

CS542200 Parallel Programming

Homework 3: All-Pairs Shortest Path

Due: Sun. Dec 10 23:59, 2023

1 GOAL

This assignment helps you manage to solve the all-pairs shortest path problem with CPU threads and then further accelerate the program with CUDA accompanied by Blocked Floyd-Warshall algorithm. In this assignment, you will realize how powerful GPUs can be. Finally, we encourage you to optimize your program by exploring different optimizing strategies for performance points.

2 REQUIREMENTS

- In this assignment, you are asked to implement 3 versions of programs that solve the all-pairs shortest path problem.
 - *CPU version (hw3-1)*
 - ◆ You are required to use **threading** to parallelize the computation in your program.
 - ◆ You can choose any threading library or framework you like (pthread, std::thread, OpenMP, Intel TBB, etc).
 - ◆ You can choose any algorithm to solve the problem.
 - ◆ You must implement the shortest path algorithm yourself. (Do not use libraries to solve the problem. Ask TA if unsure).
 - *Single-GPU version (hw3-2)*
 - ◆ Should be optimized to get the performance points (20%).
 - *Multi-GPU version (hw3-3)*
 - ◆ Must use 2 GPUs. Single GPU version is not accepted and will get 0 for correctness and performance score in hw3-3 (even if you get AC on scoreboard).

3 BLOCKED FLOYD-WARSHALL ALGORITHM

Given an $V \times V$ matrix $W = [w(i, j)]$ where $w(i, j) \geq 0$ represents the distance (weight of the edge) from a vertex i to a vertex j in a directed graph with V vertices. We define an $V \times V$ matrix $D = [d(i, j)]$ where $d(i, j)$ denotes the shortest-path distance from a vertex i

to a vertex j . Let $D^{(k)} = [d^{(k)}(i, j)]$ be the result which all the intermediate vertices are in the set $\{0, 1, 2, \dots, k-1\}$.

We define $d^{(k)}(i, j)$ as the following:

$$d^{(k)}(i, j) = \begin{cases} w(i, j) & \text{if } k=0; \\ \min(d^{(k-1)}(i, j), d^{(k-1)}(i, k-1) + d^{(k-1)}(k-1, j)) & \text{if } k \geq 1 \end{cases}$$

The matrix $D^{(V)} = d^{(V)}(i, j)$ gives the answer to the all-pairs shortest path problem.

In the blocked all-pairs shortest path algorithm, we partition D into $[V/B] \times [V/B]$ blocks of $B \times B$ submatrices. The number B is called the *blocking factor*. For instance, in figure 1, we divide a 6×6 matrix into 3×3 submatrices (or blocks) by $B = 2$.

