Department of Physics & Astronomy
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UNIVERSITY OF CALGARY
FACULTY OF SCIENCE

COURSE OUTLINE

1. **Course:** PHYS 581, Computational Physics III - Winter 2024

Lecture 01 : T 11:00 - 11:50 in ST 026

Instructor	Email	Phone	Office	Hours
Dr David Feder	dfeder@ucalgary.ca	403 220-3638	SB 535	

To account for any necessary transition to remote learning for the current semester, courses with in-person lectures, labs, or tutorials may be shifted to remote delivery for a certain period of time. In addition, adjustments may be made to the modality and format of assessments and deadlines, as well as to other course components and/or requirements, so that all coursework tasks are in line with the necessary and evolving health precautions for all involved (students and staff).

In Person Delivery Details:

This course will be offered in an entirely in-person delivery mode.

Course Site:

D2L: PHYS 581 L01-(Winter 2024)-Computational Physics III

Note: Students must use their U of C account for all course correspondence.

Equity Diversity & Inclusion:

The University of Calgary is committed to creating an equitable, diverse and inclusive campus, and condemns harm and discrimination of any form. We value all persons regardless of their race, gender, ethnicity, age, LGBTQIA2S+ identity and expression, disability, religion, spirituality, and socioeconomic status. The Faculty of Science strives to extend these values in every aspect of our courses, research, and teachings to better promote academic excellence and foster belonging for all.

The Physics and Astronomy EDI Committee acknowledges there are persistent barriers that prevent such accessibility and hinder our progress towards EDI. Our representatives (faculty, postdocs, graduate and undergraduate students) are committed to addressing any concerns and work towards proactive solutions that enact necessary change within the department. To submit anonymous questions, comments or concerns regarding EDI related issues, please reach out to our Associate Head EDI, Claudia Gomes da Rocha (claudia.gomesdarocha@ucalgary.ca)

2. **Requisites:**

See section 3.5.C in the Faculty of Science section of the online Calendar.

Prerequisite(s):
Physics 481; and Mathematics 433, Physics 435 or Physics Engineering 435.

3. **Grading:**

The University policy on grading and related matters is described in F.1 and F.2 of the online University Calendar.

In determining the overall grade in the course the following weights will be used:

Course Component	Weight	Due Date (duration for exams)	Modality for exams	Location for exams
Assignments (approximately 5, every two weeks)	50%	Ongoing		
Midterm	25%	Feb 15 2024 at 11:00 am (90 Minutes)	in-person	In Class
Registrar Scheduled Final Exam	25%	Will be available when the final exam schedule is released by the Registrar	in person	Will be available when the final exam schedule is released by the Registrar

Each piece of work (reports, assignments, quizzes, midterm exam(s) or final examination) submitted by the student will be assigned a grade. The student's grade for each component listed above will be combined with the indicated weights to produce an overall percentage for the course, which will be used to determine the course letter grade.

The conversion between a percentage grade and letter grade is as follows.

	A+	A	A-	B+	B	B-	C+	C	C-	D+	D
Minimum % Required	94 %	90 %	86 %	82%	78%	74 %	70 %	66%	62%	58 %	54 %

Note that the grade-to-letter conversion scale is NOT the one that is often used; your numerical grades need to generally be better in order to achieve the same letter grade.

This course will have a Registrar Scheduled Final exam that will be delivered in-person and on campus. The Final Examination Schedule will be published by the Registrar's Office approximately one month after the start of the term. The final exam for this course will be designed to be completed within 2 hours.

The combined weight of the midterm and final exams is 50%. Though they are both nominally worth 25% each, your final grade will also be calculated using a 20%-30% and 30%-20% split. Whichever grade is most advantageous to you will be the one used to obtain the final letter grade.

The University of Calgary offers a flexible grade option, Credit Granted (CG) to support student's breadth of learning and student wellness. Faculty units may have additional requirements or restrictions for the use of the CG grade at the faculty, degree or program level. To see the full list of Faculty of Science courses where CG is not eligible, please visit the following website: https://science.ucalgary.ca/current-students/undergraduate/program-advising/flexible-grading-option-cg-grade

4. **Missed Components Of Term Work:**

   In the event that a student legitimately fails to submit any online or in-person assessment on time (e.g. due to illness, domestic affliction, etc...), please contact the course coordinator, or the course instructor if this course does not have a coordinator to arrange for a re-adjustment of a submission date, or possible exemption and reweighing of components. Absences not reported within 48 hours will not be accommodated. Students may be asked to provide supporting documentation (Section M.1) for an excused absence, See FAQ.

