyze the results of the benchmark that was run in order to compare the two aforementioned implementations. To begin with, the benchmarked implementations will be briefly summarized along with the specifications of the platform that the benchmarks were run on. Then, the set of matrices used in the benchmarks will be presented. Finally, the results of the benchmark will be presented and analyzed.

3.1 Benchmarked Implementations TO

The implementations in the *Decomposition* project that were benchmarked are the following:

- *Crout method* (CM) - This implementation is only available for the CPU. At its core, it is a sequential algorithm that delivers a decomposition of the input matrix in one pass.
- *Iterative Crout method* (ICMx) - This implementation is available only for the GPU. At its core, it is an iterative and parallelizable algorithm that converges to an approximate decomposition of the input matrix. This implementation was further divided into three different configurations of threads per block (denoted by x): 8×8 (ICM8), 16×16 (ICM16), and 32×32 (ICM32); ICMx refers to all three configurations.

¹HELIOS cluster documentation URL: <http://helios.fjfi.cvut.cz/>

3.2 Benchmark Platform Specifications TO

The benchmark was run on the RCI (Research Center for Informatics in CTU Prague) Cluster² which is a HPC (High Performance Computing) infrastructure intended for use mainly by researchers. It is made up of CPU, GPU, and SMP nodes that are interconnected by a 100Gbit low-latency network [3]. The hardware and software specifications of the cluster node that the benchmarks were run on can be found in Table 3.1.

CPU	AMD EPYC 7543@3.1GHz (32 cores, 64 threads)
RAM	32GB RAM
GPU	Nvidia Tesla A100 40GB HBM2 (1.6 TByte/s memory bandwidth)
Operating System	CentOS 8 Linux
Compiler	GCC 10.3
CUDA	CUDA 11.4.1

Table 3.1: Specifications of the `gpu` RCI Cluster node that the benchmarks were run on. Taken from *RCI Cluster Hardware* [3] and the configuration of the computation job.

3.3 Matrices Used for Benchmarks TO

The benchmarks for the implementations were run on a set of 63 matrices. The number of matrices used is comparatively smaller compared to the set of matrices used in the benchmarks of the author's bachelor thesis *Formats for storage of sparse matrices on GPU* [42]. The lack of matrices in this benchmark is due to the fact that the current version of the *Decomposition* project does not support decomposition of matrices that are not strongly regular, i.e. matrices that require a permutation matrix for a successful decomposition - described in Section 1.3. This means that any matrices used in the benchmark had to be checked for the aforementioned requirement which made the selection process lengthy. Furthermore, since some dense matrices were included in the set, the drive space required was nearing the limit of what was feasible to move between servers and store in a compute node's scratch memory.

The majority of matrices from the set used are sparse as they were obtained from the *SuiteSparse Matrix Collection* [2]. The remaining matrices are dense - they were randomly generated using the Python script shown in Listing D.1 in Attachment D. The dimensions of the matrices in the set ranged from 27×27 to $10,793 \times 10,793$ and, in general, their nonzero elements were mostly located along the main diagonal with some exceptions. For the direct comparison of results 14 matrices were selected from the set of 63. The chosen matrices were selected to represent a wide variety of characteristics: density/sparsity, nonzero element structure, and dimensions. The 14 selected matrices can be found in Table 3.2.

3.4 Benchmark Results TO

This section will present and analyze the benchmark results obtained from decomposing the matrices shown in Table 3.2 using the implementations mentioned in Section 3.1 on the platform described in

²RCI homepage URL: <http://rci.cvut.cz/>

Matrix	Rows	Columns	Nonzeros	Avg. nonzeros per row
bcsstk03	112	112	640	5.7
494_bus	494	494	1,666	3.4
LeGresley_2508	2,508	2,508	16,727	6.7
Cejka2842	2,842	2,842	8,076,964	2,842.0
rail_5177	5,177	5,177	35,185	6.8
c-31	5,339	5,339	78,571	14.7
s3rmt3m3	5,357	5,357	207,123	38.7
s1rmq4m1	5,489	5,489	262,411	47.8
Na5	5,832	5,832	305,630	52.4
Cejka5943	5,943	5,943	35,319,249	5,943.0
fp	7,548	7,548	834,222	110.5
Cejka7580	7,580	7,580	57,456,400	7,580.0
bundle1	10,581	10,581	770,811	72.8
Cejka10793	10,793	10,793	116,488,849	10,793.0

Table 3.2: Set of 14 selected matrices from the *The university of Florida sparse matrix collection* [2] and randomly generated dense matrices (labeled *Cejka<num_rows>*) that was used for the direct comparison of implementations.

Section 3.2. The benchmark subroutine described in Section 2.2.3 assumed that each matrix is decomposed once, however, in this benchmark run, in order to minimize anomalous behaviors and assure the quality of presented results, each matrix was decomposed 100 times. Then, the data collected across all 100 runs (execution time, bandwidth, speedup, etc.) was averaged and subsequently logged. First, the terminology that will be used during the analysis will be introduced for clarity. Then, benchmark results for both single and double precision comparing the bandwidths achieved by CM and different ICMx implementations will be presented. Following that, the comparison of speedup between CM and ICMx will be detailed for both single and double precision. Last but not least, benchmark results across the entire set of 63 matrices will be briefly shown, along with the accuracy of results for all matrices. Finally, the benchmark results measured during development for the optimizations described in Section 2.3 will be shown. Full benchmarks results - including logs - are available upon request, or they can be found in the CD attached.

Benchmark Terminology The terminology used in the analysis of the benchmark results is both common and adjusted to this project. It will be briefly explained in the context of the benchmark below:

- **Bandwidth** - The amount of data that can be read from or written to device memory by the device within a specified time interval [1]. This rate of data transfer is measured in Bytes per second (Byte/s), however, given the evolution in computation it is most-often measured in Gigabytes (GByte/s) - or even Terabytes (TByte/s) with the recently launched Nvidia A100 as shown in Table 1.1. According to Section 8.2.2 in *CUDA C++ Best Practices Guide* [1] effective bandwidth is defined as

$$\frac{(B_r + B_w) / 10^9}{\text{execution_time}},$$

where B_r refers to the number of bytes read per kernel, B_w is the number of bytes written per kernel, and the unit of measurement for *execution_time* is seconds. Since the implementations all

read from three instances of `DenseMatrix` and the write to two during computation (not counting loops), then the numerator can be generalized as:

$$\frac{mtx_rows \cdot mtx_cols \cdot 5 \cdot \text{sizeof}(Real)}{10^9}.$$

Where `mtx_rows` represents the number of rows of the input matrix; `mtx_cols` represents the number of columns of the input matrix; `Real` denotes the precision, which is either single (`float`) or double (`double`). The '5' signifies the reading from three matrices (`A`, `Z`, and `Znew`) and writing to two matrices (`Z` and `Znew`).

- **Time** - The execution time of the `CroutMethodIterative::decompose()` method. In other words, not only the kernel, but also the setup of the computation and copying the required data from the host to device was incorporated into execution time.

3.4.1 Bandwidth of the Implementations TO

The bandwidth of the decomposition implementations on the set of matrices using single and double precision is shown in Figure 3.1 - note that the graphs in the figure have a log-scaled vertical axis for clearer presentation of differences between the individual implementations.

Overall, no implementation outperformed the rest on all matrices. However, there seems to be a trend in ICM16 and ICM32 achieving a higher bandwidth on average for both single and double precision. The highest bandwidths achieved for single precision were 12.01 GByte/s by ICM16 and 11.92 GByte/s by ICM32 on the `s1rmq4m1` matrix, and 10.70 GByte/s by ICM16 on the `Na5` matrix. In terms of double precision the highest bandwidths achieved were 16.87 GByte/s by ICM32, 14.29 GByte/s by ICM16, and 11.38 GByte/s by ICM8 - all on the `s1rmq4m1` matrix. Matrices `s1rmq4m1` and `Na5` are shown in Figure 3.2.

As can be seen from Figure 3.2a, matrix `s1rmq4m1` has nonzero elements on and near its main diagonal. Thus, the matrices arising from the decomposition (\mathbb{L} and \mathbb{U} , or \mathbb{Z}) will also have elements mainly around their main diagonals. From the perspective of ICMx this means that the majority of elements requiring computation are found within diagonal sections, therefore, more iterations are required to converge them. On the other hand, non-diagonal sections do not require as many iterations to converge as they contain mostly zeros. Consequently, ICMx is able to leverage the fact that each diagonal section has the device's resources available to itself and that non-diagonal sections converge in fewer iterations which results in a fast decomposition of the input matrix. In other words, ICMx is efficient at decomposing n-diagonal sparse matrices, i.e. matrices that have a small number (n) of nonzero diagonals near the main nonzero diagonal. For the `s1rmq4m1` matrix - using either precision - the optimal number of threads per block is either 16×16 or 32×32 .

Similarly, the `Na5` matrix (Figure 3.2b) has more so an n-diagonal nonzero element structure with minor protrusions in the center. However, the protrusions do not impact the performance severely since the concentration of nonzero elements on the main diagonal is greater than that of the outer diagonals. Therefore, ICMx also benefits from the fact that, overall, fewer iterations are required to converge to an approximate solution.

Conversely, ICMx achieved its lowest bandwidth across all dense matrices when using double precision. Since the dense matrices used contain only nonzero elements, every section needed many iterations to be converged which in turn meant that, overall, more iterations were needed to converge the entire matrix. For context, the `Cejka5943` dense matrix was decomposed by ICM32 in 44.53 seconds (using

