Ivan Theodor-Adrian - DSWT II 1A
Savin Vlad-Mihai - DSWT II 1B

PI computation GPU acceleration using Monte Carlo simulation on CUDA

General description

The number π is a mathematical constant. Originally defined as the ratio of a circle's circumference to its diameter, it now has various equivalent definitions and appears in many formulas in all areas of mathematics and physics. It is approximately equal to 3.14159.

Monte Carlo methods are a broad class of computational algorithms that rely on repeated random sampling to obtain numerical results. One of the basic examples of getting started with the Monte Carlo algorithm is the estimation of π.

The idea is to simulate random (x, y) points in a 2-D plane with domain as a square of side 1 unit. Imagine a circle inside the same domain with same diameter and inscribed into the square. We then calculate the ratio of number points that lied inside the circle and total number of generated points.

We know that area of the square is 1 unit sq while that of circle is:

$$\pi * (\frac{1}{2})^2 = \frac{\pi}{4}$$

Now for a very large number of generated points,

$$\frac{\text{area of the circle}}{\text{area of the square}} = \frac{\text{no. of points generated inside the circle}}{\text{total no. of points generated or no. of points generated inside the square}}$$

that is,

$$\pi = 4 * \frac{\text{no. of points generated inside the circle}}{\text{no. of points generated inside the square}}$$

Parallelization methods

Naive approach

In our first implementation, we used a naive approach to distribute the computation of the value of π on CUDA blocks.

On the host device, we generated two vectors with random (x, y) pairs.

Then we copied the vectors into the memory of the graphics device. After that, we launched the CUDA kernel, which had the task of counting how many points land inside the circle and write the value of the counter in the **sampleCountPerThreads** shared vector. The first thread from each block then sums up the values from the thread counter and stores the result in a **device_sampleCountPerBlock** vector. The host device then does the computation of π, after summing up the values from the **device_sampleCountPerBlock** vector.

Deficitary aspects and optimizations

The first and most important optimization would be generating the random samples directly on the GPU threads. This would eliminate the severe overhead on the CPU.

Hardware & software devices used

CPU	GPU	OS	CUDA version
Intel Core i7-4790 @ 3.6 GHz	GeForce GTX 660, 2048MB	Windows 10 Pro	10.2

Results analysis

No. of samples	CPU version (ms)		GPU version (ms)				Acceleration
	Samples generation	Pi computation	Samples generation	Copy data host -> device	Kernel computation	Copy data device -> host	
10^5	**13**	**1**	**12**	**0.2975**	**159.7696**	**0.0945**	**0.08**
10^6	**125**	**7**	**127**	**1.7931**	**159.7395**	**0.0543**	**0.46**
10^7	**1238**	**62**	**1235**	**16.0672**	**160.0351**	**0.0619**	**0.92**
10^8	**12255**	**510**	**12274**	**162.6636**	**203.5319**	**0.2047**	**1.01**

```
Generating host X samples...
Generating host Y samples...
Generated vectors in 12255.000000 ms
pi = 3.141531
Pi calculus took 512.000000 ms
Whole process took 12767.000000 ms
```

Output for the CPU version

```
Generating host X samples...
Generating host Y samples...
Generated vectors in: 12274.000000 ms
Device malloc randX...
Device malloc randY...
Copying randX from host to device...
Copying randY from host to device...
Malloc and copy from --proc-- to --graphics card-- time: 162.663620
Device malloc sampleCountPerBlock...
Launching kernel...
Kernel execution time: 203.531998
Copying sampleCountPerBlock from device to host...
Copy from --graphics card-- to --proc-- time: 0.204768
pi = 3.141514
```

Output for the GPU version

Optimizations

1. **Generate samples per threads**

We refactored the code to generate the random samples on the device threads instead of the host. The setup parameters are:
NUM_BLOCKS=2048,
NUM_THREADS_PER_BLOCK=32 and
NUM_SAMPLES_PER_THREAD=2000

Each thread generates NUM_SAMPLES_PER_THREAD samples. The number of samples in circle per thread are then stored in a shared memory zone. We then select a master thread per block, which sums up all the counters from the threads. Those sums are stored in a vector on the device, which is then copied to the host. The host applies a simple algorithm to estimate pi, based on the values from the vector.

