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 and 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;// Width of the area
const int ny = 200;// Height of the area
const float a = 0.5;// Diffusion constant
const float h = 0.005;// h=dx=dy  grid spacing
const int numSteps = 100000;// Number of 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

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, with some adaptations.[1]

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 5.43% of the execution time dedicated to kernel execution. The program spends 50.73% of time copying data from the host to the device and 43.84% from the device to the host. The complete results are available at `results/v1/nvprof_results`.

C. V2 Version

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

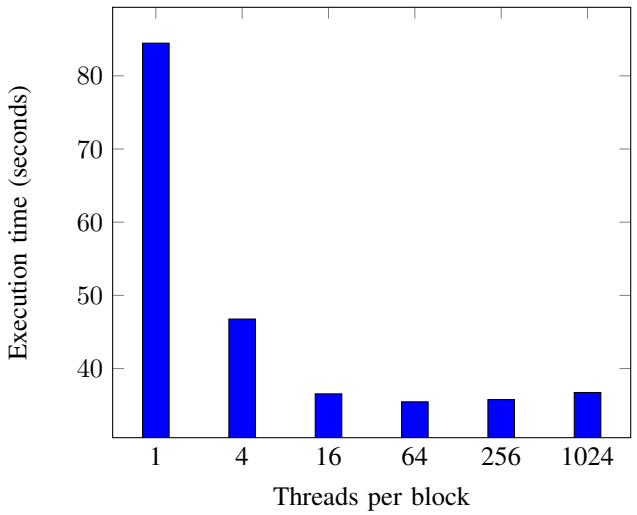


Fig. 1: Execution time of different grid configurations for V1

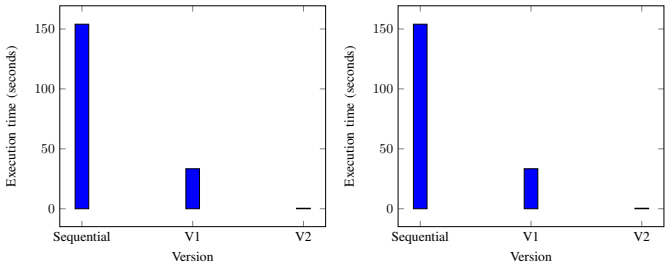
in the previous version. In this problem, there aren't any computations needed between the steps so we don't need to transfer the data to the host between steps.

As expected we got a huge improvement in execution time. This version has an average execution time of 0.424355 seconds. Using `NVPROF` we can see that now the kernel is executing 99.98% of the total execution time. The full report is in `results/v2/nvprof_results`.

we decided from now on to increase the complexity of the problem by increasing the amount of work. So the new parameters are:

```
const int nx = 200;              // Width of the
    area
const int ny = 200;              // Height of the
     area
const float a = 0.5;             // Diffusion
    constant
const float h = 0.005;           // h=dx=dy  grid
     spacing
const int numSteps = 100000;     // Number of
    time steps to simulate (time=numSteps*dt)
const int outputEvery = 100000; // How
    frequently to write output image
```

III. Results



(a) Execution time of sequential version, V1 e V2

(b) Execution time of V2, V3, V4 and V5

Fig. 2: Execution time of the different versions

References

[1] "Solving heat equation with CUDA — OpenACC/CUDA for beginners." (), [Online]. Available: https://enccs.github.io/OpenACC-CUDA-beginners/2.02_cuda-heat-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).