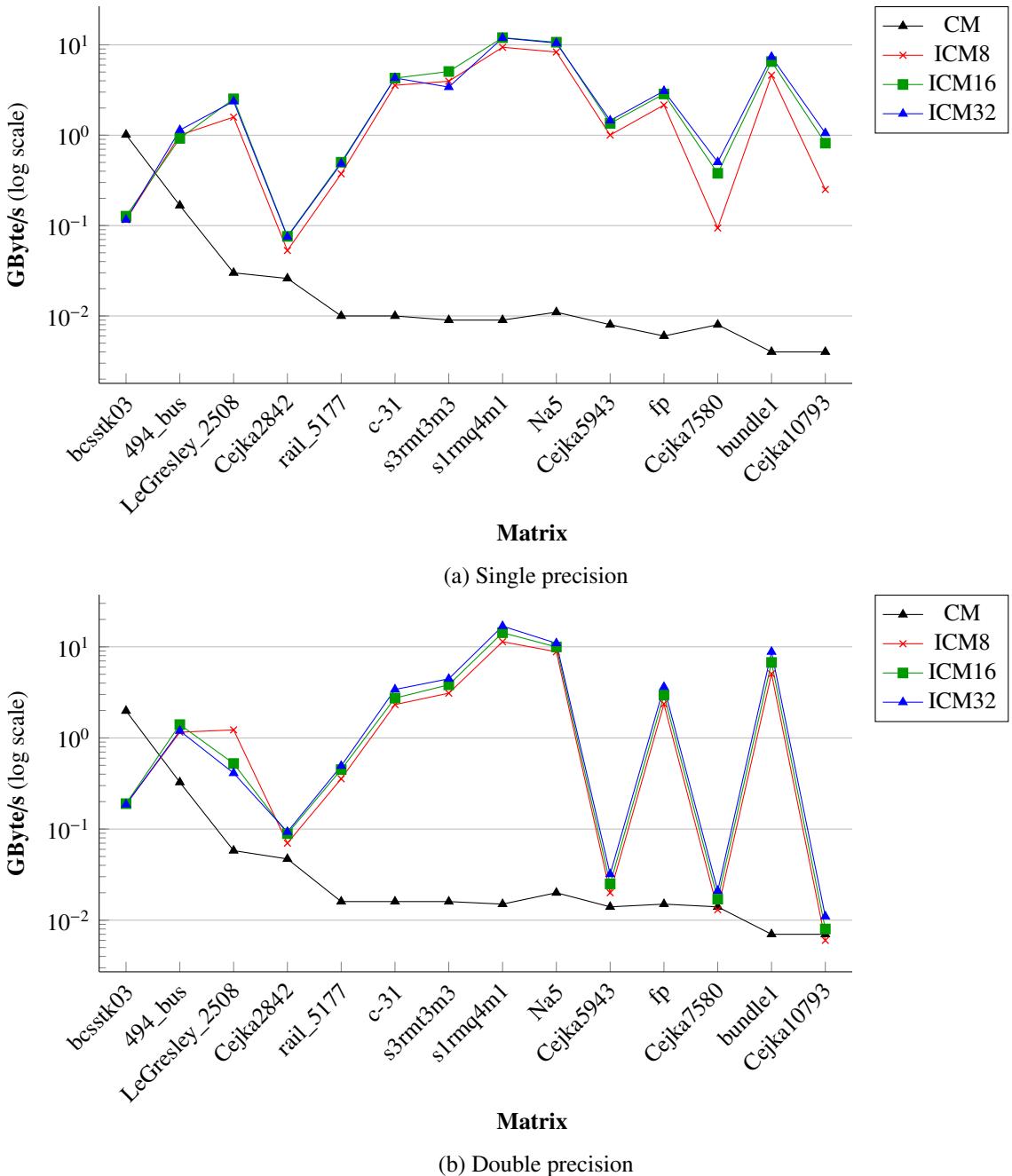
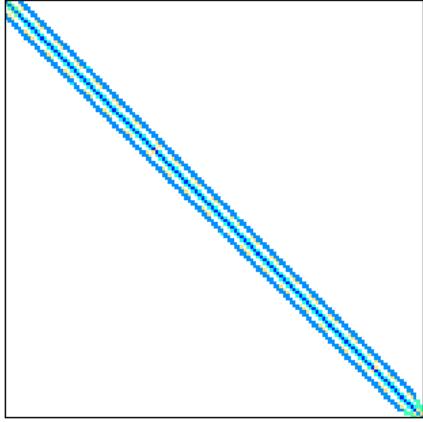
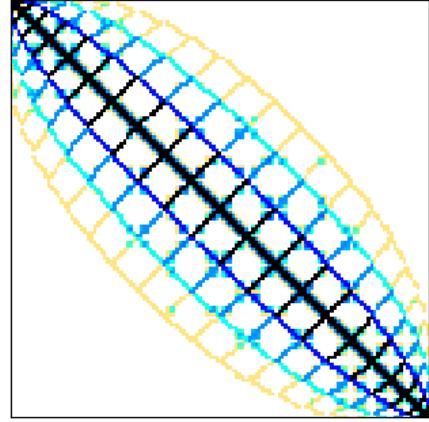


Figure 3.1: Bandwidth achieved by the decomposition implementations on the set of matrices (Table 3.2) using single and double precision. The vertical axis is log-scaled for better visibility of differences between implementations.

double precision), whereas the *Na5* matrix was decomposed in 0.12 seconds. On the other hand, when single precision was used, the noticeable difference in performance between sparse and dense matrices was not as prominent. While the reason behind the stark performance difference between single and double precision for $ICMx$ on dense matrices remains unproven, high-speed shared memory access and generally faster operations using single precision are suspected to be the root causes.



(a) s1rmq4m1

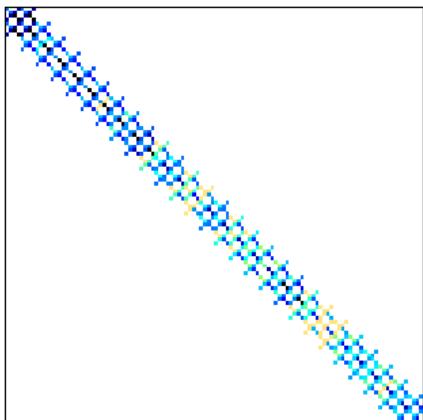


(b) Na5

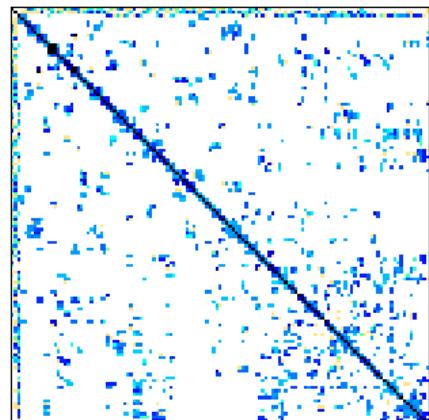
Figure 3.2: Nonzero element pattern of the *s1rmq4m1* and *Na5* matrices. Taken from the *The university of Florida sparse matrix collection* [2].

ICMx achieved higher bandwidths on all sparse matrix with the exception of the *bcsstk03* (Figure 3.3a) and *rail_5177* (Figure 3.3b) matrices despite the former's nonzero element structure being favorable to ICMx. As Table 3.2 lists, the dimensions of the *bcsstk03* matrix are 112×112 which is advantageous for the sequential implementation of CM, as there are fewer steps to perform. Furthermore, since the matrix was already present in host memory, CM's decomposition procedure began without delay. On the other hand, for ICMx, the matrix first had to be copied to device memory and, additionally, the pre-kernel overhead subroutine of ICMx took - in this case - relatively valuable time to complete. This, combined with the fact that the strength of the iterative algorithm lies in the GPU's ability to process larger datasets, indicates that CM is more suitable for decomposing smaller matrices.

When it comes to the *rail_5177* matrix (Figure 3.3b), irrespective of the fact that its main diagonal is heavily populated with nonzero elements, there are other nonzero elements interspersed in a seemingly random fashion throughout the matrix. Therefore, similarly to dense matrices, the non-diagonal sections of this matrix also require more iterations to converge.



(a) bcsstk03



(b) rail_5177

Figure 3.3: Nonzero element pattern of the *bcsstk03* and *rail_5177* matrices. Taken from the *The university of Florida sparse matrix collection* [2].

The performance of ICM8 - as shown in Figure 3.1 - brings some interesting results. In general, its performance follows that of ICM16 and ICM32, however, some anomalous behavior is present in both single and double precision. For the former, bandwidths achieved seem to be slightly lower for the first 10 matrices (*bcsstk03* to *Cejka5943*), however, they are considerably lower the larger the matrix dimensions become. This behavior is most likely a result of global memory access becoming a greater bottleneck for single precision when decomposing larger matrices. Consequently, as non-coalesced global memory access is more common for ICM8 than for ICM16, or ICM32 (detailed further in Section 3.4.2), its performance is proportionately lower. For double precision, ICM8 retains the relative performance difference compared to single precision. This is true even when it comes to the *LeGresley_2508* matrix (Figure 3.4) which cannot be said about ICM16 and ICM32.

When comparing the differences in performance over all matrices between single and double precision for ICM16 and ICM32, the results seem consistent with the exception of certain dense matrices and the *LeGresley_2508* matrix (Figure 3.4). When double precision is used, the performance of the mentioned implementations decreased drastically compared to single precision and compared to the decrease in performance of ICM8. Since 1/10 of the matrix dimensions are 250.8, `sectionSize` is set to 256 - the edge of the interval. Thus, `sectionSize` is the same for ICM8, ICM16, and ICM32 as their respective `BLOCK_SIZE` is a divisor of 256. Therefore, from the perspective of software, the only difference between the implementations in this instance - except for the precision - is the different `BLOCK_SIZE`. It can be argued that ICM8 performed better due to the greater granularity of its thread blocks combined with the smaller size of the matrix. The greater granularity stems from the fact that ICM8 had 32 blocks assigned to each SM, whereas ICM16 had 8 and ICM32 had 2 - the A100 has a maximum of 2048 threads (64 warps; 32 blocks) per SM [38]. This means that if the GPU would run out of resources in terms of concurrently active threads, then ICM8 would fair better as its smaller blocks could fill up the remaining resources more tightly (detailed in *Grid* in Section 1.2.2). This effect is only observed when decomposing smaller matrices which have a nonzero element structure similar to that of *LeGresley_2508*, i.e. matrices with nonzero elements on the main diagonal and nonzero elements interspersed elsewhere. Figure 3.8b further confirms this suspicion for certain matrices where ICM8 outperforms ICM16 and ICM32 when double precision is used. For matrices with larger dimensions this effect would be mitigated since being able to utilize a few additional blocks would not amount to such a drastic difference in performance. Furthermore, the non-coalesced global memory access present for ICM8 (more so than ICM16) becomes apparent when decomposing larger matrices - especially when using single precision.

Other than the notable bandwidth achieved on the *bcsstk03* matrix, in general, the performance of CM was lower than that of ICMx - especially when single precision was used. Conversely, when double precision was used, its performance on dense matrices was comparable to that of ICMx. Specifically, the bandwidth achieved for matrices *Cejka2842*, *Cejka5943*, *Cejka7580*, and *Cejka10793* by CM and ICM32 (best ICMx for the matrices mentioned) can be seen in Table 3.3.

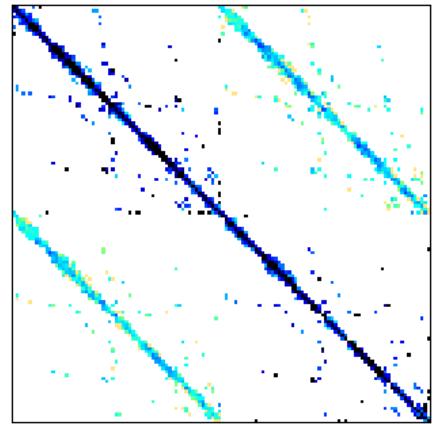


Figure 3.4: Nonzero element pattern of the *LeGresley_2508* matrix. Taken from the *The university of Florida sparse matrix collection* [2].

Figure 3.4 shows the nonzero element pattern of the *LeGresley_2508* matrix. The matrix is represented as a grid of colored dots, primarily blue and yellow, forming several diagonal bands that intersect at the center. The pattern is highly symmetric and sparse, with most non-zero elements concentrated along the main diagonal and a few off-diagonal bands. This pattern is characteristic of a banded matrix, which is a common type of sparse matrix used in numerical linear algebra.

The *LeGresley_2508* matrix is a square matrix with dimensions 2508x2508. It has approximately 10,000 non-zero elements. The matrix is stored in a compressed sparse row (CSR) format, which is a common way to store sparse matrices in memory. The CSR format consists of three arrays: a row index array, a column index array, and a value array. The row index array contains the starting index of each row in the value array. The column index array contains the column indices of the non-zero elements. The value array contains the values of the non-zero elements.

The nonzero element pattern of the *LeGresley_2508* matrix is shown in Figure 3.4. The pattern is highly symmetric and sparse, with most non-zero elements concentrated along the main diagonal and a few off-diagonal bands. This pattern is characteristic of a banded matrix, which is a common type of sparse matrix used in numerical linear algebra.

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The nonzero element pattern of the *LeGresley_2508* matrix is shown in Figure 3.4. The pattern is highly symmetric and sparse, with most non-zero elements concentrated along the main diagonal and a few off-diagonal bands. This pattern is characteristic of a banded matrix, which is a common type of sparse matrix used in numerical linear algebra.

