DEPARTMENT: MECHANICAL ENGINEERING	
COURSE #: EMA 4813 3 credits Course Web Delivery System	**COURSE TITLE:** Computational Material Physics
TYPE COURSE: Technical Elective	**TERMS OFFERED:** Fall
CATALOG DESCRIPTION: This course covers numerical simulation techniques for predicting various physical properties of conventional materials, nanomaterials, and biomaterials. Example properties include elasticity, viscosity, thermal conductivity, diffusivity, wettability, phase transition temperatures, etc. The goal is to use computational material physics tools (molecular dynamics, Monte Carlo, Brownian dynamics, density functional theory, and etc.) to understand, predict, and design new materials and guide experimental studies at the atomistic level.	**PREREQUISITES:** Junior or Senior standing and instructor's permission
AREA COORDINATOR: Dr. William Oates **RESPONSIBLE FACULTY:** Dr. Shangchao Lin **INSTRUCTOR OF RECORD:** Dr. Shangchao Lin Building, Office room number AME 214; (850) 645-0138 slin@eng.famu.fsu.edu Office Hours: make appointments via email **DATE OF PREPARATION:** 06/20/2017 (SL)	**CLASS SCHEDULE:** **Class:** Two times weekly for 1 hr. and 15 min. **Lab:** No
TEXTBOOKS/REQUIRED MATERIAL: 1. Not required. All course materials are based on lecture notes **References, Additional Resources:** • Andrew R. Leach, *Molecular Modelling: Principles and Applications*, Prentice Hall, 2011 • M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids*, Oxford Science Publications, 1989 • D. C. Rapaport, *The Art of Molecular Dynamics Simulation*, Cambridge University Press, 2004, • Daan Frenkel and Berend Smit, *Understanding Molecular Simulation: From Algorithms to Applications*, Academic Press, 2001 • Markus J. Buehler, *Atomistic Modeling of Materials Failure*, Springer, 2008	**SCIENCE/DESIGN (%):** 75% / 25% **CONTRIBUTION TO MEETING THE PROFESSIONAL COMPONENT:** 75% engineering science 25% engineering design
COURSE TOPICS: The topics to be covered includes (not necessarily in the order shown) 1. Introduction of atomistic structures of materials 2. Statistical mechanics and Monte Carlo (MC) simulations 3. Molecular dynamics (MD) simulations 4. Model atomistic interactions with “force fields” 5. Free Energy Calculation Methods	**ASSESSMENT TOOLS:** **Undergraduate:** 1. Homework without Additional Assignments (30%) 2. Midterm Exam (30%) 3. Final Team Project (40%)

6. Brownian dynamics (BD) and dissipative particle dynamics (DPD)
7. Analyzing MD simulation results
8. Brief Introduction to Quantum Mechanics Calculations
9. Case study I: solid and fracture mechanics
10. Case study II: phonon heat transfer
11. Case study III: phase change and thermodynamics
12. Case study IV: fluid mechanics and interfacial phenomena

Student Learning Objectives for FSU Curriculum File Syllabus	At the end of the course the student should be able to 1. Select the appropriate computational material physics tools for specific materials and material properties of interest. 2. Carry out numerical simulations using online nanoHUB modules. 3. Collect, visualize, and analyze data using basic computer programming skills. 4. Determine the structural, transport, and mechanical properties of materials. 5. Work as a team to complete a well-written final project report and oral presentation with clearly expressed motivations, introductions of methods, discussions of results, and conclusions.
Justification for addition or change	Computational Material Physics is a new course (originally under EML4930/5930 as a special topic course in ME) which aims to serve as an elective core course in the “Computational Methods for Materials” topic area in the MS&E program. Offering of similar courses in this topic area has been missing for many years.

Level of computer usage: None ☐ Elementary ☑ Intermediate ☐ Advanced ☐
Modes of Instruction: Lecture ☑ Lab ☐ DIS ☐ Discussion ☐ Other ☐
Core Curriculum Course: Yes ☐ No ☑
Availability to other Majors: Yes ☑ No ☐

