short course

TMS2012
141st Annual Meeting & Exhibition

March 11 – 15, 2012 • Walt Disney World Swan & Dolphin Resort • Orlando, Florida

Atomistic Simulations Using Standardized Interatomic Potentials

Sunday, March 11, 2012 • 8:30 a.m. – 4:30 p.m.

Member fee: **$525**	Nonmember fee: **$575**	Cancellation fee: **$50**
Late Member fee: **$600**	Late Nonmember fee: **$650**	Cancellation fee: **$50**

Course Description and Objectives:
Atomistic or molecular simulations of materials have the potential to play a key role in the development of innovative technology to address many problems the world is currently facing (including climate change, energy generation and distribution, and terrorism). In order to model the large numbers of atoms required for many applications, and to be able to study their dynamics over reasonable time scales, it is generally necessary to develop approximate models of interatomic bonding, referred to as "interatomic potentials" or "interatomic models". Once such a model is at hand, one can theoretically use it to predict almost any mechanical property, thermal property or behavior of the element (or elements) it purports to describe.

This short course will introduce participants to atomistic simulation techniques and to a current international effort to establish the "Knowledgebase of Interatomic Models," (KIM), which attempts to address some of the practical limitations of this approach. The KIM project (http://openKIM.org) has the following main objectives: (1) development of an online resource for standardized testing, long-term warehousing and easy retrieval of interatomic potentials and data. This includes the development of application programming interface (API) standards for coupling simulation codes and interatomic potential subroutines written in different languages; and (2) development of a quantitative theory of interatomic potential transferability providing rigorous criteria for selecting potentials for given applications and error bounds on results. The course will include theoretical lectures as well as hands-on experience performing atomistic simulations and learning about the KIM API.

Participants in the course will receive a copy of the book *Modeling Materials: Continuum, Atomistic and Multiscale Techniques* by Ellad B. Tadmor and Ronald E. Miller (Cambridge University Press, 2011). For more information, visit http://www.modelingmaterials.org

Who should attend:
Professors, postdoctoral fellows and graduate students with an interest in computational atomistic modeling. No prior knowledge in atomistic simulations is required, although participants are expected to have the equivalent of an undergraduate degree in one of the science or engineering disciplines. Proficiency in one or more of the following computer languages is required: C, C++, FORTRAN 77, Fortran 90 or Fortran 2003. Participants should bring a laptop computer with wireless internet capabilities for use during the hands-on part of the course.

Instructors:
Prof. Ellad Tadmor, Prof. Ryan Elliott **and** ***Dr. Valeriu Smirichinski*** - Department of Aerospace Engineering and Mechanics, University of Minnesota, USA

Prof. Ronald Miller - Department of Mechanical and Aerospace Engineering, Carleton University, Canada

For more information please contact Ellad Tadmor by email at **tadmor@aem.umn.edu**

Fee for this course includes a copy of the book *Modeling Materials Continuum, Atomistic, and Multiscale Techniques* by Ellad B. Tadmor and Ronald E. Miller (Cambridge University Press, 2011) for each registrant."