Implementation	Cejka2842	Cejka5943	Cejka7580	Cejka10793
CM	0.047	0.014	0.014	0.007
ICM32	0.093	0.032	0.021	0.011

Table 3.3: Bandwidth achieved (in GByte/s) when decomposing the subset of dense matrices from Table 3.2 by CM and ICM32 using double precision.

Since the algorithm used for CM is sequential and computes every element of the resulting decomposed matrix \mathbb{Z} regardless of its value, then there is no difference in how it computes matrices with distinct nonzero element structures. However, it can be argued that - especially when double precision is used - sparse matrices are, in general, decomposed slightly faster than dense matrices with the same dimensions. This is due to the fact that the multiplication and addition operations performed will be working with zeros in the majority of cases. Nevertheless, it can be concluded that the performance of CM is determined more so by the dimensions of a matrix, rather than its nonzero element structure.

3.4.2 Speedup Comparison Between CM and different ICMs TO

As the bandwidth results shown in Figure 3.1 are presented with a log-scaled vertical axis, it can be difficult to see the performance differences between implementations. Therefore, to put the results into perspective, this section presents the speedup comparison between the implementations listed in Section 3.1. Specifically, as mentioned in *Implementation requirements* in Section 2.2.2 one of the goals of this project was to "*measure the acceleration of the GPU version of the LU decomposition against the CPU version*". For that reason, speedup from the CM (host) implementation to the ICMx (device) implementations will be compared. The comparison - using single and double precision - on the set of matrices listed in Table 3.2 is shown in Figure 3.5.

ICM16 and ICM32 Similarly to the bandwidth results, overall, ICM16 and ICM32 were the best-performing implementations. For single precision, the three highest speedups compared to CM were 2030.30 by ICM32 and 1803.08 by ICM16 on the *bundle1* matrix (Figure 3.6a), and 1352.55 by ICM16 on the *s1rmq4m1* matrix (Figure 3.2a). In terms of double precision, the highest speedups compared to CM were 1337.53 and 1137.98 achieved by ICM32 on matrices *bundle1* and *s1rmq4m1* respectively, and 1022.01 achieved by ICM16 on the *bundle1* matrix.

Nevertheless, there are exceptions to the greater performance of ICM32. One such exception is the speedup compared to ICM8 on the *s3rmt3m3* matrix (Figure 3.6b) when single precision is used. For this matrix, ICM32 achieved a speedup of 368.14, whereas ICM8 achieved 427.55. As can be seen from Figure 3.6b the nonzero element structure of the *s3rmt3m3* matrix comprises of a strong concentration of nonzero elements along the main diagonal and six nonzero-element lines aimed away from the main diagonal. The reason mentioned for the higher performance on the *Na5* matrix describes that a matrix with a similar nonzero element structure should not require many iterations to decompose for ICMx as the main diagonal has most of the nonzero elements and only a few other nonzero elements are found outside it. However, since the nonzero elements found outside the main diagonal are located much further from it than that of the *Na5* matrix pictured in Figure 3.2b, then the non-diagonal sections needed more iterations to converge.

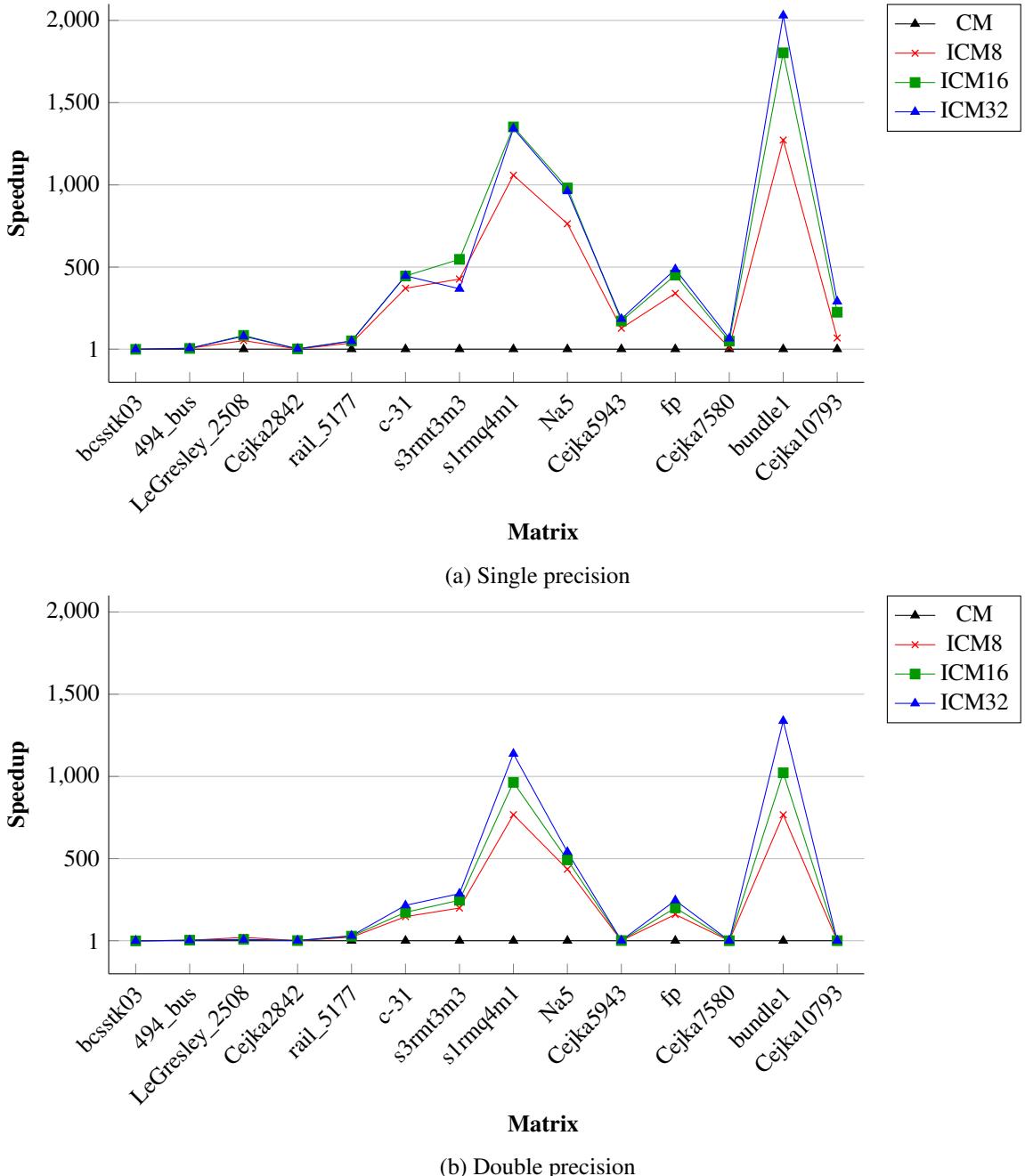


Figure 3.5: Speedup comparison between the decomposition times of CM and the ICM x implementations on the set of matrices (Table 3.2) using single and double precision.

Another noteworthy sparse matrix on which ICM x struggled - relative to the rest - was the *fp* matrix (Figure 3.7). It can be seen that the nonzero element structure is similar to that of the *rail_5177* matrix (Figure 3.3b). In other words, nonzero elements are concentrated on the main diagonal and other nonzero elements are interspersed throughout the rest of the matrix. Consequently, the lack of performance by ICM x is due to more iterations required to converge the non-diagonal sections.

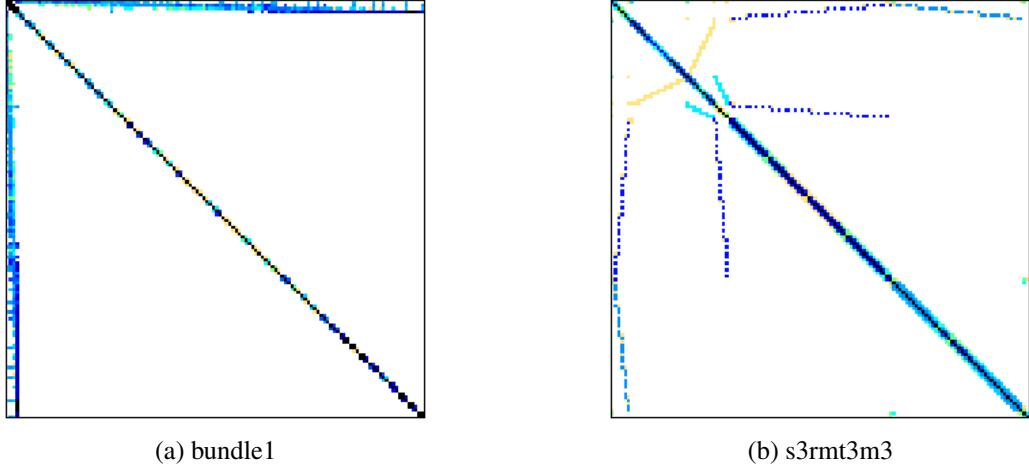


Figure 3.6: Nonzero element pattern of the *bundle1* and *s3rmt3m3* matrices. Taken from the *The university of Florida sparse matrix collection* [2].

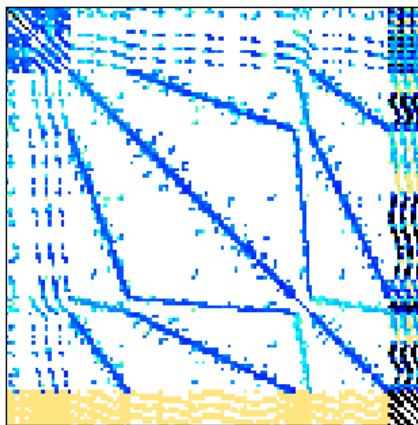


Figure 3.7: Nonzero element pattern of the *fp* matrix. Taken from the *The university of Florida sparse matrix collection* [2].

ICM8 In general, ICM8 was faster than CM, however, when its speedup is compared to that of ICM16 and ICM32, there is a difference in performance. This difference is noticeable especially for matrices that required few iterations to decompose the entire matrix, for example, *s1rmq4m1*, *Na5*, and *bundle1*. Since the decomposition time for these matrices was - at worst - 0.9 seconds for each, loading elements from global to shared memory became a bottleneck. The reason behind this stems from the fact that threads in blocks are divided into warps by their `threadIdx.x` index. Thus, when reading from shared memory threads in a warp should - ideally - access neighboring global memory addresses. Since elements of the `DenseMatrix` instance are stored in row-major order on the GPU, each warp in ICM8 loads elements from global memory in the following way: first 8 threads of the warp read data from neighboring addresses, the next 8 threads of the warp also read from other neighboring addresses, in other words, they are not found near the first 8 addresses (unless the matrix dimensions are 8×8) - this is non-coalesced access to memory. In this instance, the non-coalesced access is the same as depicted in the upper image of Figure 1.12b. Therefore, as mentioned in the figure's caption, instead of the threads in a warp performing one transaction to global memory, they will perform $32/8 = 4$ sequential transactions (detailed further in *Global memory* in Section 1.2.3).

This means that non-coalesced access to global memory occurs for ICM8 and ICM16, however, the latter will only perform $32/16 = 2$ sequential transactions. On the other hand, this defect is not present for ICM32 as the threads of a warp access `BLOCK_SIZE = 32` neighboring addresses in global memory. This effect is apparent in Figure 3.5 (ICM32 performed better than ICM16 which outperformed ICM8), especially when decomposing the previously-mentioned matrices: *s1rmq4m1*, *Na5* and *bundle1* using double precision.