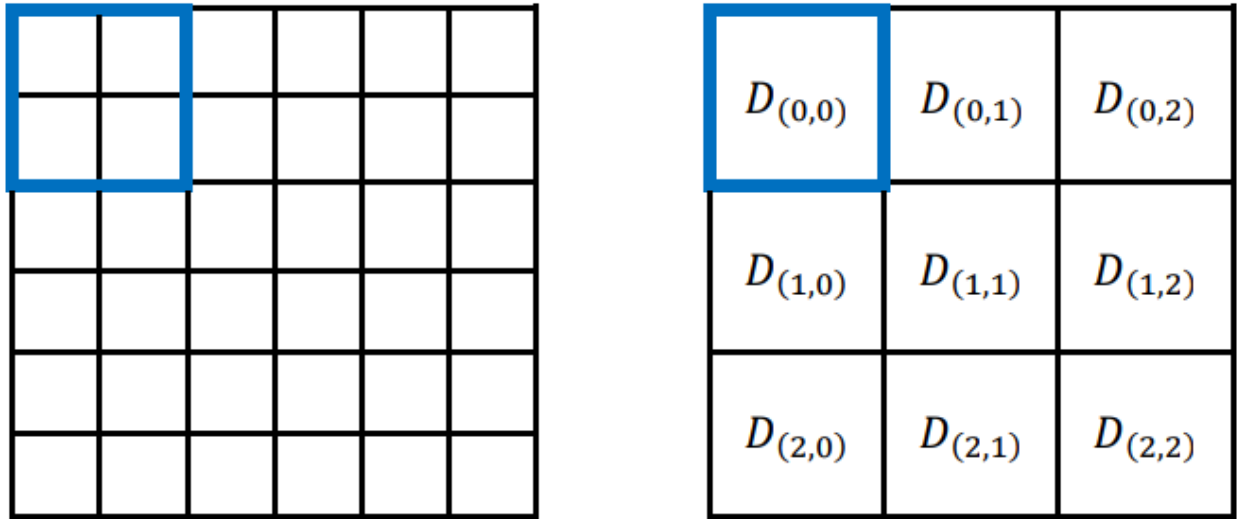


Figure 1: Divide a matrix by $B = 2$

The blocked version of the Floyd-Warshall algorithm will perform $[V/B]$ rounds, and each round is divided into 3 phases. It performs B iterations in each phase.

Assuming a block is identified by its index (I, J) , where $0 \leq I, J < [V/B]$. The block with index (I, J) is denoted by $D_{(I, J)}^{(k)}$.

In the following explanation, we assume $N = 6$ and $B = 2$. The execution flow is described step by step as follows:

- **Phase 1:** self-dependent blocks.

In the k -th round, the first phase is to compute the $B \times B$ pivot block $D_{(k-1, k-1)}^{(k \cdot B)}$.

For instance, in the 1st round, $D_{(0,0)}^{(2)}$ is computed as follows:

$$d^{(1)}(0, 0) = \min(d^{(0)}(0, 0), d^{(0)}(0, 0) + d^{(0)}(0, 0))$$

$$d^{(1)}(0, 1) = \min(d^{(0)}(0, 1), d^{(0)}(0, 0) + d^{(0)}(0, 1))$$

$$d^{(1)}(1, 0) = \min(d^{(0)}(1, 0), d^{(0)}(1, 0) + d^{(0)}(0, 0))$$

$$d^{(1)}(1, 1) = \min(d^{(0)}(1, 1), d^{(0)}(1, 0) + d^{(0)}(0, 1))$$

$$d^{(2)}(0, 0) = \min(d^{(1)}(0, 0), d^{(1)}(0, 1) + d^{(1)}(1, 0))$$

$$d^{(2)}(0, 1) = \min(d^{(1)}(0, 1), d^{(1)}(0, 1) + d^{(1)}(1, 1))$$

$$d^{(2)}(1, 0) = \min(d^{(1)}(1, 0), d^{(1)}(1, 1) + d^{(1)}(1, 0))$$

$$d^{(2)}(1, 1) = \min(d^{(1)}(1, 1), d^{(1)}(1, 1) + d^{(1)}(1, 1))$$

Note that the result of $d^{(2)}$ depends on the result of $d^{(1)}$ and therefore cannot be computed in parallel with the computation of $d^{(1)}$.

- **Phase 2:** pivot-row and pivot-column blocks.

In the k -th round, it computes all $D_{(h,k-1)}^{(k \cdot B)}$ and $D_{(k-1,h)}^{(k \cdot B)}$ where $h \neq k - 1$.

The result of pivot-row / pivot-column blocks depend on the result in phase 1 and itself.

For instance, in the 1st round, the result of $D_{(0,2)}^{(2)}$ depends on $D_{(0,0)}^{(2)}$ and $D_{(0,2)}^{(0)}$:

$$d^{(1)}(0, 4) = \min(d^{(0)}(0, 4), d^{(2)}(0, 0) + d^{(0)}(0, 4))$$

$$d^{(1)}(0, 5) = \min(d^{(0)}(0, 5), d^{(2)}(0, 0) + d^{(0)}(0, 5))$$

$$d^{(1)}(1, 4) = \min(d^{(0)}(1, 4), d^{(2)}(1, 0) + d^{(0)}(0, 4))$$

$$d^{(1)}(1, 5) = \min(d^{(0)}(1, 5), d^{(2)}(1, 0) + d^{(0)}(0, 5))$$

$$d^{(2)}(0, 4) = \min(d^{(1)}(0, 4), d^{(2)}(0, 1) + d^{(1)}(1, 4))$$

$$d^{(2)}(0, 5) = \min(d^{(1)}(0, 5), d^{(2)}(0, 1) + d^{(1)}(1, 5))$$

$$d^{(2)}(1, 4) = \min(d^{(1)}(1, 4), d^{(2)}(1, 1) + d^{(1)}(1, 4))$$

$$d^{(2)}(1, 5) = \min(d^{(1)}(1, 5), d^{(2)}(1, 1) + d^{(1)}(1, 5))$$

Phase 3: other blocks.

In the k -th round, it computes all $D_{(h_1, h_2)}^{(k \cdot B)}$ where $h_1, h_2 \neq k - 1$.

The result of these blocks depends on the result from phase 2 and itself.

For instance, in the 1st round, the result of $D_{(1,2)}^{(2)}$ depends on $D_{(1,0)}^{(2)}$ and $D_{(0,2)}^{(2)}$:

$$d^{(1)}(2, 4) = \min(d^{(0)}(2, 4), d^{(2)}(2, 0) + d^{(2)}(0, 4))$$

$$d^{(1)}(2, 5) = \min(d^{(0)}(2, 5), d^{(2)}(2, 0) + d^{(2)}(0, 5))$$

$$d^{(1)}(3, 4) = \min(d^{(0)}(3, 4), d^{(2)}(3, 0) + d^{(2)}(0, 4))$$

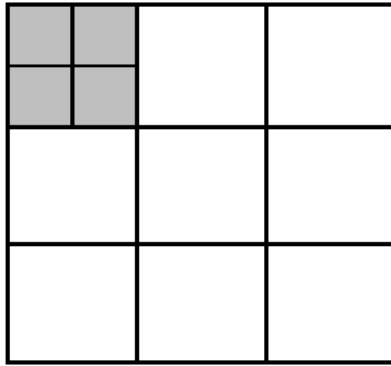
$$d^{(1)}(3, 5) = \min(d^{(0)}(3, 5), d^{(2)}(3, 0) + d^{(2)}(0, 5))$$

$$d^{(2)}(2, 4) = \min(d^{(1)}(2, 4), d^{(2)}(2, 1) + d^{(2)}(1, 4))$$

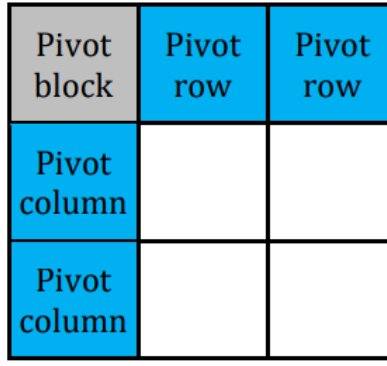
$$d^{(2)}(2, 5) = \min(d^{(1)}(2, 5), d^{(2)}(2, 1) + d^{(2)}(1, 5))$$

$$d^{(2)}(3, 4) = \min(d^{(1)}(3, 4), d^{(2)}(3, 1) + d^{(2)}(1, 4))$$

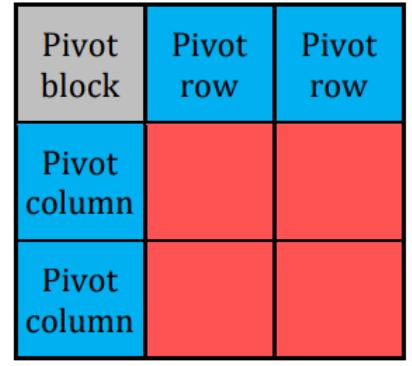
$$d^{(2)}(3, 5) = \min(d^{(1)}(3, 5), d^{(2)}(3, 1) + d^{(2)}(1, 5))$$



