Physics 540 COMPUTATIONAL PHYSICS Fall Term, 2006

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REQUIRED TEXT: The reading assignments for Physics 540 come from *Computation and Problem Solving in Undergraduate Physics* (*CPSUP*). You will perhaps find all of *CPSUP* useful, and there are two hard-bound copies of the 9 February 2004 printing of the *entire* opus in the CPL for your reference, though you should keep in mind that a fair number of edits have been made in the time since those copies were printed. Assignments will direct you explicitly to parts of Chapters 7, 8, 10, 13, 14, and 15.[1] All but Chapter 15 are in the notebooks delivered to you at the first class meeting. Chapter 15 will come along in due time. There will be no charge for these materials.

For reference, you will probably also want to locate your copy of the *Local Guide* (*LG*), though all existing versions—including the ones in the CPL—are a bit out of date and a new version is not likely to be generated until I prepare for Physics 225 in the winter term.

Furthermore, those of you who took *Computational Mechanics* two years ago may find it prudent to spend a bit of time familiarizing yourself with the HP workstations, especially if you haven't yet worked on those platforms very much. Working through Section 2 of the 2 January 2006 printing of the *LG*, copies of which are in the CPL, should get you started. Everything still should work on the old SGI machines, but you should plan to work with the newer LINUX machines instead.

SCHEDULE: The schedule for this course is included with this fact sheet. *Nominally*, we meet three times a week. Because of the intensity of computer work in this course, however, we will not *actually* meet as a class in *all* of those times. Some classes will be cancelled—see schedule—to compensate for the time you will spend at the keyboard. It really won't take me very long to lay out in class topics and approaches that will be quite capable of keeping you busy at the workstations for quite a while.

OFFICE HOURS: Though they may require adjustment once one or two further scheduling items settle for the term, at the moment I set the following office hours:

7:00–9:00 PM most Sundays
9:30–11:00 AM Tuesdays
1:30–3:00 PM Fridays
other times by appointment

CONSULTING SCHEDULE: Since this course is the highest level course in computational physics offered at Lawrence and none of the students who took the course at its first offering two years ago is still on campus, you and I together are on our own. Consult with one another and don't hesitate to consult with me.

STRUCTURE: In most sessions when we actually meet as a class, I will summarize the topic of the day and illustrate it with various segments of code or whole programs. Three times during the term (see schedule), a class meeting will be devoted to student presentations of particular exercises. In the first two of these sessions, each student will present a brief (15-minute) discussion of an assigned exercise. That exercise will also serve as the basis for a substantial written solution to be submitted to me a couple of days after the presentation.

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[1] You already have Chapters 7 and 8, but they have suffered significant edits since the copies you have were printed.

In the third session, which will occur in the last week of the term and probably will require more than one class period, each student will present a 25–30 minute discussion of an exercise of that student's choice (related, of course, to the course itself—and subject to my prior approval). That exercise will be more extensive than the first two, and it will be the subject of a thorough written paper, longer than the first two papers, due at the end of the term. That project will be each student's primary responsibility during the last two weeks of the term.

ASSIGNMENTS: At the end of this fact sheet you will find a description of the several assignments to be made during the term. Each assignment identifies readings in *CPSUP* and—most importantly—designates several exercises that you should solve as a test that you understand the material covered by the assignment. Exercises are divided into two groups. You should give some thought to and make an effort to solve all exercises labeled 'Try'. The exercises labeled 'Hand-In'—a subset of those labeled 'Try'—are to be written up *carefully*, *thoroughly*, and *neatly* and handed in at the beginning of the class meeting indicated on the schedule. A day or two after each assignment is due, I will try to place solutions for at least some of the exercises on that assignment in a notebook in Y104/CPL, but I may not be able to live up to that promise, since solutions to only a few of the exercises actually exist at this time. *In the interests of your keeping abreast of the course and of my efficient grading, I ask that you turn in at each due date whatever of the assignment you have completed; do not withhold an entire assignment solely because you have not completed some of the exercises.*