   If an excused absence is approved, options for how the missed assessment is dealt with is at the discretion of the coordinator or course instructor. Some options such as an exemption and pro-rating among the components of the course may not be a viable option based on the design of this course.

   The weight of excused missed assignments will be transferred to other assignments so that the total term weight of all submitted assignments remains at 50%. The weight of an excused missed midterm will be transferred to the final exam.

5. **Scheduled Out-of-Class Activities:**

   There are no scheduled out of class activities for this course.

6. **Course Materials:**

   Lecture notes will be posted to D2L.

   In order to successfully engage in their learning experiences at the University of Calgary, students taking online, remote and blended courses are required to have reliable access to the following technology:

   - A computer with a supported operating system, as well as the latest security, and malware updates;
   - A current and updated web browser;
   - Webcam/Camera (built-in or external);
   - Microphone and speaker (built-in or external), or headset with microphone;
   - Current antivirus and/or firewall software enabled;
   - Stable internet connection.

   For more information please refer to the UofC ELearning online website.

7. **Examination Policy:**

   Somewhat unusually for a course in computational physics, the midterm and final exams will be entirely pen-and-paper, no actual coding. I don't want you to be in a situation where you're trying to complete a timed exam, and you end up spending all of your time debugging. How would I be able to assess your understanding in that case? So the exams will instead focus on your comprehension of the fundamental concepts and the underlying mathematical, algorithmic, and architectural frameworks, and not on the coding part itself which will be adequately assessed on assignments.

   Students should also read the Calendar, Section G, on Examinations.

8. **Approved Mandatory And Optional Course Supplemental Fees:**

   There are no mandatory or optional course supplemental fees for this course.

9. **Writing Across The Curriculum Statement:**

   For all components of the course, in any written work, the quality of the student's writing (language, spelling, grammar, presentation etc.) can be a factor in the evaluation of the work. See also Section E.2 of the University Calendar.

10. **Human Studies Statement:**

    Students will not participate as subjects or researchers in human studies.

    See also Section E.5 of the University Calendar.

11. **Reappraisal Of Grades:**

    A student wishing a reappraisal, should first attempt to review the graded work with the Course coordinator/instructor or department offering the course. Students with sufficient academic grounds may request a reappraisal. Non-academic grounds are not relevant for grade reappraisals. Students should be aware that the grade being reappraised may be raised, lowered or remain the same. See Section I.3 of the University Calendar.

    a. **Term Work:** The student should present their rationale as effectively and as fully as possible to the Course coordinator/instructor within **ten business days** of either being notified about the mark, or of the item's return to the class. If the student is not satisfied with the outcome, the student shall submit the Reappraisal of Graded Term work form to the department in which the course is offered within 2 business days of receiving the decision from the instructor. The Department will arrange for a reappraisal of the work within the next ten business days. The reappraisal will only be considered if the student provides a detailed rationale that outlines where and for what reason an error is suspected. See sections I.1 and I.2 of the University Calendar

    b. **Final Exam:** The student shall submit the request to Enrolment Services. See Section I.3 of the University Calendar.

12. **Other Important Information For Students:**

    a. **Mental Health** The University of Calgary recognizes the pivotal role that student mental health plays in physical health, social connectedness and academic success, and aspires to create a caring and supportive campus community where individuals can freely talk about mental health and receive supports when needed. We encourage you to explore the mental health resources available throughout the university community, such as counselling, self-help resources, peer support or skills-building available through the SU Wellness Centre (Room 370, MacEwan Student Centre, Mental Health Services Website) and the Campus Mental Health Strategy website (Mental Health).

    b. **SU Wellness Services:** For more information, see their website or call 403-210-9355.

    c. **Sexual Violence:** The Sexual Violence Support Advocate, Carla Bertsch, can provide confidential support and information regarding sexual violence to all members of the university community. Carla can be reached by email (svsa@ucalgary.ca) or phone at 403-220-2208. The complete University of Calgary policy on sexual violence can be viewed here.

    d. **Student Ombuds Office:** A safe place for all students of the University of Calgary to discuss student related issues, interpersonal conflict, academic and non-academic concerns, and many other problems.

    e. **Student Union Information:** SU contact, Email your SU Science Reps: science1@su.ucalgary.ca, science2@su.ucalgary.ca, science3@su.ucalgary.ca,

    f. **Academic Accommodation Policy:**

       It is the student's responsibility to request academic accommodations according to the University policies and procedures listed below. The student accommodation policy can be found at: https://www.ucalgary.ca/legal-services/sites/default/files/teams/1/Policies-Student-Accommodation-Policy.pdf

       Students needing an accommodation because of a disability or medical condition should communicate this need to Student Accessibility Services in accordance with the Procedure for Accommodations for Students with Disabilities: https://www.ucalgary.ca/legal-services/sites/default/files/teams/1/Policies-Accommodation-for-Students-with-Disabilities-Procedure.pdf.

