Multiscale Material Design: from Atoms to Structures

Crosslisted as *MEEM 550C, ENGR 657, PHYS 657, MSNT 511, MSNT 657, MSE 557C*

Time and Location: TR 12-1:50 — BOGH304

Instructor: Dr. Kasra Momeni
Phone: (318) 257-2407
e-mail: kmomeni@latech.edu
website: www.knanosys.com
Office: BOGH 250
Office Hours: T 02:00pm-04:00pm;
W 10:00am-12:00pm;
or use email to schedule a time

Course Topics:
Introducing the materials modeling, terminology and fundamentals of modeling/simulations in engineering systems, modeling materials at atomic scales using molecular dynamics techniques, statistical methods, mesoscale simulations using phase field, largescale simulations using continuum mechanics and finite element method, getting familiar with the software tools – e.g. COMSOL, LAMMPS, VMD, ParaView. Students are expected to develop models across different scales, run programs, and to analyze the results.

Textbooks: No textbook is required.

Recommended Books:

Molecular Dynamics: D. Frenkel and B. Smit, Understanding Molecular Simulation, 2nd ed. (Academic Press, 2001).
Phase Field Method: The Diffuse Interface Approach in Materials Science (Springer Berlin Heidelberg, Berlin, Heidelberg, 2003).
Continuum Mechanics: P. Chadwick, Continuum Mechanics (Courier Corporation, 2012).
Finite Element Method: T. J. R. Hughes, The Finite Element Method (Courier Corporation, 2012).

Laptop: You must have your own laptop for this course.

Software: Open-source software packages will be used in most part of this course, except the finite element simulations that are performed using COMSOL. An educational version of COMSOL is freely available for the LATech students on computer labs at Nethken Hall. The open-source software packages can be installed following their instructions:

- Cygwin (Linux virtual machine for Windows): https://www.cygwin.com
- LAMMPS (for molecular dynamics simulations): http://lammps.sandia.gov/doc/Section_start.html
  - For windows installation see http://rpm.lammps.org/windows.html
- VMD (Visualization of molecular dynamics simulations): http://www.ks.uiuc.edu/Research/vmd/
- ParaView (visualizing the scientific data): http://www.paraview.org

Grading:

Undergraduate Students		Graduate Students	
Homework	60%	Homework	40%
Review Article	30%	Term Project	40%
Final Presentation	10%	Final Presentation	20%

There are no exams in this course, however, there might be extra credit quizzes in the class.

Homework
The key element of learning in this class is the Homework. It is designed to help students to learn step by step and gain experience in problem solving and critical thinking, to better grasp the materials taught in the class. The homework should be turned in *no later than a week from the date it was posted*. The students are expected to turn in their homework individually. However, the undergraduate students may have discussions among themselves and share ideas while graduate students are expected to work alone.

Review Article/Term Project
The students will be assigned a specific topic based on their interest and background. The *undergraduate students* are expected to read at least 7 articles on that particular subject and prepare a review summarizing the key points of the articles they read. The final review must at least 4 pages (excluding the references) and follow the format of ACS journals (such as ACS Nano). The graduate students will be required to select a modeling technique based on the assigned topic, implement the proper numerical model, and generate results. They should prepare a final report in a form of a paper following the format of ACS journals (such as ACS Nano).

Final Presentation
There will be a final presentation during the last week of the class that is limited to 10 min for undergraduates and 15 min for graduate students. The *final reports' due* is *May 11, 2017*.

Grading Scale:

A	90 - 100%	(highest degree of excellence)
B	80 - 89%	(superior)
C	70 - 79%	(average)
D	60 – 69%	(poor, class must be repeated)
F	< 60%	(failure)

Honors Code (same as what you had in youe ENGR120):
Louisiana Tech has established an Honor Code to ensure the "highest standard of conduct in academic affairs." By enrolling at Louisiana Tech, you have agreed to the Honor Code that states, "Being a student of a higher standard, I pledge to embody the principles of academic integrity." Students who cheat during an exam, plagiarize another person's work, obtain or distribute copies of exams without the instructor's permission, falsify documents, or steal property or electronic information will be considered in violation of the Honor Code. It is also considered a violation of the Code to assist a person in any of the above actions. For the first infraction, a

student who violates the Code will be given a grade of "zero" on the assignment in question. A second infraction will result in an "F" for the class. All violations will be reported to the Honor Council as required by the University. For a complete copy of the Honor Code go to the following web page: http://www.latech.edu/documents/honor-code.pdf

The following statement must be attached and SIGNED for all assignments:

On my honor, I promise that I have not received inappropriate assistance on this assignment. SIGNATURE

Inappropriate assistance for homework: Copying off another person's or group's paper, copying information from the solution of homework from previous quarters or posted to the web, and any sort of computer file sharing.
Inappropriate assistance on quizzes and exams: All work must be your own (no looking at other people's paper, no talking, no cheat sheets, and no use of electronic information).
Inappropriate assistance on projects: All aspects of a project should be completed by the group submitting the project for a grade (don't copy design features, purchase the same parts as other groups unless specifically allowed by the instructor, . . .)