You all, of course, already know—but I will repeat it anyway—that I believe a solution to an exercise is FAR more than a mere answer, that the method by which you solve an exercise is more important than the end result. All submitted solutions must be *complete*, i.e., they must contain not only the answer, not only a succession of equations, but—and most importantly—enough narrative to make clear how you thought your way carefully and logically from first principles. Especially with solutions arrived at numerically, they must contain enough exploration to convince me that your solution is in fact accurate. It is your job in your submitted work to convince me that you have identified the applicable starting point, worked your way step-by-step from that starting point to a solution, and defended its accuracy. Pay attention not only to the substance of your solution but also to its exposition. Solutions that look like your first draft on a sheet of scrap paper are not acceptable. *All work in this course is to be submitted as output generated from LaTeX source files.*

Further, with computer-related exercises, your solutions need to include not only explicit, detailed coding but also some narrative description of what the coding is supposed to accomplish and, perhaps as an appendix, a complete listing of the final program. When you include computer-produced graphs, your solution will be incomplete unless the accompanying narrative describes how you produced the graphs and indicates the specific statements you submitted to whatever visualization program you used.

EXAMINATIONS: There will be no examinations, either hour or final, in this course.

GRADING: Your grade in this course will be based on your oral presentations, your written papers on the three major exercises, and your diligence and overall success in working the other assigned exercises.

HONOR SYSTEM: Each student is expected to present only her or his own work on the three talks/papers. In contrast, students are encouraged to work together on the other exercises. Each student is expected to write up her or his own assignments, but working together to solve the exercises can be a valuable learning aid. I establish only two ground rules: (1) Working together will be most effective if all individuals contribute more or less equally to the group effort; you should be wary if you are always on the receiving end in such effort, for ultimately you will be expected to perform on your own. At the very least, once you have finished solving an exercise in a group, make sure that you could solve a similar exercise on your own. (2) Where substantial help has been received through conversation with another, I ask that you follow common scientific courtesy and acknowledge that help briefly in your submitted work.

Physics 540 SCHEDULE Fall Term, 2006

Abbreviations used in this schedule are C for conference session, N for no class, L for lecture, E for exercises related to the topic of the day, R for reading assignments, S for special event, and *CPSUP* for *Computation and Problem Solving in Undergraduate Physics*. Unless otherwise noted, assignments are due at the start of class on the indicated days. Details of each assignment are tabulated after this schedule.

20 Sep	We	L: Programming Structures and Strategies R: *CPSUP* Sections 7.1, 7.2, and 7.3.1 E: *CPSUP* Exercises 7.2, 7.7, 7.9
22 Sep	Fr	L: Programming in FORTRAN and IDL R: *CPSUP* Sections 7.4, 7.5, 7.8 E: *CPSUP* Exercises 7.12, 7.13, 7.16

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25 Sep	Mo	L: Analytic/Physical Derivation of PDEs R: *CPSUP* Section 13.1.1–13.1.5 E: *CPSUP* Exercises 13.2, 13.3
27 Sep	We	L: Finite Difference Methods (FDMs): Part I R: *CPSUP* Section 13.1.6–13.1.8, 13.2 E: *CPSUP* Exercises 13.6, 13.8
28 Sep	Th	S: (11:10 AM Y-115) *Department Town Meeting*
29 Sep	Fr	ASSIGNMENT 1 DUE L: Driving Programs for LSODE: Part I R: *CPSUP* Sections 10.1, 10.3, 10.5 E: *CPSUP* Exercises 10.1, 10.6, 10.8

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02 Oct	Mo	L: Driving Programs for LSODE: Part II R: *CPSUP* Sections 10.4, 10.6 E: *CPSUP* Exercises 10.12, 10.13, 10.15 S: (5:30–7:00 PM) *Department Picnic*
04 Oct	We	N: No class; work on assignment.

