COMPUTATION IN THE LAWRENCE PHYSICS CURRICULUM

A Report to the National Science Foundation,
the W. M. Keck Foundation, and Departments of Physics
on Twenty Years of Curricular Development at Lawrence University

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Executive Summary

With support from the National Science Foundation, the W. M. Keck Foundation, and Lawrence University, we in the Department of Physics at Lawrence University have for two decades been developing the computational dimensions of our curriculum, both at the introductory and at the intermediate and advanced levels. We have equipped our introductory laboratory with computers, assorted sensors, and suitable software; we have built a Computational Physics Laboratory (CPL) that makes a wide spectrum of hardware and software available to students; we have developed a curricular approach that introduces students to these resources and to prototypical applications; we have incorporated computational dimensions into our advanced laboratory offerings; and we have drafted several hundred pages of instructional materials, some of which have in the last few years been published. This report describes the history of these developments at Lawrence, the computational components of our curriculum, and the text written to support these components.

Based on the premise that twenty-first century physicists cannot function fully if they are unaware of the role that computation can play in both theoretical and experimental endeavors and if they lack at least some skill in applying computational approaches when appropriate, we have structured a curriculum that

- introduces freshmen to computer-based statistical data analysis, curve fitting, graphical visualization, and on-line data acquisition,
- requires sophomores to take a course called *Computational Mechanics*, in which they learn classical mechanics at an intermediate level, apply symbolic and numerical computation for solving ordinary differential equations, evaluating integrals, and generating graphical displays, and use LaTeX for preparing documents,
- expects students to use computational resources on their own initiative during the rest of their time at Lawrence (and encourages that use by granting 24/7 access to the CPL);
- directs students to use computational resources in several upper-level courses;
- offers an elective junior/senior course that focuses on finite difference and finite element approaches to partial differential equations; and
- supports the use of computers for the conduct of senior independent studies.

By the time of graduation, all physics majors at Lawrence have developed a comfortable familiarity with computational approaches to problems and some have become quite adept at sophisticated applications.

Among the outcomes of our two-decade long effort is a text, *Computation and Problem Solving in Undergraduate Physics*, which has grown along with our curriculum but has also expanded beyond our curriculum to include, as options, use of software packages different from those chosen at Lawrence. This book is now available in several different versions to support inclusion of computation in undergraduate physics curricula at institutions other than Lawrence.

Preface and Acknowledgments

The primary purpose of an undergraduate program in physics is to generate a full realization of the beauty, breadth, and power of the discipline and to develop both an understanding of fundamental concepts and the skills to use a variety of tools—both theoretical and experimental—to apply and test those concepts. In the last two or three decades of the twentieth century, computational approaches to addressing both theoretical and experimental problems have taken their place alongside the more traditional approaches. The twenty-first century physicist unfamiliar with computational approaches lacks skills that are now critical to the successful pursuit of the field.

To be sure, computers have been used in undergraduate programs in departments of physics at many institutions for quite some time. The overwhelming majority of these applications, however, has focused on introductory courses, in which—typically—students either run instructor-written programs or access web-based resources, both of which are designed to support the teaching of the concepts of physics. Valuable though uses of computers to support the teaching of physics have been and continue to be, the exposure of undergraduate physics majors to computation cannot be limited to those applications. The important objective for physics majors at the beginning of the twenty-first century is not so much to learn how to use programs written by others to reinforce fundamental concepts as to learn how to use whatever tools are appropriate and available to create their own computer-based solutions. To this end, contemporary curricula must assure that graduates are familiar with the capabilities—and limitations—of available tools, are introduced to an assortment of standard algorithms applied in physical contexts to standard problems and, by the time of graduation, are able to use computers not only for the *learning* of physics but even more for the *doing* of physics.

In the last few years, computation has indeed begun to find its way into upper-level courses in computational physics or as an inclusion in individual courses on other topics. Unfortunately, these courses often come along late in the student's undergraduate program, and students therefore do not encounter computational approaches early enough for those approaches to become almost second-nature by the time of graduation. Further, single courses, wherever they occur during the students' undergraduate days, are decoupled from the rest of the curriculum and typically introduce only those resources needed for the specific course; they do not foster a broad appreciation of the versatility and scope of computational approaches.

In the last couple of years, a systematic and cooperative effort to explore ways to enhance the use of computation in upper-level undergraduate physics and to provide materials to support that effort has finally begun to emerge. At the 2005 summer meeting of the American Association of Physics Teachers (AAPT) in Salt Lake City, UT, for example, Bruce Mason, founder of ComPADRE, Norman Chonacky, editor of *Computers in Science and Engineering* (*CiSE*), and David Winch, Professor of Physics Emeritus at Kalamazoo College, convened an informal crackerbarrel session on the topic "Building a Physics Computing Community for Undergraduate Education". The session was attended by key early adopters of computational physics who expressed many varied perspectives on experiences to date and prospects for the future. With support from *CiSE*, Robert Fuller, Professor of Physics Emeritus at the University of Nebraska, was commissioned to conduct a survey of all uses of computation in undergraduate physics programs throughout the country. That survey produced baseline national data and led to the identification of invitees for contributions both to a session of invited papers and to a poster session at the 2006 summer meeting of the AAPT in Syracuse, NY. Further, the September/October 2006 (Volume 8, Number 5) issue of *CiSE* was devoted to the theme "Computation in Physics Courses". It included the results of Professor Fuller's survey, five articles about several approaches (texts based on the invited papers delivered at the Syracuse meeting), and—as a sidebar to Guest Editor Professor Winch's introduction—abstracts of the seventeen invited posters mounted at the poster session at the same meeting. The posters themselves are available from links at the *CiSE* website, specifically

`http://opac.ieeecomputersociety.org/opac?year=2006&volume=8&issue=5&acronym=cise`

On the eve of the invited sessions at the Syracuse meeting and sponsored by *CiSE*, a dinner discussion among a dozen and a half of the current major players launched a collaborative effort to develop ways to include more computation in undergraduate physics programs. As next steps, *CiSE* Editor Chonacky is spearheading that effort by offering *CiSE* support to continue the national discussion and by seeking the support of professional societies and outside foundations for a development project. The theme issue of *CiSE* is an example of publicizing the effort. In November, 2006, the Shodor Educational Foundation convened a meeting of selected players to brainstorm about and plan the next steps toward such a project.

The Department of Physics at Lawrence University has been ahead of the pack. In the mid 1980s, we recognized the growing importance of computation to the serious physicist. Since that time, we have been striving to embed the use of general purpose graphical, symbolic, and numerical computational tools throughout our curriculum. Developed over more than two decades, our approach involves

- introducing freshman to tools for on-line data acquisition, statistical data analysis and curve fitting;
- introducing sophomores to the simulation of electronic circuits in *Electronics*,
- introducing sophomores to computer-based symbolic, numerical, and visualization tools in a required course titled *Computational Mechanics*, which develops classical mechanics at an intermediate level while giving particular attention to uses of computational resources in application to mechanics problems that involve graphical visualization, ordinary differential equations, integrals, eigenvalues, and eigenvectors, and to introducing the use of LaTeX for the preparation of documents and reports;
- incorporating computational approaches alongside traditional approaches to problems in many intermediate and advanced courses, most of which list *Computational Mechanics* as a prerequisite;
- providing more exposure to on-line data acquisition, data analysis, graphical visualization of data, and report writing in a required junior course titled *Advanced Laboratory*;
- offering juniors and seniors the elective course *Computational Physics*, which has *Computational Mechanics* as a prerequisite and focuses on numerical solution of the wave, diffusion, and Laplace equations by finite difference and finite element methods.
- making computational resources available and, through 24/7 access to the Computational Physics Laboratory, encouraging students to use these resources routinely *on their own initiative* whenever that use seems appropriate.

In the twenty-plus years since the start of this endeavor, numerous materials have been drafted and redrafted and tested and retested. These materials have now been assembled into a flexible text that is customizable to reflect many different choices of hardware and software. Details about the Lawrence curricular approach and about this text, titled *Computation and Problem Solving in Undergraduate Physics*, are described in this report and also posted on the project web site at `www.lawrence.edu/dept/physics/ccli`.

This report, which is being distributed to all domestic departments of physics that offer the bachelor's degree, embodies a progress report on a project that began slowly at Lawrence University in the late 1960s and has been more consciously and vigorously pursued since the mid 1980s. While the project will continue to evolve, it is now sufficiently well developed that documenting its current state and some of the underlying motivations seems in order. The author hopes that this report may prove useful to the steadily increasing numbers of departments that are giving serious thought to including computational physics in their undergraduate curricula. Comments, suggestions, and requests for additional copies should be directed to the author.

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Chapter 1

Introduction

1.1 Underlying Convictions

Practicing physicists routinely confront a variety of tasks that support their research but are peripheral to their main objectives. While physicists in different subareas will probably disagree about the relative importance of particular tasks, most will agree that the more important and most frequent of these tasks involve

- visualizing functions of one, two, and three variables graphically,
- solving algebraic equations,
- solving ordinary differential equations,
- solving partial differential equations,
- evaluating integrals,
- finding roots, eigenvalues, and eigenvectors,
- acquiring data,
- displaying data graphically,
- performing statistical analyses of data,
- fitting theoretically expected functions to data,
- processing images, and/or
- preparing reports and papers.

More often than not, pursuit of these tasks symbolically and analytically is at best tedious, difficult, and prone to error and at worst essentially impossible. In many cases, however, these tasks can be addressed by exploiting computational approaches. To facilitate their use of such approaches, practicing physicists of the twenty-first century must be acquainted with[1]

- a common operating system, preferably some flavor of UNIX or LINUX,
- a good text editor, e.g. `nedit`[1] or `xemacs`[2],
- a spreadsheet program, e.g., *Excel*[3],
- an array/number processor, e.g., IDL[4], MATLAB[5], or OCTAVE[6],
- a symbolic manipulator, e.g., MAPLE[7], *Mathematica*[8], or MAXIMA[9],
- a visualization tool, e.g. *Kaleidagraph*[10] and (IDL, MATLAB, or OCTAVE),

[1]Citations in square brackets refer to items in the bibliography, which can be found starting on page 69.

