MASSACHUSETTS INSTITUTE OF TECHNOLOGY

1.021/3.021/10.333/22.00 – Introduction to Modeling and Simulation

Spring 2018

Lectures:	Tuesdays and Thursdays, 3:00-4:30 PM, Room 4-231
Recitations:	Mondays and Fridays, 4:00-5:00 PM, Room 8-205
Lecturers:	Markus J. Buehler (1-290, phone x2-2750, mbuehler@MIT.EDU) Rafael Gomez-Bombarelli (office 13-5037, x3-5632, rafagb@mit.edu)
Recitation instructor:	Francisco Martin-Martinez (office 1-235, fmartinm@mit.edu)
Simulation tools:	Most tools to be used will be on the nanoHUB website (http://nanohub.org/)
Stellar site:	https://stellar.mit.edu/S/course/1/sp18/1.021/index.html

LOGISTICS

This subject provides an introduction to modeling and simulation (IM/S), covering continuum methods, atomistic and molecular simulation (e.g. molecular dynamics) as well as quantum mechanics. These tools play an increasingly important role in modern engineering. You will get hands-on training in both the fundamentals and applications of these methods to key engineering problems. The lectures will provide an exposure to areas of application, based on the scientific exploitation of the power of computation. We will use web-based applets for simulations and thus extensive programming skills are not required.

Instructors: The subject will be taught by two instructors, each covering approximately one half of the subject. Each lecturer will teach a set of 13 lectures (Part I, lectures 1-13, Markus Buehler, particle and continuum methods; Part II, lectures 14-26, Rafael Gomez-Bombarelli, quantum and related methods). The two parts will be based on one another and are integrated. Francisco Martin-Martinez will teach recitations throughout the semester.

Lectures: Lectures will meet Tuesday and Thursday 3-4:30PM (classroom 4-231). The lectures will start at 3:05 to allow you adequate time to be there on time. Lecture notes will be distributed for each lecture, usually covering the material discussed in class. On occasion, detailed notes on "theoretical" aspects (derivations, formulas, algorithms, concepts etc.) or research papers will be distributed. The subject content is defined by the material presented in lectures, recitations and reading assignments, so regular attendance is advisable.

Recitations: There will be recitations each week on Monday and Friday 4-5PM (classroom 8-205). Recitations will illustrate and/or expand concepts presented in lectures by working through numerical example problems, or by showing how to use the simulation codes. Material covered in recitations is often related to the problem sets and is considered part of the subject content, so regular attendance is advisable.

Lecture notes: Each instructor will distribute his own lecture notes and details about the format will be announced at the beginning of each part.

Homework: We will assign a total of 4-5 problem sets, focused on simulation work and data analysis. Each problem set is designed to build upon the material covered in the preceding lectures and recitations. Students are free to work in teams, and can hand in one solution per team. **The solution must state each member of the team, and must state that each member contributed actively to the solution**. The teams must be the same throughout the semester. You may use any material to complete the solution. However, it is important that you properly reference the material used (e.g. books, website, journal articles).

Due dates for problem sets are firm. The homework assignments will be graded and solutions will be provided quickly after the due date.

Exams: **There will be two in-class 1.5 hour exams, on Thursday March 22, 2018, and May 10, 2018.** All exams are open-book, but bear in mind to develop an appropriate exam strategy. The exams typically cover theoretical material and important concepts related to the two parts.

Office hours: You can meet us at any time, just set up an appointment by email or by phone call. Regular office hours of the instructors will be announced in class. The TA will offer weekly office hours, to be announced as well.

Grading scheme: The final grade will be based on: Homework (50%) and in-class exams (50%). Additional projects can be used to improve your overall score.

Prerequisites: 18.03 or 3.016, or permission of instructor. Please contact us if you have any questions.

Stellar Site: Lecture and Recitation Notes, Homework Assignments (with solutions added after due dates), etc. will be posted on: https://stellar.mit.edu/S/course/1/sp18/1.021/index.html