Performance enhancement using CUDA in a simulation of heat diffusion

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I. Introduction

This assignment aims to optimize a base code, written in C, that computes a simulation for heat diffusion. For the optimization, we seek to take advantage of GPU programming using CUDA, and explore several alternatives to find the most efficient one.

To find the best performance we will explore different approaches, namely analyzing different configurations, exploring the impact of using shared memory, and the difference between using streams or not.

Knowing that the architecture of the system influences the performance obtained, the first step of our work is to understand the architecture of the system where our program will run. So we present the characteristics below:

```
Device: NVIDIA GeForce GTX 1050 Ti
CUDA Driver Version: 11.4
Runtime Version: 11.2
CUDA Capability Major/Minor version number: 6.1
6 Multiprocessors (SM)
Max Grid sizes: 2 147 483 647, 65 535, 65 535
Max Block sizes: 1024, 1024, 64
Max Blocks per SM: 32
Max threads per Block: 1024
Warp size: 32
Total global memory: 4 137 024 MB
Shared Mem per SM: 98 304
Max ShMem per Block: 49 152
```

II. RESULTS

To accurately compare the different versions all the tests were performed in the university cluster and averaged the execution times over ten execution. The parameters chosen were:

```
const int nx = 200;
    area
const int ny = 200;
    area
const float a = 0.5;
    constant
const float h = 0.005;
    spacing
const int numSteps = 100000;
    time steps to simulate (time=numSteps*dt)
const int outputEvery = 100000; // How
    frequently to write output image
```

A. Sequential Verion

We start by analyzing and profiling the sequential version to understand what improvements can be done, and what parts are the more problematic.

By a quick analysis of the code, we expect the cycle present in the main function to be the biggest problem. This assumption is supported by the reports of the profiling tools. The output of these tools can be seen in the files results/sequential/gprof and results/sequential/perf.

The average execution time obtained with this version is 153.979 seconds.

B. V1 Version — CUDA

Next, we make a naive translation of the sequential code to CUDA code, which can be found in proj1/v1.cu. This implementation was based on the tutorial provided with the project[1], with some adaptations.

With this version, we experimented with a variety of grid configurations. We follow Nvidia recommendations[2]:

- Threads per block should be a multiple of warp size to avoid wasting computation on under-populated warps and to facilitate coalescing.
- A minimum of 64 threads per block should be used, and only if there are multiple concurrent blocks per multiprocessor.
- Between 128 and 256 threads per block is a good initial range for experimentation with different block sizes.

So we start with a configuration having 256 threads per block and we test until the maximum of 1024 threads per block. We didn't find significant differences between these configurations.

For the sake of completeness, we tested with blocks smaller than 68 threads, and, as expected, we got worse results. The results are summarized in Figure 1

Analyzing this version using the profiling tool NVPROF we can conclude that the majority of execution time is spent in communication between the host and the device, with only 22.19% of the execution time dedicated to kernel execution. The program spends 41.74% of time copying data from the host to the device and 36.07% from the device to the host. The complete results are available at results/v1/nvprof_results. From this iteration,

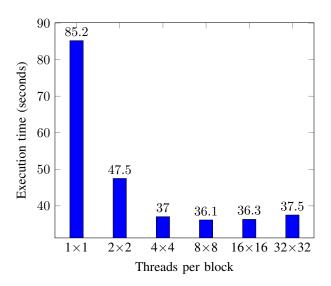


Fig. 1: Execution time of different grid configurations for V1

we concluded that the better configuration is to use 16×16 threads. We will use this configuration in the next versions.

C. V2 Version — Better comunication

In this version, we intend to improve the previous naive implementation, reducing the communication between the host and the device, which we detect to be a big problem in the previous version. In this problem, there aren't any computations needed between the steps so we don't need to transfer the data to the host between steps.

As expected we got a huge improvement in execution time. This version has an average execution time of 2.172697 seconds. Using NVPROF we can see that now the kernel is executing 100.00% of the total execution time. The full report is in results/v2/nvprof_results.

We want to understand the impact that this new communication profile is affected by the number of threads so we conduct an analysis similar to the previous one, showing the results in Figure 2.

We maintain the use of the 16×16 configuration as the default for this version.

D. V3 Version — Shared Memory

Looking deeper into our current solution we realize that the same array position is accessed by five different threads, thus revealing a great opportunity for the use of shared memory.

In this version, we take advantage of the shared memory between threads of the same block. Each thread starts by coping a value to the shared memory and after synchronization, the thread computes the designated value.

This version had an average execution time of 2.206946 seconds, which doesn't show any improvement compared with the previous version. This may be because of the overhead introduced by copying each element and the threads' synchronization is not balanced by faster access to the shared memory.

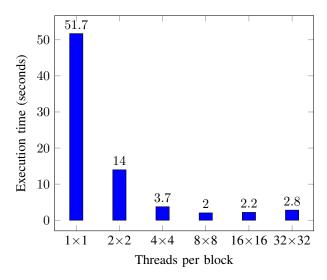


Fig. 2: Execution time of different grid configurations for V2

E. V4 Version — Streams with shared memory

After analyzing our version with shared memory we decided to add streams to this version despite not expecting any big improvement when working with a small grid.

Our implementation adds streams that allow the device to run as soon as the first partition of our table is downloaded. Since our function works with smaller squares we have a twodimension cycle in order to copy the necessary data.

We were already expecting the results we got, an average execution time of 2.203838 seconds when using 16 streams (4×4) . This time is similar to the time obtained by V3, it's to be expected because of a few factors, which the biggest is that the majority of the time is spent on the execution of steps, so, the time saved in the execution of the first step e relatively small.

