

Physics 305
Computational Physics
Fall 2010
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Welcome to Physics 305, Computational Physics. This is a course on using computers to solve physics problems. As such, it combines an introduction to computer programming, some elementary numerical methods, and some aspects of physics that you probably haven't seen before.

Prerequisites for this course include two semesters of introductory physics, which here at the University of Arizona usually means 141-142 or 161-162. You should also have completed second semester calculus, or Math 129, and be concurrently enrolled in differential equations. Phys 105A is also a prerequisite, although we suspect that many of you will not have had this, and we will begin the course with a review (Or maybe it's an introduction) to programming. Those of you who already are good at programming may find the first part of the course is familiar material. If so, be patient — there is a good chance that the later material will be new and challenging.

This course is different from introductory physics classes in that each assignment will have many steps, and the later parts depend on the earlier parts. This means that you need to organize your work accordingly. **Do not wait until the night the assignment is due to start it!** Generally, assignments will be due on Mondays. As a rule of thumb, this means that you should have your computer programs working by Friday, so that you have time to explore the results and write your report.

1. Class meetings are at 12:30 AM on Tuesday and Thursday in room Social Sciences 224. Generally I will lecture for about 45 minutes, and use the rest of the class period to give individual assistance as you work on the assignments.
2. There is a computer lab in room 272 of the physics building which is available to you. This room contains computers that are similar to those in Social Sciences 224, although the procedure for logging in and starting up your connection to faraday is somewhat different. It is possible to do all of your course work in this lab, although many of you will also want to work from your home or other remote locations. We will try our best to give you advice on this. **PLEASE NOTE that if there is some problem with the physics department equipment that prevents people from doing their work, we will make reasonable adjustments. But if your home computer goes up in smoke, and you didn't make backups, that's your tough luck.**
3. "Office hours" will be after each class — this means that I will stay after class if anyone needs help then. Also, there will be an office hour Thursday at 2:00 in my office, in

room PAS 386a. You are also welcome to come by my office at other times — you can either make an appointment or just drop in. We encourage you to contact us by electronic mail: `doug@physics.arizona.edu` and `wfreeman@physics.arizona.edu`, either to ask questions or to make appointments.

4. Students requiring accommodations in testing or note taking should consult with me during the first week of classes.
5. **DON'T HESITATE** to ask for help. It's surprisingly easy to get far enough behind that it is difficult to catch up. When you ask for help, think about your question beforehand. If you are emailing us, don't just say "My program doesn't work". Attach the program, and explain what it is doing that convinces you it is wrong. This will help us to give a sensible response.
6. Our goal is to learn to analyze a problem, figure out what algorithms are appropriate, write a computer program to do the necessary calculations, test the program, run the program and then interpret the results. At the end of the course, this sequence should be familiar and natural to you. To this end, there will be lots of assignments, and each assignment is likely to require writing, testing and understanding more than one program. But don't be intimidated — most of these programs will be quite short, and many will be modifications of an earlier program.
7. The major part of this course will be the weekly homework assignments, and these will count for 70% of your grade. There will be frequent unannounced in-class quizzes, which will count for 20% of the grade. The final exam will count for the remaining 10%. As a rough idea of the grading standards, if your overall average in the course is 80% or better you are guaranteed an A; if it is less than 50% you are guaranteed an E. Between these two lines, adjustments may be made to accommodate obvious divisions in the class, etc. For example, the cutoff line for "A" may actually be lower than 80%. I generally grade problems on a ten point scale, where 10 means you got it right, 8 or 9 means only minor errors or omissions, 6 and 7 is the right idea, and 5 is barely passing.
8. I encourage students to talk with your classmates about the homework problems, and to consult other books. However, after you have discussed the problem, you must go home and do it yourself to turn in. **The work that you turn in must be your own.** This applies to the code in your computer programs in the same way that it applies to the text of your reports. When you use any source other than your own notes or the class notes, **you must give credit to your sources.** Do this whether the source is another textbook, something you found on the web, something you did for another class or something you got from the student next to you. Remember that

a computer program is a piece of intellectual work just as is an essay in your English class.

When you turn in work to us, you are representing that the work is your own. The easy way to stay out of trouble is simply to explain where anything that is not your own work comes from. An exception to the rule about always acknowledging your sources is that you can always get help with the text editors or with unix commands from your fellow students or from manuals without making an acknowledgement. These are necessary skills, but are not part of the scientific content of the course, and not one of the things we want to grade you on.