These are the results of the run:

```
Device malloc sampleCountPerBlock...
Launching kernel (0)...
Kernel execution time: 2480.241943
Copying sampleCountPerBlock from device to host...
Copy from --graphics card-- to --proc-- time: 0.068288
Device memory used: 500Mb
Total processing time: 2572.000000 ms
Number of samples: 131072000
pi = 3.141555
```

We can notice by far how much faster this version is. We had a total processing time of about 12.4 seconds for 1e8 samples on the previous version, and now we managed to obtain 2.5 seconds for 1.3 * 1e8 samples.

2. **Optimized memory using Unified Memory**

We optimized the usage of the vector of sums stored on the device, by using *cudaMallocManaged* . Now both the CPU and GPU have direct access to the vector, so there's no need in copying it from the device to the host. This would mean losing some processing time.

The results showed us that we are wrong.

```
Launching kernel (0)...
Kernel execution time: 2483.098145
Device memory used: 500Mb
Total processing time: 3142.000000 ms
Number of samples: 131072000
pi = 3.141440
```

We noticed that the kernel execution time is approximately the same, we don't waste time on transferring data from the device to the host, but we have a higher total processing time.

This optimization would have been better on the previous implementation, where we transferred heavy data from the host to the device. Using Unified Memory, the data would have been brought to the device before calling the kernel (prefetch).

3. **Local reduction on gpu with warp shuffle at the beginning**

After adding warp shuffle reduction to count the number of samples in circle / block, we had a better result:

```
Launching kernel (0)...
Kernel execution time: 2471.587402
Device memory used: 500Mb
Total processing time: 3055.000000 ms
Number of samples: 131072000
pi = 3.141530
```

We then reverted the Unified memory changes, and this is what we got:

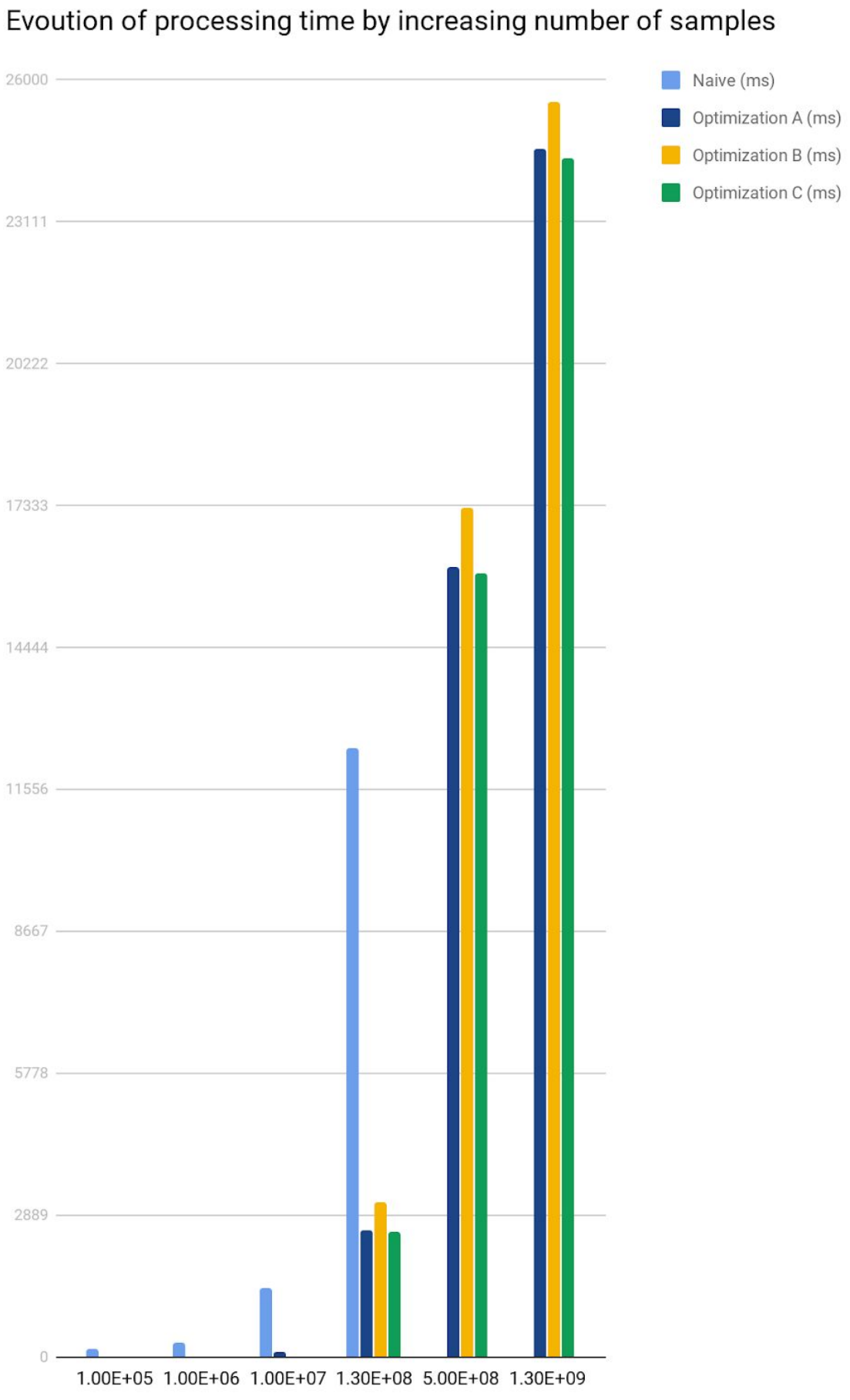
```
Device malloc sampleCountPerBlock...
Launching kernel (0)...
Kernel execution time: 2471.448242
Copying sampleCountPerBlock from device to host...
Copy from --graphics card-- to --proc-- time: 0.082112
Device memory used: 500Mb
Total processing time: 2548.000000 ms
Number of samples: 131072000
pi = 3.141598
```

