

Advancing materials simulations on Summit via RAPIDS

The Science

DCA++, an ORNL-developed code to simulate correlated quantum materials. Researchers develop optimized algorithm and parallelization strategies for the implementation of new science capabilities in DCA++ using the performance and visualization tool, TAU (Tuning and Analysis Utilities). TAU is a scalable and portable profiling and tracing toolkit for the analysis of parallel programs developed under SciDAC's RAPIDS Institute.

The Impact

Collaborating via the RAPIDS Institute, a joint research team from ORNL and the University of Oregon has harnessed TAU's performance feedback to assist the DCA++ team in exploiting the GPUs on ORNL's Summit supercomputer. Specifically, TAU has enabled DCA++ developers to improve the code's performance on the Summit system and increase GPU utilization.

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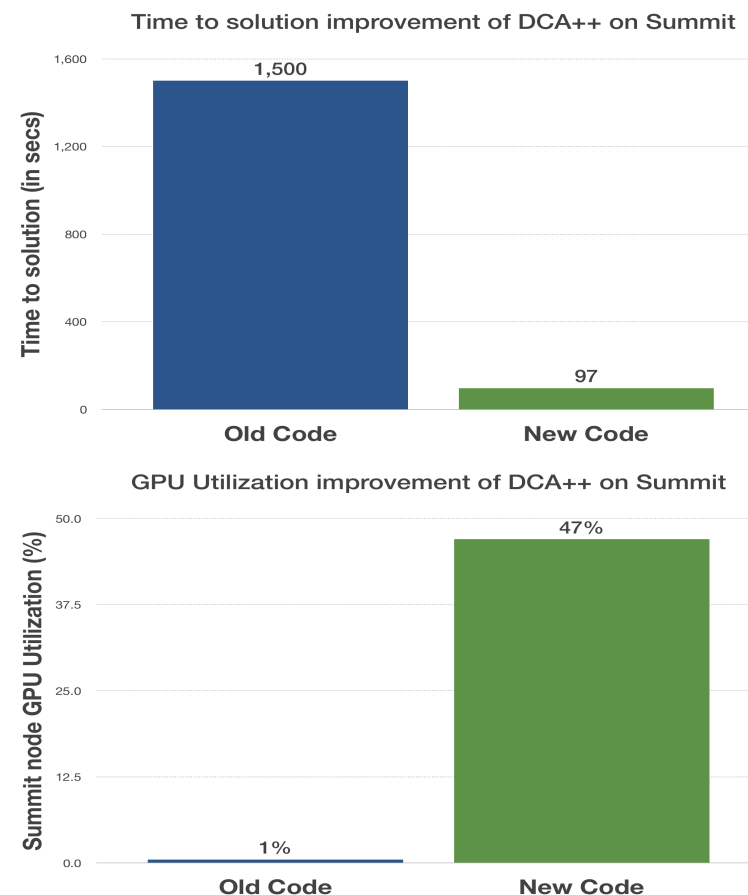


Figure: Four way comparison between the old code and new code, with respect to the time to solution and GPU utilization of the codes on Summit. These numbers were obtained from the profiling of DCA++. We notice a **speedup of 15x** over the old code, and **47x** increase in the **GPU utilization** of over the old code.

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