CME 213, Introduction to parallel computing
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Spring 2024

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Project Final Assignment

Total number of points: 100.

Most of the code has been written during previous homework assignments. In this assignment, you will focus on analyzing and discussing the performance of the code. This assignment is more open-ended than the previous ones, and you will receive less guidance. You are responsible for submitting a PDF to Gradescope. Although you may want to develop some new code to test new ideas, code submission is not required for this assignment.

When including figures, tables, etc., to make a point, ensure that each figure/table is useful. They should be referenced in the text and have a caption. The caption should be informative and self-contained. Figures should be easy to understand without reading the text. The same applies to tables and code snippets. You should comment on each figure and table in the text. The code snippets should be short and relevant. They should be referenced in the text and commented on. Avoid including material that is not commented on and is simply included for archival purposes.

Warning: Because this homework requires using the cluster for longer periods of time, please be respectful of other students and cluster usage. Make sure to use `squeue` to check the status of your jobs. Use `scancel [jobid]` to kill jobs that run for too long. Do not submit more than 1 script or job at a time.

Starter code information

In the starter code we provide, we have added several `MPI_Barrier`, `cudaDeviceSynchronize`, and `nvtxRangePushA` and `nvtxRangePop` calls to help profile the code using Nsight Systems. Please refer to the online documentation for information about NVTX. For this homework, you will need to install Nsight Systems on your local machine by following these instructions.

In summary, `nvtxRangePushA` will start a new range in the timeline, and `nvtxRangePop` ends the range. You can use these calls to profile the code and understand where time is spent. They will create ranges in the profiler, as shown in Figure 1. This is very useful for facilitating the analysis of the code and better understanding the profiler output.

`MPI_Barrier` is not required for correctness and will affect performance to some extent. But it helps simplify and clarify the profiling. For example, if you call `MPI_Allreduce` it may look like some processes take a lot of time to complete that command. In reality, because `MPI_Allreduce` is a synchronous collective operation, the process is mostly waiting for the other processes to complete. By adding a barrier, you can see the time spent in the `MPI_Allreduce` operation more clearly.

`cudaDeviceSynchronize` is used to synchronize the CPU with the GPU. Without this, the NVTX information may be inaccurate.

The starter code contains the tests that were previously used in Homework 6. They are contained in the `gtestTrain` test suite. At the end, you will find a different test: `gtestProfile`. This test is a little different. The code is similar to the one in Homework 6 except that we additionally load a test set for the MNIST data set. This test set is used to evaluate the precision of your DNN model.

Recall that precision is defined as:
precision = total number of labels correctly predicted / total number of labels

You can adjust the size of the hidden layer (`hidden_size`) and the number of epochs in order to train your model.

You will see the precision only if `test_size` is non-zero. See `main.cpp` for more details.

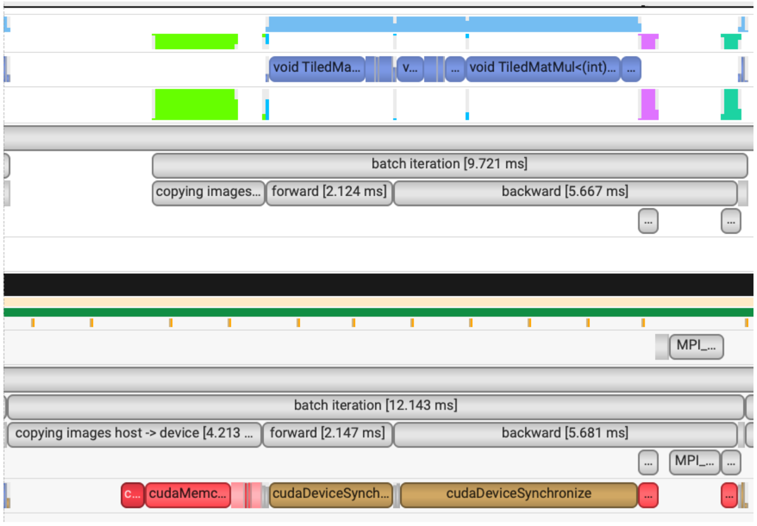


Figure 1: Sample Nsight Systems screenshot

Problem 1 Convergence of your model

Question 1.1

(5 points) First test the code to make sure that it is correct. Run:

```
make clean && srun make -j && salloc -n 4 -p gpu-turing mpirun ./main
```

Run your code again in double precision:

```
make clean && CXXFLAGS=-DUSE_DOUBLE srun make -j && salloc -n 4 -p gpu-turing mpirun ./main
```

Please report on the output. Does your code pass all the tests?

Focus now on the test

```
TEST(gtestProfile, nsys)
```

You may run this test only using the command:

```
salloc -n 4 -p gpu-turing mpirun ./main --gtest_filter=gtestProfile.*
```

You can use a similar-looking command in a batch script as well. Note that you can also get rid of the color in the google unit test output using the command:

```
salloc -n 4 -p gpu-turing mpirun ./main --gtest_filter=gtestProfile.* --gtest_color=no
```

This may clean up your output in some cases.

