SCC 2017 Reproducibility Challenge

Your team is taking on the challenge of reviewing an article for reproducibility entitled: *The Vectorization of the Tersoff Multi-Body Potential: An Exercise in Performance Portability*, which will be referred to as "the Tersoff paper". Grading will be based on an interview (30%) and a written report (70%). The outline of the report is described in the following section: *Report Instructions*.

In addition to the input files supplied by the source code, we are adding one more input file named *in.porter*. This input file was used in the paper: *Empirical bond-order potential description of thermodynamic properties of crystalline silicon* by Porter, Yip, Yamaguchi, Kaburaki, and Tang. The paper is included in the input files of the competition server. We will ask a few simple questions about this paper during the interview. However, more in depth questions will be asked about the Tersoff paper during the interview.

Good luck to you all!

Report Instructions

Produce a report in English with the following outline. Use the ACM template available at http://www.acm.org/publications/proceedings-template-16dec2016
The report must be 4 pages or less and in PDF format. Only the first four pages will be read. Any parts of the report not on the first four pages will not count toward your score. You may omit author information to save space, but please indicate your team name on the report.

Report Outline

- Abstract: 5 points
    - Write two or three sentences describing this manuscript. Include goals of the report and a description of the platform on which the work is done.
- Introduction: 10 points
    - Give a brief description of the Tersoff paper, and the claims from the paper you are trying to reproduce.
- Machine description: 5 points
    - Describe the details of your cluster including:
        - Number of Nodes
        - Memory, CPU, and GPU (if exists) information per node
        - Vendor
        - Network interconnect
        - Operating system with version number
- Compilation/Run description: 5 points
    - Describe the steps to compile/run the software for your machine.

    - Include compiler and MPI name/version number used to compile and run the tests.
    - Include LAMMPS version and location pulled from (i.e. from Tersoff repository or official LAMMPS repository).
- Accuracy study: 10 points
    - Do an accuracy study like the one done to produce Figure 3, but compare both single to double and mixed to double precision.
    - Use the input file: *in.tersoff-acc*.
- Compare performance differences: 20 points
    - Compare the performance of the different optimizations described in the paper on your system. If using a CPU or KNL, reproduce results for Figures 4 and 5. If using a GPU, reproduce results for Figure 6.
    - For Figure 4, use the input file: *in.tersoff*.
    - For Figure 5 or 6, use the input files: *in.tersoff_bench* and *in.porter*.
    - Report results for both *in.tersoff_bench* and *in.porter*.
    - To report the results, run each case 5 times for *in.tersoff_bench* (use the second performance number from each run) and only once for *in.porter* since this file runs several cases already. Display the maximum, minimum, and average ns/day for each case on a graph. This can be reported on your graph by using error bars. However, you may report this data in any visual format you choose.
- Strong scaling study: 10 points
    - Do a strong scaling study like the one in Figure 9 using the input files *in.tersoff_bench and in.porter*.
    - Again, display on a graph: maximum, minimum, and mean ns/day using the same number of runs as the *Compare performance differences* section.
    - Since some clusters have only a few very powerful nodes, you may need more data points than a strong scaling per node can yield. To get more data points, you can do a strong scaling study by core or socket for CPUs and by individual accelerator for GPUs.
- Conclusions: 5 points
    - Conclude whether you are able to reproduce the results from the paper. Give an explanation of why the results were reproduced or why they were not. If the results are different, please include a summary and information about your platform or software stack describing why the results are different.