       Students needing an accommodation in relation to their coursework or to fulfil requirements for a graduate degree, based on a Protected Ground other than Disability, should communicate this need, by filling out the Request for Academic Accommodation Form and sending it to Dr. David Feder by email phas.ahugrd@ucalgary.ca preferably 10 business days before the due date of an assessment or scheduled absence.

    g. **Misconduct:** Academic integrity is the foundation of the development and acquisition of knowledge and is based on values of honesty, trust, responsibility, and respect. We expect members of our community to act with integrity. Research integrity, ethics, and principles of conduct are key to academic integrity. Members of our campus community are required to abide by our institutional Code of Conduct and promote academic integrity in upholding the University of Calgary's reputation of excellence. Some examples of academic misconduct include but are not limited to: posting course material to online platforms or file sharing without the course instructor's consent; submitting or presenting work as if it were the student's own work; submitting or presenting work in one course which has also been submitted in another course without the instructor's permission; borrowing experimental values from others without the instructor's approval; falsification/fabrication of experimental values in a report. Please read the following to inform yourself more on academic integrity:

Student Handbook on Academic Integrity
Student Academic Misconduct Policy and Procedure
Faculty of Science Academic Misconduct Process
Research Integrity Policy

Additional information is available on the Student Success Centre Academic Integrity page

h. **Copyright of Course Materials:** All course materials (including those posted on the course D2L site, a course website, or used in any teaching activity such as (but not limited to) examinations, quizzes, assignments, laboratory manuals, lecture slides or lecture materials and other course notes) are protected by law. These materials are for the sole use of students registered in this course and must not be redistributed. Sharing these materials with anyone else would be a breach of the terms and conditions governing student access to D2L, as well as a violation of the copyright in these materials, and may be pursued as a case of student academic or non-academic misconduct, in addition to any other remedies available at law.

i. **Freedom of Information and Privacy:** This course is conducted in accordance with the Freedom of Information and Protection of Privacy Act (FOIPP). Students should identify themselves on all written work by placing their name on the front page and their ID number on each subsequent page. For more information, see Legal Services website.

j. **Surveys:** At the University of Calgary, feedback through the Universal Student Ratings of Instruction (USRI) survey and the Faculty of Science Teaching Feedback form provides valuable information to help with evaluating instruction, enhancing learning and teaching, and selecting courses. Your responses make a difference - please participate in these surveys.

Course big picture

This is the fourth and last course in scientific computing / computational physics, from CPSC 217 / DATA 211 through PHYS 381 and 481. Ostensibly, the main point of this course is to expose you to advanced methods in computing for physics applications. In many aspects, it will do just that, by picking up where you left off in PHYS 481 (solving partial differential equations) to learn advanced techniques for representing spatial data and effecting its evolution in time. So we'll be studying other ways of representing spatial data by focusing on functions including Lagrange interpolating polynomials, splines, orthogonal polynomials, and finite elements; and exploring other (implicit and explicit) approaches to time dynamics, including split-step operators, variable timestep Runge-Kutta and its extensions, and Bulirsch-Stoer, as well as multistep / predictor-corrector methods such as Adams-Bashforth and Adams-Moulton. The priority will be on balancing efficiency with accuracy, to give you the tools you need to quickly generate solutions that you can trust for large problems. For this reason we will also explore approaches to parallelization of your code on both shared and distributed memory architectures.

While Python is an excellent language for algorithm design, given its simple and forgiving syntax, and for readily solving problems, given the huge repository of packages constantly under development that can be used for almost any conceivable purpose, it has one major disadvantage for scientific computing: it runs slowly. Python is an interpreted language, which means that it interprets commands while executing them, which leads to poor performance. Compiled languages, on the other hand, run much faster (by orders of magnitude for some problems), which can make the difference between a code that takes minutes to run compared to a week. Another issue is that most high-performance computing environments like Compute Canada don't readily accommodate interpreted languages, because the jobs are run in the background after waiting in queues. And Python doesn't readily parallelize in these kinds of distributed-memory systems. Last, for many applications that involve huge datasets, you need to be very careful about memory (especially when deciding on the kinds of queues you want your jobs submitted to), but Python doesn't offer any control over memory allocation.

