Computational Science on Many-Core Architectures Exercise 5

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The code for all tasks can be found at: $\label{local_model} $$ $ TUWIEN/tree/main/WS2023/Many-Core%20Architectures/e5 $$

1 Performance Modeling: Parameter Identification

1.1 a)

For measuring PCIE latency of cudaMemcpy, I copied a very small package of data (1 double). I repeated the measurement 10 times - I would have done this way more often, but I did not want to clutter the online environment with that many requests (also I often received [errno:16] device busy). From these initial times I omitted the lowest and highest 2 times each before averaging - I think because the current load on the online environment was high, there were some "exceptional" runs in the data that were possibly caused by the server lagging, which were thus avoided. Also I benchmarked these values for a "warm" CUDA device - I noticed it makes a big difference running these instructions as one of the first lines in the codes as opposed to running them 10000 times before performing the actual benchmark (for this particular task for example, the latency for an early/cold cudaMemcpy was about 14μ s for me).

Also, this measurement is possibly not all too accurate; this is because I am not sure how exactly cudaMemcpy() works here - surely for each call we have a latency that should be constant, and then a term dependant on the data. I could have assumed here that that latter term stays constant for increasing N, in which case I could have made a second measurement run with a bigger amount of data, then solving the resulting system for this dependant term and as such calculate the latency. But since I have no idea if that dependency is actually linear (I have the feeling it is not) I just used this more simple approach.

My findings concluded in the PCIE latency for cudaMemcpy being $\approx 6.7 \mu s$. This is roughly in line with the data from the lecture slides, with the actual value possibly being a bit smaller due to the above.

1.2 b)

For measuring the latency of a CUDA kernel call, I tried to model the launch of an "empty kernel", such as

```
__global__ void empty() {}
```

This has one problem in that the compiler will optimize the calling of this kernel away - at least in theory, it did not seem that way when I tested it. I still left the following in: The way that I decided to tackle this with was by initializing a volatile variable within the kernel:

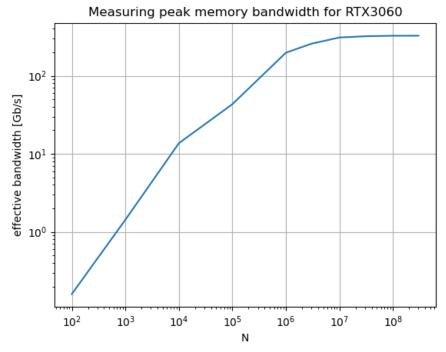
```
__global__ void empty() {volatile int a = 0;}
```

This should result in the call not being optimized because the volatile flag tells the compiler that it might be accessed from placed that are out of scope on compile level. I initially received a launch latency of $\approx 0.01s$. This is way beyond the expected $\approx 10\mu s$. I ran the kernel using my "anti-optimized" version as well as with a completely empty kernel for checking, both resulted in these times.

It only dawned on me in the end that I might be also measuring some kind of "CUDA device initialization", since my code was not using any cuda related calls before the kernel launch. And indeed, CUDA uses lazy initialization - when I then added a single cudaMalloc line before my kernel launch (and also some more runs before to warm up the kernel, as stated above), I received the more expected $\approx 1.7 \mu s$.

1.3 c)

For measuring the practical peak bandwidth, I basically repeated what we already did in earlier exercises - saturating the kernel with a high enough system size for a kernel call - I used here a simple copy kernel. For added accuracy, I also ran a reference kernel that runs through the same instructions apart from the copying step and subtracted that from the actual kernel run time, to minimize the amount of overhead that got included in the data.