06 Oct	Fr	ASSIGNMENT 2 DUE L: FDMs: Part II R: *CPSUP* Sections 13.3, 13.5, 13.12 E: *CPSUP* Exercises 13.4, 13.5, 13.10, 13.22, 13.23

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09 Oct	Mo	L: FDMs: Part III R: *CPSUP* Sections 13.13, 13.15 E: *CPSUP* Exercises 13.21, 13.24, 13.34
11 Oct	We	N: No class; work on assignment
13 Oct	Fr	N: No class; work on assignment.

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16 Oct	Mo	C: Oral presentation of FDM exercises
18 Oct	We	ASSIGNMENT 3 DUE L: MUDPACK and Multigrid Techniques: Part I R: *CPSUP* Sections 14.1, 14.2 E: *CPSUP* Exercises 14.2, 14.4
20 Oct	Fr	L: MUDPACK and Multigrid Techniques: Part II R: *CPSUP* Sections 14.3, 14.4 E: *CPSUP* Exercises 14.6, 14.8

Note: The somewhat unusual arrangement of sessions in this week and next week reflects the fact that DMC will be out of town from Thursday morning, 26 October, until shortly before noon on Tuesday, 31 October. The schedule is designed to keep the course moving as smoothly as possible during his absence.

23 Oct	Mo	L: Finite Element Methods (FEMs): Introduction R: *CPSUP* Sections 13.7, 13.8 E: *CPSUP* Exercises 13.9, 13.11, 13.12. 13.13
24 Oct	Tu	DMC available most of the day for consultation as you complete Assignment 4.
25 Oct	We	L: FEMs: Part II R: *CPSUP* Sections 13.10, 13.17 E: *CPSUP* Exercises 13.14, 13.16 ASSIGNMENT 4 DUE at 3:00 PM
27 Oct	Fr	MID-TERM READING PERIOD; NO CLASS

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30 Oct	Mo	N: No class, work on assignment.
01 Nov	We	L: FEMs: Part III R: *CPSUP* Sections 13.18, 13.20 E: *CPSUP* Exercises 13.18, 13.35
03 Nov	Fr	N: No class, work on assignment.

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06 Nov	Mo	ASSIGNMENT 5 DUE L: FEMs with MARC/MENTAT: Part I R: *CPSUP* Chapter 15, Sections 1–7 E: *CPSUP* Exercise 15.1
08 Nov	We	L: FEM with MARC/MENTAT: Part II R: *CPSUP* Sections 8–14 E: *CPSUP* Exercises 15.2, 15.4, 15.5
10 Nov	Fr	PROJECT PROPOSAL DUE N: No class; work on assignment
13 Nov	Mo	C: Oral presentation on FEM exercises
15 Nov	We	ASSIGNMENT 6 DUE at noon; START FINAL PROJECTS N: No class; work on projects
17 Nov	Mo	N: No class; work on projects
20 Nov	Mo	N: No class; work on projects
22 Nov	We	THANKSGIVING BREAK
24 Nov	Fr	THANKSGIVING BREAK
27 Nov	Mo	N: No class; work on projects
29 Nov	We	C: Oral presentation of projects
01 Dec	Fr	C: Oral presentation of projects
02 Dec	Sa	(noon) ASSIGNMENT 7 DUE

NO FINAL EXAMINATION

ASSIGNMENT 1 (due Friday, 29 September)

Reading:	*CPSUP* Sections 7.1, 7.2, 7.3.1, 7.4, 7.5, 7.8, 13.1, 13.2
Try:*	*CPSUP* Exercises 7.2, 7.7, 7.9, 7.12, 7.13, 7.16; 13.2, 13.3, 13.6, 13.8
Hand In:†	*CPSUP* Exercises 7.9, 7.13, 13.3, 13.6, 13.8

Note: All computer programs for this assignment are to be written in FORTRAN.

* All exercises in the group labeled 'Try' should be attempted.

† The exercises in the group labeled 'Hand In' are to be written up in good form using LaTeX and, unless otherwise noted, are to be handed in at the beginning of class on the due date for the assignment.

