PHYS 6230: Computational Physics II

Syllabus

Teachers: Dr. Harald W. Griesshammer, Samson Hall 317, 202-994-3849, hgrie@gwu.edu; Dr. Glen MacLachlan, Corcoran Hall 211, machlach@gwu.edu; Dr. Helmut Haberzettl, helmut@gwu.edu.

Hours: Friday 15:30 to 16:20 in Corcoran Hall 212B. The class will be held in a lab/studio format; discussion of weekly project progress at these times, or as arranged with individual lecturers.

Bring your laptop to all lab/studio classes!

Web-site: http://home.gwu.edu/~hgrie/lectures/edyn12/edyn12.html for up-to-date course information, .pdf-files of Problem Sheets, suggested reading, corrections, etc.

Prerequisites: PHYS 6110 (Mathematical Methods), 6120 (Mechanics), 6130 (Computational Physics I).

Co-requisite/Coordinated with PHYS 6210: Electrodynamics (Griesshammer), PHYS 6220: Quantum Mechanics I (Haberzettl). Second of a series of three courses, tied-in with the lectures of semesters 1 to 3.

Goals/Learning Objectives: Introduction to Scientific Computing with problems accompanying the parallel course lectures. Focus on skill-building: clean and reproducible, well-documented and efficiently written code. This semester, focus is on applying efficient code-development tools (meta-language, debuggers, plotting, etc.); conceptual enrichment of parallel course lectures; visualisations; proficiency to assess usefulness and limits of numerical techniques. Final goals by semester 3 are proficiency in Scientific Computing on an advanced level, with the ability to: efficiently develop and document complex codes; critically assess powers and limitations of codes; be able to study more advanced and specialised numerical techniques on their own and as their research will necessitate. The tools and tricks we discuss form the indispensable back-bone of graduate life.

Style: 4 projects which are interlaced with the parallel course lectures Electrodynamics and Quantum Mechanics. The grades in Computational Physics do not count towards the grades in these courses, and vice versa. Each project spans 3-4 weeks and has intermediate, weekly deadlines. Two projects will be associated with Electrodynamics, 2 projects with Quantum Mechanics. A completed project consists of the submission of

- a stand-alone package which contains the complete code and all sub-routines/depending programmes, written for a common, standard, non-commercial compiler;
- the running executable;
- sample output;
- technical report/documentation in \LaTeX describing the workings of the code, including which implementation was chosen and why, and its limitations;
- further requirements as specified in the project descriptions.

While structures are quite common, two programming languages account for nearly 99% of all code written or used in Physics: Fortran and C. As understanding them is essential, projects have to be completed in either, as specified in the Project Descriptions.

Solutions must be sent by email as .pdf file of documentation and results plus source code plus executable to Drs. MacLachlan (maclach@gwu.edu), Griesshammer (hgrie@gwu.edu) and Haberzettl (helmut@gwu.edu) as specified in the project descriptions.

Grading policy: The course will be graded on an absolute scale. The final grade is based on the grades in the projects. In order to pass, you need at least 50% of all points. An excellent score usually starts at 80% of all points. No exam. Graded solutions are returned and discussed during class.
While it is necessary to have the correct answer for full credit, it is not sufficient. Indeed, it may serve you only one point. What you hand in should be a tidy and efficiently short presentation of your results and how they come about, which can be understood and reproduced by your peers. Imagine it is not homework, but a research problem whose solution you are asked to explain to your peers. Electronic submission is no excuse for leaving out sketches. 

I reserve the right to award zero points for any illegible, chaotic or irreproducible section of your homework. Homework serves several purposes, e.g.: expand and solidify your “tool-chest”, and deepen your understanding by applying what you learned. I encourage you to form study groups to discuss and attack projects as team. Nothing helps you understand better than interacting with your peers. However, the solution you hand in must be your own alone. Do not share code.

You can best study and check your progress if you regularly discuss your project progress with the respective lecturer. Office hours are the prime tool to gauge progress and revisit material not fully digested yet.

Typical workload for this course: 2 to 3 hours per week, in addition to lectures and surgery hours.

A note on academic integrity: You like Physics, or you would not be here. Thus, it is trivial that you will abide by the GW Code of Academic Integrity in all graded work. An excerpt: “Academic dishonesty is defined as cheating of any kind, including misrepresenting one’s own work, taking credit for the work of others without crediting them and without appropriate authorization, and the fabrication of information.” For the remainder of the code, see: http://www.gwu.edu/~ntegrity/code.html. You are encouraged to collaborate on your homework and even be inspired by a good textbook, but make sure you have understood what you hand in as your solution. Do not offend your own (and my) intelligence by copying other people’s work (especially without referencing). The web-site, all problems and solutions are for your personal use only. Please do not pass solutions or problems on to any student who has not taken the course (yet). Noncompliance with these rules is a breach of integrity and will be dealt with accordingly. If you have any questions about what constitutes academic dishonesty, ask me.

Absences and Excuses follow standard GW policy. It is your own responsibility to make sure you fulfil the criteria for passing. The only way around is to submit in writing documentation that you were unable to perform homework for more than half the semester due to reasons out of your control, as outlined in the GW policy on absences and excuses.

If you see a conflict between religious observances and the class schedule, you will bring them to my attention in advance, in the first week of the semester. It is University policy to extend to these students the courtesy of absence without penalty on such occasions, including permission to make up examinations.

Some Suggested Reading

There is no required reading for this course. You will not be able to find all aspects explained well in only one textbook. Moreover, it is an essential part of the learning process to view the same topic from different angles, i.e. using different textbooks. Here is a list of those which we found most useful. If you discover others, tell us. In addition, each Project Description may list additional recommended readings.

Overview of Available Literature

Scientific Computing


Specific Programming Languages: C


[ANSIC] International Standard ISO/IEC: *ISO/IEC 9899:TC3 (n1256)* The ANSI specifications for the 1999 version of C, which is the most widely used flavour. It is in fact readable which is a bit surprising for a technical specification. This is the last word in C.

Specific Programming Languages: Fortran


Miscellaneous


Security In the case of an emergency, if at all possible, the class should shelter in place. If the building that the class is in is affected, follow the evacuation procedures for the building. After evacuation, seek shelter at a predetermined rendezvous location.

Disability Support Services (DSS) Any student who may need an accommodation based on the potential impact of a disability should contact the Disability Support Services office at 202-994-8250 in the Marvin Center, Suite 242, to establish eligibility and to coordinate reasonable accommodations. For additional information please refer to: http://gwired.gwu.edu/dss/.

The University Counseling Center (UCC) assists you in addressing personal, social, career, and study problems that can interfere with your academic progress and success. Services for students include:

- Crisis Consultations at 202-994-5300 open day and night, not only for emergency.
- Confidential assessment, counseling services (individual and small group), and referrals: http://gwired.gwu.edu/counsel/CounselingServices/AcademicSupportServices
- Academic Support and Peer Tutoring Services: http://gwired.gwu.edu/counsel/AcademicSupport
- Podcasts and Self-Help: gwired.gwu.edu/counsel/PodCast, gwired.gwu.edu/counsel/OutreachSelfHelp

They are also very good when you need to review your habits, like learning and exam strategies. It’s never too early to get help.