(a) Phase 1

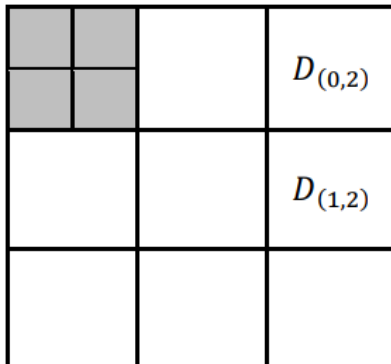


(b) Phase 2

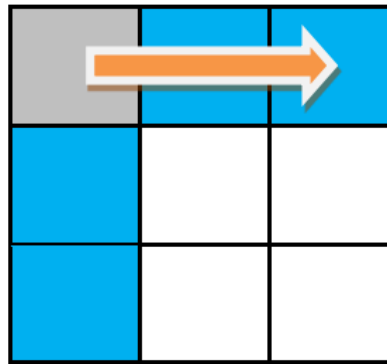


(c) Phase 3

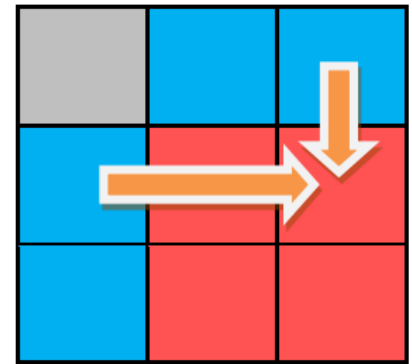
Figure 2: The 3 phases of the blocked FW algorithm in the first round.



(d) Phase 1



(e) Phase 2



(f) Phase 3

Figure 3: The computations of $D_{(0,2)}^{(2)}$, $D_{(1,2)}^{(2)}$ and their dependencies in the first round.

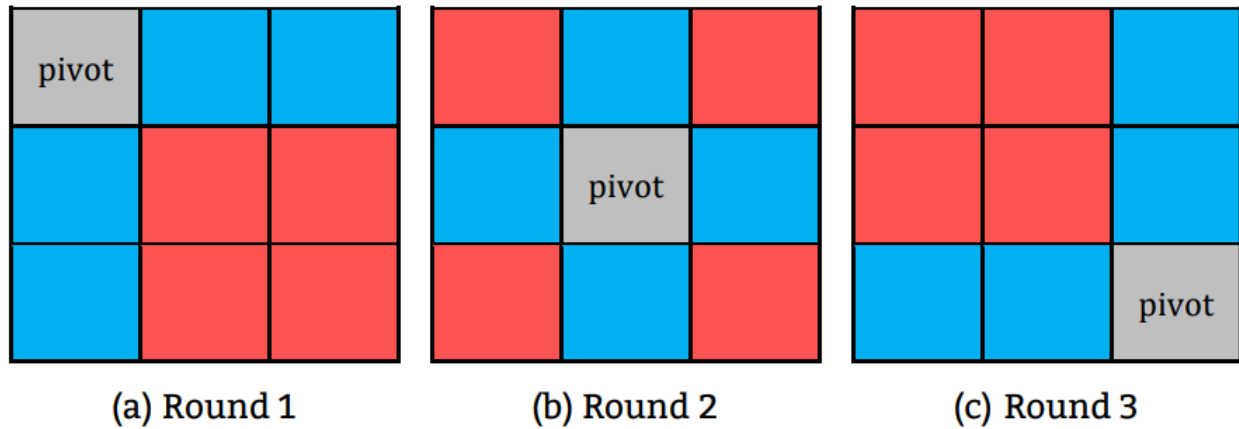


Figure 4: In this particular example where $V = 6$ and $B = 2$, we will require $\lceil V/B \rceil = 3$ rounds.

4 RUN YOUR PROGRAMS

- **Command line specification**

```
# CPU
srun -N1 -n1 -cCPUS ./hw3-1 INPUTFILE OUTPUTFILE

# Single-GPU
srun -N1 -n1 --gres=gpu:1 ./hw3-2 INPUTFILE OUTPUTFILE

# Multi-GPU
srun -N1 -n1 -c2 --gres=gpu:2 ./hw3-3 INPUTFILE OUTPUTFILE
```

- CPUS: Number of CPUs, specified by TA.
- INPUTFILE: The pathname of the input file. Your program should read the input graph from this file.
- OUTPUTFILE: The pathname of the output file. Your program should output the shortest path distances to this file. CPUS: Number of CPUs, specified by TA.