ASSIGNMENT 2 (due Friday, 6 October)

Reading:	*CPSUP* Sections 10.1, 10.3, 10.4, 10.5, 10.6
Try:	*CPSUP* Exercises 10.1, 10.6, 10.8, 10.12, 10.13, 10.15
Hand In:	*CPSUP* Exercises 10.8, 10.12, 10.13

Note: All computer programs for this assignment are to be written in FORTRAN and are to use LSODE.

ASSIGNMENT 3 (due Wednesday, 18 October)

Reading:	*CPSUP* Sections 13.3, 13.5, 13.12, 13.13, 13.15
Try:	*CPSUP* Exercises 13.4, 13.5, 13.10, 13.21, 13.22, 13.23, 13.24, 13.34
Hand In:	*CPSUP* Exercises 13.4, 13.34, and your assigned Big Exercise #1

Note: I will identify your assigned Big Exercise after the term is underway and has settled into a routine. For this assignment, you may choose whether you want to write your programs in FORTRAN or IDL—or perhaps do some of both.

ASSIGNMENT 4 (due Wednesday, 25 October, at 3:00 PM)

Reading:	*CPSUP* Sections 14.1, 14.2, 14.3, 14.4
Try:	*CPSUP* Exercises 14.2, 14.4, 14.6, 14.8
Hand In:	*CPSUP* Exercises 14.4, 14.8

ASSIGNMENT 5 (due Monday, 6 November)

Reading:	*CPSUP* Sections 13.7, 13.8, 13.9, 13.10, 13.17, 13.18, 13.19
Try:	*CPSUP* Exercises 13.9, 13.11, 13.12, 13.13, 13.14, 13.16, 13.18, 13.35
Hand In:	*CPSUP* Exercises 13.9, 13.14*, 13.18, 13.35*

* Use either IDL or FORTRAN—you're choice.

PROJECT PROPOSAL (due Friday, 10 November, at noon)

ASSIGNMENT 6 (due Wednesday, 15 November)

Reading:	*CPSUP* Chapter 15
Try:	*CPSUP* Exercises 15.1, 15.2, 154.4, 15.5
Hand In:	*CPSUP* Exercises 15.4 and your assigned Big Exercise #2

ASSIGNMENT 7 (due Saturday, 02 December, at noon)

For this assignment you will conduct a project of your choice, present a 25–30 minute oral report on that project during the last week of the term, and submit a detailed paper at the very end of the term. A fuller statement defining this assignment and suggesting possible topics is presented at the end of this fact sheet.

Big Exercise #1 (Assignment 3)

The first of the individualized assignments in Physics 540 is Assignment 3, the written portion of which is due on Wednesday, 18 October. Completion of this assignment involves

- Reading Sections 13.3, 13.5, 13.12, 13.13, and 13.15 in *CPSUP*, which deal with the use of FDMs for fully discretized 1D and 2D PDEs.
- Solving and writing out solutions to Exercises 13.4 and 13.34 in *CPSUP*, and
- Putting a special effort into solving the first "big" exercise of the term. As announced in the course fact sheet, each student will do *one* of the following exercises, and I will assign exercises to students not later than the due date for Assignment 2. Your tasks with respect to the assigned exercise are
  - To generate a solution.
  - To write a carefully written document in which you
    - Describe in some detail how you set up and solved the problem (including a discussion of any particular wrinkles—anticipated or unanticipated—that you had to address),
    - Defend the accuracy of your solution,
    - Explore the solution in as many ways—be creative—as you think of and, in particular, as a function of any parameters—if any—in the exercise,
    - Make any other comments that seem appropriate, and
    - Discuss the features of your solution and its dependence on the parameters.

  Your written solution is due at class on Wednesday, 18 October. As with all other submitted work, this paper is to be prepared with LaTeX. Please pay attention not only to substance but also to style. I will be happiest with a well written paper that has been carefully proofread, reads smoothly, and is neat and attractive and uncluttered on the page.