Optimization conclusions

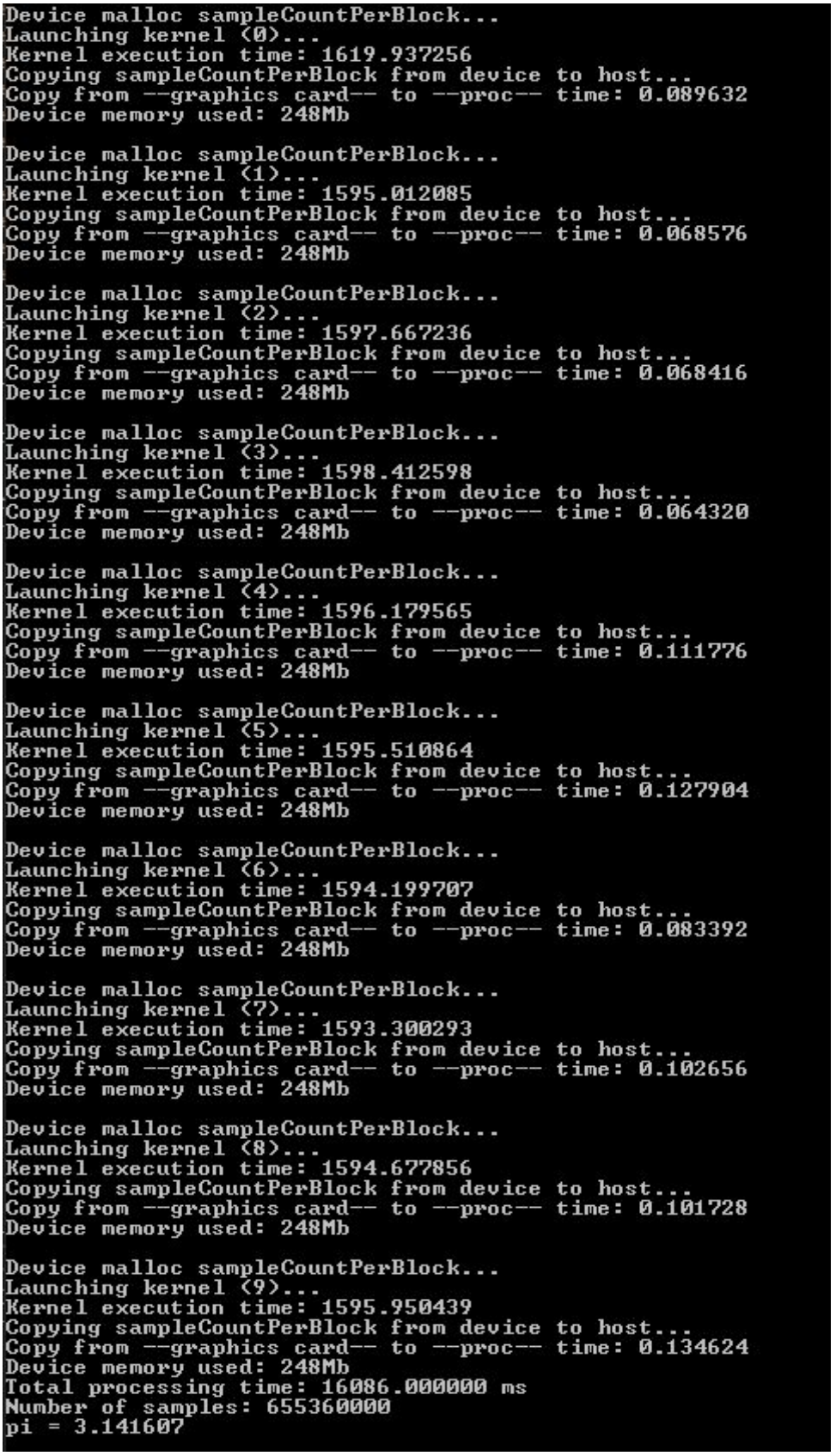
The most important optimization in terms of acceleration was the generation of the samples on the device. Then, one more optimization with a very little impact was the warp shuffling used for vector reduction on the array containing the counters of each thread. As expected, the unified memory didn't produce any improvement because we only have one CPU and one GPU and there is no need for high level abstraction of memory management.

GPU optimization method	CPU & memory transfer operations time (ms)	Kernel computation time (ms)	Total time (ms)	Acceleration	Number of samples
Naive	**12436**	**203**	**12640**	-	1e8
A	**91**	**2480**	**2572**	**4.91**	1.3e8
B	**659**	**2483**	**3142**	**4.02**	1.3e8
C	**77**	**2471**	**2548**	**4.96**	1.3e8