- a standard computational language, e.g., FORTRAN or C or C++, at least sufficient to support comfortable use of subroutine packages like Numerical Recipes[11], ODEPACK[12]. and MUDPACK[13],
- a program for circuit simulation, e.g., *Multisim 7*[14] or SPICE[15];
- a program for data acquisition, e.g. *LabView*[16],
- a technical publishing system, e.g., LaTeX[17],
- a drawing program for creating publication quality figures and diagrams, e.g., Tgif [18], and
- a presentation program, e.g., *PowerPoint*[19].

Undergraduate curricula that do not provide physics majors with at least an orientation to the applicable algorithms and a reasonable spectrum of the appropriate computational tools are failing to prepare their graduates for the activities that practicing scientists will find themselves doing frequently and extensively in the twenty-first century.

Beyond the substance of the approaches introduced, a curriculum that responds to these convictions must also make sure that students

- are aware of the hazards associated with doing finite-precision arithmetic on floating-point numbers.

- are introduced to computational resources early enough so that they can continue to use these resources at subsequent points in their undergraduate careers, thereby reinforcing the universality and broad applicability of those resources. An upper-level course in computational physics is a valuable curricular inclusion, but students need to become acquainted with computational resources long before they have either the mathematical or the physical background to profit from a rigorous course in computational physics.

- use computational resources throughout the curriculum, again to emphasize the wide variety of contexts in which computational resources can be a valuable aid to the conduct of careful science. The point is best made—and the skills most reliably developed—if use of these resources permeates the entire curriculum.

- focus *initially* on the tools themselves. To be sure, numerous examples drawn from physical contexts must be used to motivate the study of techniques and tools, but the focus at first must be on the features and capabilities of the tools. Otherwise, knowledge of the tools ends up being limited to the capabilities needed for the specific problems encountered. Simply put, encountering computational tools as an appendix to tasks of higher priority leads to a narrow, unsystematic, and incomplete understanding of the capabilities of the tools and does not fully set the stage for career-long, confident use of the tools in wider—and possibly unrelated—contexts.

In the broadest of terms, by graduation (and, with any luck well before that time), each student should have developed not only the ability to recognize when a computational approach may have merit but also the skill to pursue that approach confidently, fluently, effectively, knowledgeably, and independently on his or her own initiative.

1.2 The Challenge

The task before the physics educator is to design a physics curriculum that, without short-changing important topics from the historical curriculum, nonetheless includes exposure to and opportunity to build skill in the use of computational approaches to a selected important set of representative problems in physics. The skills must, of course, be developed within the context of numerous specific problems from several areas of physics. The end objective, however, is not so much the results of the analyses of those problems as the development of generalizable skills that prepare the student to apply appropriate computational tools to other problems as they arise during the course of a career and that provide a solid foundation on which the student can readily learn new computational techniques as the need arises.

1.3 Overview of the Lawrence Response

The response in the Department of Physics at Lawrence University to the challenge posed in Section 1.2 involves building infrastructure (i.e., acquiring hardware and software), revising curricula, and drafting instructional materials—all of which contribute to our moving towards a full addressing of the goals laid out in Section 1.1. More specifically, we have

- equipped our introductory and advanced laboratories with appropriate hardware and software —see Sections 3.2 and 3.4.2, respectively—and built a Computational Physics Laboratory (CPL)—see Appendix A.
- introduced computer acquisition of data, statistical analysis of data, and least squares fitting in the introductory laboratories, as described in Section 3.2.
- introduced simulation of electronic circuits in *Electronics*, as described in Section 3.3.1.
- introduced *Computational Mechanics*, a required sophomore course that orients majors to the CPL, as described briefly in Section 3.3.2 and more extensively in Section 4.1.
- introduced relaxation methods for Laplace's equation in *Electromagnetic Theory*, as described in Section 3.3.3.
- reinforced techniques for graphical visualization and for numerical and symbolic solution of ordinary differential equations, evaluation of integrals, and finding of eigenvalues and eigenvectors in *Quantum Mechanics*, as described in Section 3.4.1.
- expanded the majors' exposure to on-line data acquisition, techniques for data analysis and curve fitting, and use of publishing software for generating reports in *Advanced Laboratory*, as described in Section 3.4.2.
- introduced *Computational Physics*, an elective junior/senior course that focuses on partial differential equations and the graphical visualization of their solutions, as described briefly in Section 3.4.3 and more extensively in Section 4.2.
- incorporated computer-based exercises in other courses, as described at the beginning of Section 3.4.
- drafted and redrafted numerous documents and, ultimately, a book, as described in Chapter 5.
- sought outside funding. A complete listing of outside support is included in the section titled *Acknowledgements* on page vii in the preface.
- publicized our efforts in a number of talks, posters, and journal articles. A full listing of these items is presented in Appendix A.6.

The Lawrence approach to developing the abilities of students to use computational resources is active; it requires students to play a personal role in their own learning; it forces students to defend their work in writing; it gives students practice in preparing and delivering oral presentations; it encourages students to work in groups; and it permeates our curriculum. More than any other objective, we encourage students to use our computational resources whenever they feel it appropriate to do so, and we expect that, by the time of graduation, students will have developed both a secure knowledge of computer-based approaches and the initiative and confidence to exploit those approaches *on their own initiative.*

In Chapters 3–5, we provide fuller detail on the several computational dimensions of the physics major at Lawrence. For background, however, we begin in Chapter 2 with a brief description of the broader institutional and departmental context.

Chapter 2

The Institutional and Departmental Context

2.1 About Lawrence

Founded in 1847 and located in Appleton, Wisconsin, Lawrence University is a nationally ranked, private, coeducational, residential liberal arts college and conservatory of music with 130 full-time faculty members and 1400 full-time students. Of the students, 1100 are pursuing the bachelor of arts degree in the college, 165 are pursuing the bachelor of music degree in the conservatory, and 135 are pursuing a five-year program leading to both degrees. About 10% of the students come from countries other than the United States. A student-faculty ratio of about 11:1 fosters personalized teaching and responsiveness to individual student needs. Small classes, specialized tutorials, and extensive faculty-student collaboration in research characterize the Lawrence program. Jill Beck is currently in her third year as president of Lawrence University, succeeding Richard Warch, who served for twenty-five years prior to his retirement in June, 2004. For the past several years, applicant pressure at Lawrence has been growing—2315 applicants,1304 admitted students, and an entering freshman class of 374 in the fall of 2006. As of 30 June 2006, endowment stood at about $200M. In the academic year 2000–01, our Departments of Chemistry and Biology moved to a new 78,000 square foot, $18.1M science building (which also houses research space for one physics faculty member) and, in the fall of 2001, the Department of Physics moved into substantially renovated spaces enlarged by 40% in Youngchild Hall, which was first occupied in 1963 but experienced a $10M renovation during the academic year 2000–01.

2.2 About the Department

The Department of Physics at Lawrence consists of five full-time faculty members. Professor David M. Cook (Ph.D., Harvard, 1965; joined the faculty in 1965), who works in mathematical and computational physics, and Professor John R. Brandenberger (Ph.D., Brown, 1968; joined the faculty in 1968), whose interests lie in experimental atomic physics, laser spectroscopy, and the foundations of quantum mechanics, will be retiring in June, 2008. Associate Professor Jeffrey A. Collett (Ph.D., Harvard, 1983; joined the faculty in 1995) is a condensed matter physicist who studies phase transitions in thin films of liquid crystals. Associate Professor of Physics Matthew R. Stoneking (Ph.D., University of Wisconsin, 1994; joined the faculty in 1997) studies non-neutral plasmas. Associate

Professor of Physics Megan K. Pickett (Ph.D., Indiana University, 1995; joined the faculty in 2006) is a computational astrophysicist and is Professor Cook's successor. In addition, Lawrence Fellow Joan P. Marler (Ph.D., University of California–San Diego, 2005; joined the faculty in 2005) is a fundamental particle physicist in the second year of a two-year appointment. Finally, the Department benefits from the services of Mr. LeRoy Frahm, electronics technician, and Mr. Thomas Hesselman, machinist and instrument maker. Searches are currently underway for Professor Brandenberger's successor and for a Ph.D. physicist to be offered a three-year appointment as a Visiting Assistant Professor of Physics, a continuing position that was created in 1996 and whose holder changes every two or three years. With those hires, the Department will be fully staffed at five FTE in the years after Professors Brandenberger and Cook retire.

In the mid 1980s, the Department of Physics adopted the goal of becoming one of the premier small undergraduate physics departments in the country. To be sure, if a department is to be included in that group, the departmental course offerings—its curriculum—must be first rate. We are convinced, however, that a departmental *program* must be much more than its *curriculum*. In particular, we strive each year to

- foster out-of-class interactions among students and between students and faculty (twice-weekly mid-afternoon teas, annual department-wide weekend retreat, fall picnic),
- involve students in hosting visitors and candidates for positions,
- discuss matters of departmental concern with students,
- actively recruit prospective students and involve current students in those efforts,
- encourage students to work together,
- provide spaces that students can call their own,
- maintain a departmental colloquium series (talks by half a dozen outside visitors each year, by faculty members, by students who conducted summer research at Lawrence or elsewhere, and by students completing independent study projects),
- engage aggressively in faculty and student/faculty research in order to extend faculty productivity and longevity so that attempts at innovation and searches for funding are based upon a continuous record of professional involvement and achievement,
- pursue outside support to nurture active research and to keep facilities and equipment up to date, and
- provide 24/7 access to student spaces, the computational laboratory, and departmental library holdings.

Our faculty offices lie side by side along a single hallway and student study spaces are near to those offices. We try to build a community in which we work together to help students grapple successfully with course material and to continue the forward-looking development of the Department.