Question 1.2

(10 points) Make changes to this test. In particular, vary:

```
hidden_size, num_epochs, learning_rate
```

Does your code report errors? This means that the weights produced by the GPU code are different from the weights produced by the CPU code. Can you explain this discrepancy? Does it matter? What precision do you get using the CPU and GPU codes?

Question 1.3

(10 points) What learning rate seems to lead to the fastest convergence? What happens when you increase or decrease this learning rate?

Question 1.4

(10 points) Train your model for many epochs. What loss are you able to achieve? Has your model converged? What is the precision of your model? Does the precision depend on `hidden_size`? What value of `hidden_size` would you recommend? What happens when you reduce or increase it?

For this question, you may want to set debug=1 in the code to print the loss at each epoch and monitor the convergence. debug is the last parameter in

```
hyperparameters{60000, 10000, 784, 64, 3200, 1, 10, 1e-4, 0.2, 1};
```

You can change the frequency of the loss printouts by changing `printout_frequency` in this line:

```
const int printout_frequency = 4;
const int printout_period = std::max(1, (hparams.num_epochs * num_batches) / printout_frequency);
print_flag = (hparams.debug == 1) && ((iter % printout_period) == 0);
```

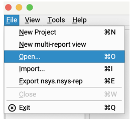
Problem 2 Performance Analysis

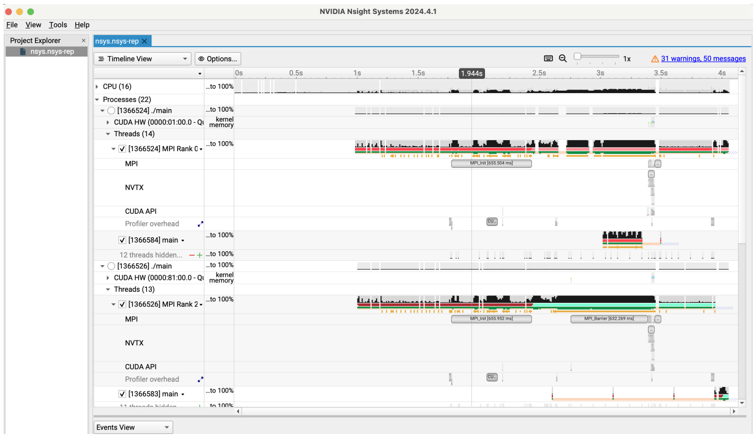
To analyze the performance, we recommend using Nsight Systems. You can use the following command to profile the code:

```
sbatch nsys.sh
```

Note that `nsys` and `mpirun` do not work properly from the command line. You have to use a batch submission. This command will produce the usual `slurm*.out` file along with a file `report*.nsys-rep`. Copy the `report*.nsys-rep` file to your local machine.

Load this file into Nsight Systems on your local machine. These screenshots may be useful to illustrate what you should see:





You will see the labels from NVTX that will guide your analysis.

Question 2.1

(10 points) In your profile, what are the steps that take the most time? Is this consistent with the analysis from Homework 6? Does this match your expectations or are there surprises?

Question 2.2

(15 points) Can you identify areas of the code that could be improved based on the profiling? What changes would you suggest?

Examples of possible changes include:

- Changing the way memory is allocated and managed.
- Changing the pattern of MPI communications and using non-blocking MPI calls.
- Using CPU pinned memory. This can be done using `cudaMallocHost`. See this blog post for more information.
- Using GPU memory pointers in MPI calls. See this blog post for more information.
- Pipelining various MPI and CUDA memcpy operations.
- Using CUDA streams. See this NVIDIA presentation for more information.
- Optimizing the CUDA kernels.

These are examples. You do not need to discuss all of them. You can focus on the ones that you think are most important.

We would like you to come up with an approximate model of the performance and arithmetic intensity of the code, similar to Homework 6, with a roofline model.

In the discussion below, all the numbers are normalized per GPU and per batch. We assume single precision. For simplicity, we only consider the case of two GPUs. This makes it easier to model the running time of MPI collective operations.

Question 2.3

(10 points) Using your profiling information, list the CUDA kernels and calculations that take a substantial amount of runtime during training. Then for these kernels, estimate the number of flops.

For memory transfers, focus on the cudaMemcpy and MPI operations. These are the slowest memory transfer operations. Estimate the number of bytes transferred.

For `MPI_Allreduce`, you can make the following assumptions. Assume we want to reduce b bytes. The reduction on 2 GPUs requires communicating b bytes. Then the result needs to be sent to the other process, requiring another b bytes. This gives a total of $2b$ bytes communicated.

You may ignore operations that are independent of the epoch, including: copying image data from one process to other processes, and copying image data from host to device memory.

Please write your estimates in terms of these variables (following Homework 6 notations):

```
D = input_size,
H = hidden_size,
C = num_classes,
B = batch_size.
```

Question 2.4

(10 points) Based on your profiling measurements, provide an estimate for the effective compute throughput P_{flops}, and the `cudaMemcpy` (P_{pci}) and `MPI_Allreduce` (P_{mpi}) memory bandwidth throughputs.