CM In Figure 3.5 it can be seen that CM took more time to decompose most of the benchmarked matrices. However, an interesting result arises when comparing CM and ICM8 for double precision. Specifically, for 3 out of the 14 matrices, ICM8 was slower than CM as it achieved the following speedups: 0.09 for *bcsstk03*, 0.92 for *Cejka7580*, and 0.96 for *Cejka10793*. While the result for *bcsstk03* is not surprising given the matrix's dimensions, the others are. The most likely reason for the lower performance is the non-coalesced access to global memory which is most prominent for ICM8.

Overall, the decomposition of matrices using single precision was faster compared to double precision. However, the difference in speed is not clearly visible from either Figure 3.1 (due to the vertical axis being log-scaled) or Figure 3.5 (due to the range of the speedup factor being too great for the values to be distinguishable). For this reason, the raw execution times for single and double precision are included in Table 3.4 and Table 3.5 respectively.

Matrix	CM	ICM8	ICM16	ICM32
<i>bcsstk03</i>	0.0002	0.0022	0.0020	0.0022
<i>494_bus</i>	0.0292	0.0049	0.0053	0.0043
<i>LeGresley_2508</i>	4.2193	0.0793	0.0498	0.0531
<i>Cejka2842</i>	6.2210	3.0391	2.1182	2.1412
<i>rail1_5177</i>	55.1124	1.4350	1.0669	1.1022
<i>c-31</i>	59.3208	0.1598	0.1330	0.1327
<i>s3rmt3m3</i>	61.9867	0.1450	0.1133	0.1684
<i>s1rmq4m1</i>	67.8509	0.0641	0.0502	0.0505
<i>Na5</i>	62.3995	0.0817	0.0636	0.0649
<i>Cejka5943</i>	90.1114	0.7035	0.5230	0.4856
<i>fp</i>	179.7054	0.5278	0.3980	0.3690
<i>Cejka7580</i>	151.7981	12.2164	3.0289	2.2853
<i>bundle1</i>	617.5120	0.4853	0.3425	0.3041
<i>Cejka10793</i>	643.3462	9.2837	2.8510	2.2107

Table 3.4: The execution time (in seconds) of decomposition for all implementations on the set of matrices (Table 3.2) using **single** precision. The fastest time for each matrix is highlighted in green.

From the results presented in Table 3.4 it could be concluded that ICM32 is the most suitable implementation for decomposing matrices using single precision. In terms of double precision the same statement could be made when looking at Table 3.5. However, since the results presented in the mentioned tables were only a small subset of all results, verification of this claim is required for the entire set of 63 matrices.

Matrix	CM	ICM8	ICM16	ICM32
bcsstk03	0.0003	0.0027	0.0026	0.0027
494_bus	0.0299	0.0084	0.0070	0.0082
LeGresley_2508	4.3542	0.2055	0.4805	0.6118
Cejka2842	6.9110	4.5995	3.6436	3.4559
rail_5177	67.9030	3.0109	2.3882	2.1754
c-31	72.3863	0.4913	0.4166	0.3349
s3rmt3m3	74.0106	0.3704	0.2997	0.2577
s1rmq4m1	81.2749	0.1059	0.0843	0.0714
Na5	67.2166	0.1543	0.1365	0.1243
Cejka5943	104.6150	70.8865	56.2768	44.5275
fp	154.8232	0.9641	0.7715	0.6287
Cejka7580	159.6421	172.9549	138.9242	107.8041
bundle1	679.3846	0.8859	0.6648	0.5079
Cejka10793	699.9634	731.9412	556.0243	419.1401

Table 3.5: The execution time (in seconds) of decomposition for all implementations on the set of matrices (Table 3.2) using **double** precision. The fastest time for each matrix is highlighted in green.

3.4.3 Performance of Implementations Across All Matrices

This section shows the bandwidth, speedup comparison, and accuracy of results - using both single and double precision - for the decomposition implementations listed in Section 3.1. The metrics were measured across the entire set of 63 matrices and the benchmarks were run on the platform specified in Table 3.1. In order to illustrate how ICMx compares to CM on matrices that increase in size, the matrices in the graphs were sorted from smallest to largest. The bandwidth results can be found in Figure 3.8, the speedup comparison between CM and ICMx can be found in Figure 3.9, and the accuracy of the results can be found in Figure 3.10. All figures in this section have a log-scaled vertical axis as the range of values was too great to present any coherent data.

Bandwidth As shown in Figure 3.8, in terms of bandwidth, the ICMx implementations achieved similar results with the exception of ICM8 that is noticeably less performant. The lack of ICM8's performance is more prominent for single precision where the issue with non-coalesced global memory access appears to be making a difference. This is further supported by the fact that after a certain point (matrix 46) ICM8 appears to be consistently falling behind ICM32 in terms of bandwidth achieved - especially noticeable for the larger dense matrices (the three dips in bandwidth after matrix 55 in Figure 3.8a).

In terms of double precision the performance of ICMx is more consistent. The general rule of ICM8 performing worse than ICM16 and ICM32 for larger matrices still stands and the performance of ICM16 for matrices past matrix 30 is - in the majority of cases - less than that of ICM32. The dips in bandwidth of ICMx for matrices past matrix 25 are caused by the dense matrices found in the set. For the majority of matrices, the bandwidth achieved during their decomposition was greater than 1 GByte/s for both single and double precision. On the other hand, Figure 3.8 shows that the bandwidth achieved by CM decreases in an almost logarithmic fashion with increasing matrix dimensions.

Contrary to what the subset of results presented in Section 3.4.1 seemed to suggest, it can be seen from Figure 3.8a (single precision) and Figure 3.8b (double precision) that CM outperformed ICMx in more

cases than just one. Although, it must be mentioned that the matrices on which CM achieved a higher bandwidth than ICM x did have dimensions between 27×27 and 415×415 .

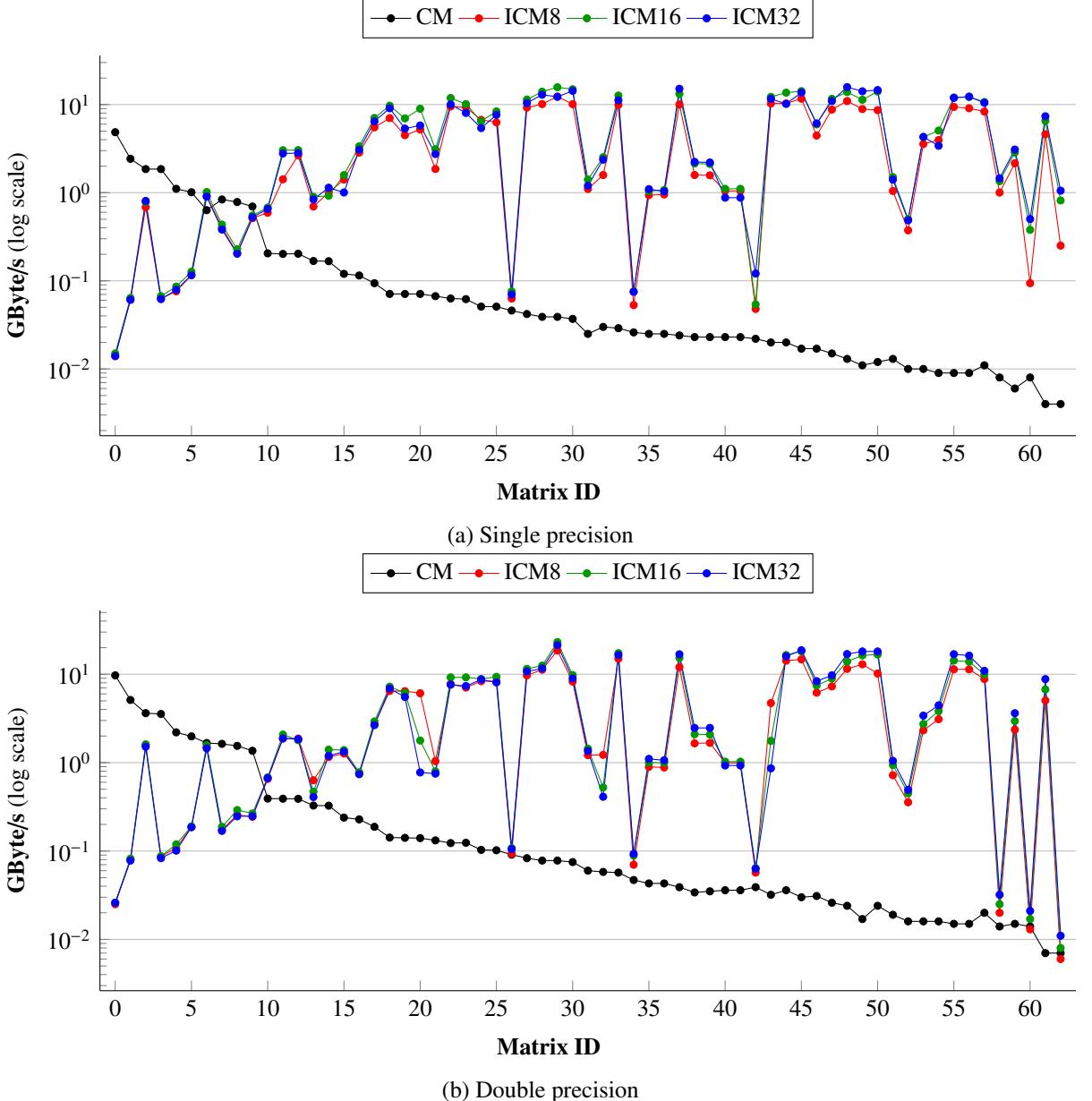


Figure 3.8: Bandwidths achieved by decomposition implementations listed in Section 3.1 on the entire set of 63 matrices using both single and double precision. Matrix ID signifies the ID of the matrices, after they have been sorted according to their dimension from smallest to largest. The vertical axis is log-scaled for better visibility of differences between implementations.

Speedup The speedup comparison in Figure 3.9 is presented for the sake of completeness and to show how much faster the ICM x implementations were compared to CM. Specifically, when single precision was used, all ICM x implementations were faster in 54/63 cases. In terms of double precision, ICM8 was

faster in 51/63 cases, and ICM32 and ICM16 were faster in 53/63. However, as mentioned before, all of the matrices (with the two exceptions for ICM8 detailed in *CM* in Section 3.4.2) that CM decomposed faster than ICM x have dimensions 415×415 or smaller.