That we have had some success in our efforts to become a premier department is attested to by several items:

- Our raising since 1987 of more than $2.5M of outside support for faculty research, curricular development, summer stipends for student researchers, travel to meetings, and dissemination of developments at Lawrence.
- Our invited presentation as one of ten case-study schools at the October, 1998, AIP-APS-AAPT national "Physics Revitalization Conference: Building Undergraduate Physics Programs for the 21st Century".
- Professor Cook's invited talk on building undergraduate physics programs, the talk delivered at the April, 2001, Washington meeting of the American Physical Society.
- Our Department's hosting in April, 2002, of a visit by a team from the National Task Force on Undergraduate Physics, a group that was seeking insight into how we have strengthened our program so as to pass that information on to departments striving to do likewise.

- Professor Brandenberger's invited talk on developing signature programs in physics, the talk delivered at the May, 2002, Quebec City meeting of the Canadian Association of Physicists.
- Professor Cook's and Professor Brandenberger's invited talks on aspects of the Lawrence physics program, the talks delivered at different sessions of the March, 2004, Montreal joint meeting of the American Physical Society and the Canadian Association of Physicists.
- Professors Brandenberger and Collett's invited workshop on signature programs, the workshop conducted at the Tenth National Conference of the Council on Undergraduate Research, held at LaCrosse, WI, in June, 2004.
- Between September, 2004, and June, 2006, two invitations to Professor Brandenberger and two separate invitations to Professor Cook to provide outside reviews to departments of physics at four different colleges, all interested in the insights gained by our experiences building a physics program.

2.3 Signature Programs

In 1986, realizing that attracting strong majors would be difficult without something exciting to attract them, Professor Brandenberger began the assembly of a unique laser facility to support course work in laser physics and optics as well as experimental independent research. In 1988, Professor Cook began the assembly of the Computational Physics Laboratory, which brought a strong computational dimension to our upper-level courses, supporting theoretical independent research and complementing experimental independent research as well. Currently, a similar effort in surface physics is emerging.

In time, we came to refer to these specialized laboratories as the central facilities supporting *signature programs*, which we define as innovative, high-visibility teaching efforts that focus on contemporary topics taught in well-equipped signature laboratories specifically designed and equipped for these programs. Because of their pedagogic dimensions, signature programs are not identical to faculty research, but the two are strongly coupled, and many of the experiments included in a signature laboratory emerge from faculty research programs. Signature programs affect the total departmental program in numerous ways: they support specialty courses that lend distinctiveness to a department; they intensify student/faculty interaction and increase the drawing power of a department; they foster departmental pride; they support student projects at several levels; they increase departmental holdings of up-to-date equipment; and—perhaps most important of all for the long-range future of a department and of physics programs nationally (see Section 2.4)—they serve as staging areas for the active recruitment of science students.

In the computational signature program—the program most relevant to the present document, the author has for the last twenty years been building the Lawrence Computational Physics Laboratory (CPL) and revamping the departmental curriculum so that majors come to use sophisticated computational tools like IDL, MAPLE, and LaTeX whenever they deem it appropriate. We have had outside support to the tune of nearly $725K for the acquisition of hardware, the conduct of summer programs in curricular development, the conduct of workshops for physics faculty from around the country, and the support of released time for writing curricular materials. In particular, the required sophomore course *Computational Mechanics* (to be described more fully in Sections 3.3.2 and 4.1) which combines intermediate mechanics with an introduction to computational approaches to problems in physics, was introduced in 2002–03 to make sure that *all* of our physics majors have developed a beginning acquaintance with our computational resources and have developed skills that will support their continued use of these resources in subsequent studies. The elective junior/senior course *Computational Physics* (to be described more fully in Sections 3.4.3 and 4.2), was introduced in 2004–05 to offer interested students an opportunity to extend their knowledge and skills to include more advanced computational topics and techniques not covered in the sophomore course. Neither of these courses would have been possible without the infrastructure of hardware and software provided by the CPL.

In retrospect, Professor Brandenberger's decade-long exploration in the 1970s and early 1980s of laboratory computing was a precursor of and perhaps provided the germ for the notion of the signature programs we conceived in the mid 1980s. Supported first by a Digital Equipment Corporation (DEC) PDP-11 laboratory computer and then a DEC MINC computer, Professor Brandenberger's pilot program explored ways in which interfacing of computers with experimental apparatus and on-line data acquisition would strengthen the undergraduate laboratory program. This project, however, may have been ahead of its time, as it faded in the early 1980s because expecting students to address the difficulties (assembly language programming to access interfaces, control of the timing of measurements, ...) associated with the then-available computers and measuring equipment was ultimately deemed to be less important than exposing them to the topics that the computational components displaced from the undergraduate laboratory experience.

2.4 Recruiting of Majors

A particularly important component of our efforts to build a strong program for physics majors entails active recruiting of able prospective students. Starting in 1987 and continuing ever since, we have hosted annual weekend workshops for prospective students. Each year, about 25–30 participants are selected from 50–75 extremely able applicants. Selection of successful applicants is difficult. Those whom we invite are especially able academically, well rounded personally, genuinely interested in careers in the sciences, and highly motivated to success. Successful applicants spend a weekend on campus, arriving in the afternoon on Friday, staying in the residence halls with current physics majors, and leaving Sunday morning. On Friday evening, participants, current majors, and faculty members enjoy a served dinner.[1] The dinner is followed by a session in which participants and faculty members introduce themselves to one another and, assisted by current students, faculty members conduct a tour of the departmental facilities. From 8:30 AM until 4:00 PM on Saturday, participants, working in teams of two and guided at each station by a current physics major, perform several half-hour hands-on experiments. In the first years, almost all the experiments involved lasers or computation. In more recent years, the spectrum has been broadened to include other areas of current interest within the Department. In the past few years, eight or nine experiments have been selected from experiments titled

- Build a Laser,
- Holography,
- Speed of Light (via time of flight of a laser pulse),
- Diffraction of Light (Schalow experiment with machinist's rule),
- Xray Diffraction from Thin Films,
- Confinement of Non-Neutral Plasmas and Plasma Oscillations,
- Motion of Electrons in Magnetic Fields,
- Transverse Electromagnetic Modes in a Laser,
- Polarization and Malus' Law,
- Scanning Tunneling Microscopy (with a bow to nanoscience),
- Computational Physics and Chaos (Lorentz attractor), and
- Atomic Spectroscopy.

[1] We try hard to persuade the prospective students that such meals are the norm at Lawrence, but then, fearing a charge of false advertising, we correct that illusion by having them go through the standard food lines for lunch on Saturday.

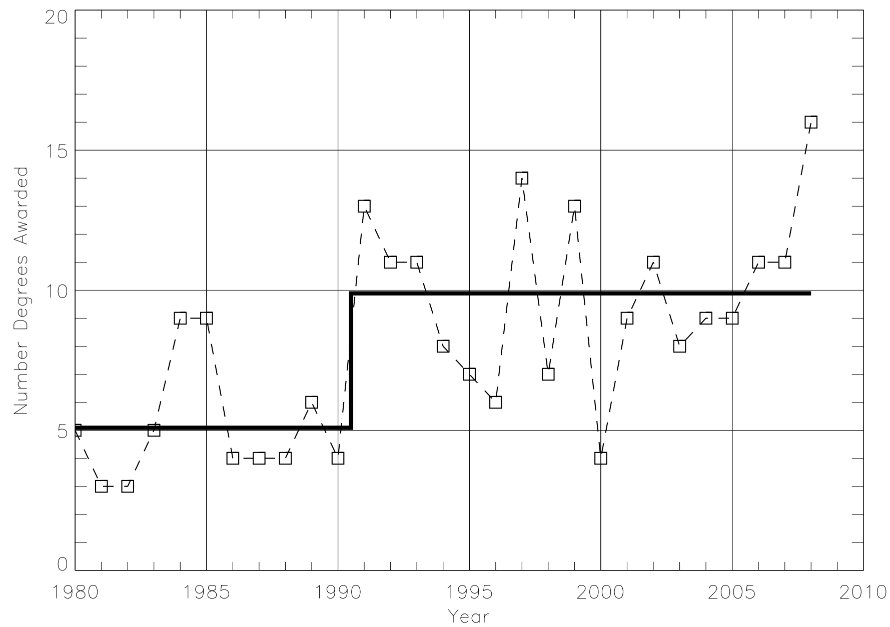

Figure 2.1: Number of Physics Graduates versus Year. Annual recruiting workshops started in 1987 began influencing this number with the class of 1991. The points for the classes of 2007 and 2008 are based on current enrollments in those classes.

Saturday is busy, fast moving, and exhausting for participants and instructors alike. The day concludes after dinner with several evening activities (watch selected videos; attend a concert or play; visit the gym for pick-up volley ball or basketball) that provide a way for participants and current majors to interact informally and socially as a complement to the intellectual and academic activities of the morning and afternoon.

These workshops, which would not have been possible without the signature laboratories described in Section 2.3, have had an enormous influence on the number and quality of physics majors choosing to attend Lawrence. Each year six to ten of the participants and another several individuals from our total applicant pool matriculate at Lawrence and pursue programs of study that anticipate a major in physics. As shown in Fig. 2.1, these recruiting efforts have resulted in our graduating an average of ten majors each year since 1991, the first year a graduating class was affected by our recruiting efforts.[2] More than half of our majors graduate with honors; more than half embark immediately on advanced studies in strong graduate programs around the country.

[2]For the sake of calibration, note that, in 2003, only 6% of the 500+ institutions in the country that offer only the bachelor's degree in physics graduated ten or more majors; only 23% graduated 5 or more majors.

Chapter 3

The Computational Components of the Lawrence Curriculum

Computers have been used in physics instruction at Lawrence since 1964 when students in the introductory courses were sent, card deck in hand, to the institution's IBM 1620 computer to solve ordinary differential equations, find energy eigenvalues for the quantum harmonic oscillator, and analyze experimental data. Teletype terminals to a time-shared computer came along in 1969 and the first institutionally owned time-shared computer—a Digital Equipment Corporation (DEC) PDP 11-45—was installed in the early 1970s. Some of these early uses were spurred by Professor Cook's first sabbatical in 1971–72 at Dartmouth College, then a leader in educational applications of time-shared computing. More consciously structured efforts to bring computing into the entire curriculum trace to the first Computational Physics Laboratory (CPL) in 1988[1] and the first equipping of the introductory laboratory with computers and hardware for on-line data acquisition in 1990.[2] Since that time, the hardware in the introductory laboratory has been changed twice and and the hardware in the CPL has been changed three times. These two facilities now provide the infrastructure for nearly all of the current uses of computers in our instructional program.