- **Input specification**

- The input is a directed graph with non-negative edge distances.
- The input file is a binary file containing 32-bit integers. You can use the `int` type in C/C++.
- The first two integers are *the number of vertices (V) and the number of edges (E)*.

- Then, there are E edges. Each edge consists of 3 integers:
 1. *source vertex id* (src_i)
 2. *destination vertex id* (dst_i)
 3. *edge weight* (w_i)
- The values of vertex indexes & edge indexes start at 0.
- The ranges for the input are:
 - $2 \leq V \leq 6000$ (CPU)
 - $2 \leq V \leq 40000$ (Single-GPU)
 - $2 \leq V \leq 60000$ (Multi-GPU)
 - $0 \leq E \leq V \times (V - 1)$
 - $0 \leq src_i, dst_i < V$
 - $src_i \neq dst_i$
 - if $src_i = src_j$ then $dst_i \neq dst_j$ (there will not be repeated edges)
 - $0 \leq w_i \leq 1000$

Here's an example:

offset	type	decimal value	description
0000	32-bit integer	3	# <i>vertices</i> (V)
0004	32-bit integer	6	# <i>edges</i> (E)
0008	32-bit integer	0	src id for edge 0
0012	32-bit integer	1	dst id for edge 0
0016	32-bit integer	3	edge 0's distance
0020	32-bit integer		src id for edge 1
...
0076	32-bit integer		edge 5's distance

- **Output specification**
 - The output file is also in binary format.

- For an input file with V vertices, you should output an output file containing V^2 integers.
- The first V integers should be the shortest path distances for starting from edge 0: $dist(0, 0), dist(0, 1), dist(0, 2), \dots, dist(0, V - 1)$; then the following V integers would be the shortest path distances starting from edge 1: $dist(1, 0), dist(1, 1), dist(1, 2), \dots, dist(1, V - 1)$; and so on, totaling V^2 integers.
- $dist(i, j) = 0$ where $i = j$.
- If there is no valid path between $i \rightarrow j$, please output with:
 $dist(i, j) = 2^{30} - 1 = 1073741823$.

Example output file:

offset	type	decimal value	description
0000	32-bit integer	0	$dist(0, 0)$
0004	32-bit integer	?	$dist(0, 1)$
0008	32-bit integer	?	$dist(0, 2)$
...
$4V^2 - 8$	32-bit integer	?	$dist(V - 1, V - 2)$
$4V^2 - 4$	32-bit integer	0	$dist(V - 1, V - 1)$

5 REPORT

Answer the questions below. You are recommended to use the same section numbering as they are listed.

1. Implementation

- Which algorithm do you choose in hw3-1?
- How do you divide your data in hw3-2, hw3-3?
- What's your configuration in hw3-2, hw3-3? And why? (e.g. blocking factor, #blocks, #threads)
- How do you implement the communication in hw3-3?

e. Briefly describe your implementations in diagrams, figures or sentences.

2. Profiling Results (hw3-2)

Provide the profiling results of following metrics on the biggest kernel of your program using NVIDIA profiling tools. NVIDIA Profiler Guide.

- occupancy
- sm efficiency
- shared memory load/store throughput
- global load/store throughput

3. Experiment & Analysis

a. System Spec

If you didn't use our `hades` server or NCHC container for the experiments, please show the CPU, RAM, disk of the system.

b. Blocking Factor (hw3-2)

Observe what happened with different blocking factors, and plot the trend in terms of Integer GOPS and global/shared memory bandwidth. (You can get the information from profiling tools or manual) (You might want to check `nvprof` and Metrics Reference)

