Elements of ICME Workshop
23–25 July • 8:30 am–4 pm • 2240 DCL

General Information

The objective of this course is to present to research engineers the foundations of and recent developments within integrated computational materials engineering (ICME). ICME promises designers and engineers the potential to shorten product and process development time using computational design methods. This workshop will focus on the fundamental engineering problems addressed by ICME, computational components (and their integration) of ICME, and both recent developments and open questions in the field. The target audience consists of materials researchers from academia and industry who desire a review of current practices, open questions, and cutting-edge techniques in computational materials science and its incorporation into ICME.

This example-driven three-day research workshop, hosted by Computational Science and Engineering (http://cse.illinois.edu) at the University of Illinois, will introduce researchers to the elements of integrated computational materials engineering (ICME). Lectures and tutorials will alternate with hands-on practical exercises, and participants are encouraged both to help one another, and to try applying what they have learned to their own research problems during and between sessions. Participants should bring their own laptops to work on for hands-on components—contact Neal Davis (mailto:davis68@illinois.edu) if you need special accommodation.

Who: The target audience for this research workshop is academic researchers—faculty, postdoctoral students, graduate students, and other researchers—who are interested in exploring the new field of ICME to further their insight into processes and structures.

Where: 2240 Digital Computer Laboratory, 1304 West Springfield Avenue, Urbana, Illinois

When: 23–25 July, 2014
8:30 am–4 pm

Contact: Please mail cse@cse.illinois.edu (mailto:cse@cse.illinois.edu) for more information.

Registration

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Tentative Agenda

Wednesday 23 July
MOTIVATION

http://uiuc-cse.github.io/icme-su14/
8:30 AM–9:30 AM  Accelerated Materials Research  
Santanu Chaudhuri  
Applied Research Institute  
University of Illinois  

9:30 AM–10:45 AM  ICME & Industry  
Jason Sebastian  
QuesTek  

11:00 AM–12:00 PM  Materials Project & Materials Genome Initiative  
Shyue Ping Ong  
Nanoengineering  
University of California at San Diego  

11:45 AM–12:45 PM  Lunch  

COMPUTATIONAL METHODS  

1:00 PM–2:00 PM  Knowledgebase of Interatomic Models  
Ryan Elliott  
Aerospace Engineering & Mechanics  
University of Minnesota  

2:15 PM–4:00 PM  Molecular Dynamics with LAMMPS  
Andrew Ferguson  
Materials Science & Engineering  
University of Illinois  

Thursday 24 July  
COMPUTATIONAL METHODS (CONTINUED)  

8:30 AM–9:30 AM  Introduction to Quantum Monte Carlo  
David Ceperley  
Physics  
University of Illinois  

9:30 AM–10:45 AM  Quantum Monte Carlo with QWalk  
Lucas Wagner  
Physics  
University of Illinois  

11:00 AM–12:00 PM  QMC Applications  
Elif Ertekin  
Mechanical Science & Engineering  
University of Illinois  

12:00 PM–1:00 PM  Lunch  

CHARACTERIZATION & ANALYSIS  

1:00 PM–2:00 PM  ICME  
Bill Wilson  
Frederick Seitz Materials Research Laboratory  
Materials Science & Engineering  
University of Illinois  

3:00 PM–4:00 PM  Mesoscale Computational Materials Science: What is it, why should I care, and how do I do it?  
Olle Heinonen  
Materials Science Division  
Argonne National Laboratory  

3:00 PM–4:00 PM  Ab Initio Computation for Materials Characterization  
Maria Chan  
Center for Nanoscale Materials  
Argonne National Laboratory  

Friday 25 July  
CHARACTERIZATION & ANALYSIS (CONTINUED)  

8:30 AM–9:30 AM  Nanomaterial Fabrication & Characterization  
SungWoo Nam  
Mechanical Science & Engineering  
University of Illinois
Virtual Machine

Install VirtualBox (https://www.virtualbox.org/). **Warning:** this file is quite large, so please download it prior to the workshop. The image will be made available as soon as all data for exercises have been gathered.

LAMMPS Molecular Dynamics

LAMMPS (http://lammps.sandia.gov/) is a classical molecular dynamics code which is highly scalable and integrable with other programs such as Quantum Espresso (http://www.quantum-espresso.org/).

LAMMPS executables are available for major platforms.

QWalk Quantum Monte Carlo

QWalk (https://code.google.com/p/qwalk/) is a program developed to perform high-accuracy quantum Monte Carlo calculations of electronic structure in molecules and solids.

OVITO Open Visualization Toolkit

OVITO (http://www.ovito.org/) is a scientific visualization and analysis software for atomistic simulation data, available for all major platforms.

VMD Visual Molecular Dynamics

VMD (https://www.s.ks.uiuc.edu/Research/vmd/) is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3D graphics and built-in scripting.

MATLAB

MATLAB (http://www.mathworks.com/products/matlab/) is a high-level language and interactive environment for numerical computation, visualization, and programming.

We will use MATLAB for scripting. As the University has already purchased a sitewide MATLAB license (https://webstore.illinois.edu/Shop/product.aspx?zpid=1271), we will use MATLAB 8.3 R2014a.

COMSOL Multiphysics

COMSOL (http://www.comsol.com/comsol-multiphysics) is a general-purpose software platform, based on advanced numerical methods, for modeling and simulating physics-based problems.

COMSOL will provide a temporary license and installation files for the latest version at the COMSOL workshop Friday afternoon.