In broad outline, freshman prospective majors encounter *LoggerPro*[20], *Kaleidagraph*, and *Excel* for data acquisition and analysis, curve fitting, and graphical visualization. Fall-term sophomores in *Electronics* encounter *Multisim 7* for circuit simulation and continue to use *Kaleidagraph* and *Excel*; winter-term sophomores in *Computational Mechanics* experience a concentrated exposure to IDL, MAPLE, and LaTeX for solving ODEs, evaluating integrals, visualizing functions graphically, and preparing neatly printed problem solutions; and spring-term sophomores in *Electromagnetic Theory* continue to use IDL and MAPLE for graphical visualization and for numerical solution of Laplace's equation. Junior/senior courses in quantum mechanics, advanced laboratory, computational physics, mathematical methods of physics, plasma physics, and advanced mechanics make further explicit use of computers, though the extent of those uses varies with the instructor. In addition, at all points in our curriculum, students are free to use the resources of the CPL whenever they deem it appropriate or useful, and many do so in *Advanced Laboratory*, senior independent projects, and many other contexts. Indeed, our primary objective in incorporating an early—and substantial—explicit introduction to computation is to make sure our students develop sufficient skills early enough in their studies at Lawrence to assure that, ultimately, they will have the necessary knowledge and the personal confidence to pursue computational approaches fluently, effectively, and independently *on their own initiative*.

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[1] The CPL is fully described in Appendix A; financial support is acknowledged on page vii in the preface.

[2] The configuration of hardware and software in this introductory laboratory is described in Section 3.2 and in footnote 3 in that section; financial support is acknowledged on page vii in the preface.

	Term I	**Term II**	**Term III**
Fresh	Freshman Studies Elective **Calculus I**	Freshman Studies ***Intro Classical Physics** **Calculus II**	Elective ***Intro Modern Physics** **Calculus III**
Soph	***Electronics** **Diff Eq/Lin Alg** Elective	***Computational Mechanics** Elective Elective	***E and M** Elective Elective
Junior	***Quantum** Elective Elective	**Physics Elective** Elective Elective	***Advanced Lab** **Physics Elective** Elective
Senior	Capstone Elective Elective	**Physics Elective** Elective Elective	Elective Elective Elective

Available Physics Electives:

Group 1: Thermal Physics, Optics, Advanced Mechanics, Advanced E and M, Mathematical Methods of Physics, Advanced Modern Physics, Plasma Physics, Solid State Physics, Laser Physics, Computational Physics, Tutorials.

Group 2: Independent Studies/Capstone.

Table 3.1: Typical Program of a Physics Major. Courses in bold type are required for a minimum major in physics; courses marked with an asterisk direct students explicitly to the computer and, in most cases, include some instruction in one or more of our computational resources.

3.1 Typical Program for Physics Majors

An efficient way to describe the Lawrence approach is to track the computational experience of matriculating freshman physics majors as they move towards graduation four years later. Each year, full-time students at Lawrence take three courses in each of three ten-week terms. Class periods are 70 minutes long, and a one-term course is treated officially as the equivalent of a 3-1/3 semester-hour course. While there are many variations, the typical program of a student pursuing a physics major is shown in Table 3.1, in which courses marked with an asterisk direct students explicitly to the computer and the ten physics and four mathematics courses shown in bold type are required for a minimum major in physics, though the occasional matriculant will have sufficient background to justify bypassing one or two introductory courses, especially in calculus. Seven to ten of the (unqualified) electives will be chosen to satisfy various general education requirements. On the order of ten electives (28% of the student's program) are completely unconstrained by the requirements for the Lawrence degree or for the major in physics, though most of our (typically) ten graduates each year will take courses in physics, mathematics, and computer science beyond the minimum required for the major. In addition, many will elect to undertake a senior capstone project which, however, is not currently required for the major.

Available physics electives, most of which are offered every other year, are also shown in Table 3.1. *Computational Physics* makes extensive use of the CPL; in the rest of these courses, students are free—and are often encouraged—to use those resources on their own initiative (and many use them regularly, particularly for graphical visualization and preparation of problem solutions and papers). Majors are *required* to take three courses from the eleven in Group 1 and *may* take as many as five more from Groups 1 and 2 before exceeding an institutionally imposed limit of fifteen courses in any single department. Tutorials and independent studies, the latter being elected by about half of all senior majors and sometimes extending over more than one term and leading to honors in independent study at graduation, offer a vehicle for students to study topics not included in our regular course offerings.

Beyond our regular curriculum during the academic year, we encourage majors to seek scientifically significant research experiences during the summers. Each summer, four to six students who are rising juniors or rising seniors will be engaged as research assistants to Lawrence physics faculty members and, occasionally, a rising sophomore will be offered that opportunity. In addition, a few (again four to six) Lawrence physics majors will accept offers to participate in REU programs at other institutions around the country or in industrial or government laboratories. These off-campus positions are usually limited to rising seniors.

3.2 The Freshman Year (Physics 150, 160)

As freshmen, prospective physics majors at Lawrence first encounter computational approaches in the introductory, calculus-based courses (Physics 150, 160). The infrastructure supporting the computational components in these courses (and, incidentally, the computational components in several introductory and outreach courses for non-majors) is housed in the introductory physics laboratory.[3] Computer-related hardware in that laboratory now consists of eight Hewlett-Packard PCs running Windows XP, a Hewlett-Packard monochrome laser printer, *LabPro*[20] interfaces and several sensors from Vernier Software and Technology, and units for gathering data on radioactive counting rates from Spectrum Technologies, Inc. Students in these courses also use the NanoSurf EasyScan scanning tunneling microscopes and atomic force microscopes that are technically part of our emerging surface physics signature laboratory. Available software includes *LoggerPro*, *Excel*, *Kaleidagraph*, the software for driving the Spectrum Technologies and Nanosurf hardware, *Multisim 7* for circuit simulation in *Electronics*, and *Praat*[21] for spectral analysis of sound waves in *Physics of Music*.

In particular, students use *LoggerPro*, *Excel*, *Kaleidagraph*, and image-processing software associated with scanning tunneling microscopes. Exercises assigned in the nine or ten three-hour laboratory sessions in each term routinely involve

[3] Computers have been used in this introductory laboratory since the late 1960s, when simple data analysis was done on a Lawrence-owned batch-mode IBM 1620 computer, then through teletype access to a remote IBM 360 computer, and then on in-laboratory terminals to a succession of Lawrence-owned DEC PDP-11 and VAX time shared computers. In 1990, an NSF grant for a project undertaken by then Assistant Professor John Gastineau, now employed at Vernier Software, supported the acquisition of the first microcomputers (MAC SE30s), Vernier ULI cards, and several sensors, and the laboratory took a large step in the direction of providing freshmen with an exposure to on-line data acquisition, statistical data analysis, and graphical visualization of experimental data. Awarded in 1997, a grant from the NSF to Professor David M. Cook provided for the replacement of the original computers with (then) state-of-the-art MAC 7300/180 and G3 computers and the acquisition of additional equipment and software for Fourier analysis. While the proposal resulting in this grant focused on up-grading the introductory laboratory to support the addition of a full laboratory to Professor Cook's course *Physics of Music*, it almost goes without saying that other introductory physics courses benefited from this upgrade. Finally, in the summer of 2004, Lawrence University underwrote the updating of the equipment in this laboratory to its current status.

- automated data acquisition in several experiments (as described in the next two paragraphs),
- statistical data analysis in essentially all experiments (*Excel* and *Kaleidagraph*),
- least squares fitting of linear and parabolic functions to experimental data in several experiments (*Excel* and *Kaleidagraph*),
- graphical visualization (*Kaleidagraph* and software special to data-gathering equipment),
- creation of images with computer-controlled NanoSurf EasyScan scanning tunneling microscopes and processing of those images, and
- radioactive counting experiments using hardware and associated software for data acquisition from Spectrum Technologies, Inc.

Physics 150, the first course in this two-term rapidly paced sequence, lists one term of calculus as a *pre*requisite—not a *co*requisite—and deals with classical physics, mostly mechanics and electromagnetic theory; its current text is Young and Freedman.[4] In the lecture portion of this course, students are occasionally assigned exercises that send them to the laboratory computers for graphing theoretical results or solving ordinary differential equations via Euler and improved Euler methods using editable *Excel* templates supplied by the instructor. By far the bulk of the exposure to computers, however, comes in the laboratory meetings, in which students perform experiments titled

- *Using the Laboratory Computers/Elements of Data Analysis*, in which students are introduced to the descriptive statistics associated with multiple measurements of single quantities and to *Excel* as a tool for recording data and doing the requisite arithmetic to determine these statistical parameters.

- *Position, Velocity, and Acceleration*, in which students explore the relationships among these kinematic quantities, learn how to work with a sonic ranger, and have their first encounter with on-line data acquisition and graphical display using *LabPro* interfaces and *LoggerPro* software.

- *Free Fall*, in which students use a spark-timer to obtain a record of position versus time for the first half-second of the motion of an object falling from rest, enter the 25–30 measured positions manually into *Excel*, use *Excel* to calculate velocities and accelerations, copy appropriate values into *Kaleidagraph*, and use several different approaches, including least squares fitting to linear and parabolic functions, to extract measured values of the acceleration of gravity *with uncertainties.*

- *Hooke's Law and Simple Harmonic Motion*, in which students explore the relationship between force and extension and the relationship between period and suspended mass for a Hooke's law spring, using *Excel* and *Kaleidagraph* to do arithmetic and least squares fitting. Then, using the sonic ranger again, a force probe, and *LoggerPro*, students return to on-line data acquisition to explore not only position, velocity, acceleration, and force as functions of time but also velocity as a function of position (phase plane), force as a function of acceleration ($F = ma$), and force as a function of extension ($F = kx$).

