International Institute for Multifunctional Materials for Energy Conversion (IIMEC)
2012 WINTER SCHOOL IN COMPUTATIONAL MATERIALS SCIENCE ACROSS SCALES
College Station, Texas, USA
January 8-17, 2012

Rationale

Throughout history, the development of technology-enabling materials has been carried out using mostly experimental approaches. Thanks to recent advances at the theory, software and hardware level, computational materials science has emerged as an extremely valuable tool in the development of new materials.

Goals

The goal of this week-and-a-half Winter School is to introduce some of the most important methods within the Computational Materials Science toolkit to undergraduate and graduate students interested in this emerging field. Since materials science studies multi-scale phenomena, this Winter School will offer modules focused on different methods used to investigate physical phenomena at multiple scales.

Target Audience

The target audience for this Winter School is composed of students and junior researchers (postdocs, faculty) interested in learning more about computational materials science, but who may not be familiar with some (or all) of the methods and techniques used to simulate the behaviors of materials at multiple scales. In a sense, this school should be considered introductory. Participants are expected to at least become aware of the potential (and limitations) of computational materials science.

Organization

The Winter School will be organized from a top-down perspective, starting with a discussion of theoretical and computational approaches to the understanding of materials phenomena at the continuum scale, working our way down through mesoscale and atomistic approaches, ending our discussions with electronic structure-level descriptions of matter.

The idea is for each day to have a theoretical section in the morning (about 3 hours with a coffee break in between), followed by hands-on laboratory exercises. The organizers (Raymundo Arroyave, Dimitris Lagoudas, Etienne Patoor, Amine Benzerga, Tahir Cagin) will provide with computational resources and software necessary to carry out the hands-on sessions based on specifications on the part of the instructors.

Winter School Curriculum

	Date	Topic	Instructor(s)
Sunday	Jan 8th	Registration	N/A
Monday	Jan 9th	Materials Simulation at the Continuum Level	Dimitris Lagoudas (Lagoudas@tamu.edu) Darren Hartl (darren.hartl@tamu.edu)
Tuesday	Jan 10th	Mechanical Properties of Materials at the Micro/nano-scale	Amine Benzerga (benzerga@tamu.edu) Etienne Patoor (patoor@lpmm.univ-metz.fr)
Wednesday	Jan 11th	Phase Stability and Thermodynamics of Materials	Raymundo Arroyave (rarroyave@tamu.edu)
Thursday	Jan 12th	Microstructural Evolution of Materials at the Mesoscale	Jonathan Guyer (jonathan.guyer@nist.gov)
Friday	Jan 13th	Computer Laboratory	TBD
Saturday	Jan 14th	Atomistic Simulation of Materials	Tahir Cagin (tcagin@tamu.edu)
Sunday	Jan 15th	Break	N/A
Monday	Jan 16th	Materials at the Electronic Structure Level	Peter Entel (entel@thp.uni-due.de)
Tuesday	Jan 17th	Multi-functional Materials Modeling at Multiple Scales Winter School Adjourns	Peter Entel Etienne Patoor
Wednesday	Jan 18th	IIMEC Third Annual Meeting	N/A
Thursday	Jan 19th	IIMEC Third Annual Meeting	N/A

Hardware/Software Available

During the Winter School, students and instructors will have access to a Linux Cluster consisting of 328 CPUs distributed in 30 nodes with 24 GB RAM each. We already have multiple computer simulation software installed (VASP, ABAQUS, LAMMPS, etc). Additional software can be installed at the request of the instructors.