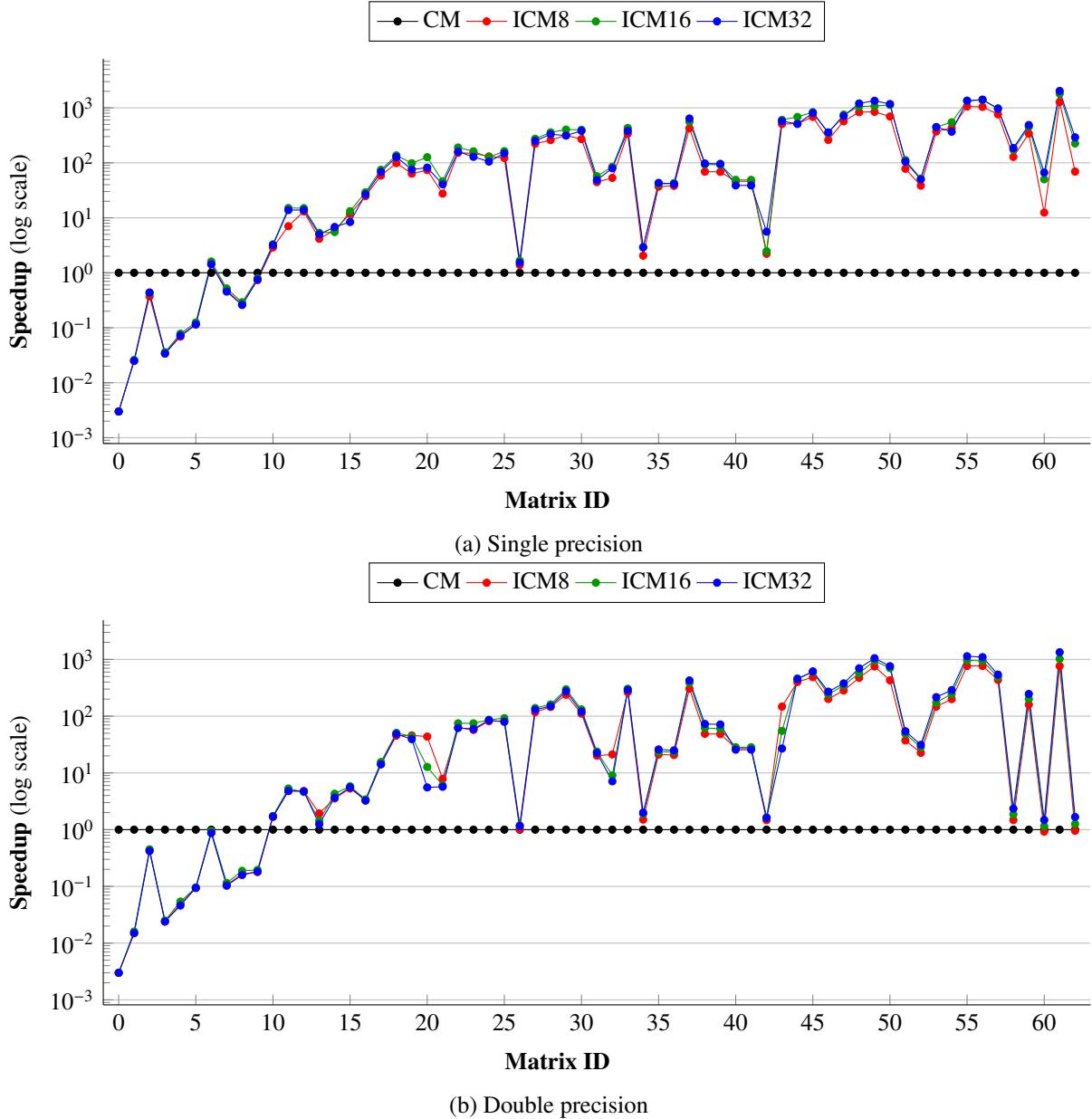


Figure 3.9: Speedup comparison between CM and ICM x implementations on the entire set of 63 matrices using both single and double precision. Matrix ID signifies the ID of the matrices, after they have been sorted according to their dimension from smallest to largest. The vertical axis is log-scaled for better visibility of differences between implementations.

Additionally, Table 3.6 shows the total time required by each implementation to decompose the set of 63 matrices using both single and double precision. The data in this table provides further support to the claim made at the end of Section 3.4.2 which stated that ICM32 is the most suitable implementation for

single and double precision.

Matrix	CM	ICM8	ICM16	ICM32
Single	2393.09	35.88	17.36	13.84
Double	2635.45	1000.27	772.29	592.19

Table 3.6: The total execution time (in seconds) taken by each implementation to decompose the set of 63 matrices (Table 3.2) on the RCI compute cluster specified in Table 3.1 using single and double precision. The fastest time for each precision is highlighted in green.

Accuracy of results While this part is the other key factor of the implementation (the first being speed of execution), it serves more as a means to verify that the presented performance does not come at the cost of drastically inaccurate results. Figure 3.10 shows the maximum difference between the input matrix \mathbb{A} and the multiplication of the decomposed matrices (\mathbb{L} and \mathbb{U} , or \mathbb{Z}), i.e.

$$\max |\mathbb{A} - \mathbb{L}\mathbb{U}| .$$

In other words, the matrix that results from multiplying the matrices obtained from the decomposition (\mathbb{L} and \mathbb{U}) should - ideally - be the same as the input matrix (\mathbb{A}). The values presented in this part are the largest differences between the actual results and the ideal results.

For the purpose of this project, the maximum difference will also be referred to as the *error*. Similarly to the previous figures, the vertical axis is log-scaled in order to present the results more clearly. This is due to the fact that the data ranged from 268,435,500 to 0 for single precision and the median of the values for double precision was 2.32831×10^{-10} with the data ranging from 2 to 0. The figure only shows data for ICMx as the accuracy of the results did not differ for the ICMx implementations.

Overall, it seems that the accuracy of results produced by both approaches (CM and ICMx) is similar, nevertheless, values for both single and double precision will be analyzed.

Single precision The statistical analysis of the accuracy of results for single precision is presented using a collection of basic statistical indexes in Table 3.7.

The values from the table present the problem of using single precision. Even though CM is a sequential algorithm and should provide the exact solution - as is required in the majority of unit tests - the results produced by it can be drastically different from those expected. Specifically, the average error for CM was 4,540,350.594 which is not usable. On the other hand, since the median is 0.125, and the smallest difference is 0 it seems that the large average was caused by a few extreme values. This claim is further supported by the maximum error achieved by CM which is 268,435,500.

For ICMx, the average error was 36,830.43 which is significantly lower than that of CM. Furthermore, the maximum error and median value of errors achieved by ICMx are all lower than that of CM. Additionally, the standard deviation is 128 times smaller than that of CM.

In summary, all of the facts mentioned for the accuracy of results when using single precision can be used to further promote the claim made at the end of *Numerical method* in Section 1.3.2: "Since Crout's

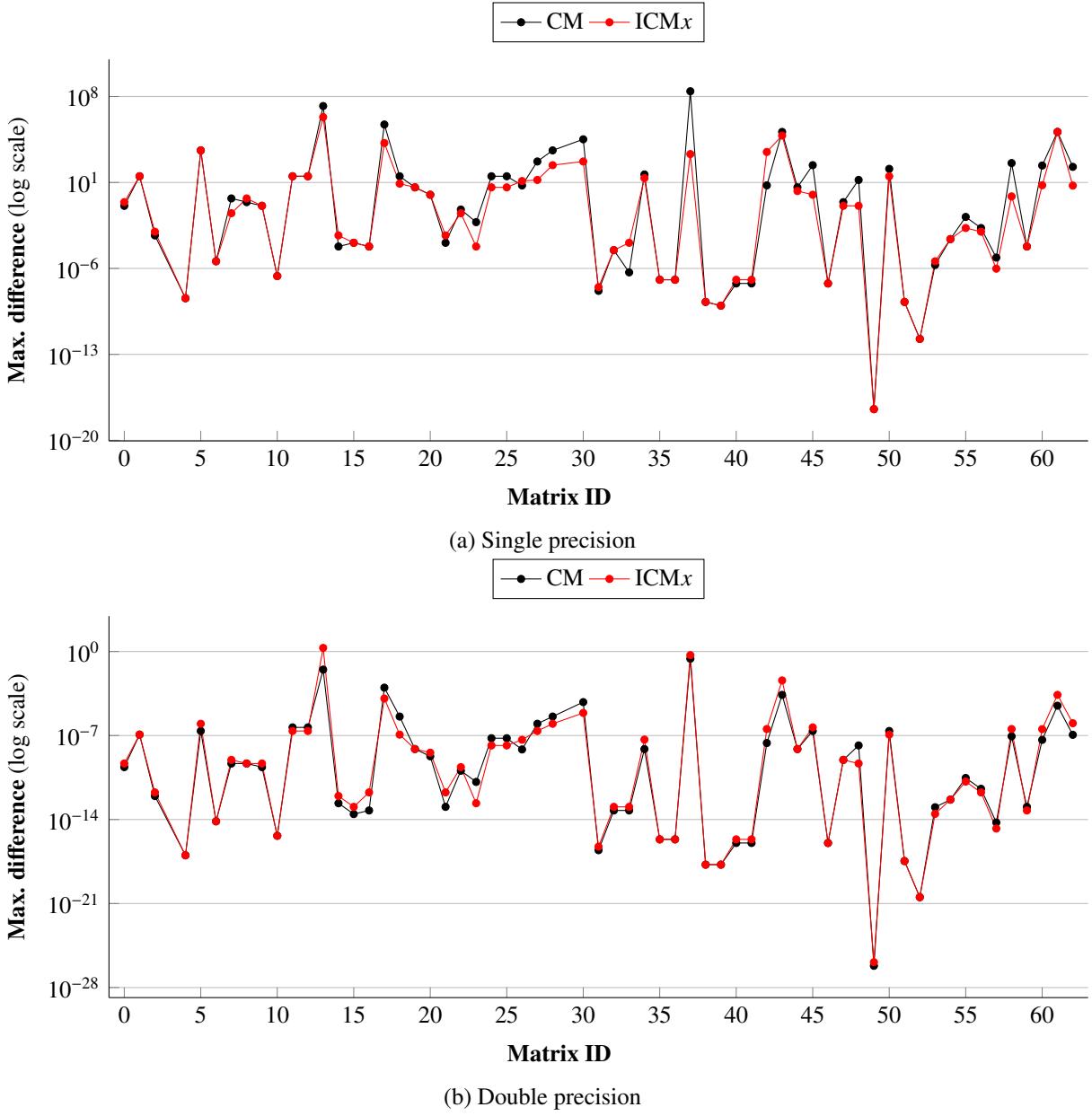


Figure 3.10: Comparison of the accuracy of results between CM and ICMx implementations on the entire set of 63 matrices using both single and double precision. In this instance "accuracy" refers to the maximum difference of $|\mathbb{A} - \mathbb{L}\mathbb{U}|$ where \mathbb{A} is the input matrix and \mathbb{L} and \mathbb{U} are the matrices obtained from the decomposition procedure. The higher the maximum difference, the lower the accuracy of the results (the higher the error). Matrix ID signifies the ID of the matrices, after they have been sorted according to their dimension from smallest to largest. The vertical axis is log-scaled for better visibility of differences between implementations. Note that the vertical axes of both graphs do not cover the same range.

method is direct, it can be theorized that rounding errors may result in it providing less accurate results compared to its numerical modification". In other words, for single precision, the results, obtained from decomposing the set of 63 matrices, suggest that ICMx is more accurate than CM. However, since the

Accuracy index	CM	ICMx
Average	4,540,350.594	36,830.430
Maximum	268,435,500.000	2,097,152.000
Minimum	0.000	0.000
Median	0.125	0.031
Std. dev.	33,580,198.190	262,296.394

Table 3.7: Statistical indexes for the accuracy of the results obtained from the decomposition procedure performed by CM and ICMx using single precision. The accuracy of the results was rounded to three decimal places as that was sufficient to portray the characteristics of the dataset.

set contained only 63 matrices, further benchmarks on larger sets are required to verify this claim.

Double precision Similarly to single precision, the statistical analysis of the accuracy of results for double precision is presented using a collection of basic statistical indexes in Table 3.8.