- *Inelastic Collisions*, in which the sonic ranger is again used to gather data on the inelastic collision of a moving cart with a stationary cart, and *Excel* and *Kaleidagraph* are used to assess (1) the applicability of conservation of linear momentum, (2) the agreement between experimentally determined and theoretically predicted graphs of final velocity versus initial velocity, and (3) the agreement between experimentally determined and theoretically predicted graphs of final kinetic energy versus initial kinetic energy.

[4] *University Physics* (11th Edition), Hugh Young and Roger Freedman (Pearson/Addison-Wesley, San Francisco, 2004, ISBN 0-8053-9179-7).

- *Ballistic Pendulum* (Cenco Apparatus), in which students use the rise of the pendulum to measure the velocity of the projectile, then predict the position *with uncertainty* at which the projectile will hit the floor when fired across the room, place a target, and then subject their prediction to experimental test. The computer plays a smaller role in this experiment than in most others, but still is used for statistical analyses of measured values.

- *Charge to Mass Ratio of the Electron*, in which students measure the currents (and hence the magnetic fields) necessary to deflect an electron beam of known energy in circles of known radii and then use least squares fitting of those measurements to extract a value for e/m *with uncertainty*.

- *The Driven String: Resonance and Standing Waves*, in which mechanical drivers and suitable signal generators acquired initially for the course *Physics of Music* are used to study standing waves in a vibrating string. Students locate a dozen or more normal modes of oscillation and use least squares fitting to extract information from graphs of frequency versus mode number and of wavelength versus mode number.

- *Interference: Wavelength of Light with a Steel Rule*, in which students scatter a laser beam off of the rulings on a machinist's scale, measure the positions of the maxima in the interference pattern on the wall, and use *Excel* and *Kaleidagraph* to reduce the data (a fairly complicated numerical process), plot a suitable graph, perform a least squares analysis, and ultimately extract a measurement of the wavelength of the light in the laser beam.

Physics 160, the second course in this two-term sequence, deals with relativity, quantum mechanics, solid state physics, and particle physics; its current text is Tipler.[5] Students are free to use the laboratory computers as they work on the weekly assignments but, again, the bulk of the exposure to computers comes in the laboratory meetings, in which students perform experiments titled

- *Speed of Light*, in which students use a pulsed laser and an oscilloscope in a time-of-flight measurement of the speed of light. *Excel* is used for reduction of the measurements.

- *Special Relativity Simulation*, in which students use Edwin F. Taylor's *SpaceTime*[22] to explore length contraction, time dilation, velocity addition, and the relativity of simultaneity. *This experiment is the only experiment in the introductory course in which students use a computer simulation rather than real physical apparatus.*

- *The Photoelectric Effect*, in which the stopping potential of photoelectrons is measured as a function of the frequency of the incident light. Least squares fitting of the data leads to a determination of Planck's constant and the work function of the photoelectric surface.

- *The Bohr Model and the Hydrogen Spectrum*, in which students use a diffraction grating to measure the wavelength of the lines in the Balmer spectrum. Those wavelengths are then correlated with the predictions of the Bohr model. *Excel* is used for reduction of the measurements.

- *Electron Impact Excitation of Helium (Franck-Hertz Experiment)*, in which students determine the excitation energies for helium initially in its ground state by measuring the current at a collecting ring as a function of the energy of the bombarding electrons, associating peaks in the resulting current with transition energies in the helium atoms. The computer plays only a small role in this experiment.

[5] *Modern Physics* (4th Edition), Paul A. Tipler and Ralph A. Llewellyn (W. H. Freeman and Company, New York, 2003, ISBN 0-7167-4345-0).

- *The Scanning Tunneling Microscope (STM)*, in which students use a computer-controlled NanoSurf EasyScan STM to generate and examine images of the surface of graphite. In this experiment, on-line data acquisition and subsequent data analysis are integrated into a single program that controls the entire process.
- *Alpha, Beta, and Gamma Radiation*, in which students use a computer-controlled Geiger counter to explore the penetration of various radiations through different distances in air and in other absorbers.
- *Radioactive Decay Rate and Half-Life*, in which students use a computer-controlled Geiger counter to measure the activity of a short-lived isotope as a function of time.
- *Gamma Spectroscopy*, in which students use a scintillation counter and computer-controlled pulse height analysis to measure the gamma ray spectrum emitted by available sources and to identify the material of those sources by its spectrum

Throughout Physics 150 and 160, students are expected to keep complete, accurate, careful records of their work while in the laboratory, and their laboratory records are graded each week not only on the accuracy and thoroughness of the physics embodied but also on the quality of the record as a record of what was done, how it was done, and what was thought along the way. Certainly, this laboratory helps students develop their experimental skills and also their skills at keeping useful records of experimental work. By the end of the freshman year, prospective majors have also begun to develop their skills in the use of computational tools, particularly that subset of such skills of particular value in the laboratory.

3.3 The Sophomore Year

Beyond the freshman year, majors—of course—continue to use *Excel* and *Kaleidagraph.* A serious introduction to "real" computation, however, emerges in the sophomore year. In that year (and thereafter), students have 24/7 access to our Computational Physics Laboratory (CPL), which is equipped—see Appendix A—with hardware and software in all the categories enumerated in Section 1.1 except *PowerPoint* and *LabView*. Fall-term sophomores are introduced explicitly to circuit simulation in *Electronics* (Section 3.3.1); winter-term sophomores see several applications in *Computational Mechanics* (Section 3.3.2); and spring-term sophomores see additional uses in *Electricity and Magnetism* (Section 3.3.3).

3.3.1 Electronics (Physics 220)

The course *Electronics* (Physics 220) meets three times a week, twice for three-hour laboratory sessions and once for a 70-minute lecture/discussion of the current topic. The bulk of the course entails constructing various circuits and using assorted measuring instruments (oscilloscopes, signal and function generators, frequency counters, digital voltmeters,and digital multimeters) to examine the properties of the circuits. About 70% of the course is devoted to analog circuits, including LRC resonant circuits and operational amplifiers, and 30% of the course is devoted to digital circuits. The texts are Horowitz and Hill[6] and Simpson,[7] the first as a primary reference and important addition to the students' personal libraries and the second for most of the reading.

[6]Paul Horowitz and Winfield Hill, *The Art of Electronics* (Cambridge University Press, Cambridge, England, 1989, ISBN 0-521-37095-7), Second Edition.

[7]Robert Simpson, *Introductory Electronics for Scientists and Engineers* (Prentice-Hall, Englewood Cliffs, NJ, 1987, ISBN 0-205-08377-3), Second Edition. This book is out of print, but several copies are available in the laboratory.

Throughout the term, students continue to hone their skills with *Excel* and *Kaleidagraph*. In addition, early in the course, students are introduced to *Multisim 7* software installed on the computers in the introductory laboratory and, subsequently, use that software to complete a number of the weekly problem assignments and, whenever they feel it appropriate, to predict or interpret experimental results. Each student maintains a careful hand-written laboratory notebook, though computer-produced graphs and spreadsheets will frequently be taped into that notebook. Towards the end of the term, each student writes a journal-quality article on one of the experiments. Most will use *Microsoft Word* for the drafting of this article but a few will by this time have learned—and will use—LaTeX. Many will use *Multisim 7* to generate theoretical predictions for comparison with their experimental results.

3.3.2 Computational Mechanics (Physics 225)

Prior to the academic year 2002–03, we offered a traditional course in intermediate mechanics, using Symon[8] or Barger and Olsson[9] as the text. In addition, we offered an *elective* course called *Computational Tools in Physics*, which used locally produced documents[10] as the text and, in that period, provided the starting point in our nurturing of our students' abilities to take full advantage of the resources of the Computational Physics Laboratory (CPL). That full-credit course was offered in three 1/3-credit segments, one in each of the three terms of our academic year, and was taken by sophomores as an overload. Its topics were coordinated with the required courses taken by sophomore majors. The first term focused on acquainting students with the rudimentary capabilities of our CPL (the UNIX operating system, array processing and graphical visualization using IDL, publishing scientific manuscripts using LaTeX and Tgif, symbolic manipulations using MAPLE, and circuit simulation using SPICE and was coordinated with *Electronics*. The second term was coordinated with the intermediate course in classical mechanics, and focused on symbolic and numerical approaches to ordinary differential equations (ODEs). The third term was coordinated with an intermediate course in electricity and magnetism[11] and focused on symbolic and numerical integration. Especially for those sophomores who did not elect *Computational Tools in Physics*, we included two short computational workshops—one on IDL and the other on MAPLE—in the *required* sophomore mechanics course. Thus, *all* sophomores had at least a small, *forced* exposure to the CPL, and some—but unfortunately not all—sophomores had a fully comprehensive introduction to the available capabilities.

Beginning in the academic year 2002–03, the course *Computational Tools in Physics* was discontinued, and the required sophomore course titled *Computational Mechanics* (Physics 225), which replaced the course in classical mechanics, became the starting point in our nurturing of our students' abilities to take full advantage of the resources of the CPL. In brief, this course combines about 60% of the material covered in a traditional course in intermediate mechanics with about 40% of the orientation to computing covered in the discontinued course *Computational Tools in Physics*. The gain lies in the incorporation of the computational elements in a course that is *required* of sophomore majors, thus assuring that all majors have an early introduction to computational approaches, making possible the assumption of that background in all subsequent courses, and supporting independent use of our computational resources even if individual faculty members in later courses do not make explicit assignments involving those resources.

Computational Mechanics does not, of course, cover all of the topics treated in its predecessor. In particular, Lagrangian mechanics and rigid body dynamics were moved to our elective

[8] Keith Symon, *Mechanics* (Addison Wesley, Reading, MA, 1971, ISBN 0-201-07392-7), Third Edition.

[9] Vernon D. Barger and Martin G. Olsson, *Classical Mechanics: A Modern Perspective* (McGraw-Hill, New York, 1995, ISBN 0-07-003734-5), Second Edition

[10] See Chapter 5.