All of this is to say that one of the learning goals of this course is to expose you to a compiled language, which I've decided will be C. C is an 'oldie but a goodie' language. Python itself is written in C! As are other interpreted languages like PHP, html, and Javascript. If you know C, learning C++, C#, objective C, Java, etc. will be easy as they all share C syntax and philosophy. C isn't object-oriented like these others, but my understanding is that you haven't really been using this aspect of Python up until now anyhow, so no loss there. C is a versatile language in that it is as high-level as Python, but you can still code at the bit-manipulation level (so it's not as low-level as Assembler, for example). Python can get you to the point where you can generate excellent working code to solve small problems, but if you're ever in a situation where running on a desktop doesn't suffice (because of memory and/or time), you'll need to translate your code into something like C. We'd be irresponsible to let you graduate without your knowing how to code a compiled language. Here's another thing: almost all of Linux (and likewise the Mac OS) is written in C, which means that C compilers and libraries are already built into the OS on the computers in the PJL. So while you learn C, you'll also learn some basic UNIX, if you don't already.

Finally, much of physics corresponds to solving math problems. One way to do that is to solve them numerically, which is the whole point of computational physics. The other way is to solve them (or at least approximate the solutions) analytically, which up until now meant working with pen on paper. But a MUCH more convenient way to do analytic work is to use a symbolic computation package. The big ones are Maple and Mathematica. If you haven't been using one of these throughout your undergraduate degree, I guarantee that you will feel some regret once you realize how much of a timesaver these could have been for you. Given that these are a core tool in the physicist's toolkit, you're all going to become familiar with Mathematica. I think that this is the superior product, sorry for not being patriotic (Maple was one of the early University of Waterloo spin-offs). To give you an idea of the importance of symbolic computation, I spend at least half of my research time working in Mathematica, and I consider myself a computational physicist!

As you can see, there is a lot to cover in this course! Fundamental techniques in computation, C, UNIX, and Mathematica. There is only one official lecture hour per week, and the remaining (lab) time is to be spent coding and performing simulations on computers. You're encouraged to work together and learn from one another. But this means that you'll be expected to study the theory, as well as work on / debug your code, outside of class time. There is more material to understand than I can possibly cover during the lectures, and your understanding of these materials will be evaluated during the midterm and final exam. You are strongly encouraged to attend all lectures and labs, so that you can clarify issues arising and to make use of the expertise of your instructor and your classmates. Otherwise, you'll fall behind quickly.

Approximate lecture schedule

Jan. 9: Introduction to the course, and to C and UNIX

Jan. 16: Review of the finite-difference approximation

Jan. 23: Introduction to Mathematica

Jan. 30: Lagrange interpolating functions

Feb. 6: Orthogonal polynomials and Gaussian quadrature

Feb. 13: The discrete variable representation; interpolation (Feb. 15 is the midterm exam)

Feb. 20: Term break, **no classes or labs**

Feb. 27: Shape functions / finite elements (Feb. 15 is the midterm exam)

March 5: Instructor away at the APS March Meeting, **no classes or labs**

March 12: Time propagators: Euler, Crank-Nicholson, Runge-Kutta; stability

March 19: Adaptive timestep methods; the split operator and fast Fourier transform

March 26: Multi-step / predictor-corrector methods

April 2: Parallelizing code on distributed-memory machines

April 9: Last class - catch up and wrap up

Course Outcomes:

- Assess how problems in physics and astrophysics can be recast into computationally solvable problems
- Construct logic and flow approaches to physical solutions to more complex physical and astrophysical problems. Determine which aspects of a physical problem are best served by computational or numerical analysis
- To understand how their graduate research will be advanced by the use of modern scientific computing skills and tools
- The ability to analyse more complex physics and astrophysics problems using more advanced numerical techniques.
- Grasp the importance of the use of random numbers in physics and astrophysics
- Master the world of Monte-Carlo techniques and its ramification to various problems in academia and beyond academia.
- Develop a keen sense of analysis of differential equations with a much wider application in physics and astrophysics
- How to use Finite-difference, Finite-volume and Finite-elements methods to problems in hydrodynamics, plasma physics and other known physical and astrophysical problems.
- How to apply of Fast Fourier Transform to a wide variety of real problems in physics, signal analysis, engineering etc …

Electronically Approved - Dec 21 2023 00:27

Department Approval