2072U Computational Science I
Course outline, Winter 2024

Instructor
Lennaert van Veen, office: UA3022.
Office hours: Wednesdays and Fridays 14:00pm–15:00pm.

Time and place
Section 1: Wednesday and Friday 17:00-18:30 in UA1120. Section 2: Mondays and Thursdays 20:00-21:30 in UA1120. First class on January 6th, last class on April 4th. There are no lectures and tutorials in the week of February 17th. Please consult MyOntarioTech for the tutorial schedule.

Prerequisites
MATH1020U, MATH1850U or MATH2050U, CSCI2000U.

Text materials
Python Programming And Numerical Methods: A Guide For Engineers And Scientists by Kong, Siauw & Bayen, Elsevier. Available at
https://pythonnumericalmethods.studentorg.berkeley.edu/notebooks/Index.html.

It is essential that you have Python and SciPy/NumPy/Matplotlib installed and ready to use. Linux-based operating systems are preferred as they are most suitable for computational science.

Online resources
In addition to Canvas, which will mainly be used for lecture slides, quizzes and grades, we will use Slack for discussions and GitHub Classroom for assignments and code written in (or in preparation for) lectures. In the first week of the course we will instruct you on setting up your repository and Slack account.

Assessment
Final 40%; assignments 40%, in-class quizzes 20%.
Late assignments will not be considered.

Course description
There are two dominant themes in this course: programming applied to scientific computing and the theory and development of numerical algorithms. Using the scientific problem-solving environment provided by PYTHON/NUMPY, we will develop an understanding of the numerical computations that arise in many scientific problems and of their mathematical analysis. In particular, we will consider for a number of basic algorithms under what conditions they provide answers, how efficiently they do so and how accurate the results are.
The topics include basic numerical linear algebra, interpolation, nonlinear root-finding, quadrature and ordinary differential equations.

Course outcomes
Upon completing this course you will be able to implement a number of basic computational algorithms in PYTHON. You will understand how to evaluate the efficiency and accuracy of these algorithms using theoretical arguments as well as visualization. The ability to numerically approximate solutions to mathematical problems and visualize data will be useful in many of your third and fourth year courses and is increasingly regarded as a requirement for entry-level jobs in data science, machine learning and other forms of industrial research and development.

Tentative schedule

Week	Topic	Python	Chapter
1	Introduction		
1–2	Solving nonlinear equations	Functions, loops, lists, branching, matplotlib.pyplot	19
3–4	Solving systems of linear equations	arrays, numpy.linalg	14
5–6	Computational complexity		8
7–8	Interpolation and least squares	scipy.interpolate	16, 17
9–10	Integration and differentiation	scipy.integrate	20, 21
11–12	Ordinary differential equations		22

Accessibility
Students who require alternative testing and examination arrangements or other academic accommodations must contact the Centre for Students with Disabilities as well as the instructor as early as possible.

Academic integrity
You are welcome to collaborate on the assignments and Slack channels will be available for that purpose. However, each student must hand in their own assignment for marking. Group submissions are not acceptable. If you submit Python code as part of an assignment, it can be the same as that of the students you collaborated with. In that case, clearly list your collaborators in the submitted files as a comment. Failure to do so may be considered plagiarism.
Refer to
http://academicintegrity.ontariotechu.ca/
for the UOIT policy in matters of academic integrity.

Final examination
The final examination will take place during the final examination period at the end of the semester. It is your responsibility to check the published Examination Schedule. You must present your valid Student ID Card at the examination venue.
Refer to
https://science.ontariotechu.ca/undergraduate/academic-advising/academic-policies.php
for procedures for requesting deferred examination on the basis of religious, medical or compassionate grounds.

Course evaluation
You will be invited through the MyCampus or Canvas web site to evaluate this course. Your opinion is important to the instructor and to Ontario Tech, please take ten minutes to formulate your opinion.

More information
Included on Canvas is an addendum to this outline that touches upon such matters as privacy, intellectual property and academic integrity.