[11] See Section 3.3.3.

junior/senior course *Advanced Mechanics*. These topics thus remain available to junior and senior majors but are not any longer encountered by *all* majors. We believe, however, that this loss is more than compensated by the acquaintance *all* of our majors now have with computational approaches and by their and our ability to exploit computational approaches at many points in our intermediate and advanced curriculum.

Computational Mechanics is discussed in fuller detail in Section 4.1.

3.3.3 Electricity and Magnetism (Physics 230)

In *Electricity and Magnetism* (Physics 230), which uses Griffiths[12] as its text, is almost always taken by students immediately after they complete *Computational Mechanics*, which is the main prerequisite. Thus, at the end of their sophomore year, majors have an immediate reinforcing of some of the computational topics addressed in *Computational Mechanics*. Though the details and the extent of computer use depend on the individual instructor, students in *Electricity and Magnetism* use the CPL for graphical visualization of problem solutions worked out by hand; use symbolic and numerical integration to evaluate electrostatic potentials, electric fields, and magnetic fields; solve the Laplace equation using instructor-supplied templates written in IDL's language; and review numerical approaches to trajectory problems (which were treated more fully in *Computational Mechanics*).

3.4 The Junior and Senior Years

With *Computational Mechanics* as a uniform background, subsequent theoretical and experimental courses alike offer students many opportunities to continue honing their computational skills and, depending on the instructor, some of these courses will direct students explicitly to the CPL for an occasional exercise. Techniques for graphical visualization are used routinely on the students own initiative in *Optics*, *Advanced Mechanics*, *Advanced Electricity and Magnetism*, *Mathematical Methods of Physics*, and *Plasma Physics*, all of which are alternate-year elective offerings. Most senior capstone projects exploit the resources of the CPL, at least for graphical visualization and preparation of reports. Some recent senior projects, notably those in fluid mechanics, musical acoustics, xray diffraction, mapping of astrophysical data, multiphoton quantum transitions, and theoretical explorations of the confinement of non-neutral plasmas, have made extensive use of these facilities. Some physics students use the CPL in conjunction with courses in other departments, particularly mathematics. Further, once students have learned to use LaTeX in *Computational Mechanics*, they routinely use that tool for preparation of written papers and reports. All of these uses are facilitated by our policy of granting sophomore, junior and senior majors 24/7 access to the CPL.

Three upper-level courses make more extensive and explicit use of the computer. Uses in *Quantum Mechanics*, *Advanced Laboratory*, and *Computational Physics* are discussed in Sections 3.4.1, 3.4.2, and Sections 3.4.3 and 4.2, respectively.

[12]David J. Griffiths, *Introduction to Electrodynamics* (Prentice-Hall, Upper Saddle River, New Jersey, 1999), Third Edition.

3.4.1 Quantum Mechanics (Physics 310)

Quantum Mechanics (Physics 310), which uses either Griffiths[13] or Cook[14] as its text, is almost always taken by students in the fall term of the junior year and, hence, provides the third term of a comprehensive, intermediate-level exposure to mechanics, electromagnetic theory, and quantum mechanics. As with *Electricity and Magnetism*, the details and the extent of computer use depend on the individual instructor. Students are always free to use the resources of the CPL on their own initiative and, by this point in their careers at Lawrence, they have acquired sufficient skill and confidence that many in fact do see ways to use the computer to support their study of quantum mechanics. When one of our more computer-oriented faculty members teaches this course, students are explicitly directed to the computer for graphical visualizations of quantum wave functions, reflection and transmission coefficients, ...; for symbolic and numerical solution of quantum eigenvalue problems (e.g., infinite and finite depth potential wells, simple harmonic oscillator); for symbolic and numerical determination of the time-evolution of Gaussian wave packets; for symbolic and numerical evaluation of integrals to find matrix elements and then, for example, explore perturbation expansions, selection rules, and the Stark effect for higher values of n than are usually addressed by hand; etc.

3.4.2 Advanced Laboratory (Physics 330)

Technically, the laboratory dimensions of our program are outside the purview of responsibility for the author of this report. Nonetheless, the exposure that majors have to computation before enrolling in *Advanced Laboratory* supports their confident use of an assortment of computational resources in that course and also provides the background that facilitates learning about new computational techniques that support experimental science to complement the techniques they have already learned in support of theoretical science.

The course *Advanced Laboratory* is required for physics majors and is usually taken by juniors either in the winter or the spring term. Students work individually, and each has exclusive access to the equipment when working on each experiment. Typically, in ten weeks, each student does three or four experiments. For the sake of a serious exposure to research, each student spends four or five weeks on the first experiment and is expected to study the pertinent literature, to do an extremely thorough job of the experiment, to contribute something new to the experiment or explore some new dimension of the physical system, to keep a careful laboratory record, to prepare a journal-quality paper on the experiment, and to give a talk to the rest of the class on that experiment. While new experiments are added and, occasionally, an experiment will be retired, the current options include the experiments listed in Table 3.2. Most of these experiments involve use of *Kaleidagraph* and other graphical visualization tools for examining acquired data, use of LaTeX or other publishing packages for preparing written reports, and use of *PowerPoint* or equivalent presentation software for preparation of talks. The laboratory is equipped with several computers having interface cards and with numerous measuring instruments that can output digital signals directly to computers, and many experiments therefore involve on-line acquisition of data and compel the student to figure out how to persuade the physical apparatus to communicate with a computer. Linear, polynomial, and non-linear least squares fitting figures in numerous experiments. Occasionally, students use numerical simulations to support comparison of theoretical predictions with experimental results.

[13]David J. Griffiths, *Introduction to Quantum Mechanics* (Prentice-Hall, Upper Saddle River, New Jersey, 2005, ISBN 0-13-111892-7), Second Edition.

[14]David M. Cook, *Non-Relativistic Quantum Mechanics*. This set of notes, whose writing was started in 1967 and which has seen numerous revisions over the years, has grown to a full—though as yet unpublished—text. A particular feature distinguishing the current version from other books at the same level is its incorporation of computational approaches alongside the more traditional analytic approaches to addressing quantum mechanical problems.

- Gamma-Gamma Correlation,
- High T_c Superconductivity,
- Mossbauer Effect,
- Muon Decay,
- Compton Effect,
- Faraday Rotation,
- Optical Pumping in Rubidium,
- Xray Diffraction,
- Quantum Beats,
- Holography,
- Child's Law,
- Saturated-Absorption Spectroscopy,
- Non-linear Quantum Optics,
- Electrical and Optical Properties of Thin Films,
- Alpha and Beta Spectroscopy,
- Electron Paramagnetic Resonance,
- Scanning Tunneling Microscopy,
- Atomic Force Microscopy,
- Raman Spectroscopy,
- Optogalvanic Spectroscopy,
- Population Dynamics in a Laser Plasma, and
- Laser Fundamentals.

Table 3.2: Experiments Available in *Advanced Laboratory*.

Those responsible for developing this course are working to incorporate *LabView* into some of the experiments, but that inclusion is not yet available to students.

3.4.3 Computational Physics (Physics 540)

The main computational techniques of importance not included in *Computational Mechanics* apply to generating and visualizing solutions to partial differential equations (PDEs). Some years ago, we tried to incorporate finite-difference and finite-element approaches to PDEs into our junior/senior electives *Advanced Electricity and Magnetism* and *Mathematical Methods of Physics*. That effort failed, first—and primarily—because the necessary sacrifice of other topics (electromagnetic radiation from accelerated particles, relativistic formulation of electromagnetic theory, Fourier analysis and complex contour integration, ...) was ultimately deemed unacceptable, and second because—at the time—only those students who had elected *Computational Tools in Physics* had the necessary background, so only a few juniors and seniors were prepared to profit from inclusion of those topics in those courses. Once *Computational Mechanics* had been introduced and taught for two years, however, all junior and senior majors then indeed had the appropriate background. Rather than resurrecting our earlier incorporation of computational approaches to PDEs into other courses, however, we introduced a new junior/senior course titled *Computational Physics* (Physics 540). This elective course lists *Computational Mechanics* as a prerequisite, so students who elect Physics 540 can move quickly to serious computation; they need not spend a portion of the course learning how to log in and out, work with a text editor and a publishing package, send files to the printer, and work with basic numerical and symbolic tools—skills that are critical to successful use of a computer but at the same time are decidedly peripheral to the computational tasks at hand. In short, to use an analogy from foreign languages, students come to Physics 540 already knowing the vocabulary and the grammar, and they can begin right away to use these skills in application to the computational topics themselves.

Computational Physics is discussed in fuller detail in Section 4.2.

Chapter 4

Central Courses

Two courses in the Lawrence physics curriculum have substantial computational components. *Computational Mechanics* is offered every year, is required in the winter term of the sophomore year, and provides *all* majors with an introduction to the resources of the Computational Physics Laboratory (CPL). *Computational Physics* is an elective junior/senior course that is offered in alternate years, lists *Computational Mechanics* as a prerequisite, and serves the 20–25% of our majors who seek a more advanced understanding of computational approaches than is provided by the sophomore course. Because these two courses are central to the computational dimensions of the Lawrence curriculum, they are described more fully in this chapter than in the previous brief description in Sections 3.3.2 and 3.4.3, respectively.

4.1 Computational Mechanics (Physics 225)

The main objectives of *Computational Mechanics* (Physics 225) are conveyed by its catalog description, which asserts that it "introduces symbolic and numerical computation through examples drawn mainly from classical mechanics but also from classical electromagnetism and quantum mechanics" and that it "emphasizes computer-based approaches to graphical visualization, the solution of ordinary differential equations, the evaluation of integrals, and the finding of eigenvalues and eigenvectors". Prerequisites for the course are *Introductory Classical Physics* and *Differential Equations and Linear Algebra*, which itself has three terms of calculus as prerequisites. The text for the mechanics component, *Notes for Computational Mechanics*,[1] is written by Professor Cook and is comparable in level and sophistication to Symon[2] or Barger and Olsson[3] but is abbreviated to include only those topics covered in the course; the text for the computational components is *Computation and Problem Solving in Undergraduate Physics* (*CPSUP*), also written by Professor Cook.[4] Over the years, the writing of successive drafts of the materials that ultimately found their way into the version of *CPSUP* used for this course and ultimately the writing of that book was supported by grants from the NSF; the actual design of the course and some of the polishing of the text was supported by the 2001 grant from the W. M. Keck Foundation.[5]

[1]While these notes may ultimately be published, as of December, 2006, they are still very much in draft form.