  Remember that, in contrast to the "small" exercises, you are expected to work on this "big" exercise on your own. If you need consultation, please have a chat with me.

  Please note also that I have not done any of the exercises enumerated below. I think they are doable in reasonable time, but I may be wrong. In any case, please be aware that my evaluation of your oral and written discussions of your exercise will turn on how well, systematically, and thoroughly you approach your exercise and how carefully and completely you document your efforts, not on whether you succeed in solving the exercise in its entirety. Please alert me to any difficulties along the way; perhaps the exercise will need modification.

- To prepare a 15-minute oral summary of your solution and its properties, perhaps with power point, and deliver that summary in class on Monday, 16 October.[2]

[2]Clearly, 15-minute presentations from all students in the class will not fit into a 70-minute class period. So, we need to talk about strategy. Do we reduce the length of the presentations to 10 minutes, making our session more like a professional meeting with strict—and quite short—time limits for each presentation, or do we find a second time—Thursday morning, 9-10:45 AM?, meet class both Friday and Monday?, . . .—when we can gather so we can have 15-minute presentations.

Note: These exercises all involve finite difference methods in one context or another.

B1.1 *CPSUP* Exercise 10.14, which uses LSODE. This exercise involves following the evolution of the temperature distribution in a two-dimensional L-shaped plate.

B1.2 *CPSUP* Exercise 10.15, which uses LSODE. This exercise involves the osclllations of a thin membrane stretched over an L-shaped frame.

B1.3 Exercise 10.16, which uses LSODE. The exercise involves tracing the time evolution of a particular quantum wave packet.

B1.4 *CPSUP* Exercise 13.5, which uses either an IDL program or a FORTRAN program. This exercise entails solving Laplace's equation in (two-dimensional) polar coordinates.

B1.5 *CPSUP* Exercise 13.22, which uses either an IDL program or a FORTRAN program. This exercise entails demonstrating that the algorithm for solving the 1D wave equation by converting it into a family of ODEs is unstable when $\alpha > 1$.

B1.6 *CPSUP* Exercise 13.23, which uses either an IDL program or a FORTRAN program. This exercise entails demonstrating that the algorithm for solving the 1D diffusion equation by converting it into a family of ODEs is unstable when $\gamma > 1/2$.

Big Exercise #2 (Assignment 6)

The second of the individualized assignments in Physics 540 is Assignment 3, the written portion of which is due on Wednesday, 15 November. Completion of this assignment involves

- Reading Sections Reading Chapter 15 in *CPSUP*, which deals with the use of MARC/MENTAT to set up and solve two-dimensional problems using finite element methods,
- Solving and writing out a solution to Exercise 15.4 in *CPSUP*, and
- Putting a special effort into solving the second "big" exercise of the term. As announced in the course fact sheet, each student will do *one* of the following exercises, and I will assign exercises to students not later than the due date for Assignment 5. Your tasks with respect to the assigned exercise are
  - To generate a solution.
  - To write a carefully written document in which you
    - Describe in some detail how you set up and solved the problem (including a discussion of any particular wrinkles—anticipated or unanticipated—that you had to address),
    - Defend the accuracy of your solution,
    - Explore the solution in as many ways—be creative—as you think of and, in particular, as a function of any parameters—if any—in the exercise,
    - Make any other comments that seem appropriate, and
    - Discuss the features of your solution and its dependence on the parameters.

  Your written solution is due at class time on Wednesday, 15 November. As with all other submitted work, this paper is to be prepared with LaTeX. Please pay attention not only to substance but also to style. I will be happiest with a well written paper that has been carefully proofread, reads smoothly, and is neat and attractive and uncluttered on the page.

  Remember that, in contrast to the "small" exercises, you are expected to work on this "big" exercise on your own. If you need consultation, please have a chat with me.

