**CUDA Implementation of a Hybrid Atomistic-continuum Model for Simulation of Short Pulse Laser Interaction with Metals**

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**Abstract**

Short pulse laser irradiation has the ability to bring materials into a state of strong electronic, thermal, phase, and mechanical non-equilibrium and trigger a sequence of structural transformations leading to the generation of complex multi-scale surface morphologies, unusual metastable phases and microstructure that cannot be produced by any other means.

The hybrid atomistic-continuum (TTM-MD) simulations [1-5] have been instrumental in providing valuable information on the microscopic mechanisms of laser melting, photomechanical spallation and ablation. Beyond the analysis of the initial dynamic material response to the fast laser energy deposition, however, there has been little progress in extending the TTM-MD simulations to the investigation of processes responsible for the formation of complex surface morphologies and microstructures of the laser-processed targets. The main factors that have been limiting the application of atomistic modeling to the analysis of the evolution of surface microstructure are the severe limitations on the time- and length-scales accessible for MD simulations.

The TTM-MD model is thus implemented into a parallel code with MPI and CUDA, exploring a hierarchy of parallelism with optimizations on communication hiding and memory access, to fully take advantage of the heterogeneous architecture of Titan at OLCF. GPU computing with CUDA implementation speeds up the code performance by ~ 8 times and an excellent scalability is observed up to the use of 21840 computer cores based on the results of strong scaling and weak scaling. Great thanks to OLCF, the access to its computing facility, for the first time, enables our petascale simulations to study the complex multi-scale processes responsible for the formation of surface morphology a