PRISM Seminar Series – Spring 2012

PRISM
NNSA Center for Prediction of Reliability, Integrity and Survivability of Microsystems

PURDUE UNIVERSITY Discovery Park

"Exascale Co-design for Materials in Extreme Environments: *Heterogeneous Algorithms for Heterogeneous Architectures*"

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3:00 pm, Birck 1001

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 (1015 operations/second) to exascale (1018 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.

Bio: Timothy C. Germann is in the Physics and Chemistry of Materials Group (T-1) at Los Alamos National Laboratory (LANL). Tim earned dual Bachelor of Science degrees in Computer Science and in Chemistry from the University of Illinois at Urbana-Champaign in 1991, and a Ph.D. in Chemical Physics from Harvard University in 1995, where he was a DOE Computational Science Graduate Fellow. At LANL, Tim has used large-scale classical MD simulations to investigate shock, friction, detonation, and other materials dynamics issues using BlueGene/L, Roadrunner, and other DOE/NNSA supercomputer platforms. He also led the development of the EpiCast large-scale epidemiological simulation model, and its use in the assessment of mitigation strategies for outbreaks of either naturally emerging or intentionally released infectious diseases, including pandemic influenza, work which directly informed the U.S. pandemic planning process. He is the Director of the DOE/ASCR "Exascale Co-Design Center for Materials in Extreme Environments," and leads the high strain-rate team in the DOE/BES "Center for Materials in Mechanical and Irradiation Extremes (CMIME)," an Energy Frontier Research Center (EFRC). Tim has co-authored over 130 peer-reviewed scientific publications with more than 2200 citations, and is currently vice-chair (becoming chair-elect in 2012 and chair in 2013) of the APS Division of Computational Physics. He has received an IEEE Gordon Bell Prize for high-performance computing (1998; also a finalist in 2005 and 2008), three LANL Distinguished Performance Awards (2005, 2007, and 2009), two NNSA Defense Programs Awards of Excellence (2006 and 2007), the LANL Fellows' Prize for Research (2006), and the LANL Distinguished Copyright Award (2007); and is a Fellow of the American Physical Society (2011).

Refreshments will be served. For further information please contact Prof. Alina Alexeenko, alexeenk@purdue.edu
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