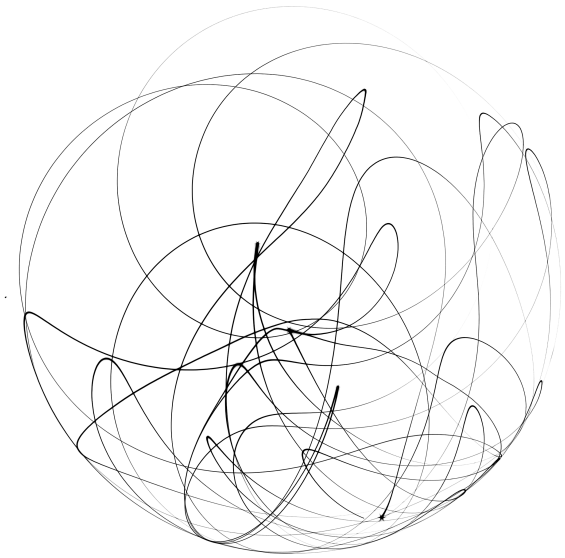
Computational Physics

PHYS-3600 (Fall 2024)

Instructor:

Name:	Dr. Jeffrey G. Rau
Title:	Assistant Professor
Office:	Essex Hall 289-1
Phone:	(519)-253-3000 ext. 2655
Email:	jrau@uwindsor.ca
Website:	https://jeffrau.ca



Office hours:

Days:	Tuesday and Thursday
Time:	2:30PM to 3:30PM
Location:	Essex Hall 289-1

Lectures:

Days:	Tuesday and Thursday
Time:	1:00PM to 2:20PM
Location:	Essex Hall 287

Assessment:

50%	Assignments (1-2 per module; lowest grade dropped, second lowest at half weight)
10%	Project proposal (pass/fail, can be resubmitted)
40%	Final project (code and report)

Materials:

Recommended text:	*Computational Physics*, M. Newman	ISBN: 1480145513
Useful resources:	*Computational Physics*, N. Giordano & H. Nakanishi	ISBN: 0131469908
	Computational Physics, S. Koonin	ISBN: 0201386232

Course information:

Website:	Brightspace (e.g. notes, discussions, assignments)
Prerequisites:	PHYS-2210, PHYS-2500, MATH-2780 and MATH-2790
Description:	An introduction to computational methods in physics, with an emphasis on applications to problems in Classical Mechanics, Electromagnetism and Quantum Mechanics. Best practices for scientific computing, data analysis and visualization. Numerical integration, differentiation, optimization; linear and non-linear equations. Techniques for initial and boundary value problems for ordinary and partial differential equations. Fast Fourier transforms. Eigenvalue problems, numerical linear algebra. Introduction to Monte Carlo methods.

Course Outline

A (tentative) course outline is given below. The content of the course is, in the end, determined by what is covered in the lectures. After a review of some foundational topics, the course is structured to revisit three of the core subjects of physics: Classical Mechanics, Electromagnetism and Quantum Mechanics through the lens of computational methods.

Foundations

- Floating point numbers, numerical error and stability; Computational complexity
- Numerical calculus; Finite differences, Simpson's rule, Gaussian quadrature
- Optimization and root-finding; Newton's method, bisection
- Solution of linear equations

Classical Mechanics

- Euler's method, Runge-Kutta method
- Symplectic integrators, Verlet method
- *Applications:*
  - Chaos; Double pendulum
  - Solar system dynamics; precession
  - Molecular dynamics; Statistical mechanics

Electromagnetism, Waves and Diffusion

- Discretization of partial differential equations; boundary conditions, time-dependence
- Poisson, diffusion and wave-equations; Classification
- Finite-difference time-domain method and relaxation; explicit and implicit methods
- *Applications:*
  - Electro- and magnetostatics
  - Simulation of Maxwell's equations
  - Kortewegde Vries equation; Solitary waves

Quantum Mechanics

- Numerical linear algebra; Jacobi method
- Time-independent Schrödinger equation; discretization, spectrum
- Time-dependent Schrödinger equation; Split-operator method, (Fast) Fourier Transform
- *Applications:*
  - Quantum billiards
  - Energy levels in periodic potentials, atoms
  - Double well potential, quantum tunnelling

Lectures

The main delivery method for the course material will be through lectures during our scheduled lecture times.

- There will be **two 80 minute sessions per week**, held during our scheduled class period (1:00PM-2:20PM, Tuesday and Thursday) in Essex Hall 287.
- During the week September 16th - 20th I will be away at a workshop and **recorded lectures will be posted** in lieu of in person delivery.

Assignments

Assignments to be done as homework will be assigned as we progress through module, with one or two assignments per module in total. Deadlines will be one to two weeks after the assignment is posted. The assignments together count for 50% of your grade.