ME COURSE OBJECTIVES* [related to ABET Student Outcomes]	(Numbers shown in brackets refer to department **Student Outcomes** – Please ask Dr. Hollis to check these numbers) http://www.eng.fsu.edu/me/about_us/accred-info.html 1. To understand the application of fundamental computational materials science tools and principles to predict, understand, and tailor material properties [1, 5]. 2. To provide a comprehensive introduction concerning applications, technological advances, and social impacts of computational materials science [7, 8, 9]. 3. To provide an overview of the guiding principles in the mechanical, thermal, transport, and thermodynamic properties of engineering, nano-, and bio-materials [1, 5]. 4. To apply basic computer programming tools to analyze results from numerical simulations and predict basic material properties [1, 5, 10]. 5. To learn and apply visualization software to probe the atomistic and molecular details in a simulated material system [1, 5, 10]. 6. To work as a team on the final project report and oral presentation to simulate materials and predict their mechanical, thermal, transport, or thermodynamic property using open-source codes or online modules [4, 7, 10]. Numbers refer to the Departmental Student Outcomes, e.g. for course objective 3, [1, 5] refers to student outcomes 1 and 5.
ME COURSE OUTCOMES* [related to ME Course Objective] **= FSU Student Learning**	*(Numbers shown in brackets are links to Course Objectives above) By the end of the semester, students should be able to: 1. Understand fundamental principles behind different numerical methods used in computational material physics and their corresponding limitations [1]. 2. Classify the appropriate MD force field to be used for modeling specific material types [1, 4]. 3. Correlate MD force field parameters to material’s structural, mechanical, and thermodynamic properties [1, 3]. 4. Apply basic computer programming skills to analyze MD simulation results based on simulated

	trajectories (positions, velocities, and forces) [3, 4, 5]. 5. Calculate radial distribution functions, mean square displacement, and autocorrelation functions and apply these results to determine the structural, transport, and stress properties of materials [3, 4]. 6. Apply the online nanoHUB simulation modules to determine the mechanical, thermal, and transport properties of example engineering materials [2, 3, 4]. 7. Be able to communicate technical findings as a team to the scientific community in a professional manner [6].

ASSESSMENT TOOL DETAILS

GRADING/ EVALUATION:

- Additional assignments: some homework assignments, appropriate to the first-year graduate student level, are optional for undergraduate students.

Grades will be based on the following breakdown of graded work:

Undergraduate:		
1.	Homework without Additional Assignments	30%
2.	Midterm Exam	30%
3.	Final Team Project	40%

Letter grades will be assigned equivalent to the following:

Undergraduate Grading Scale	
Numerical Score	**Letter Grade**
90 - 100	A
80 - 89	B
70 - 79	C
60 - 69	D
0 - 59	F

Departmental policy is that a grade of C or better is required to pass this course.

College of Engineering Undergraduate Policy:

1. It is the policy of the College not to assign "plus and minus (+/-)" grades for undergraduate engineering courses. http://www.eng.fsu.edu/current/undergraduate/guide.html, see Grading Policies.
2. Students are required to be familiar with Academic Policies and Requirements as outlined in the COE Student Handbook http://www.eng.fsu.edu/current/undergraduate/guide.html page 11.

ASSIGNMENTS/RESPONSIBILITIES:

Student Responsibilities

- Participation Attendance
- Homework
- Projects
- Exams

Assessment Tools:

1. Project reports
2. Project presentation
3. Homework
4. Exams

Examinations:

The date of all exams will be announced at least one (1) week in advance.

Instructional Method(s)

The primary instructional method is a traditional in-class lecture. There will also be extensive use of the Course Web Delivery System for distribution of course assignments and other materials. Course materials available from the textbook publisher may also be used. The use of online simulation modules (nanoHUB) will be introduced.