[2]Keith Symon, *Mechanics* (Addison Wesley, Reading, MA, 1971, ISBN 0-201-07392-7), Third Edition.

[3]Vernon D. Barger and Martin G. Olsson, *Classical Mechanics: A Modern Perspective* (McGraw-Hill, New York, 1995, ISBN 0-07-003734-5), Second Edition

[4]Both the development of this book and its customizable structure are described more fully in Chapter 5.

[5]See the section titled *Acknowledgments* on page vii in the preface for more details on these grants.

Week 01	Orientation to LINUX (including text editor) Kinematics/Dynamics of Translation/Rotation Impulse/Momentum/Work/Kinetic Energy Gravity/Electromagnetic Force/Friction/Tension
Week 02	Orientation to IDL/TGIF (basic capabilities, visualization)
Week 03	Equations of motion (constant force/torque, force dependent only on t, ... only on x, ... only on v) Potential energy, SHM, and equilibrium Work and potential energy in 3D
Week 04	Velocity-dependent forces Damped and driven SHM Resonance Coupled and small amplitude oscillation
Week 05	HOUR EXAMINATION Orientation to LaTeX Central Forces/Effective Potential Energy, Orbital Equations
Week 06	Planets, Satellites, Comets MID-TERM READING PERIOD
Week 07	Orientation to MAPLE Using MAPLE to solve ODEs Algorithms to solve ODEs numerically
Week 08	Using IDL to solve ODEs numerically
Week 09	HOUR EXAMINATION Symbolic Evaluation of Integrals
Week 10	Algorithms to Evaluate Integrals Numerically Using IDL to Evaluate Integrals Numerically
Week 11	FINAL EXAMINATION

Table 4.1: Weekly Schedule for *Computational Mechanics*.

4.1.1 Outline of the Course

As is evident from the catalog description, *Computational Mechanics* has two distinct but intertwined topics, mechanics and computation. The schedule for this course is displayed in Table 4.1. The course begins with a tutorial exercise to acquaint students with the features of the workstations in the CPL and with the LINUX operating system. Concurrently, students review and extend their introductory studies of translational and rotational kinematics and dynamics, impulse, momentum, work, kinetic energy, and common forces. They spend the second week of the term entirely in the CPL becoming acquainted with the general capabilities of IDL, especially for graphical visualization of scalar functions of one, two, and three variables, and with Tgif for generating drawings. In the third and fourth weeks, the course returns to the fundamental laws of mechanics to set up and solve the usual problems in one-dimensional motion via standard analytic techniques, and to extend the definition of potential energy and conservative forces to three dimensions. Then, in the fifth and sixth weeks, after a pause for evaluation, students encounter the elements of LaTeX and spend several days on the standard analytic approaches to the central force problem. The remainder of our ten-week term is spent mostly in computationally related activities, including an orientation to MAPLE, a discussion of numerical algorithms for solving ordinary differential equations (ODEs) and evaluating integrals, and an introduction to routines built into IDL for solving ODEs and evaluating integrals. Examples include many of the problems already discussed analytically but also introduce non-linear and chaotic systems. Sample integrals are found in the evaluation of potential energies, moments and products of inertia, and electric and magnetic fields and potentials. In the rearrangement that generated *Computational Mechanics* from its predecessor, a more traditional intermediate course in classical mechanics, only Lagrangian mechanics and rigid-body dynamics were omitted to provide the time for the addition of the computational topics. In the Lawrence curriculum, these two topics are included in an elective alternate-year, junior/senior elective titled *Advanced Mechanics*.

Computational Mechanics is a rapidly paced and intensive course. Students in the course spend quite a bit of time in the CPL. Especially during the first few weeks of the term, when students are inexperienced with the available computational tools, we arrange for a more experienced student—often a student who had worked as a research assistant to Professor Cook in the previous summer—to be available in the CPL for four to six scheduled hours each week to help students in the course strengthen their wings so that, later in the term, they can be expected to fly more confidently on their own.

4.1.2 Sample Problems from Assignments

Because they refer to chapters and exercises from the texts, detailed syllabi for this course would not be particularly meaningful and are not included in this report. Instead, to give a bit of the flavor of the course, several representative problems assigned during the term are collected in Appendix B. Note that, after students have learned a bit of LaTeX in week 5, they are required to complete their solutions to one or two problems each week using that publishing tool.

4.1.3 Examinations from a Recent Offering

The examinations given in a recent offering of this course also convey something of the expectations. In each offering, there are two one-hour examinations and one three-hour final examination. The second of the two hour examinations typically contains both an in-class, closed-book timed part and an out-of-class, open-book but closed-classmate, at-the-computer part. The first hour examination may or may not have an at-the-computer component and, because the enrollment in the course exceeds the available equipment, the final examination will not involve any work at the computer. The first hour examination and the final examination, however, may well ask students to lay out what they *would* do were they able to access a computer. Copies of the three examinations from the winter, 2006, offering of *Computational Mechanics* are contained in Appendix C.

4.2 Computational Physics (Physics 540)

The main objectives of this alternate-year offering are conveyed by its catalog description, which asserts that it "treats computational approaches to problems in physics with particular emphasis on finite-difference and finite-element methods for solving partial differential equations as they arise in electromagnetic theory, fluid mechanics, heat transfer, and quantum mechanics, and on techniques for graphical visualization of the solutions". The prerequisite for the course is *Computational Mechanics*, which simple statement hides the several physics and mathematics prerequisites for the stated prerequisite course. The text for the course is Professor Cook's *CPSUP*, supplemented with assorted documentation for the various programs used during the course. The development of this course and the drafting and revising of the portions of *CPSUP* used in this course were supported by the 2001 grant from W. M. Keck Foundation.[6]

4.2.1 Outline of the Course

The daily schedule for *Computational Physics* is compiled in Table 4.2. Because students spend quite a lot of time at the workstations in the CPL and because it usually doesn't take very long in class to set the stage for lengthy exercises at the computer, this course meets for lecture on average 1.5 times per week. At other times, students work on the regular assignments, which are common to all students and involve (relatively) straightforward exercises that invoke the computational strategy of the week. The course begins by orienting students, all of whom have taken *Computational Mechanics* but most of whom have *not* taken a formal course in programming, to the elements of structured programming, first in pseudocode (which allows focusing on concepts rather than syntactic details) and then in FORTRAN and IDL.

After spending a day and a half deriving the standard second-order partial differential equations of mathematical physics (wave equation, diffusion equation, Laplace equation) and discussing the multitude of physical contexts in which one or another of these equations appears, the course introduces finite difference methods and applies them to

- discretize the diffusion equation in the spatial coordinate(s) but not the temporal coordinate, yielding a possibly large set of first-order ordinary differential equations to be solved simultaneously subject to appropriate initial and boundary conditions. (The solution of ODEs using IDL was treated in *Computational Mechanics*; in *Computational Physics*, students review use of IDL but then move to using the large FORTRAN solver LSODE, which gives them their first experience writing driving programs to invoke existing and well tested subroutines.)
- discretize the wave equation in the spatial coordinate(s) but not the temporal coordinate, yielding a possibly large set of second-order ordinary differential equations to be solved simultaneously subject to appropriate initial and boundary conditions.
- discretize the Laplace equation in all coordinates, yielding a possibly large set of algebraic equations to be solved by an iterative approach. Students first follow a supplied template to write programs, either in IDL or FORTRAN or C, to implement the standard iteration for a variety of different boundary conditions and geometries. Later in the term, students learn about multigrid approaches to speed the convergence of the iteration and, instead of trying to code this more difficult approach themselves, encounter again the need to write driving programs to invoke existing subroutines, this time MUD2SP and MUD3SP from the MUDPACK package of solvers for elliptic partial differential equations in two and three dimensions.
- discretize the wave and diffusion equations in all coordinates, obtaining a set of algebraic equations that support the systematic stepping of the initial values indefinitely into the future and, following templates developed in lectures and the text, write their own IDL or FORTRAN or C code to solve a number of problems with different initial and boundary conditions.

About 35% of the time in our ten-week term is devoted to this segment of the course.

The final topic of the course, to which about 30% of the time is devoted, addresses finite element approaches to partial differential equations though, for simplicity of the initial development,

[6] See the section titled *Acknowledgements* on page vii in the preface for more details on these grants.

Day 01	Programming Structures and Strategies
Day 02	Programming in FORTRAN and IDL
Day 03	Analytic/Physical Derivation of PDEs (wave, diffusion, Laplace, and fluid dynamics equations)
Day 04	Finite Difference Methods (Part I)
Day 05	ASSIGN 1 DUE; Driving Programs for LSODE (Part I)
Day 06	Driving Programs for LSODE (Part II)
Day 07	No class; Work on Assignment 2
Day 08	ASSIGN 2 DUE; Finite Difference Methods (Part II)
Day 09	Finite Difference Methods (Part III)
Day 10	No Class; Work on Assignment 3
Day 11	No Class; Work on Assignment 3
Day 12	Oral presentations on Assignment 3
Day 13	ASSIGN 3 DUE; MUDPACK/Multigrid Techniques (Part I)
Day 14	MUDPACK/Multigrid Techniques (Part II)
Day 15	No Class; Work on Assignment 4
Day 16	ASSIGN 4 DUE; Finite Element Methods (Part I)
Day 17	Finite Element Methods (Part II)
Day 18	Finite Element Methods (Part III)
Day 19	MID-TERM READING PERIOD; No Class
Day 20	No Class; Work on Assignment 5
Day 21	ASSIGN 5 DUE; FEMs with MARC/MENTAT (Part I)
Day 22	FEMs with MARC/MENTAT (Part II)
Day 23	Project Proposal Due; No Class; Work on Assignment 6
Day 24	Oral Presentations on Assignment 6
Day 25	ASSIGN 6 DUE; No Class; Work on Projects
Day 26	No Class; Work on Projects
Day 27	THANKSGIVING VACATION
Day 28	THANKSGIVING VACATION
Day 29	No Class; Work on Projects
Day 30	No Class; Work on Projects
Day 31	Oral Presentations on Projects; Final Paper Due
	No Final Examination

Table 4.2: Daily Schedule for *Computational Physics*. The vertical blocking corresponds to the weeks of the term, which happened to start on a Friday in the year to which this schedule applies.

the approach is first applied to ordinary differential equations. In both one and two dimensions, the development of the technique focuses on a general second-order, self-adjoint, linear, inhomogeneous equation. The overall strategy is laid out, and templates for coding in FORTRAN and IDL are worked out for specific examples of such equations, and students then modify those templates to adapt them to other examples. After the technique has been described and practice with very simple examples completed, the course spends two days describing how to use a pair of commercial programs called MARC (a venerable solver of partial differential equations by finite element methods) and MENTAT[23] (a more contemporary GUI interface for defining problems, automeshing the geometry, creating the input file for MARC, and examining the output produced by MARC). Students then complete an assignment that asks them to adapt strategies illustrated in the class discussion of MARC/MENTAT to slightly different situations.