  Please note also that I have not done any of the exercises enumerated below. I think they are doable in reasonable time, but I may be wrong. In any case, please be aware that my evaluation of your oral and written discussions of your exercise will turn on how well, systematically, and thoroughly you approach your exercise and how carefully and completely you document your efforts, not on whether you succeed in solving the exercise in its entirety. Please alert me to any difficulties along the way; perhaps the exercise will need modification.
- To prepare a 15-minute oral summary of your solution and its properties and deliver that summary in class on Monday, 13 November.[3]

[3] Clearly, all of your 15-minute presentations will not fit into a 70-minute class period. I suggest that we plan to do two or three presentations on 13 November and that, contrary to the published schedule, we meet on Wednesday, 15 November, for the remainder of the presentations.

Note: These exercises all involve finite element methods in one context or another.

B2.1 *CPSUP* Exercise 13.12, which involves working out the integrals for the elemental equations when triangular elements are used in a finite element method.

B2.2 *CPSUP* Exercise 13.16, parts (b) and (c), which involves developing some of the background for use of finite element methods in two dimensions with triangular elements. Do not bother to do part (a); simply accept Eqs. (13.189)–(13.190)—or whatever numbers they have in your copy.

B2.3 *CPSUP* Exercise 14.6, which involves using MUDPACK to find the electrostatic potential in a particular two-dimensional space with an inhomogeneous equation.

B2.4 *CPSUP* Exercise 14.7, which involves using MUDPACK to find the electrostatic potential in a particular two-dimensional space with an inhomogeneous equation.

B2.5 *CPSUP* Exercise 15.5, which involves MARC/MENTAT for to find the steady-state temperature in an irregular geometry.

B2.6 *CPSUP* Exercise 15.7, which uses MARC/MENTAT to find the electrostatic potential in the geometry of the example in Chapter 15, except that the inner circle bounds a region inside of which there is a uniform charge density.

Suggested Really Big Exercises for Assignment 7

Your last obligation—there is no final examination—to Physics 540 is to complete an extended project of your choice (but subject to my approval), present an oral report on that project in the last week of the term, and hand in a carefully written paper on the project by noon on Saturday, 2 December. A brief written project proposal is due on Friday, 10 November. I offer the following suggestions to stimulate your thinking about this project. Within each general topic, you can, of course, find a wide spectrum of specific geometries. Consequently, two or more members of the class can work on projects in the same general area provided that the specific problems elected differ in some respect (geometry, boundary conditions, . . .).

Possible Topics for Final Project

1. The normal modes of oscillation of a square membrane. This problem can be approached by using finite difference methods *a la CPSUP* Chapter 13 to generate an equivalent matrix eigenvalue problem and then solving that problem numerically to obtain both the lowest several eigenvalues (natural frequencies) and the shapes of the membrane in each mode. This exercise would involve writing your own IDL or FORTRAN code to implement the numerical solution, though you would want to find and use IDL routines or Numerical Recipes routines for the actual solution once you had set up the matrix whose eigenvalues and eigenvectors are to be found.

2. A three-dimensional example whose solution would involve using `mud3sp.f`. Examples in *CPSUP* Sections 14.5, 14.6, and 14.7 may provide a starting point, but the problem you select should be a bit more elaborate than any of those examples. A Cartesian translation of Exercise 14.15 might be one possibility, though you could try to do the exercise itself with `mud3.f`.

3. *CPSUP* Exercise 14.5, which entails using MUDPACK to solve the two-dimensional Laplace equation in cylindrical coordinates.

4. *CPSUP* Exercise 14.9, which asks about the temperature disribution inside a cylindrically invariant geometry. This exercise should be doable with `mud2sp.f`.

5. The normal modes of oscillation of an irregularly shaped two-dimensional membrane, which would involve learning about some features of MARC/MENTAT not discussed in Chapter 15. Exercises 15.8, 15.9, and 15.10 in *CPSUP* describe possible geometries for that membrane, but others may attract your attention as well.

6. *CPSUP* Exercise 15.11 (or some similar situation), which entails using MARC/MENTAT to set up and solve a situation in a fairly simple three-dimensional geometry.

I am, of course, willing to listen to—and to help refine—any other proposals that you might have.