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GPU Acceleration of the Locally Selfconsistent Multiple Scattering Code for First Principles Calculation of the Ground State and Statistical Physics of Materials MARKUS EISENBACH, Oak Ridge National Laboratory — The Locally Self-consistent Multiple Scattering (LSMS) code solves the first principles Density Functional theory Kohn-Sham equation for a wide range of materials with a special focus on metals, alloys and metallic nano-structures. It has traditionally exhibited near perfect scalability on massively parallel high performance computer architectures. We present our efforts to exploit GPUs to accelerate the LSMS code to enable first principles calculations of O(100,000) atoms and statistical physics sampling of finite temperature properties. Using the Cray XK7 system Titan at the Oak Ridge Leadership Computing Facility we achieve a sustained performance of 14.5PFlop/s and a speedup of 8.6 compared to the CPU only code. This work has been sponsored by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Material Sciences and Engineering Division and by the Office of Advanced Scientific Computing. This work used resources of the Oak Ridge Leadership Computing Facility, which is supported by the Office of Science of the U.S. Department of Energy under contract no. DE-AC05-00OR22725.

Markus Eisenbach
Oak Ridge National Laboratory

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