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 $\{0, 1, 2,..., k - 1\}$.

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

$$d^{(k)}(i,j) = \begin{cases} w(i,j) & if\ k=0; \\ min(d^{(k-1)}(i,j),d^{(k-1)}(i,k-1)+d^{(k-1)}(k-1,j)) & if\ k\geq1 \end{cases}$$

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 $B = 2$.
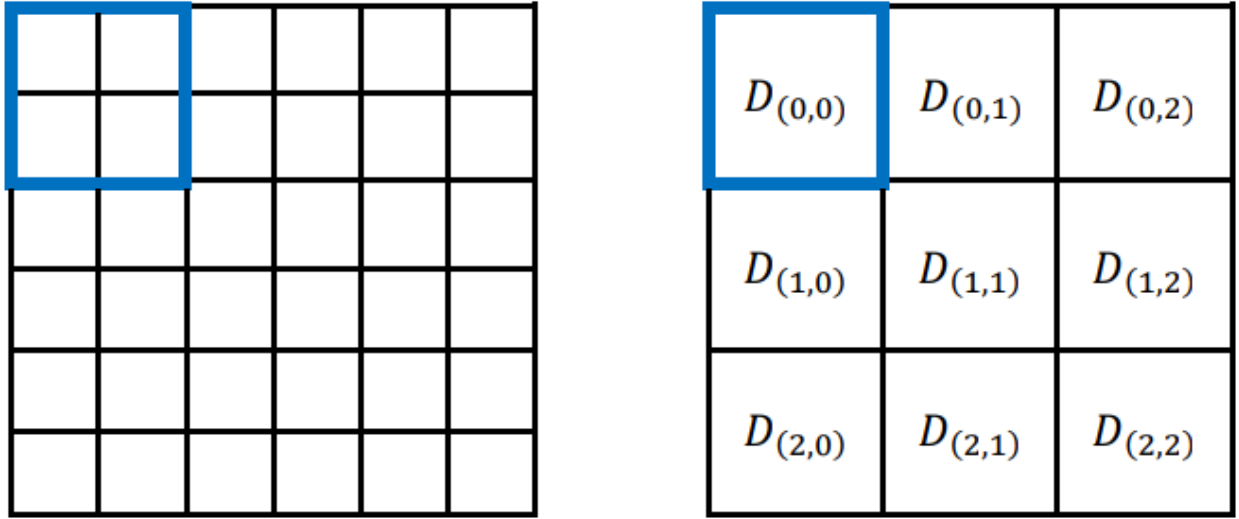

Figure 1: Divide a matrix by B = 2

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 $D^{(k \cdot B)}_{(h,k-1)}$ and $D^{(k \cdot B)}_{(k-1,h)}$ 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 $D^{(2)}_{(0,2)}$ depends on $D^{(2)}_{(0,0)}$ and $D^{(0)}_{(0,2)}$:

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

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

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

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

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

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

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

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

Phase 3: other blocks.

In the k-th round, it computes all $D^{(k \cdot B)}_{(h_1,h_2)}$ 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 $D_{(0,2)}^{(2)}$:

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

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

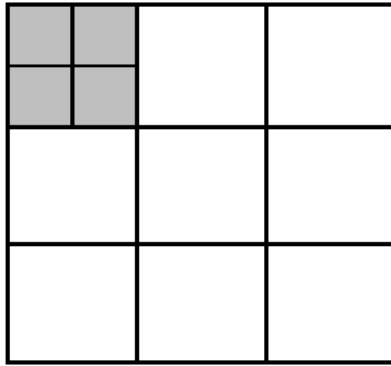$$d^{(1)}(3,4) = min(d^{(0)}(3,4), d^{(2)}(3,0) + d^{(2)}(0,4))$$

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

$$d^{(2)}(2,4) = min(d^{(1)}(2,4), d^{(2)}(2,1) + d^{(2)}(1,4))$$
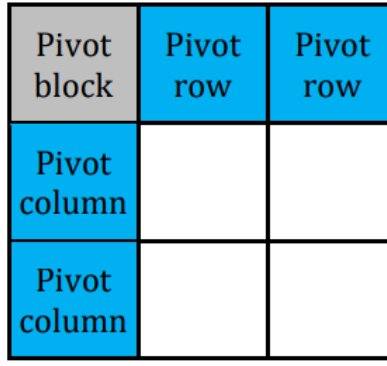
$$d^{(2)}(2,5) = min(d^{(1)}(2,5), d^{(2)}(2,1) + d^{(2)}(1,5))$$