Accommodations for Students with Disabilities:
The students whom are in need of testing or classroom accommodations based on a disability are urged to discuss their needs with the class instructor at their earlies convenience. Please contact the Department of Testing and Disability Services, 318-257-4221, www.latech.edu/ods for For more information regarding the eligibility and further assistance.

Attendance:

- University attendance policies are provided at http://www.latech.edu/administration/policies-and-procedures/2206.php; regular and punctual class attendance is expected.
- Students with three or more unexcused absences will be dropped from the class roster.
- Students are responsible for notifying the instructor prior to excused absences that are planned (jury duty, military obligations, etc.).
- Excuses for emergency absences must be submitted within three class days following the student's return to class.
- An unexcused absence for an assignment, quiz, or project presentation will result in a zero grade.

Emergency Notification System:
All Louisiana Tech students are encouraged to enroll and update their contact information in the Emergency Notification System to ensure receiving important text and voice alerts in the event of a campus emergency. For more information on the Emergency Notification System, please visit: http://www.ert.latech.edu.

Class	Topic
1 - 03/09/2017	***Course Overview*** Basic and introductory topics (Modeling vs Simulation, theory vs. experiment, etc)
2 - 03/14/2017	***Atomistic Simulations*** Newtonian Dynamics; Fundamentals of Molecular Dynamics (Initialization, Unit cells, Equilibration, and Production)
3 - 03/16/2017	***Atomistic Simulations*** Interatomic Potentials; Numerical Algorithms for MD; Neighboring Lists; Cutoff
4 - 03/21/2017	***Atomistic Simulations*** Harmonic oscillator; Conservation laws; Analysis (connection to thermodynamics, free energy, Averaging, Binning, Correlation)
5 - 03/23/2017	***Atomistic Simulations*** Long-range interactions; Convergence; Ewald sum; Fast multipole method; Spherically-truncated potential
6 - 03/28/2017	***Atomistic Simulations**** Introduction to LAMMPS Building atomistic models, Tutorials, Sample problem
7 - 03/30/2017	***Atomistic Simulations**** Hands on Experiment with LAMMPS and VMD
8 - 04/04/2017	***Statistical Simulations*** Connecting statistical models to deterministic models; Diffusion problem; Random walk; Mean square displacement
9 - 04/06/2017	***Statistical Simulations*** Basic statistics; probability; Binning; Moving to 3D; Diffusion of Vacancies;
10 - 04/11/2017	***Statistical Simulations*** Monte Carlo method; Macro/Micro states; Ensembles; Metropolis algorithm;
11 - 04/13/2017	***Statistical Simulations*** Ising model; spin-spin correlation function; Lennard-Johns system
12 - 04/18/2017	***Meso-scale Simulations*** Functional; Fundamentals of the Phase Field Method; Auxiliary Variables (Order Parameters); Conserved/nonconserved Variables;
13 - 04/20/2017	***Meso-scale Simulations**** Developing models in COMSOL; Model geometry; Adding different physics; Initial/Boundary conditions; Solvers; Visualization/Analysis
14 - 04/25/2017	***Meso-scale Simulations*** Local Free Energy; Nonlocal Free Energy (Interface Energy); Governing equations; Allen-Cahn Eq; Cahn-Hilliard Eq;
15 - 04/27/2017	***Meso-scale Simulations*** Interface width; Interface energy; Grain growth model;
16 - 05/02/2017	***Meso-scale Simulations*** Implementation in COMSOL
17 - 05/04/2017	***Large-scale Simulations*** Continuum Mechanics; Strong (classical) Form; Weak (variational) Form;
18 - 05/09/2017	***Large-scale Simulations*** Galerkin Approximation; Assembling of Stiffness Matrix
19 - 05/11/2017	***Large-scale Simulations*** Reports due Modeling in COMSOL; Implementing strong/weak forms
20 - 05/16/2017	***Presentations***