Computational Methods in Materials Science – NANO 3600
Fall 2017

Instructor
Alex Gezerlis (MacN 219, gezerlis@uoguelph.ca)

Teaching Assistant
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Lectures
ALEX 259
Monday, Wednesday, Friday 8:30 am – 9:20 am

Lab
THRN 1319; Friday 2:30 pm – 5:20 pm

Required textbook
There is no required textbook. I will be posting my lecture notes onto courselink at the end of every week.

Recommended texts

- Mark Newman, *Computational Physics* (Rev. ed., CreateSpace, 2013)
- R. H. Landau, M. J. Paez, and C. C. Bordeianu, *Computational Physics: Problem Solving with Python* (3rd edition, Wiley, 2015 – custom volume ISBN: 9783527807512)
- Morten Hjorth-Jensen, *Computational physics online lecture notes*

Online resources on Unix and Python

- Matt Might, *Survival guide for Unix newbies*
- Michael Stonebank, *UNIX Tutorial for Beginners*
- *The Python Tutorial*
- Allen B. Downey, *Think Python*

Lecture Content
This is a first course on what is known as *computational science* or *scientific computing*. We will focus on the interplay between science problem, mathematical formulation, and computational implementation. Previous exposure to programming is not required but will certainly be beneficial. We will cover the essentials of the following subjects:

- Unix shell basics
- Programming in Python
- Precision and errors
- Differentiation
- Integration
- Monte Carlo calculations
- Dealing with matrices
- Solving algebraic equations
- Data fitting
- Ordinary differential equations

Grading

40% Assignments+Labs
20% Midterm exam (October 27th, 2:30 pm)
40% Final exam (December 9th, 8:30 am)

If the final exam mark is greater than that of the midterm, the midterm will be dropped and the final exam mark will be weighted as 60% of the final mark.

Since one learns programming by doing, the lab is an integral part of this course. Thus, 5% of the overall grade will be based on lab attendance and performance.

Office Hours

- Mondays, 9:30 am—11:30 am, in my office (MacN 219)
- Feel free to approach me before and after class to discuss scientific computing
- Alternative arrangements can be made by appointment (gezerlis@uoguelph.ca)

Course policy regarding grading

Each homework assignment should be handed in on the due date before the lecture begins. There will be a significant penalty for late assignments, unless special arrangements are made ahead of time.

Course policy regarding use of electronic devices and recording of lectures

Electronic recording of classes is expressly forbidden without consent of the instructor. When recordings are permitted they are solely for the use of the authorized student and may not be reproduced, or transmitted to others, without the express written consent of the instructor.

Academic Consideration

When you find yourself unable to meet an in-course requirement because of illness or compassionate reasons, please advise the course instructor in writing, with your name, id#, and e-mail contact.
See the academic calendar for information on regulations and procedures for Academic Consideration.

Academic Misconduct

The University of Guelph is committed to upholding the highest standards of academic integrity and it is the responsibility of all members of the University community, faculty, staff, and students to be aware of what constitutes academic misconduct and to do as much as possible to prevent academic offences from occurring.

University of Guelph students have the responsibility of abiding by the University's policy on academic misconduct regardless of their location of study; faculty, staff and students have the responsibility of supporting an environment that discourages misconduct. Students need to remain aware that instructors have access to and the right to use electronic and other means of detection.

Please note: Whether or not a student intended to commit academic misconduct is not relevant for a finding of guilt. Hurried or careless submission of assignments does not excuse students from responsibility for verifying the academic integrity of their work before submitting it. Students who are in any doubt as to whether an action on their part could be construed as an academic offence should consult with a faculty member or faculty advisor.

The Academic Misconduct Policy is detailed in the Undergraduate Calendar:

Accessibility

The University of Guelph is committed to creating a barrier-free environment. Providing services for students is a shared responsibility among students, faculty and administrators. This relationship is based on respect of individual rights, the dignity of the individual and the University community's shared commitment to an open and supportive learning environment. Students requiring service or accommodation, whether due to an identified, ongoing disability or a short-term disability should contact the Centre for Students with Disabilities as soon as possible.

For more information, contact CSD at 519-824-4120 ext. 56208 or email csd@uoguelph.ca or see the website: http://www.csd.uoguelph.ca/csd/

Course Evaluation Information

Please refer to the Course and Instructor Evaluation Website

Drop date

The last date to drop one-semester courses, without academic penalty, is November 3, 2017. For regulations and procedures for Dropping Courses, see the Undergraduate Calendar.