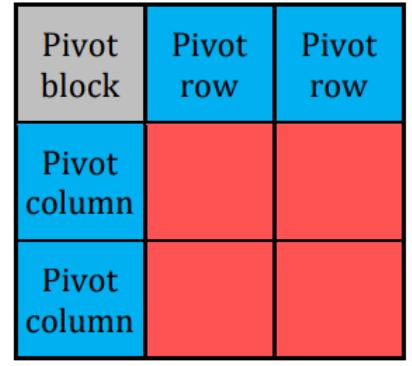$$d^{(2)}(3,4) = min(d^{(1)}(3,4), d^{(2)}(3,1) + d^{(2)}(1,4))$$

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

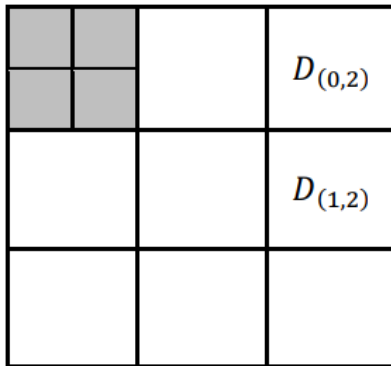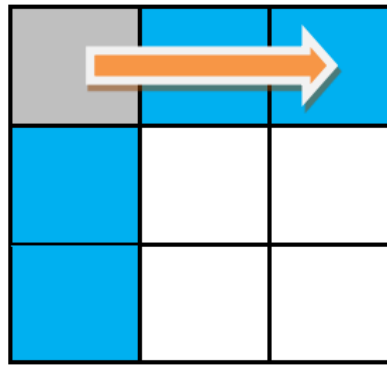(a) Phase 1   (b) Phase 2   (c) Phase 3
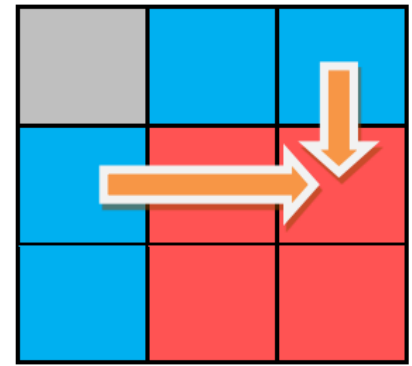
Figure 2: The 3 phases of the blocked FW algorithm in the first round.

(d) Phase 1   (e) Phase 2   (f) Phase 3

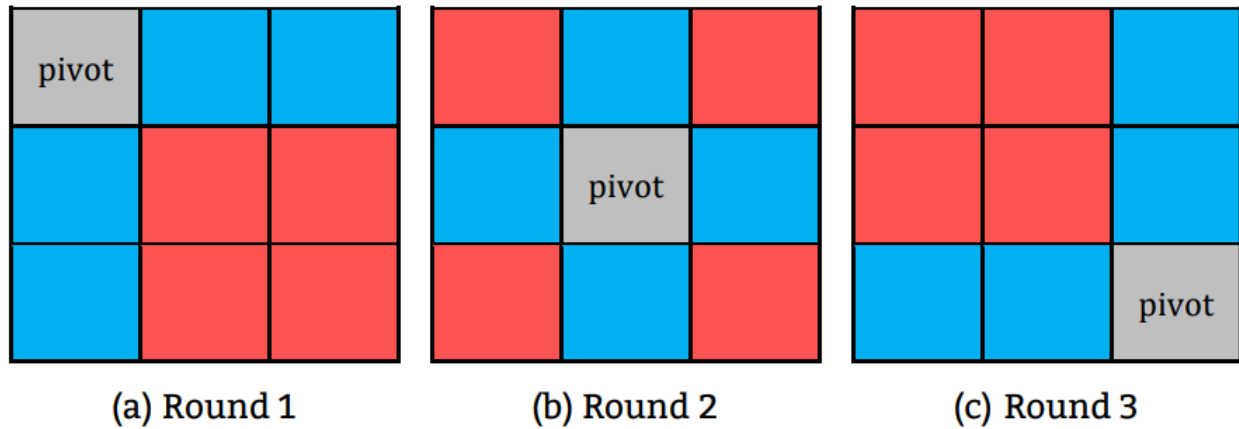Figure 3: The computations of $D_{(0,2)}^{(2)}$, $D_{(1,2)}^{(2)}$ and their dependencies in the first round.