You are expected to adhere to the University of Arizona codes on conduct and academic integrity. These codes, along with a description of what can happen if you violate them, can be found online at <http://deanofstudents.arizona.edu/policiesandcodes/>.

9. Assignments should be submitted by electronic mail, sent to `p305@physics.arizona.edu`

Your report can be a plain text file, which is the simplest option. If you wish, you can send LaTeX, Word or PDF files. This report can be either the body of your email message or an attachment. Graphs should be sent as attachments, usually in PostScript or PDF. Don't worry if you don't know how to do this; it will be covered in class.

10. Homework problems will be assigned weekly and will be due by 10:00 pm on the day before we begin the next topic. Usually this will mean on Monday.

Note: We will accept late homework up to the two days after their due date and it will be worth 50% of full credit. We strongly advise starting the homework early — don't risk running out of time and being unable to finish the assignment. If there are unavoidable conflicts, such as attending a professional conference, arrangements should be made with the instructor **before** the date of the conflict. If you are absent because of illness, we will make arrangements for you to turn the work in late.

11. The correct answer matters! If you hand in code which clearly doesn't do what it is supposed to do, *let us know that you know this is so*, and at least speculate on what kept you from getting the correct answer. Don't try to foist garbage on us in hopes that we won't notice — we will!

The correct answer is required but not sufficient! A big part of this course is making *sure* that the answer you get is correct and providing evidence of its correctness.

Since the purpose of this course is to learn about the entire process of solving a problem, and also to learn some math and physics, your homework submission is not just a computer program. Instead it is a report, somewhat like a lab report in your earlier

classes. Computer programs, graphs, and possibly tables of output are parts of this report. Exactly what the report contains will depend on the problem, but here is a list of likely ingredients:

- What is the problem, and why is it important?
- What algorithms were used?
- What codes did you write? You should send complete computer codes as attachments to your email, and you will probably need to embed fragments of code in your discussion.
- How did you test your code? This is essential - why should we believe your answers? There are many ways to do this, but testing cases where you know the answer is the most common one. For example, in the planetary orbits assignment, do you get a circular orbit for the expected initial conditions?
- What results did you get? This includes discussion of how well your algorithms performed (did you see the expected dependence of error on step size, for example) and the physics answers.
- What did you learn about computational methods? What did you learn about physics?

Style matters. Your grade depends not only on whether your computer code compiles and runs, but on our judgment of how well you understand the material. So a clear, coherent and complete explanation is important.

It often happens that we will need to compile and run your programs, sometimes to make sure they work and sometimes to fix some small error and see if that helps. To help us do this, use a header comment in each source code file telling us how to do this. In any event, this is always good practice. A suitable header might look something like this:

```
// midpoint.c  -- integrate a function by the midpoint rule
// Joe Student,  9/10/2010
//
// Use the midpoint rule (class notes section 99.2) to
// integrate a function.
// the function is named "myintegrand()" and is in a separate file.
// to compile:  cc -o midpoint midpoint.c myfunction.c -lm
// to run: midpoint  (prompts for input: integration limits and
// number of bins )
```

```
\#include <stdio.h>
```

```
...
```

All work *must* be submitted by email to the address p305@physics.arizona.edu. Further description of this procedure will be given in class.

This table summarizes the planned assignments. However, this schedule will be changed as necessary.

Assign	Lectures	Due	Topic
0	8/24	8/25	survival skills: email, editor, files
1	8/26	8/30	programming introduction or review
2	8/31,9/2	9/6	more programming, numerical integration
3	9/7,9/9	9/13	numerical integration 2: higher order methods
4	9/14,9/16	9/20	solving equations
5	9/21,9/23	9/27	first order D.E. (coffee cooling)
6	9/28,9/30	10/4	falling bodies
7	10/5,10/7	10/11	planetary orbits 1
8	10/12,10/14	10/18	planetary orbits 2
9	10/19,10/21	10/25	chaotic motion
10	10/26,10/28	11/1	iterative methods, Laplace's equation
11	11/2,11/4	11/8	matrices and least squares fitting
12	11/9,11/16	11/17	eigenvectors and normal modes
13	11/18,11/23	11/29	random numbers, random walks
14	11/30,12/2	12/6	molecular dynamics 1
–	12/7	12/8	molecular dynamics 2

Note that two assignments are due on Mondays at the end of holiday breaks (Labor Day and Thanksgiving). You might want to consider doing these assignments before the breaks, so that you can enjoy the vacations.