F. V5 Version — Streams

After V4 we already knew that since we weren't solving any of the major issues listed earlier we would get similar results, however, for the sake of verifying our expectations, we decided that the work implementing the same stream system as before but without the shared memory could be justified.

This version was executed in node17 and had an average execution time of 3.369381 seconds not showing any improvements when compared to the V2, that when executed in the same node had an average execution time of 3.355694 seconds.

In conclusion, we confirmed our predictions without any improvements whatsoever.

G. V6 Version — Streams to copy output

We expect streams to prove advantageous when we want the output in intermediate steps, allowing the communication to overlap with the computation of the next step. To perform this analysis we compare the V2 and V6 versions, varying the parameter outputEvery to values of 1000, 100, 10, and 1. For larger values of outputEvery, we cannot see significant differences revealing that the costs required for synchronization are not balanced by the overlap of communication with synchronization. But with lower values, we have begun to see the advantages of the use of streams. We can see the results in Figure 3.

With the results on every step is where we see the better improvement allowed by streams, in the end of every step we can overlap the execution of the next step with the transfer of the previous result and its writing on a host file.

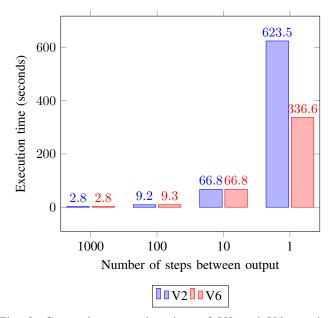


Fig. 3: Comparing execution time of V2 and V6, varying outputEvery

Another situation in that streams may be helpful is when we have a larger amount of data to transfer between the host and the device. To prove this hypothesis we vary the grid size and compare the different versions, showing the results in Figure 4.

As we can see the use of streams does not appear to improve the performance when using larger data sets. This may be because the communication time is greater than the execution time of each kernel.

H. V7 and V8 - Streams

In V7 and V8 we took the first version and developed these versions under the assumption that it would be necessary to copy data from the device to the host and from the host to the device at each step.

To achieve improvements relative to V1 we propose the use of streams. The idea of the two versions is to test the different ways of launching the kernel and the streams, as shown in CUDA documentation[3], and understand how that impacts the performance.

However, we have not been successful in developing these versions, and some errors cause longer execution times and erroneous results. Due to this fact, these versions will be excluded from our analyses.

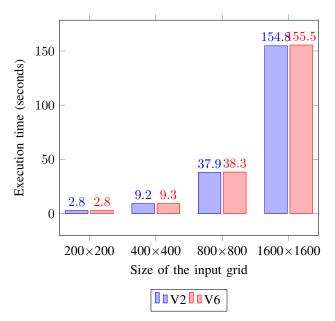


Fig. 4: Comparing execution time of V2 and V6, varying the input size

I. V9 and V10 Versions - More Work per Thread

Being a bit more creative in our approach for version V9, we decided to have a different evaluation process. In this version, we went back to our V2 and changed it for each thread to process more than a single point of the table. V10 was supposed to do the same as V9 but with the help of shared memory.

The idea was to see if increasing the amount of work and consequently, memory access, makes the use of shared memory justified by improving performance.

Unfortunately, we ran into illegal memory access and we didn't have time to correct our implementations, so we don't have results for these versions.

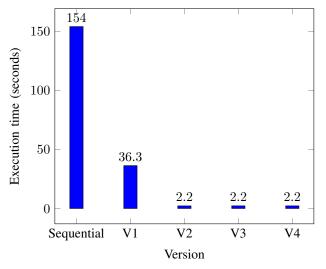
III. DISCUSSION

Throughout this report, we analyzed many different implementations of the heat equation taking advantage of the GPU.

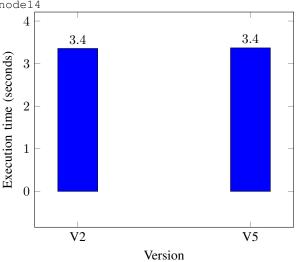
In Figure 5 we can see the execution times of our versions using the same parameters. Due to a change in the method of measuring execution time and a problem in node14 of the DI cluster, it was not possible to run all the versions in the same node. Version V5 was only executed in node17. To better compare the versions we rerun V2 in this node and we show the results of the different versions executed in node17 in Figure 5b

With this report, we could see how many strategies influence the performance of a problem and understand that not all solutions are fit for all problems. High-performance computing requires careful analyses of the problem size, structure, and requirements to find the best strategy to parallelize it.

In this problem, and with our implementation we didn't find any advantage in the usage of streams or shared memory, this may due to the fact that the extra work necessary to launch



(a) Execution times of sequential version, V1, V1, V3 and V4 in node 14



(b) Execution times of V2 and V5 node17

Fig. 5: Execution time of the different versions

these versions is not compensated by the performance gains. So to this problem, we considered V2 as the best version.

IV. COMPILATION AND EXECUTION INSTRUCTIONS

Our best version, V2, can be compiled and executed with the following command, from inside the folder /projl:

This will execute ten iterations to measure the average execution times and the results of the heat equation will be saved in the folder images/v2.

REFERENCES

[1] "Solving heat equation with CUDA — OpenACC/CUDA for beginners." (), [Online]. Available: https://enccs.github.io/OpenACC-CUDA - beginners/2.02_cudaheat - equation/?utm_source = pocket_saves (visited on 11/09/2022).

- [2] "CUDA C++ Best Practices Guide." (), [Online]. Available: https://docs.nvidia.com/cuda/cuda-c-best-practices-guide/index.html (visited on 11/09/2022).
- [3] "How to Overlap Data Transfers in CUDA C/C++," NVIDIA Technical Blog. (), [Online]. Available: https://developer.nvidia.com/blog/how-overlap-data-transfers-cuda-cc/ (visited on 11/13/2022).