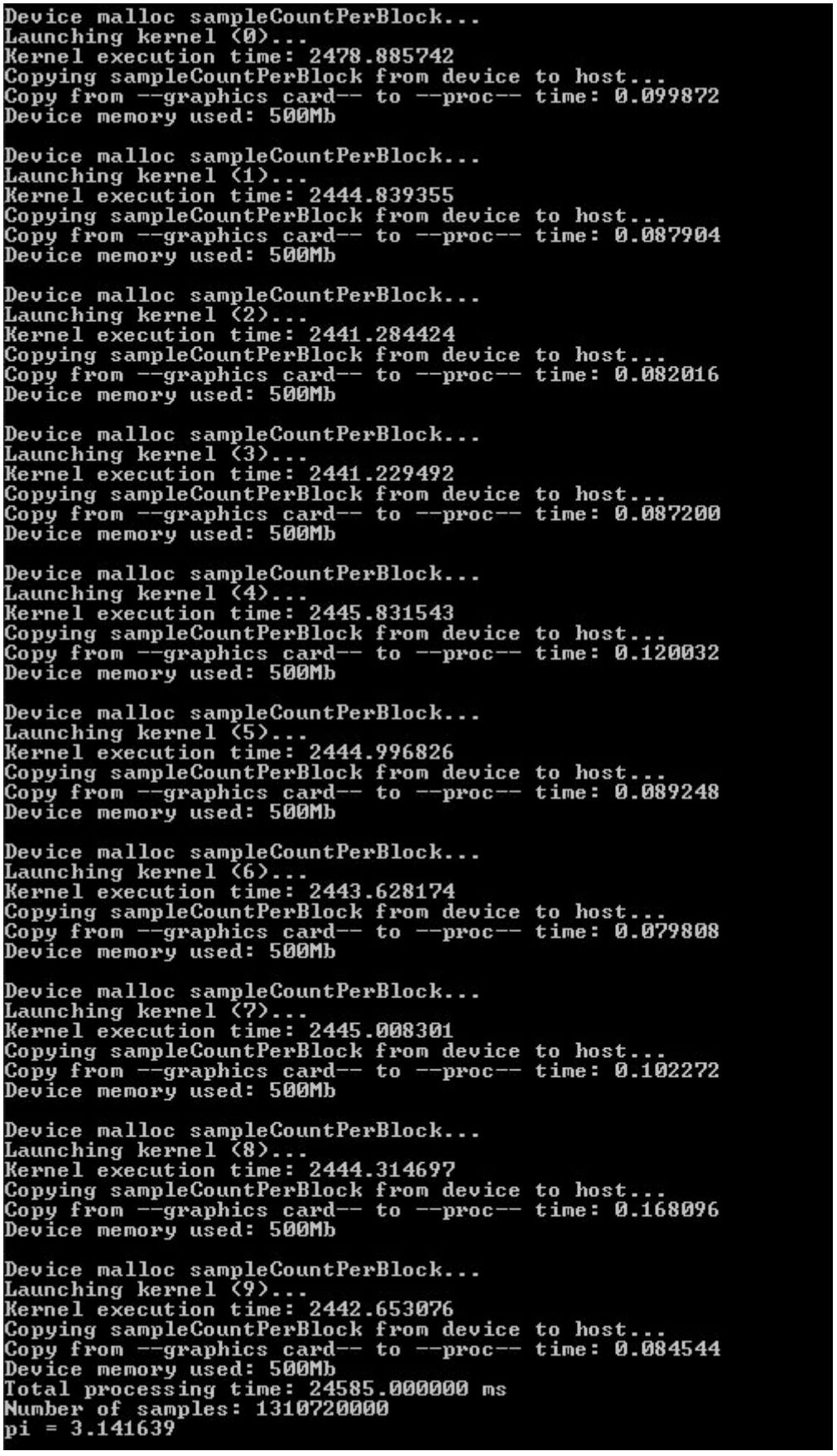
A - *Sample generation on device*
B - *Sample generation on device* with *unified memory*
C - *Sample generation on device* with *warp shuffle* and *without unified memory*


Evoution of processing time by increasing number of samples
Naive (ms)
Optimization A (ms)
Optimization B (ms)
Optimization C (ms)
26000
23111
20222
17333
14444
11556
8667
5778
2889
0
1.00E+05
1.00E+06
1.00E+07
1.30E+08
5.00E+08
1.30E+09