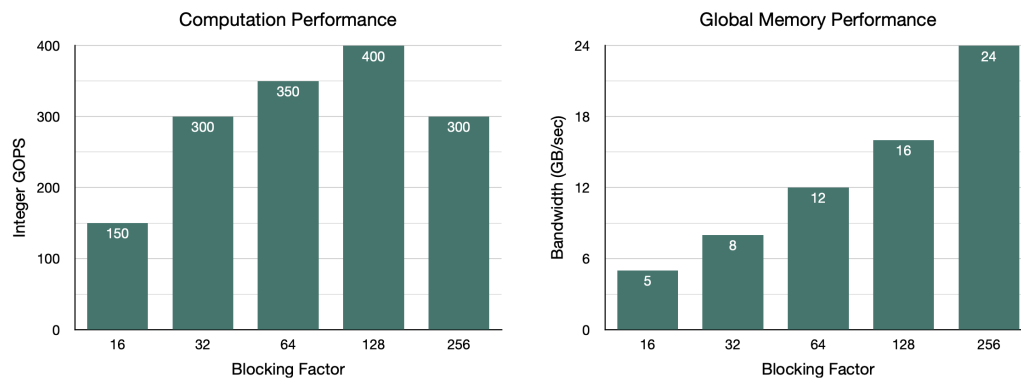


Figure 5: Example chart of performance and global memory bandwidth trend w.r.t. blocking factor

Note:

To run `nvprof` on `hades` with flags like `--metrics`, please run on the slurm partition `prof`. e.g. `srun -p prof -N1 -n1 --gres=gpu:1 nvprof --metrics gld_throughput ./hw3-2 /home/pp23/share/hw3-2/cases/c01.1 c01.1.out`

Please note that nvprof is only available for the GTX 1080. You need to use nsight-compute (command: `ncu`) on NCHC for RTX 3070 GPU.

For more details, please refer to the [Nvprof Transition Guide](#).

c. Optimization **(hw3-2)**

Any optimizations after you port the algorithm on GPU, describe them with sentences and charts. Here are some techniques you can implement:

- Coalesced memory access
- Shared memory
- Handle bank conflict
- CUDA 2D alignment
- Occupancy optimization
- Large blocking factor
- Reduce communication

■ Streaming

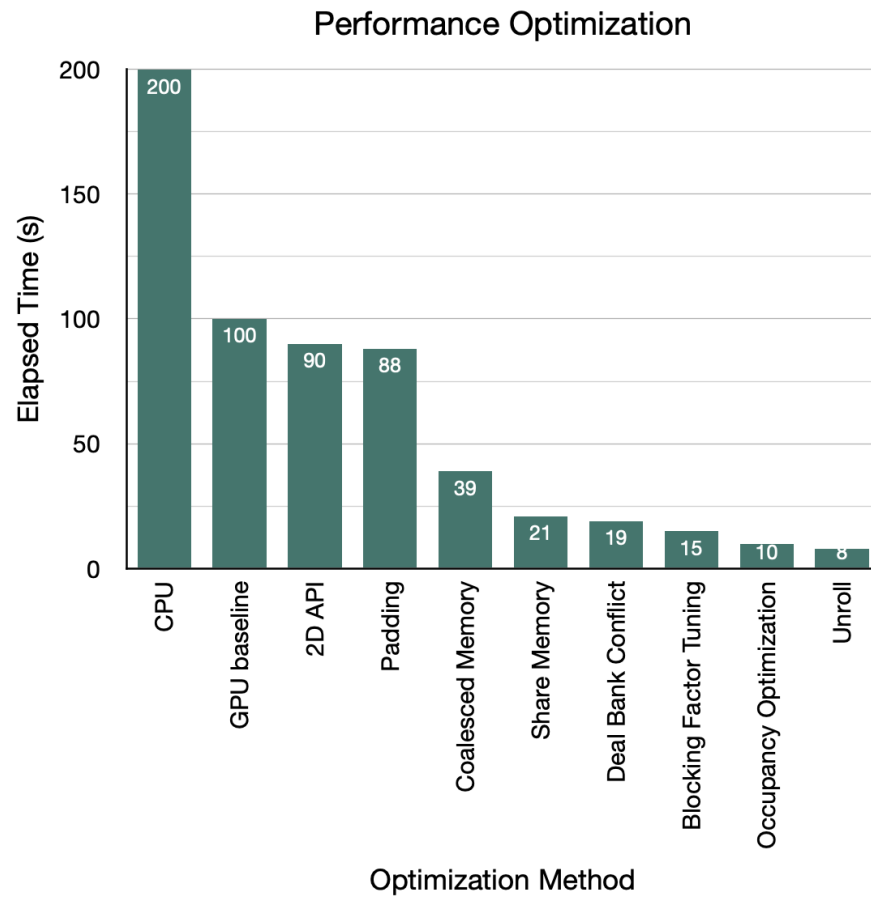


Figure 6: Example chart of performance optimization¶

d. Weak scalability (**hw3-3**)