Accuracy index	CM	ICMx
Average	0.0045	0.0398
Maximum	0.2500	2.0000
Minimum	0.0000	0.0000
Median	2.3283×10^{-10}	4.6566×10^{-10}
Std. dev.	0.0314	0.2566

Table 3.8: Statistical indexes for the accuracy of the results obtained from the decomposition procedure performed by CM and ICMx using double precision. The accuracy of the results was rounded to four decimal places to portray the characteristics of the dataset. Furthermore, some values were simply too small and as such they were listed using scientific notation.

Unlike the errors present for single precision, the results achieved using double precision were less erroneous. The average error in the results produced by CM was 0.0045, the maximum error was 0.25 and the minimum error was 0. Furthermore, the median error was at a very accurate 2.33×10^{-10} . However, the most drastic difference when comparing the errors of CM between single and double precision is the standard deviation. For the former, the deviation of errors was 33,580,198.19, whereas for the latter it was 0.0314.

When comparing CM to ICMx for double precision, it can be seen that the roles have switched and that ICMx is now the less-accurate implementation across all indexes. For ICMx, the average error is 8 times larger than that of CM. Similarly, the median of ICMx is twice that of CM. Interestingly, the standard deviation of errors for ICMx is also 8 times greater than that of CM.

Ultimately, it can be concluded that CM is the format that produces more accurate matrices when using double precision. However, the performance of CM remains to be multitudes lower than that of ICMx.

Further benchmarks on real-life problems are required to determine whether the errors achieved by ICM x are too severe, or if the speedup compared to CM is worth the slightly more inaccurate results.

3.4.4 Comparison of Optimizations [TO](#)

This section aims to show the evolution of the ICM x implementations throughout the development process. Since the benchmarks for each optimization were executed during the development process, they were run on a different platform than the results presented in Sections 3.4.1, 3.4.2, and 3.4.3. The platform used during development was one of the compute servers available to students and staff of the Faculty of Nuclear Sciences and Physical Engineering of the Czech Technical University in Prague. The specifications of the GP7 platform are listed in Table 3.9.

CPU	Intel(R) Core(TM) i9-9900KF CPU @ 3.60GHz (8 cores, 16 threads)
RAM	62GB RAM
GPU	2× Nvidia GeForce RTX 3060 12GB GDDR6 (360 GByte/s memory bandwidth)
Operating System	Arch Linux (Kernel Version: 5.18.8)
Compiler	GCC 12.1.1
CUDA	CUDA 11.7

Table 3.9: Specifications of GP7 compute server that the benchmarks were run on during development.

Furthermore, a subset of the 63 set of matrices was used for measuring the performance of implementations during development. The reasons for this were the following:

- The initial implementations on the GPU were egregiously slow, thus, only sparse matrices smaller than $6,000 \times 6,000$ were used at the time.
- The final set of 63 matrices underwent numerous changes as newly-found matrices were added throughout the development process. Only once the GPU implementation became adequately performant, larger and dense matrices were added. Once the set was completed, there was an attempt to re-do the benchmark results for key optimizations, however, the compute cluster time limit was not sufficient as the decomposition of some dense matrices would require up to 2 days with the initial implementations.

The set of matrices that was used to measure performance during development comprised of 50 sparse matrices with dimensions ranging from 27×27 to $5,832 \times 5,832$.

Other than the key optimizations mentioned in Section 2.3, two other will be described in order to show the effect that the value of `sectionSize` can have on both the speed of the computation and the accuracy of the results. Specifically, the key optimizations that will be presented are the following:

- **Base** - The naive implementation (mentioned in *Initial naive implementation* in Section 2.3).
- **SM** - The first version of the implementation that used shared memory (mentioned in *Calculation by tiles using shared memory* in Section 2.3).
- **SM opt.** - The optimized version of the shared-memory implementation (mentioned in *Elimination of conditions* in Section 2.3).

- **ConvRow005** - The initial implementation of convergence by sections: convergence by sections of 512 rows with $tol = 0.005$.
- **ConvRow0** - The upgraded version of convergence by row sections where $tol = 0$.
- **ParSecGPU** - The version of convergence by parallel sections where `sectionSize` was limited by the capabilities of the GPU (mentioned in *Section size dependent on maximum active threads* in Section 2.3).
- **ICM32** - The final version of the implementation (mentioned in *Iterative Crout method* in Section 2.2.2).

Note that the *Base*, *SM*, and *SM opt.* optimizations all had their tolerance value tol set to 0.005.

Execution times The results will be presented only for double precision and for `BLOCK_SIZE` set to 32. The reason behind this is that the results are shown in order to detail the evolution of the implementation, rather than compare differences in thread-per-block configurations. The execution times for the decomposition of the set of 50 matrices for the optimizations listed above are shown in Figure 3.11 (vertical axis is log-scaled for clarity) and the total time taken for each optimization to decompose the set of 50 matrices is shown in Table 3.10.

As can be seen from Figure 3.11 the *Base* optimization (orange line) is found at the top of the other optimizations for majority of matrices, which indicates that it took the most time to decompose each individual matrix. This fact is further supported by the total time taken by *Base* to decompose the entire set of 50 matrices, which is shown in Table 3.10. According to the graph, it would seem that the *SM* and *SM opt.* optimizations achieved similar times, however, as can be seen in Table 3.10, they were almost 3 and 4 times faster, respectively, than *Base*.

Optimization	Base	SM	SM opt.	ConvRow005	ConvRow0	ParSecGPU	ICM32
Time [s]	2140.83	745.15	514.91	57.79	143.68	89.91	43.88

Table 3.10: The total execution time (in seconds) taken by each optimization to decompose the set of 50 matrices.

It may be difficult to discern the performance of the remaining optimizations in Figure 3.11. However, the results in Table 3.10 show that ICM32 was the fastest overall. In general, the table effectively shows how each optimization helped improve the speed of decomposition - specifically the total execution time decreased almost 50 times from *Base* to ICM32. For reference, the total execution time required for ICM32 to decompose this subset of 50 matrices on the RCI compute cluster node (presented in Table 3.1) was 5.02 seconds. It can be seen that the total execution time for *ConvRow005* was 57.79 seconds, which is significantly faster than the remaining optimizations (apart from ICM32). The reason behind this is that *ConvRow005* had its tolerance value tol set to 0.005, thus, as can be seen in Table 3.11 the accuracy of the results it produced from the set of 50 matrices was not as good as that of ICM32.

Accuracy In terms of accuracy, Table 3.11 shows that *ConvRow0* achieved the most accurate decomposition results with an average error of 0.0397 and standard deviation of 0.1752. This is due to the fact that the optimization decomposed the input matrix by converging by sections comprised of 512 rows.

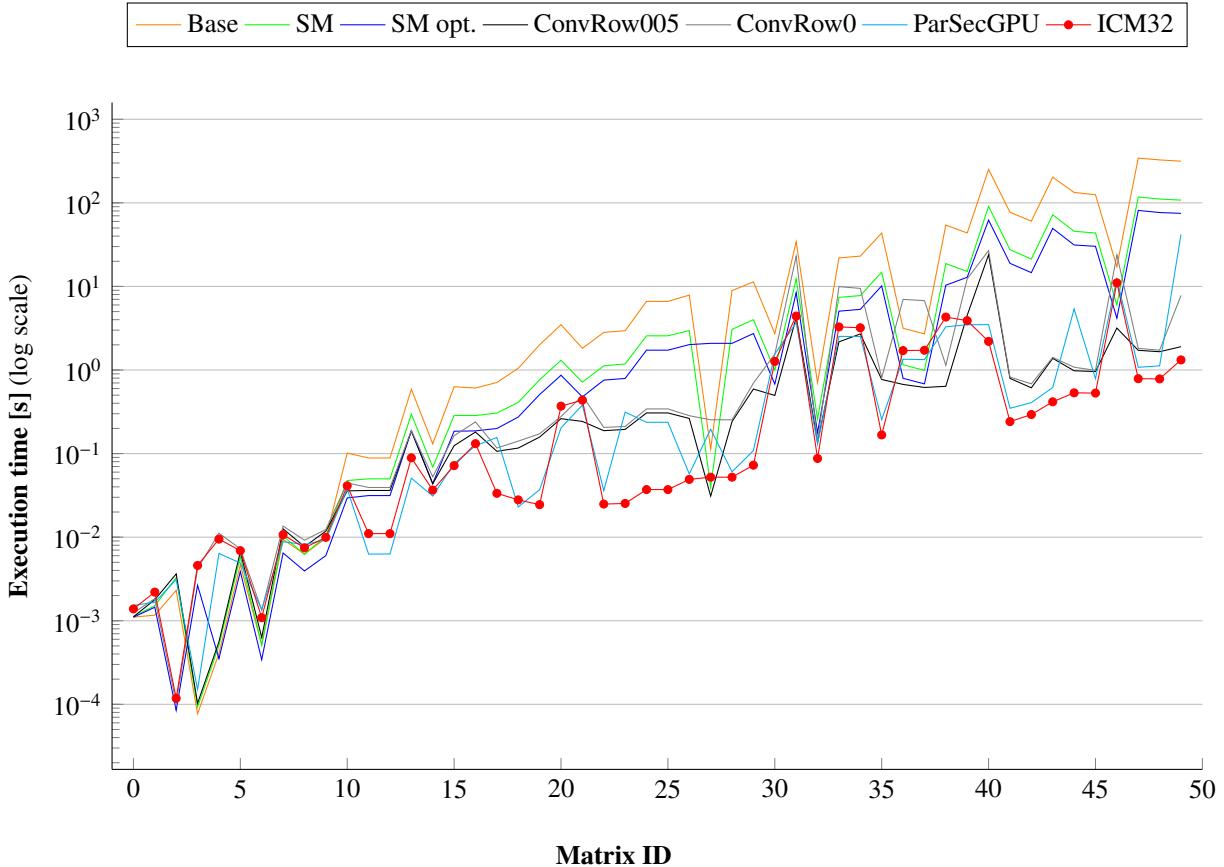


Figure 3.11: The execution times (in seconds) taken by each decomposition optimization listed above to decompose the set of 50 matrices using double precision and with 32×32 threads per block. Matrix ID signifies the ID of the matrices, after they have been sorted according to their dimension from smallest to largest. The vertical axis is log-scaled for better visibility of differences between optimizations.

This means that if the tolerance value *tol* was set to zero, then the optimization would perform many iterations before converging. However, this gain in accuracy reflected on the relatively poor performance - shown in Table 3.10. Specifically, *ConvRow0* required 143.68 seconds to decompose all 50 matrices.

Accuracy index	ConvRow005	ConvRow0	ParSecGPU	ICM32
Average	0.1559	0.0397	0.7004	0.0595
Maximum	5.6900	1.0000	29.7813	2.0000
Minimum	0.0000	0.0000	0.0000	0.0000
Median	8.57963×10^{-5}	1.25712×10^{-10}	4.07454×10^{-10}	1.25712×10^{-10}
Std. dev.	0.8097	0.1752	4.1742	0.2979

Table 3.11: Statistical indexes for the accuracy of the results obtained from the decomposition procedure performed by the optimizations listed at the beginning of this section. The procedure was done using double precision and with `BLOCK_SIZE` set to 32.

When both speed and accuracy were taken into account, the ICM32 optimization excelled more so in speed, than in accuracy. However, as mentioned before, since the execution time of the most-accurate optimization (*ConvRow0*) was insufficient the procedure used in ICM32 was selected as the optimal choice out of all the optimizations.