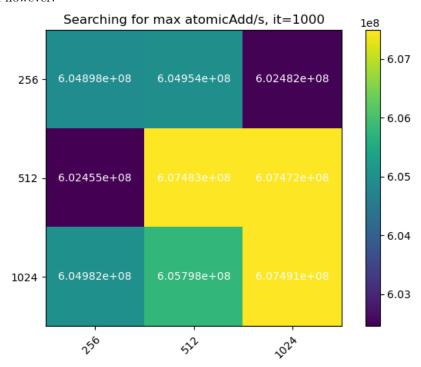
We can see that we reach the peak bandwidth at about $N=10^7$, where we receive $\approx 330 \frac{\text{GB}}{\text{s}}$ (in the plot there is a typo on the y axis label). Considering the given memory clock of 1,875GHz on 8b of GDDR6 memory, yielding 15Gb/s of effective memory clock on a 192bit bus, which results in $(15\text{Gb/s} \cdot 192/8)$ 360GB/s memory bandwidth, this result seems reasonable.

1.4 d)

For measuring the maximum amount of atomicAdds to a single address, I used a simple kernel that lets each thread call an atomicAdd to that address multiple times:

```
__global__
void atomicAddKernel(double *dest, int it){
   for (unsigned int i = 0; i<it; i ++) {
       atomicAdd(dest,1);
   }
}</pre>
```

The total amount of atomic adds was then devided by the time taken, which results in a max amount of about $6 \cdot 10^8$ atomicAdds per second. I checked this for several constellations of grid- and blocksizes because I was interested if there would be any significant change between them. The results are quite uniform however.



1.5 e)

Lastly I measured the peak floating point rate using multiply-add for testing. The kernel used was

```
__global__
void copyKernel(int N, double src1, double src2){
  volatile double res = 0;
  for(int i = 0; i < 1000; i ++){
    res += src1 * src2;
  }
}</pre>
```

To this kernel I passed two random constants and added to a volatile double again in hopes of avoiding optimizations, as that result is never used. I tried to avoid unnecessary memory accesses here as much as possible, also again I subtracted the runtime of a reference kernel. The peak rates were interestingly obtained for a high grid size of 4096 and the max block size of 1024, and resulted in about 170 GFlOPs/s - I did not produce a grid plot for this one as well to save some time, as I was (as written above) often times kicked from the machine which forced me to rerun the code, and I was already running low on time.

2 Conjugate Gradients

2.1 a)

The matrix-vector product was implemented akin to the lecture slides as:

```
__global__ void csr_matvec_product(int N, int *rowoffsets, int *colindices, double *values, double *x, double *y) {
    for (int row = blockDim.x * blockIdx.x + threadIdx.x; row < N; row += gridDim.x * blockDim.x) {
        double val = 0;
        for (int jj = rowoffsets[row]; jj < rowoffsets[row+1]; ++jj) {
        val += values[jj] * x[colindices[jj]];
        }
        y[row] = val;
    }
}
```

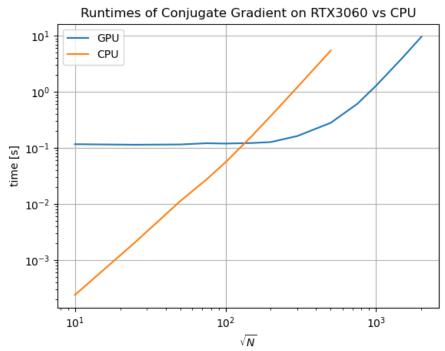
2.2 b)

I procured two kernels, with the dot kernel basically just reduced from last exercise. dot (...) takes care of the dot products, while vecIterate (...) takes care of the vector addition kernel calls in lines 7, 8, and 12.

```
__global__ void dot(int N, double *x, double *y, double *results) {
    double alphai(0);
    for(int j = blockIdx.x * blockDim.x * threadIdx.x; j < N; j += blockDim.x*gridDim.x) {
        alphai += x[j] * y[j];
    }
    for (int j=warpSize/2; j>0; j=j/2) {
        alphai += __shfl_xor_sync(0xffffffff, alphai, j);
    }
    if (threadIdx.x % warpSize == 0) {
        atomicAdd(results, alphai);
    }
}
__global__ void vecIterate(int N, double *out, double *ini, double *in2, double mod) {
        for (int i = blockIdx.x * blockDim.x * threadIdx.x; i < N; i += blockDim.x * gridDim.x) {
            out[i] = ini[i] + mod * in2[i];
        }
}</pre>
```

2.3 c)