Observe weak scalability of the multi-GPU implementations

e. Time Distribution (**hw3-2**)

Analyze the time spent in:

- computing
- communication
- memory copy (H2D, D2H)
- I/O of your program w.r.t. input size.

f. Others

Additional charts with explanation and studies. The more, the better.

4. Experience & conclusion

- a. What have you learned from this homework?
- b. Feedback (optional)

6 GRADING

1. [40%] Correctness

An unknown number of test cases will be used to test your implementation.

- CPU (15%)
 - You get 15 points if you passed all the test cases, $\max(0, 15 - k)$ points if there are k failed test cases.
 - Time limit for each case: (960 seconds) / (number of CPU cores).
- Single-GPU (15%)
 - You get 15 points if you passed all the test cases, $\max(0, 15 - k)$ points if there are k failed test cases.
- Multi-GPU (10%)
 - There are 5 test cases, each case worth 2 points. When judging, we will use hidden test cases similar to `/home/pp23/share/hw3-3/cases/c[01-05].1`.

2. [20%] Performance (*Single-GPU version only*)

- We have 30 performance test cases named pXXk1. $XX = 11 \sim 40$
- Each test case has a 30s time limit.
- Basically, larger XX test cases require longer time.
- You will get “ $\max(XX-10, 0)$ ” points if you pass test cases p11k1 ~ pXXk1. Otherwise, zero.
- For example, if you pass test cases p11k1 ~ p23k1, p25k1 and fail other test cases. You will get 13 points.
- If $XX > 20$, then extra points will still count. (but the max point of this homework is still 100)

3. [20%] Demo

- A demo session will be held remotely. You'll be asked questions about the homework.

4. [20%] Report

- Grading is based on your evaluation, discussion and writing. If you want to get more points, design or conduct more experiments to analyze your implementation.

7 SUBMISSION

Upload the files below to eeclass. (**DO NOT COMPRESS THEM**)

- hw3-1.cc
- hw3-2.cu
- hw3-3.cu
- Makefile (optional)
- hw3_{student_ID}.pdf

8 FINAL NOTES

- Type `hw3-1-judge(apollo)`, `hw3-2-judge`, `hw3-3-judge` to run the test cases. **NCHC also supports the judge commands.**
- If you want to submit your Makefile, **please combine it into a single file**. All of your code should be compiled by `make hw3-1`, `make hw3-2` and `make hw3-3` with the same Makefile.
- Scoreboard:
 - <https://apollo.cs.nthu.edu.tw/pp23/scoreboard/hw3-1/>
 - <https://apollo.cs.nthu.edu.tw/pp23/scoreboard/hw3-2/>
 - <https://apollo.cs.nthu.edu.tw/pp23/scoreboard/hw3-3/>
- Use the `hw3-cat` command to view the binary test cases in text format.
- Resources are provided under `/home/pp23/share/hw3-*/` on **Hades and Apollo**, and `/tmp/dataset-nthu-pp23/pp23/share/hw3-*/` on **NCHC**:
 - `Makefile` - example Makefile
 - `cases/` - sample test cases
- **We suggest writing your code on NCHC**, because it has more resources.
- **However, the final result is based on Hades (GTX 1080)**, so please make sure to fine tune your performance on Hades.
- Contact TA via pp@lsalab.cs.nthu.edu.tw or eeclass if you find any problems with the homework specification, judge scripts, example source code or the test cases.
- You are allowed to discuss and exchange ideas with others, but you are required to write the code on your own. You'll get **0 points** if we found you cheating.