COURSE SCHEDULE

Week	Topics to be covered (not necessarily in the order shown)
1	Introduction to the Class: Atomistic Structures of Materials, Continuum-to-Atomistic Models, Example Applications Introduction to Statistical Mechanics: Ensemble Averaging, Distribution Functions (Ideal Gas, Boson, Fermion)
2	Monte Carlo (MC) Simulations: Metropolis-Hasting Algorithm (Importance Sampling), Arrhenius Law Introduction to Molecular Dynamics (MD) Simulations: Equations of Motion, Numerical Method Flow Chart, Temperature and Virial Pressure at the Atomistic Level
3	Computer Lab 1: Introduction to the “nanoHUB” Online Computing Platform (Nanowire Tensile Deformation Study) Pseudocode for MD Simulations: Initial Conditions (Velocity, Temperature), Periodic Boundary Conditions, Force Calculations and Bookkeeping
4	Strategy for Efficient MD Simulations: Neighbor Lists, Domain Decompositions, Parallel Supercomputing Energy Minimization in MD: Steepest Descent, Conjugate Gradient; Introduction to MD Engines and Software
5	Overcome Timescale Limitations: Transition State Theory, Hyperdynamics, Parallel Replica Dynamics, Temperature-Accelerated Dynamics, Replica Exchange Dynamics Introduction to “Force Field”: Pairwise Potential, Lennard-Jones Potential, Harmonic Potential, Electrostatic Potential
6	Many-Body Potentials: Metallic Bonding (Embedded-Atom Method), Organic Polymers (CHARMM Potential) Computer Lab 2: Use “nanoHUB” Platform to Study Temperature-Accelerated Dynamics
7	Bond-Order Potentials for Chemical Reactions: Tersoff, REBO/AIREBO, ReaxFF, COMB Coarse-Grained Potentials: Bead-Spring Model for Polymers, MARTINI Force Field, Implicit Water Model
8	Free Energy Calculation Methods: Potential of Mean Force, Umbrella Sampling, Thermodynamic Integration Brownian Dynamics, Langevin Dynamics, and Dissipative Particle Dynamics (DPD)
9	Analyzing Simulation Results for Diffusivity and Structure: Mean Square Displacements, Radial Distribution Functions Analyzing Simulation Results for Diffusivity, Viscosity, and Thermal Conductivity: Autocorrelation Functions
10	Brief Introduction to Quantum Mechanics Calculations: Basic Quantum Mechanics, Electron Wave Functions and Schrödinger’s Equation, Density Functional Theory Midterm Exams
11	Case Study I, Solid and Fracture Mechanics: Brittle Fracture, Crack Model, Fracture Modes, Energy Theory for Crack Initiation and Propagation Case Study I, Solid and Fracture Mechanics: Cauchy-Born Rule, Hyper-Elasticity, Ductile Fracture, Dislocations
12	Case Study I, Solid and Fracture Mechanics: Biomechanics, Hierarchical Protein Structures, Intermediate Filament, Spider Silk, Collagen, Hydrogen Bonding, the Bell Model Case Study II, Phonon Heat Transfer: Heat Conduction, Lattice Dynamics and Vibrations, Phonon Modes and Branches

13	Case Study II, Phonon Heat Transfer: Phonon Density of States, Debye and Einstein Model, Dispersion Relation, Kinetic Theory of Phonon Transport Case Study II, Phonon Heat Transfer: Predicting Thermal Conductivity via Non-Equilibrium MD Simulations or the Green-Kubo Method, Spectral Phonon Properties
14	Case Study III, Phase Change and Thermodynamics: Predicting Phase Diagrams, Free Energy of Mixing, Homogenous and Heterogeneous Nucleation
15	Case Study IV, Fluid Mechanics and Interfacial Phenomena: Newtonian and Non-Newtonian Fluids, Surface Wetting, Surface and Interfacial Tensions, Nanoscale Transport Final Individual and Team Project Presentations

COURSE POLICIES:

Attendance Policy:

First day attendance is mandatory for FSU students, and first week attendance is mandatory for FAMU students. Students not in class during the first day (FSU) or first week (FAMU) are to be dropped from the course.

Excused Absences: Excused absences include documented illness, deaths in the immediate family and other documented crises, call to active military duty or jury duty, religious holy days, and official University activities. These absences will be accommodated in a way that does not arbitrarily penalize students who have a valid excuse Consideration will also be given to students whose dependent children experience serious illness.

Please note that the College of Engineering has a restrictive interpretation of what is considered a valid excuse for an absence. See: http://www.eng.fsu.edu/current/undergraduate/guide.html p. 5. If an absence is to be excused, make sure you check beforehand. In case of excused absence, the instructor will work with you to help you make up for missed time and catch up.

Unexcused Absences: A student having more than four unexcused absences will be dropped from the course and assigned the grade F. No exceptions. Tests and exams missed because of unexcused absence receive the grade 0. No exceptions.

Other projects and activities missed completely receive the grade 0 for those projects or activities. No exceptions.

Other Regulations

Note that the penalties for copying work may result in a failing grade for the course. If you are uncertain, please check with the instructor who assigned the work. Working together is encouraged in this course, but blatant copying is not.

Departmental Policy:

A student may continue in the B.S. in ME degree program unless one or more of the following conditions arise;

a. A grade below C in the second attempt of the same engineering course http://www.eng.fsu.edu/me/resources/pdf/ME_Prerequisite_Policy.pdf
b. More than three (3) repeat attempts in engineering courses. http://www.eng.fsu.edu/me/resources/pdf/ME_Excessive_Repeat_Policy.pdf
c. Violation of academic honor code as defined in university bulletin or catalog
d. Use of grade forgiveness (currently available for FAMU students only) in more than two (2) courses.