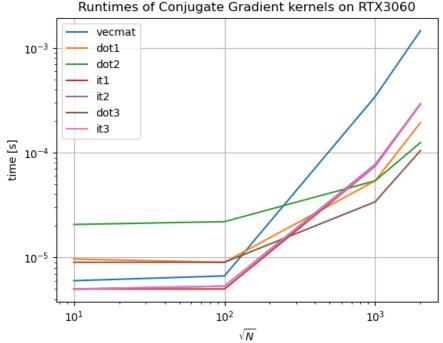
I compared the time of my implementation to the pure-CPU implementation - the GPU becomes faster than the CPU version quite swiftly. There is one little bump in the plot for the GPU, where my approach of discarding some of the lowest and highest times combined with averaging still had one outlier in. Because there were so many calls to the online environment (often getting [errno:16], device busy), I only did 7 runs for each N here - of course more would have been better, but I wanted to get this done more quickly. The bump should be interpreted as a measuring error.



Sadly I could also not test much bigger system sizes. Of course my kernel is not the fastest, but a lot of time was also lost in the setting up of the problem, especially for larger sizes.

2.4 d)

Here are the runtimes of each individual kernel:



We can see the dot products are a bit slower in comparison for small systems, but are then the fastest for bigger systems. The matrix-vector multiplication has the steepest ascent for big system sizes, and should be further optimized when mainly working on those. The vecIterate kernels start the fastest but also become more expensive quickly with rising system sice and should then also be further optimized.

3 Bonus Point: The Need for Speed

I optimized the kernel in a first step by omitting all the settings of CPU variables for the dot product; instead I set it to 0 within the kernels such as

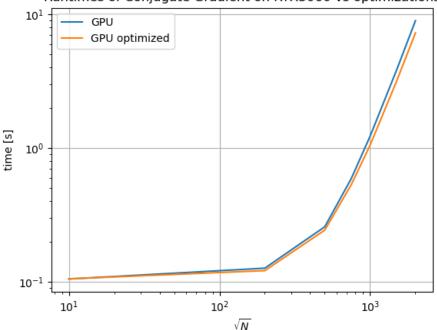
```
__global__ void dot(int N, double *x, double *y, double *results) {
double alphai{0};
unsigned int thread_id = blockIdx.x * blockDim.x + threadIdx.x;
if (thread_id == 0) *results = 0;
```

I did not do a full per-optimization benchmark for each aspect I improved, but this yielded a relatively (although low, see below) good improvement. I checked different grid/block-sizes, and, after a lot of reading up on theory regarding occupancy (and lots of trial and error, of course) I found that <<<128,128>>> yielded the best results. I also wanted to account more for the tail effect (as

found here https://developer.nvidia.com/blog/cuda-pro-tip-minimize-the-tail-effect/) but tuning kernel launches in an averaged fashion for my different problem sizes was not something I wanted to further do since this exercise was already quite lengthy and with a short time bound. Especially settings the block size to 128 seems to have had a big impact - as another optimization, I computed lines 7 and 8 in the same kernel. Since my original version initializes the csr_* cuda arrays (including copying etc.) within the conjugate_gradient (...) function (which is the function I timed), I also thought about moving these outside the function, but ultimately decided against it, as that would only be a "ghost-optimization" without any real time save. Also I tried to be a bit more frugal with variables and their assignments, which saved about 3 assignments per iteration. Sadly these optimizations did not lead to as much of a decrease in runtime as compared to the "unoptimized" version as I had initially hoped - both versions however save on one calculation of pAp (the dot product of p with Ap) per iteration already, by calculating it initially once before the while-loop, and then using

the updated value next, so that is one optimization that is not tracked here.

Runtimes of Conjugate Gradient on RTX3060 vs optimizations



While the improvements are negligible and within fluctuactions for small systems, for the largest tested system size $\sqrt{N}=2000$ I achieved a runtime decrease of $\approx 19\%$. With even bigger systems, an even larger gap should be expected. Still I am quite sure that I missed a lot of potential improvements. *Note:* I would be very glad if a truly optimized version could be uploaded to TUWEL; I would like to see what improvements could have still been made.