Conclusion TODO

Put my conclusion text here (1-3 pages, do not divide it into sub-pages) or insert it from a separate file using: `\input{conclusion.tex}`.

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Appendix A

CUDA matrix multiplication benchmark code

The full code for the matrix multiplication benchmark is shown in Listing A.1 (file `matrixMul.cu`).

```
1 /**
2 * Copyright 1993–2015 NVIDIA Corporation. All rights reserved.
3 *
4 * Please refer to the NVIDIA end user license agreement (EULA) associated
5 * with this source code for terms and conditions that govern your use of
6 * this software. Any use, reproduction, disclosure, or distribution of
7 * this software and related documentation outside the terms of the EULA
8 * is strictly prohibited.
9 *
10 */
11
12 /**
13 * Matrix multiplication: C = A * B.
14 * Host code.
15 *
16 * This sample implements matrix multiplication which makes use of shared memory
17 * to ensure data reuse, the matrix multiplication is done using tiling
18 * approach. It has been written for clarity of exposition to illustrate various
19 * CUDA programming principles, not with the goal of providing the most
20 * performant generic kernel for matrix multiplication. See also: V. Volkov and
21 * J. Demmel, "Benchmarking GPUs to tune dense linear algebra," in Proc. 2008
22 * ACM/IEEE Conf. on Supercomputing (SC '08), Piscataway, NJ: IEEE Press, 2008,
23 * pp. Art. 31:1–11.
24 */
25
26 // System includes
27 #include <assert.h>
28 #include <stdio.h>
29
30 // CUDA runtime
31 #include <cuda_runtime.h>
32
33 // Helper functions and utilities to work with CUDA
34 #include <helper_cuda.h>
35 #include <helper_functions.h>
```

```

37 template <int BLOCK_SIZE>
38 _global__ void MatrixMulCUDAGlobal(float *C, float *A, float *B, int wA, int wB) ←
39 {
40     // Each thread computes one element of C by accumulating results into Cvalue
41     float Cvalue = 0;
42     int row = blockIdx.y * blockDim.y + threadIdx.y;
43     int col = blockIdx.x * blockDim.x + threadIdx.x;
44     for( int i = 0; i < wA; ++i )
45         Cvalue += A[row * wA + i] * B[i * wB + col];
46
47     C[row * wB + col] = Cvalue;
48 }
49 /**
50 * Matrix multiplication (CUDA Kernel) on the device: C = A * B
51 * wA is A's width and wB is B's width
52 */
53 template <int BLOCK_SIZE>
54 _global__ void MatrixMulCUDA(float *C, float *A, float *B, int wA, int wB) {
55     // Block index
56     int bx = blockIdx.x;
57     int by = blockIdx.y;
58
59     // Thread index
60     int tx = threadIdx.x;
61     int ty = threadIdx.y;
62
63     // Index of the first sub-matrix of A processed by the block
64     int aBegin = wA * BLOCK_SIZE * by;
65
66     // Index of the last sub-matrix of A processed by the block
67     int aEnd = aBegin + wA - 1;
68
69     // Step size used to iterate through the sub-matrices of A
70     int aStep = BLOCK_SIZE;
71
72     // Index of the first sub-matrix of B processed by the block
73     int bBegin = BLOCK_SIZE * bx;
74
75     // Step size used to iterate through the sub-matrices of B
76     int bStep = BLOCK_SIZE * wB;
77
78     // Csub is used to store the element of the block sub-matrix
79     // that is computed by the thread
80     float Csub = 0;
81
82     // Loop over all the sub-matrices of A and B
83     // required to compute the block sub-matrix
84     for (int a = aBegin, b = bBegin; a <= aEnd; a += aStep, b += bStep) {
85         // Declaration of the shared memory array As used to
86         // store the sub-matrix of A
87         _shared__ float As[BLOCK_SIZE][BLOCK_SIZE];
88
89         // Declaration of the shared memory array Bs used to
90         // store the sub-matrix of B
91         _shared__ float Bs[BLOCK_SIZE][BLOCK_SIZE];
92
93         // Load the matrices from device memory

```

```

94     // to shared memory; each thread loads
95     // one element of each matrix
96     As[ty][tx] = A[a + wA * ty + tx];
97     Bs[ty][tx] = B[b + wB * ty + tx];
98
99     // Synchronize to make sure the matrices are loaded
100    __syncthreads();
101
102    // Multiply the two matrices together;
103    // each thread computes one element
104    // of the block sub-matrix
105    #pragma unroll
106
107    for (int k = 0; k < BLOCK_SIZE; ++k) {
108        Csub += As[ty][k] * Bs[k][tx];
109    }
110
111    // Synchronize to make sure that the preceding
112    // computation is done before loading two new
113    // sub-matrices of A and B in the next iteration
114    __syncthreads();
115}
116
117    // Write the block sub-matrix to device memory;
118    // each thread writes one element
119    int c = wB * BLOCK_SIZE * by + BLOCK_SIZE * bx;
120    C[c + wB * ty + tx] = Csub;
121}
122
123 void ConstantInit(float *data, int size, float val) {
124     for (int i = 0; i < size; ++i) {
125         data[i] = val;
126     }
127 }
128
129 /**
130 * Run a simple test of matrix multiplication using CUDA
131 */
132 int MatrixMultiply(int argc, char **argv, int block_size, const dim3 &dimsA,
133 const dim3 &dimsB) {
134     // Allocate host memory for matrices A and B
135     unsigned int size_A = dimsA.x * dimsA.y;
136     unsigned int mem_size_A = sizeof(float) * size_A;
137     float *h_A;
138     checkCudaErrors(cudaMallocHost((void **)&h_A, mem_size_A));
139     unsigned int size_B = dimsB.x * dimsB.y;
140     unsigned int mem_size_B = sizeof(float) * size_B;
141     float *h_B;
142     checkCudaErrors(cudaMallocHost((void **)&h_B, mem_size_B));
143     cudaStream_t stream;
144
145     // Initialize host memory
146     const float valB = 0.01f;
147     ConstantInit(h_A, size_A, 1.0f);
148     ConstantInit(h_B, size_B, valB);
149
150     // Allocate device memory
151     float *d_A, *d_B, *d_C;

```

```

152
153 // Allocate host matrix C
154 dim3 dimsC(dimsB.x, dimsA.y, 1);
155 unsigned int mem_size_C = dimsC.x * dimsC.y * sizeof(float);
156 float *h_C;
157 checkCudaErrors(cudaMallocHost((void **) &h_C, mem_size_C));
158
159 if (h_C == NULL) {
160     fprintf(stderr, "Failed to allocate host matrix C!\n");
161     exit(EXIT_FAILURE);
162 }
163
164 checkCudaErrors(cudaMalloc(reinterpret_cast<void **>(&d_A), mem_size_A));
165 checkCudaErrors(cudaMalloc(reinterpret_cast<void **>(&d_B), mem_size_B));
166 checkCudaErrors(cudaMalloc(reinterpret_cast<void **>(&d_C), mem_size_C));
167 // Allocate CUDA events that we'll use for timing
168 cudaEvent_t start, stop;
169 checkCudaErrors(cudaEventCreate(&start));
170 checkCudaErrors(cudaEventCreate(&stop));
171
172 checkCudaErrors(cudaStreamCreateWithFlags(&stream, cudaStreamNonBlocking));
173
174 // copy host memory to device
175 checkCudaErrors(
176 cudaMemcpyAsync(d_A, h_A, mem_size_A, cudaMemcpyHostToDevice, stream));
177 checkCudaErrors(
178 cudaMemcpyAsync(d_B, h_B, mem_size_B, cudaMemcpyHostToDevice, stream));
179
180 // Setup execution parameters
181 dim3 threads(block_size, block_size);
182 dim3 grid(dimsB.x / threads.x, dimsA.y / threads.y);
183
184 // Create and start timer
185 printf("Computing result using CUDA Kernel...\n");
186
187 // Performs warmup operation using matrixMul CUDA kernel
188 if (block_size == 16) {
189     MatrixMulCUDA<16>
190     <<<grid, threads, 0, stream>>>(d_C, d_A, d_B, dimsA.x, dimsB.x);
191 } else {
192     MatrixMulCUDA<32>
193     <<<grid, threads, 0, stream>>>(d_C, d_A, d_B, dimsA.x, dimsB.x);
194 }
195
196 printf("done\n");
197 checkCudaErrors(cudaStreamSynchronize(stream));
198
199 // Record the start event
200 checkCudaErrors(cudaEventRecord(start, stream));
201
202 // Execute the kernel
203 int nIter = 10;
204
205 for (int j = 0; j < nIter; j++) {
206     if (block_size == 16) {
207         MatrixMulCUDA<16>
208         <<<grid, threads, 0, stream>>>(d_C, d_A, d_B, dimsA.x, dimsB.x);
209     } else {

```

```

210     MatrixMulCUDA<32>
211     <<<grid, threads, 0, stream>>>(d_C, d_A, d_B, dimsA.x, dimsB.x);
212 }
213 }
214
215 // Record the stop event
216 checkCudaErrors(cudaEventRecord(stop, stream));
217
218 // Wait for the stop event to complete
219 checkCudaErrors(cudaEventSynchronize(stop));
220
221 float msecTotal = 0.0f;
222 checkCudaErrors(cudaEventElapsedTime(&msecTotal, start, stop));
223
224 // Compute and print the performance
225 float msecPerMatrixMul = msecTotal / nIter;
226 double flopsPerMatrixMul = 2.0 * static_cast<double>(dimsA.x) *
227 static_cast<double>(dimsA.y) *
228 static_cast<double>(dimsB.x);
229 double gigaFlops =
230 (flopsPerMatrixMul * 1.0e-9f) / (msecPerMatrixMul / 1000.0f);
231 printf(
232 "Performance= %.2f GFlop/s, Time= %.3f msec, Size= %.0f Ops,"
233 " WorkgroupSize= %u threads/block\n",
234 gigaFlops, msecPerMatrixMul, flopsPerMatrixMul, threads.x * threads.y);
235
236 // Copy result from device to host
237 checkCudaErrors(
238 cudaMemcpyAsync(h_C, d_C, mem_size_C, cudaMemcpyDeviceToHost, stream));
239 checkCudaErrors(cudaStreamSynchronize(stream));
240
241 printf("Checking computed result for correctness: ");
242 bool correct = true;
243
244 // test relative error by the formula
245 // |<x, y>_cpu - <x,y>_gpu| / |x|, |y| < eps
246 double eps = 1.e-6; // machine zero
247
248 for (int i = 0; i < static_cast<int>(dimsC.x * dimsC.y); i++) {
249     double abs_err = fabs(h_C[i] - (dimsA.x * valB));
250     double dot_length = dimsA.x;
251     double abs_val = fabs(h_C[i]);
252     double rel_err = abs_err / abs_val / dot_length;
253
254     if (rel_err > eps) {
255         printf("Error! Matrix[%05d]=%.8f, ref=%.8f error term is > %E\n", i,
256               h_C[i], dimsA.x * valB, eps);
257         correct = false;
258     }
259 }
260
261 printf("%s\n", correct ? "Result = PASS" : "Result = FAIL");
262
263 // Clean up memory
264 checkCudaErrors(cudaFreeHost(h_A));
265 checkCudaErrors(cudaFreeHost(h_B));
266 checkCudaErrors(cudaFreeHost(h_C));
267 checkCudaErrors(cudaFree(d_A));