Make-up Examinations and Assignments

A make-up examination may be granted to students with a valid excused absence. However, you must notify me one week in advance if your absence involves a planned event or observance of a religious holy day. If an emergency prevents you from attending a scheduled examination, you must notify me at your earliest opportunity. You must obtain a valid excused absence for the emergency to be eligible for a make-up examination. Students with a valid excused absence will not be arbitrarily penalized for missing an assignment.

Students without a valid excused absence are not entitled to a make-up examination. However, certain class assignments may be accepted late, with penalty, without a valid excused absence.

Homework Policy:

Neatness and completeness are CRITICAL! Analysis that cannot be understood, interpreted, or checked by others, is of no value. While a correct answer is the goal of any problem solution, we are equally interested in the path that you took to obtain the solution. A correct answer that does not follow from the analysis that precedes it will not be accepted as correct.

Solve each problem on a separate sheet by itself. Put your name, the title of the homework assignment, and the problem number on the top of each page. If you are using more than one page for a problem, write "continued" next to the problem number. Use only one side of paper.

Draw a box around the solution at the end of the problem. If the problem has multiple parts, summarize them at the bottom within one box.

When grading your work, it is very important that all of your work is clearly described in your solution. In the case of an incorrect final answer, this can help the instructor determine where the conceptual or computational error is in the solution.

The important elements of a good problem-solving technique are:

i. Correct problem set-up.
ii. Correct analysis.
iii. Correct numbers and units.
iv. Correct interpretation of the answer (both units and direction).

The class schedule will have a list of homework assignments and due dates. Students will be responsible to submit the designated homework problems on the day they are due. Submitting a wrong set of problems will invalidate the homework and a grade of "0" will be given.

Homework will be due at the beginning of the class period on the date that it's due. NO LATE HOMEWORK will be accepted.

Homework should be solved separately, discussion with other students is recommended, but copying from each other is NOT allowed. A grade of "0" will be assigned for the two parties of the copied homework.

Exam Policy:

The problems on the exam will be based on homework problems, problems discussed in class, and lecture notes.

All exams will be closed book and closed notes. The instructor will provide a formula sheet. Your approach to the problem is important. You will be graded upon the approach as well as correct numerical manipulations.

There are NO makeup exams except under extenuating circumstances.

Cheating will not be tolerated. Students caught cheating on the exam will be awarded a letter grade "F" and reported for the Dean's office according to the Academic Honor Policy.

Final Project Policy:

Every team of 2-3 undergraduate students is required to complete a team project. The objective of this task is that each student obtains hands-on experience in solving practical/theoretical problems using either the nanoHUB tools or any simulation software (LAMMPS, GROMACS, etc.). The project can be applied to any engineering, physical, or chemical problems. Undergraduates are recommended to use the nanoHUB tools for their projects. All students are encouraged to select projects from their own research areas (e.g., undergraduate theses). If the students do not have specific projects in mind, please discuss it with the instructor. Here is also a list of suggested projects:

1. Predictions of material (metals, ceramics, polymers, etc.) structures under various phases.
2. Nanoscale phonon heat transfer in materials and across material interfaces.
3. Fracture mechanics, stiffness, and toughness of biomaterials and nanomaterials.
4. Molecular diffusion and viscosity (Newtonian or Non-Newtonian).
5. Phase change (melting or evaporating) temperatures of materials.

Note: Please choose a (tractable) problem that you can analyze in depth in the limited time available.

The project work should involve the following steps:

• Choose a problem and consider a simple mathematical model of the problem (geometry, materials structure, boundary conditions) such that in the first instance you can compare your analysis results with some analytical results.

• Solve this “simple” problem using simulation tools and software of your choice. Obtain an accurate solution and compare with theory.

• Now increase the complexity of the problem and re-solve the problem. Obtain an accurate solution using different boundary conditions, materials structures, etc. Ask “what if” questions and experiment with the simulation tools.

• In each case, interpret the calculated response through comparisons with engineering knowledge (e.g., data, material or physical limits, theory).

Deliverables for the Final Project:

1) A short, typed description (< 400 words) of the project you would like to select. (due in the ~ 6th week of the semester)

2) Final report (≤10 pages including figures, tables, and references, 1.15 spacing, 12 font size) due 1 week before the finals week, 60% of the term project grade.