(a) Round 1   (b) Round 2   (c) Round 3

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≤V≤6000 **(CPU)**
    - 2≤V≤40000 **(Single-GPU)**
    - 2≤V≤60000 **(Multi-GPU)**
    - 0≤E≤V×($V − 1$)
    - 0≤$src_i, dst_i < V$
    - $src_i ≠ dst_i$
    - if $src_i = src_j$ then $dst_i ≠ dst_j$ (there will not be repeated edges)
    - 0≤w_i≤1000

Here's an example:

offset	type	decimal value	description
0000	32-bit integer	3	# $vertices$ (V)
0004	32-bit integer	6	# $edges$ (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: $dist(0, 0), dist(0, 1), dist(0, 2), ..., dist(0, V - 1)$; then the following V integers would be the shortest path distances starting from edge 1: $dist(1, 0), dist(1, 1), dist(1, 2), ..., dist(1, V - 1)$; 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**
   a. Which algorithm do you choose in hw3-1?
   b. How do you divide your data in hw3-2, hw3-3?
   c. What's your configuration in hw3-2, hw3-3? And why? (e.g. blocking factor, #blocks, #threads)
   d. 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)
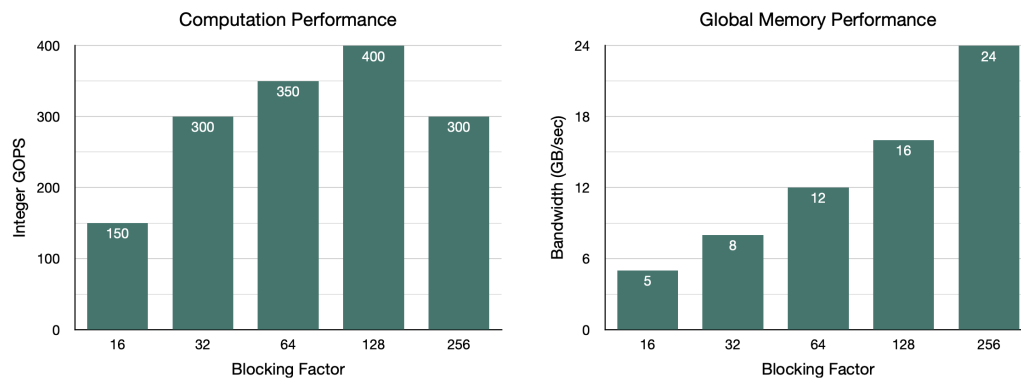

Figure 5: Example chart of performance and global memory bandwidth trend w.r.t. blocking factor

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
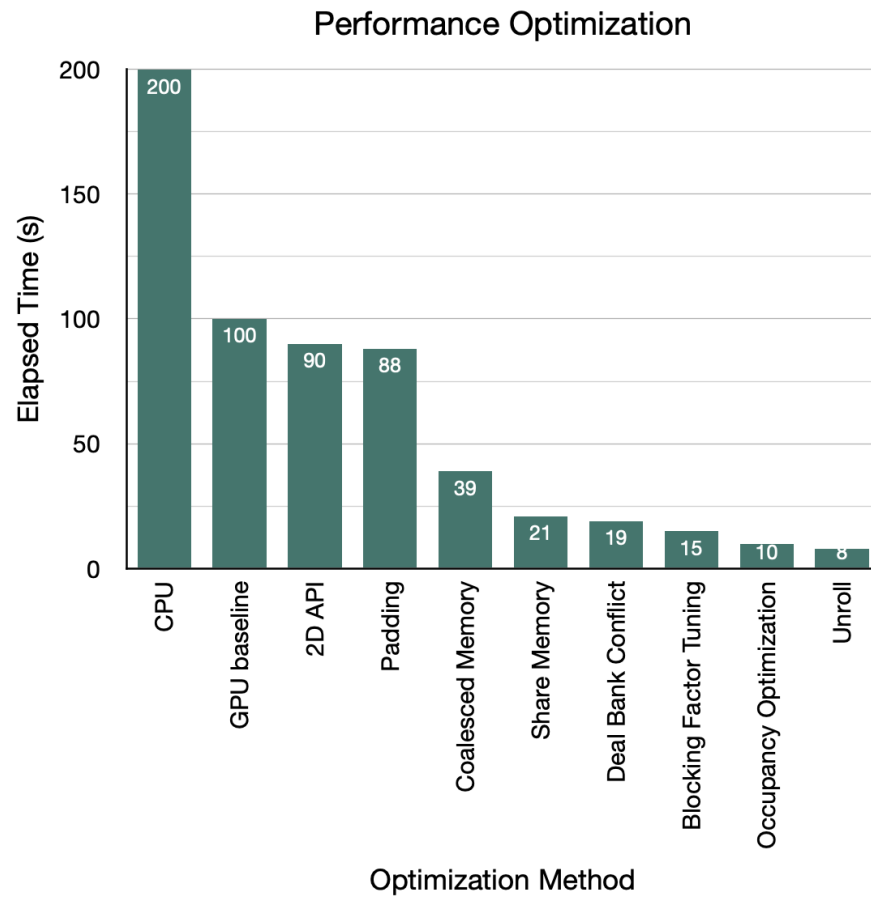- Large blocking factor
- Reduce communication

■ Streaming

Performance Optimization

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 ~ 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.