```

```

268 checkCudaErrors(cudaFree(d_B));
269 checkCudaErrors(cudaFree(d_C));
270 checkCudaErrors(cudaEventDestroy(start));
271 checkCudaErrors(cudaEventDestroy(stop));
272 printf(
273     "\nNOTE: The CUDA Samples are not meant for performance"
274     " measurements. Results may vary when GPU Boost is enabled.\n");
275
276 if (correct) {
277     return EXIT_SUCCESS;
278 } else {
279     return EXIT_FAILURE;
280 }
281 }
282
283 /**
284 * Program main
285 */
286 int main(int argc, char **argv) {
287     printf("[Matrix Multiply Using CUDA] - Starting...\n");
288
289     if (checkCmdLineFlag(argc, (const char **)argv, "help") ||
290         checkCmdLineFlag(argc, (const char **)argv, "?")) {
291         printf("Usage -device=n (n >= 0 for deviceID)\n");
292         printf("      -wA=WidthA -hA=HeightA (Width x Height of Matrix A)\n");
293         printf("      -wB=WidthB -hB=HeightB (Width x Height of Matrix B)\n");
294         printf(
295             " Note: Outer matrix dimensions of A & B matrices"
296             " must be equal.\n");
297
298     exit(EXIT_SUCCESS);
299 }
300
301 // This will pick the best possible CUDA capable device, otherwise
302 // override the device ID based on input provided at the command line
303 int dev = findCudaDevice(argc, (const char **)argv);
304
305 int block_size = 32;
306
307 int mul = 10;
308
309 dim3 dimsA(mul * block_size, mul * block_size, 1);
310 dim3 dimsB(mul * block_size, mul * block_size, 1);
311
312 // width of Matrix A
313 if (checkCmdLineFlag(argc, (const char **)argv, "wA")) {
314     dimsA.x = getCmdLineArgumentInt(argc, (const char **)argv, "wA");
315 }
316
317 // height of Matrix A
318 if (checkCmdLineFlag(argc, (const char **)argv, "hA")) {
319     dimsA.y = getCmdLineArgumentInt(argc, (const char **)argv, "hA");
320 }
321
322 // width of Matrix B
323 if (checkCmdLineFlag(argc, (const char **)argv, "wB")) {
324     dimsB.x = getCmdLineArgumentInt(argc, (const char **)argv, "wB");
325 }

```

```

326
327 // height of Matrix B
328 if (checkCmdLineFlag(argc, (const char **)argv, "hB")) {
329     dimsB.y = getCmdLineArgumentInt(argc, (const char **)argv, "hB");
330 }
331
332 if (dimsA.x != dimsB.y) {
333     printf("Error: outer matrix dimensions must be equal. (%d != %d)\n",
334         dimsA.x, dimsB.y);
335     exit(EXIT_FAILURE);
336 }
337
338 printf("MatrixA(%d,%d), MatrixB(%d,%d)\n", dimsA.x, dimsA.y, dimsB.x,
339         dimsB.y);
340
341 int matrix_result = MatrixMultiply(argc, argv, block_size, dimsA, dimsB);
342
343 exit(matrix_result);
344 }
```

Listing A.1: Matrix multiplication benchmark code. Taken from Nvidia's samples located in the users home directory by default: `$HOME/NVIDIA-samples/0_Introduction/matrixMul/`.

Appendix B

Decomposition project build script arguments

The `build` script arguments, i.e. the usage instructions are shown in Listing B.1 (file `build`).

```
1  usage: $0 [options] [target ...]
2
3  By default, the script does not select any target. Build targets available for
4  selection are listed below. If the --install option is used, the Decomposition ←
5      header
6  files as well as the selected targets will be installed into the directory
7  specified by the --prefix option.
8
9  Targets:
10   all          Special target which includes all other targets.
11   benchmark    Compile the 'src/Benchmark' directory.
12   tests        Compile unit tests in the 'src/UnitTests' directory.
13
14  General options:
15   --help         Write this help list and exit.
16   --verbose      Enables verbose build.
17   --install=yes/no  Enables the installation of Decomposition ←
18       files. '$INSTALL' by default.
19   --prefix=PATH  Prefix for the installation directory. '←
20       $HOME/.local' by default.
21
22  Options affecting all targets:
23   --offline-build=yes/no  Disables online updates during the build. ←
24       '$OFFLINE_BUILD' by default.
25   --build=Debug/Release    Build type.
26   --build-jobs=NUM         Number of processes to be used for the ←
27       build. It is set to the number of available CPU cores by default.
28   --cmake=CMAKE            Path to the cmake command. '$CMAKE' by ←
29       default.
30   --cmake-only=yes/no     Run only the cmake command, don't actually←
31       build anything. '$CMAKE_ONLY' by default.
32   --compiler=gcc/clang/icc Selects the compiler to use. '$COMPILER' ←
33       by default.
34   --with-mpi=yes/no       Enables MPI. '$WITH_MPI' by default (←
35       OpenMPI required).
```

```

27 --with-cuda=yes/no                      Enables CUDA. '$WITH_CUDA' by default (←
28   CUDA Toolkit is required).               $WITH_CUDA' by default.
29 --with-cuda-arch=all/auto/3.0/3.5/...    Chooses CUDA architecture. '←
30   $WITH_CUDA_ARCH' by default.
31 --with-openmp=yes/no                     Enables OpenMP. '$WITH_OPENMP' by default.
32 --with-gmp=yes/no                       Enables the wrapper for GNU Multiple ←
33   Precision Arithmetic Library. '$WITH_GMP' by default.
34 Options for the 'tests' and 'matrix-tests' targets:
35 --run-tests=yes/no                      Runs unit tests if they were compiled. '←
   $RUN_TESTS' by default.
36 --tests-jobs=NUM                         Number of processes to be used for the ←
   unit tests. It is $TEST_JOBS by default.
37 --with-system-gtest=yes/no                Use GTest installed in the local system ←
   and do not download the latest version. '$WITH_SYSTEM_GTEST' by default.

```

Listing B.1: Decomposition project's `build` script usage. Taken from the Decomposition project repository on GitLab⁴.

Appendix C

Crout method implementation for the CPU

The Crout method implementation for the CPU using matrices \mathbb{L} and \mathbb{U} is shown in Listing C.1 and using matrix \mathbb{Z} in Listing C.2.

```
1 template< typename Matrix1, typename Matrix2, typename Matrix3 >
2 void CroutMethod::decompose( Matrix1& A, Matrix2& L, Matrix3& U )
3 {
4     using RealType = typename Matrix1::RealType;
5     using IndexType = typename Matrix1::IndexType;
6
7     IndexType num_rows = A.getRows();
8     IndexType num_cols = A.getColumns();
9
10    TNL_ASSERT_EQ( num_rows, num_cols, "Matrix A must be a square matrix!" );
11
12    IndexType i, j, k;
13    RealType sum = 0;
14
15    for( j = 0; j < num_rows; ++j )
16    {
17        for( i = j; i < num_rows; ++i )
18        {
19            sum = 0;
20            for( k = 0; k < j; ++k )
21                sum = sum + L.getElement( i, k ) * U.getElement( k, j );
22
23            L.setElement( i, j, A.getElement( i, j ) - sum );
24        }
25
26        for( i = j; i < num_rows; ++i )
27        {
28            TNL_ASSERT( L.getElement( j, j ) != 0,
29                        std::cerr << "L( " << i << ", " << j <<
30                        " ) = 0. Cannot divide by 0." << std::endl );
31            sum = 0;
32            for( k = 0; k < j; ++k )
33                sum = sum + L.getElement( j, k ) * U.getElement( k, i );
34
35            U.setElement( j, i, ( A.getElement( j, i ) - sum ) / L.getElement( j, j ) );
36        }
37    }
```

Listing C.1: Implementation of the Crout method on the CPU using matrices \mathbb{L} and \mathbb{U} . All matrix and variable types are obtained from template arguments of the method. Taken from the Decomposition project repository on GitLab⁴.

```

1 template< typename Matrix1, typename Matrix2 >
2 void CroutMethod::decompose( Matrix1& A, Matrix2& Z )
3 {
4     using RealType = typename Matrix1::RealType;
5     using IndexType = typename Matrix1::IndexType;
6
7     IndexType num_rows = A.getRows();
8     IndexType num_cols = A.getColumns();
9
10    TNL_ASSERT_EQ( num_rows, num_cols, "Matrix A must be a square matrix!" );
11
12    IndexType i, j, k;
13    RealType sum = 0;
14
15    for( j = 0; j < num_rows; ++j )
16    {
17        for( i = j; i < num_rows; ++i )
18        {
19            sum = 0;
20            for( k = 0; k < j; ++k )
21                sum = sum + Z.getElement( i, k ) * Z.getElement( k, j );
22
23            Z.setElement( i, j, A.getElement( i, j ) - sum );
24        }
25
26        for( i = j; i < num_rows; ++i )
27        {
28            if( j == i ) continue;
29
30            TNL_ASSERT( Z.getElement( j, j ) != 0,
31                        std::cerr << "Z( " << j << ", " << j <<
32                        " ) = 0. Cannot divide by 0." << std::endl );
33            sum = 0;
34            for( k = 0; k < j; ++k )
35                sum = sum + Z.getElement( j, k ) * Z.getElement( k, i );
36
37            Z.setElement( j, i, ( A.getElement( j, i ) - sum ) / Z.getElement( j, j ) );
38        }
39    }
40 }
```

Listing C.2: Implementation of the Crout method on the CPU using matrix \mathbb{Z} . Taken from the Decomposition project repository on GitLab⁴.

Appendix D

Random Dense Matrix Generator Script

The Python script used to generate random dense matrices that were later decomposed in the benchmark can be seen in Listing D.1.

```
1 import numpy as np
2
3 num_mtx_files = 3
4 num_rows_cols_range = [2000, 5000]
5 elements_range = [-1000, 1000]
6
7 mtx_files = np.random.randint(low=num_rows_cols_range[0], high=num_rows_cols_range[1], size=num_mtx_files)
8
9 for num_rows_cols in mtx_files:
10     dense_mtx_filename = f"Cejka{num_rows_cols}.mtx"
11
12     header_lines = [
13         "%MatrixMarket matrix coordinate real general",
14         "%-----",
15         "% Cejka Dense Matrix Collection , Lukas Cejka",
16         "% Insert URL here",
17         f"% name: Cejka/{dense_mtx_filename}",
18         "% date: 2022",
19         "% author: L. Cejka",
20         "% kind: Random Dense Matrix",
21         "%-----",
22     ]
23     header_lines = [line + "\n" for line in header_lines]
24
25     mtx_info = f"{num_rows_cols} {num_rows_cols} {num_rows_cols*num_rows_cols}\n"
26
27     rand_floats = np.random.uniform(low=elements_range[0], high=elements_range[1], size=(num_rows_cols*num_rows_cols))
28     rand_floats = [flt+1 if flt == 0 else flt for flt in rand_floats]
29     rand_floats = [str(flt) + "\n" for flt in rand_floats]
30
31
32     with open(dense_mtx_filename, 'w') as f:
33         f.writelines(header_lines)
34         f.write(mtx_info)
35         for col in range(1, num_rows_cols):
```

```
36     for row in range(1, num_rows_cols):
37         f.write(f'{row} {col} {rand_floats[(col-1)*num_rows_cols + row - 1]}')
```

Listing D.1: Python script for generating random dense matrices in the *SuitSparse Matrix Collection* [2] format. On line 28 it can be seen that any zeros were incremented which was done to assure that the matrices produced would be both strongly regular and composed only of nonzero elements.