CHIMaD | **Center for Hierarchical Materials Design**

SPECIAL SEMINAR

The Exascale Co-design Center for Materials in Extreme Environments (ExMatEx)*

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May 27, 2014 (Tuesday)
COOK Hall, Rm 2058 | **12.00pm-1.00pm**
Pizza will be provided for lunch

ABSTRACT Computational materials scientists have been among the earliest and heaviest users of leadership-class supercomputers. The codes and algorithms which have been developed span a wide range of physical scales, and have been useful not only for gaining scientific insight, but also as testbeds for exploring new approaches for tacking evolving challenges, including massive (nearly million-way) concurrency, an increased need for fault and power management, and data bottlenecks. Multiscale, or scale-bridging, techniques are attractive from both materials science and computational perspectives, particularly as we look ahead from the current petascale era towards the exascale platforms expected to be deployed by the end of this decade. In particular, the increasingly heterogeneous and hierarchical nature of computer architectures demands that algorithms, programming models, and tools must mirror these characteristics if they are to thrive in this environment. Given the increasing complexity of such high-performance computing ecosystems (architectures, software stack, and application codes), computational "co-design" is recognized to be critical as we move from current petascale (10^{15}operations/second) to exascale (10^{18} operations/second) supercomputers over the next 5-10 years. The Exascale Co-design Center for Materials in Extreme Environments (ExMatEx) is an effort to do this by initiating an early and extensive collaboration between computational materials scientists, computer scientists, and hardware manufacturers. Our goal is to develop the algorithms for modeling materials subjected to extreme mechanical and radiation environments, and the necessary programming models and runtime systems (middleware) to enable their execution; and also influence potential architecture design choices for future exascale systems

James Belak *Co-Leads (along with Tim German from LANL) the DOE/ASCR Exascale Co-design Center for Materials in Extreme Environments whose goal is to establish the interrelationship between software and hardware required for materials simulation at the exascale while developing a multi-physics simulation framework for modeling materials subjected to extreme mechanical and radiation environments. Jim Belak has been a staff physicist in Condensed Matter and Materials Division at Lawrence Livermore National Laboratory since 1989. Jim has worked to apply materials simulation (molecular dynamics, Monte Carlo, phase-field, microstructure evolution, and continuum mechanics) and synchrotron x-ray techniques (3D tomography, small-angle scattering and in situ diffraction) to quantify dynamic material behavior in extreme conditions*