- Homework must be prepared in a professional and legible manner and must be turned in either as a *hard-copy* or *electronically* through Brightspace. If submitting electronically, handwritten pages must be scanned and uploaded as a *single* PDF file. If prepared electronically, the final output format must be a single PDF file. **Parts of assignments submitted as code should be in the form of Jupyter notebooks**.
- The lowest one and half homework grades will be dropped. Explicitly: the lowest grade will be dropped and the second grade lowest will count with half the weight as the remaining assignments.
- **No late homework will be accepted** – after the deadline it will be given a mark of zero.
- While discussing the problems with your peers is encouraged, homework is to be written and submitted *individually* and should represent *your own work*.
- Copying from other students or from *any other source* is *not allowed*. Plagiarism and academic dishonesty are serious offences and will be addressed using university guidelines and policies. The use of generative AI *is* permitted in this course as a tool to aid and enhance understanding, but not as a substitute for learning or as a substitute for producing original work. All submitted homework should reflect your own thoughts, ideas and reasoning and (if necessary) students may be held responsible for defending their solutions.

Project Proposal (Due: October 1st, 2024, Resubmit by: October 22nd, 2024)

A one to two page document that outlines your proposed project topic, the computational methods you will use to approach it, and the questions you will explore and try to answer using these methods.

- Grade assigned on pass/fail basis. If initial submission is not satisfactory, feedback will be provided and it can be resubmitted (before the resubmission deadline). Once satisfactory, you get the full credit, worth 10% of your final grade.
- Each student must choose a different topic; if there are collisions, topics will be assigned on a first come first serve basis.

- A list of potential topics with a starting references will be provided. If you have your own ideas for a potential project topic I encourage you to discuss them with me; if I deem that the ideas are, or can be, made appropriate for the course and its objectives then you may use this as your final project.

Final project (Due: TBD, Comments if submitted by November 28th, 2024)

A significant portion of your grade (40%) will be from a final project that you submit at the end of the term. This will be on a topic in computational physics related to those we have covered which you will explore in detail. It will be completed in two main parts, each with their own weights:

- *Code (15%):* The computer code used to implement your computational methods and documents the exploratory calculations that you carried out. Comments are required.
- *Report (25%):* A written report (8-12 pages) covering the problem you are tackling, the questions you are trying to answer and summarizes and discusses your computational results.

Since this project accounts for a large fraction of your grade in the course I strongly encourage you to start early, and if you lack direction or are confused about some point make sure to ask for help. Your completed proposal should serve as a guide to what you are going to cover and in how much detail. Some further logistical details:

- Late projects will only be allowed with acceptable and verifiable medical (or equivalent compassionate) reasons, handled through official University of Windsor channels and procedures.
- Since the project is the summative evaluation for the course, it will be due by **the end of our exam day (TBD)**. If you send me a draft of your project (in any stage of completion) by November 28th, 2024, I will provide comments and suggestions (on any initiated parts) on how to improve the work.
- The final project must be written and submitted *individually* and should represent *your own work*. Copying from other students or from *any other source* is *not allowed*. The use of generative AI *is* permitted in this course as a tool to aid and enhance understanding, but not as a substitute for learning or as a substitute for producing original work. The submitted project should reflect your own thoughts, ideas and reasoning and (if necessary) students may be held responsible for explaining or defending their report and code.

Technical

- All email correspondence must be from your University of Windsor email address; email from other addresses will be ignored. Please include the course number (PHYS-3600) in the subject line any emails so I can get to it quickly.
- If you have a conflict with the posted office hours, you are also free to ask me questions at any time via email (though I will not guarantee a response rate, I will try my best). Alternatively, you can also arrange a scheduled time.
- Files submitted electronically should have a filename that indicates the course number (PHYS-3600), what is being submitted and your full name.

- For scanning of hand-written pages there are many good smartphone applications that directly produce PDFs. Some examples include Office Lens (Android, iOS) and Adobe Scan (Android, iOS).

Miscellaneous

- *Voluntary withdrawal deadline*: **November 13th, 2024**
- *Reading week:* **October 12th, 2024 - October 20th, 2024**
- For a medical absences students should follow current policies, including use of the self-report of illness interface.
- As per senate rules, grades are percentages, reported as whole numbers.
- The content of the course is, in the end, determined by what is covered in the lectures and not by the outline provided in the syllabus.
- The Student Perceptions of Teaching (SPT) be administered in the final two weeks of the semester. Instructions are available here.
- Students in need of university-recognized accommodations (via student accessibility services) should make themselves known to the instructor at the beginning of the course and discuss what arrangements are needed and how they might be accommodated.
- University of Windsors student code of conduct provides that all students are expected to commit to a code of behavior based on dignity and individuality, and respect for the rights and property of others.
    - Anyone exhibiting disruptive behavior during lectures will be asked to leave. Disciplinary actions will be taken for failure to follow directions.
    - Plagiarism and academic dishonesty are serious offences and will be addressed using university guidelines and policies.
- For help addressing mental or physical health concerns, refer to Student Health, Counselling and Wellness Services for a full list of on-and off-campus resources available to students.