For example, let's say you want to multiply two square matrices of size n. The total number of flops is $2n^3$. If you measure a running time of t seconds, the effective compute throughput is $2n^3/t$ flops/second.

Similarly, the memory transfer for a square matrix is $4n^2$ (4 bytes per float) and the effective memory throughput is $4n^2/t$ bytes/second.

This estimate will be more useful than the peak performance listed by the manufacturer.

Similar to the previous question, **you may ignore** `copying images host -> device` and `train setup` since these are independent of the epoch.

Question 2.5

(10 points) As in Homework 6, we want to plot FLOPS/sec vs arithmetic intensity. Assume that FLOPS is the total number of flops that you estimated and that Bytes is the total number of bytes transferred. The arithmetic intensity is defined as FLOPS/Bytes. Following the example in Homework 6, provide a theoretical estimate of the roofline model. The y-axis is FLOPS/sec and the x-axis is arithmetic intensity. The answer will involve P_{flops}, P_{pci}, and P_{mpi}. Plot this function in a way similar to Homework 6.

Question 2.6

(10 points) Similar to Homework 6, we now want to compare the theoretical estimate with experimental values. For this purpose, calculate the FLOPS/sec. The FLOPS is based on your estimate of the flops performed by the CUDA kernels. The running time should be based on the profiling information.

For the arithmetic intensity, you may use the formula from Question 2.5.

The main difference with Question 2.5 is that you replace your theoretical estimate of the running time with the actual running time.

Run a few experiments with different values of H and B. Plot your experimental values along with the roofline model. Discuss the results. What trends do you observe? What is required to increase the arithmetic intensity and the FLOPS/sec performance? Give your answer in terms of D, H, C, and B. Do the theoretical and experimental estimates agree? Why/why not? Comment on the difference. Explain how you would improve your theoretical roofline model to better represent the experimental results.

3 Optional questions

Depending on your time and interest, you may want to consider the following questions. These will not be graded but they may help you better understand the material and improve your programming skills.

1. You could implement one or two of the optimizations suggested in Question 2.2.
2. Analyze and improve the performance of your CUDA kernels using the Nsight Compute profiler.
3. You could implement the model parallel approach instead of the data parallel approach we have used so far. This will reduce considerably the amount of bytes transferred.
4. Alternatively, you could simply do a theoretical estimate of the running time of the model parallel approach compared to the data parallel approach using the data from Question 2.5.

More information on the model parallel approach is provided below.

Model parallel approach

Let's simplify the problem by considering the following simplified situation. We can think of the feedforward phase as a series of matrix-matrix multiplications. In our case, since we have two layers, we can simplify our analysis and define the feedforward pass as $y = W^{(2)}W^{(1)}x$ where x is the input data and y is the output. The number of columns of x is the batch size. The number of rows of y is 10.

Similarly, the backpropagation phase corresponds to a series of matrix-matrix multiplications. In our case, it can be simplified to $[W^{(2)}]^T y$. The NN weights are then updated using a sum of rank-1 matrices of the form $\Delta W = \sum_i d_i a_i^T$, where the sum is over all the input images. The vector d_i (from image sample i) is the "gradient" vector from the backpropagation (e.g., $[W^{(2)}]^T y$) at layer l while a_i is the activation for layer $l - 1$.

The goal is then to subdivide or block the data and operations in such a way that communication is minimized. In the current approach, we split the input sample x into column blocks and assign one block to each processor. Then we do a reduction of all the $d_i a_i^T$ contributions from all processes. Since the size of the matrix ΔW is quite significant, this approach leads to a large MPI overhead.

To reduce the communication time, a common optimization is to partition the NN coefficient matrices W across different processes. This is called model parallelism as opposed to data parallelism. Data parallelism corresponds to splitting the input "data" across different processes, while model parallelism corresponds to splitting the NN coefficients W because the NN is our model in this problem. Model parallelism typically splits the weights along a certain dimension, and synchronization occurs when outputs from other parts of the model are required. Splitting weights across different dimensions results in different operations when synchronization is required.

In an abstract manner, let's focus on a general matrix-matrix product AB and write it out as

$$\sum_k A_{ik} B_{kj}$$

For each triplet (i, k, j) there is one multiplication and addition to perform. We can map all the triplets onto a parallelepiped Ω whose dimensions are given by the dimensions of A and B (namely the number of rows in A, the number of columns in A, and the number of columns in B). The question is then, generally speaking, how to partition this set of triplets Ω across the different processes to minimize communication.

You can experiment with different ideas to reduce the amount of data that needs to be communicated using MPI.

For example, as we perform many iterations, the input data is fixed across iterations (the input images). Therefore for the first layer, you can experiment with splitting $W^{(1)}$ along the rows (index i) and sharing the input images across all processes (which needs to be done only once).

Similarly, $W^{(2)}$ is a very wide matrix with only 10 rows (the 10 labels). You can therefore experiment with splitting this matrix along its columns (index k).

See for example this documentation page from Hugging Face for your information on this topic.