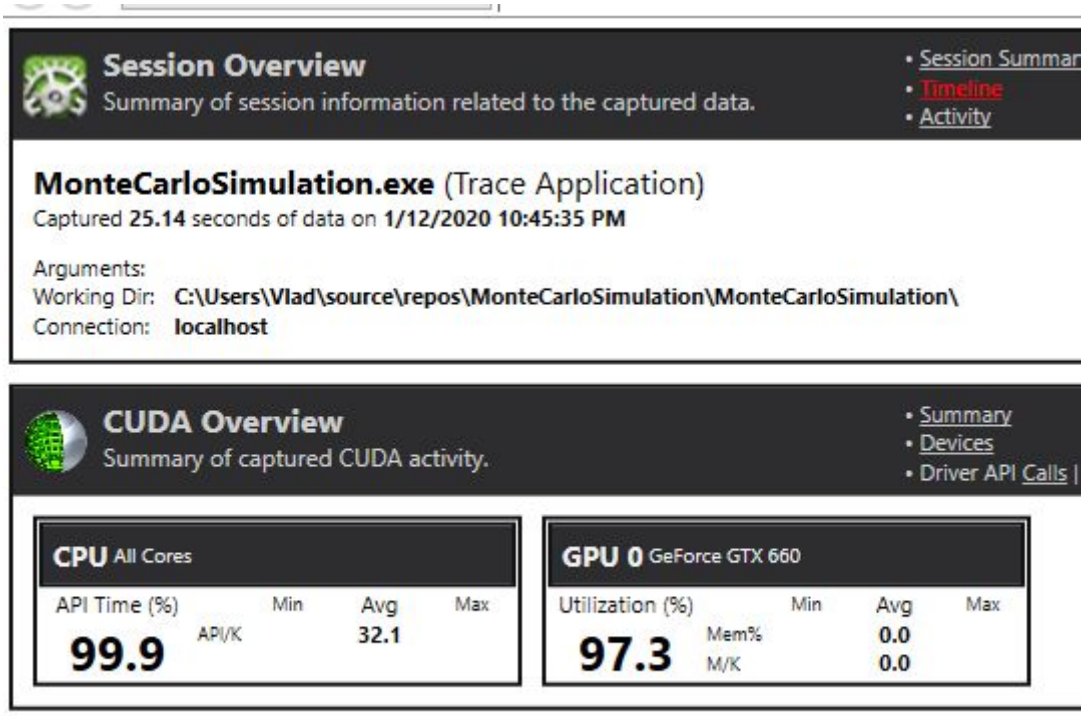
Appendix



Trial 1 - with 248Mb of samples, we called the kernel several times, to increase the accuracy of the result, but we lost the advantage in the Total processing time side.



Trial 2 - with 500Mb of samples, we called the kernel several times, to increase even more the accuracy of the result, and we noticed that the Total processing time did not double.



Nsight output for Trial 2

```
Launching kernel (0)...
Kernel execution time: 2467.950928
Device memory used: 500Mb
Launching kernel (1)...
Kernel execution time: 2443.187500
Device memory used: 500Mb
Launching kernel (2)...
Kernel execution time: 2444.209961
Device memory used: 500Mb
Launching kernel (3)...
Kernel execution time: 2444.368896
Device memory used: 500Mb
Launching kernel (4)...
Kernel execution time: 2443.156006
Device memory used: 500Mb
Launching kernel (5)...
Kernel execution time: 2442.818848
Device memory used: 500Mb
Launching kernel (6)...
Kernel execution time: 2442.350830
Device memory used: 500Mb
Launching kernel (7)...
Kernel execution time: 2443.999268
Device memory used: 500Mb
Launching kernel (8)...
Kernel execution time: 2443.906982
Device memory used: 500Mb
Launching kernel (9)...
Kernel execution time: 2444.862549
Device memory used: 500Mb
Total processing time: 25528.000000 ms
Number of samples: 1310720000
pi = 3.141577
```

Trial 3 - After using the **Unified Memory** optimization strategy, with *cudaMallocManaged* instead of copying a vector from device to host, we noticed that the total processing time stays approximately the same.