3) In class project presentation (PowerPoint slides) during the last lecture, 40% of the term project grade. Each team of undergraduate students has 20 minutes for the presentation and 5 minutes for Q&A.

The project presentation and final report will be graded on technical content, coherency of writing, level of fundamental understandings and clearness. The results must be without technical errors and thoroughly illustrate mastery of the computational materials method through numerical validation and comparison with theory or data. Comparison with theory (in some cases, simplified initial validation problems) or comparison with data is very important. The technical content will be weighed heavier than writing style; however, the final paper must be coherent, free of grammatical mistakes and easy to understand for full credit. Points will be taken off if it is unclear what has been done. It is recommended to have someone not familiar with the project proof read your final reports.

DEPARTMENTAL STUDENT OUTCOMES

The department's student outcomes can be found at http://www.eng.fsu.edu/about/accreditation/program_outcome.html?ID=215&agency=ABET

Program Outcomes/Student Learning Outcomes

Student learning outcomes for students majoring in engineering may be found at http://www.eng.fsu.edu/outcomes

Location of Academic Learning Compacts (ALC)

COE: http://www.eng.fsu.edu/about/accreditation/program_outcome.html?ID=217&agency=ALC
FAMU: http://www.famu.edu/index.cfm?Assessment&CurrentALCs#engineering
FSU: http://learningforlife.capd.fsu.edu/smalcs/learningCompact.cfm?smalcId=62534

ACADEMIC HONOR POLICY

Students are expected to uphold the University Student Code of Conduct and/or University Academic Honor Code

> The Florida A&M University is committed to academic honesty and its core values which include scholarship, excellence, accountability, integrity, fairness, respect, and ethics. These core values are integrated into its academic honesty policy. Being unaware of the Academic Honesty Policy is not a defense to violations of academic honesty. Academic Honesty Policy violations shall be reported and appropriate actions taken by the Department Chair and Associate Dean for Student Affairs and curriculum. The complete Florida A&M Student Code of Conduct - Regulation 2.012 (8a) can be found on (p. 5) http://www.famu.edu/judicialAffairs/Regulation%202_012%20Student%20Code%20of%20Conduct.pdf and in the Student Handbook "The Fang" p. 61 http://www.famu.edu/Students/STUDENT%20HANDBOOK%20%28FANG%29%202012-2014.Updated%208.22.13.pdf p 61
>
> The Florida State University Academic Honor Policy outlines the University's expectations for the integrity of students' academic work, the procedures for resolving alleged violations of those expectations, and the rights and responsibilities of students and faculty members throughout the process. Students are responsible for reading the Academic Honor Policy and for living up to their pledge to ". . . be honest and truthful and . . . [to] strive for personal and institutional integrity at Florida State University." (Florida State University Academic Honor Policy, found at http://fda.fsu.edu/Academics/Academic-Honor-Policy.)

AMERICANS WITH DISABILITIES ACT

During the first week of class students with disabilities needing academic accommodation should:

1) register with and provide documentation to the FAMU **LDEC** or FSU **SDRC**; and
2) bring a letter to the instructor indicating the need for accommodation and what type.

Please note that instructors are not allowed to provide classroom accommodation to a student until appropriate verification from the Student Disability Resource Center has been provided.

For more information about services available to FAMU students with disabilities, contact **The Learning Development and Evaluation Center (LDEC)**

677 Ardelia Court Florida A&M University Tallahassee, FL 32310 Nathaniel Holmes, Director Donna Shell, Asst. Director	599-3180 (phone) 561-2512 (fax) 561-2783 (TDD) http://www.famu.edu/index.cfm?a=EOP&p=ADA

For more information about services available to FSU students with disabilities, contact the:
Student Disability Resource Center (SDRC)

874 Traditions Way 108 Student Services Building Florida State University Tallahassee, FL 32306-4167	(850) 644-9566 (voice) (850) 644-8504 (TDD) sdrc@admin.fsu.edu http://www.disabilitycenter.fsu.edu/

This syllabus and other class materials are available in alternative format upon request.

UNIVERSITY'S NON-DISCRIMINATION POLICY STATEMENT

FAMU: http://www.famu.edu/index.cfm?EOP&NON-DISCRIMINATIONPOLICYSTATEMENT
FSU: http://www.hr.fsu.edu/PDF/Publications/diversity/EEO_Statement.pdf

SYLLABUS CHANGE POLICY:

Except for changes that substantially affect implementation of the evaluation (grading) statement, this syllabus is a guide for the course and is subject to change with advanced notice.