4.2.2 The Projects

Because they refer to chapters and exercises from the texts, detailed syllabi would not be particularly meaningful and are not included in this report. Further, no examinations are given in this course. Beyond the weekly written assignments (which all students complete using LaTeX), students also complete two medium-length projects, the first (a component of Assignment 3) an assigned project using finite difference techniques and the second (a component of Assignment 6) an assigned project using finite element techniques. At the end of the term (the entirety of Assignment 7), each student completes a final, longer project of his or her choice but subject to the instructor's advance approval. On each of these projects, each student prepares an oral presentation (15 minutes for the first two projects; 25–30 minutes for the end-of-term project) delivered to the class and also a written paper. The general level of the course and the types of problem that students are expected to be able to address are conveyed by the portions of the assignments describing these three projects. Those portions of Assignments 3, 6, and 7 are presented in Appendix D.

Chapter 5

CPSUP

The computational components of the Lawrence curriculum and the text which is the topic of this chapter evolved together, and the text has played an important role in supporting our curricular developments. Titled *Computation and Problem Solving in Undergraduate Physics* (*CPSUP*),[1] the text had its origins in the mid 1980s when, as has been detailed in the previous chapters of this report, we at Lawrence decided that, to be properly prepared for their future careers in physics, our majors needed to have a substantial exposure to computational approaches to problems alongside the more traditional analytic approaches and they needed to have that exposure early enough so that we could require them to use computational resources in subsequent courses and so that they would have the knowledge and confidence to use those resources *on their own initiative* whenever it seemed to them appropriate to do so. In the first decade of this project, activities focused on acquiring hardware and software, developing a succession of curricular modifications, and generating numerous—ultimately 65 or 70—documents that described the features of the operating system and the several acquired software packages and illustrated how to apply those software packages—both symbolic and numeric—to selected representative problems drawn from several different subareas of physics.

By late 1998, it was clear that developments at Lawrence might well be of interest to the wider community—a realization that prompted the submission of a proposal to the Educational Materials Development (EMD) track of the CCLI program of the NSF.[2] The objectives of the proposed activity were

- to standardize the format of and expand the extensive library of instructional materials developed at Lawrence into a flexible publication to support introduction of uses of computational resources into the upper-level undergraduate physics curriculum;
- to conduct week-long summer workshops for physics faculty from around the country, not only for evaluation and assessment but also for dissemination; and
- to publish the final product.

The bulk of the writing took place during the summers of 2000, 2001, and 2002 and during a sabbatical year early in that period. In the summers, student assistants drafted solutions to representative exercises. Thus, the end result is not only a book, which runs to about 900 pages if *all* components

[1]Greater detail about *CPSUP* can be found at the URL `http://www.lawrence.edu/dept/physics/ccli`. A review was published in the *American Journal of Physics*, Vol. 74, No. 7 (July, 2006), pp. 653–655.

[2]See NSF Grant DUE-9952285 as listed in the section titled *Acknowledgements* on page vii in the preface.

are included, but also an accompanying manual containing solutions to nearly 200 representative exercises.

In this chapter, the text itself is described in fuller detail. While the writing of this text was prompted by the absence of curricular materials appropriate to what we wanted to do at Lawrence, the attempt in the final version was to create a text that would have potential use in a variety of contexts. In this chapter, we state the challenges, describe the structure of the resulting book, speculate about possible uses of *CPSUP*, describe the strategy adopted for meeting the publishing challenge, and outline the future growth of *CPSUP*.

5.1 The Challenges

That different departments use different hardware and software poses a major challenge to the writing of a widely useful text. The variety of options and combinations is so great that any single choice (or coordinated set of choices) is bound to limit the usefulness of the end result to a small subset of all potentially interested users. The strategy adopted by *CPSUP* to address this challenge involves assembling different versions of the basic materials from a wide assortment of components, some of which—the generic components—will be included in all versions and others of which—those specific to particular software packages—will be included only if the potential user requests them. Thus, the specific software and hardware treated in any particular version will be microscopically "tailor-able" to the spectrum of resources available at the user's site. One version, for example, could include the generic components and only the components that introduce the features of and apply IDL, MAPLE, C, and LaTeX while another might include the generic components and the components that introduce the features of and apply MATLAB, MATHEMATICA, and FORTRAN (including Numerical Recipes).

A second challenge arises because, even among sites that use the same hardware and software, some aspects of local environments are still unique to individual sites. Rules of citizenship, practices and policies regarding accounts and passwords, the features and elementary resources of the operating system, the structuring of public directories, backup schedules, after-hours access, licensing restrictions in force on proprietary software, and numerous other aspects are subject to considerable local variation. *CPSUP* itself makes no attempt to address this challenge and does not constrain local options in these matters. Throughout the book, individual users are directed to a publication called the *Local Guide* for site-specific particulars. A suggested template for that guide will be provided. This guide will have to be created at each site, though a template for that guide—specifically, the guide used at Lawrence—accompanies *CPSUP*.

Third and fourth challenges are consequences of the microscopic customizability. The market for any single version is likely to be small. Thus, any potential publisher must be able not only to assemble and print the desired version on demand (the third challenge) but also (the fourth challenge) to respond economically to orders for relatively small numbers (5–10) of copies of a particular version. The author's way to address these challenges is laid out in Section 5.5.

5.2 The Structure of *CPSUP*

The essential idea for the book emerged from a recognition that the background for and setup of particular problems to be addressed with a computer are independent of the specific hardware on which and software package with which the solutions would be pursued. It ought therefore to be possible to create a *single* book that could be produced in various versions. The book would be assembled from generic components that would be common to all versions and software-specific

Chapter	1.	Preliminaries
Chapter	2.	Introduction to IDL
Chapter	3.	Introduction to MATLAB
Chapter	4.	Introduction to MACSYMA
Chapter	5.	Introduction to MAPLE
Chapter	6.	Introduction to *Mathematica*
Chapter	7.	Introduction to Programming
Chapter	8.	Introduction to Numerical Recipes
Chapter	9.	Solving Ordinary Differential Equations
Chapter	10.	Introduction to LSODE
Chapter	11.	Evaluating Integrals
Chapter	12.	Finding Roots
Appendix	A.	Introduction to LaTeX
Appendix	B.	Introduction to TGIF

Table 5.1: Top-Level Table of Contents for *CPSUP*.

components, different subsets of which would appear in different versions. At the coarsest level, that flexibility is illustrated in the top-level table of contents in Table 5.1. Chapter 1 stands alone; Chapters 2 and 3 introduce the general features of two common array processors; Chapters 4, 5, and 6 introduce the features of three different computer algebra systems; Chapters 7 and 8 introduce a programming language and the numerical recipes library; Chapters 9, 10, 11, and 12 address several important categories of computational processing; and the appendices introduce a publishing system and a program for producing drawings. Any particular version would include at least one of Chapters 2 and 3 and one of Chapters 4, 5, and 6, and Chapters 9, 11, and 12—though these last three would be assembled with only those components that illustrate the programs included in the selections from Chapters 2–6. Chapters 7, 8, and 10, the associated sections in Chapters 9, 11, and 12, and the appendices would be included only if desired by the end user. While the pedagogic objective is for students to become fluent in the use of a spectrum of computational tools, and the chapters are organized by program or by computational technique, the focus throughout is on physical contexts.

The top-level table of contents, however, does not accurately convey the full structure of the text. Chapters fall into two groups. Each of Chapters 2, 3, 4, 5, 6, 8, and 10 and Appendices A and B, for example, focuses on the basic features of a particular application program. Though these chapters draw their examples from physical situations and conclude with numerous physically oriented exercises, they still focus on the capabilities of the application program rather than on the physics illustrated in the examples. Their format reflects a conviction that students must first focus attention on the application program itself before being ready to use the program to address problems in physics. For example, Chapter 3, the table of contents of which is shown in Table 5.2, is representative of chapters in this group. Specifically, Chapter 3 introduces the main features of MATLAB, a program for processing arrays of numbers and creating graphical visualizations of one-, two-, and three-dimensional data sets. The other chapters in this group have a similar structure. Many of the sections in these chapters are structured as tutorials that lead the reader through the main features of the corresponding program, are to be studied *at a computer*, and lean in some measure on vendor-supplied documentation and on-line help to encourage and guide self-study.

Shown in Table 5.3, the structure of Chapter 11 on evaluating integrals exemplifies the structure of the chapters in the second group, each of whose members focuses on a particular computational technique. Presumably, before approaching any particular section in this chapter, the student would have studied the relevant sections in earlier chapters. The first section in each of these chapters (here Section 11.1) sets several physical problems, the successful addressing of which

Section	3.1	Beginning a Session with MATLAB
Section	3.2	Basic Entities in MATLAB
Section	3.3	A Sampling of MATLAB Capabilities
Section	3.4	Properties, Objects, and Handles
Section	3.5	Saving and Retrieving a MATLAB Session
Section	3.6	Loops, Logical Expressions, and Conditionals
Section	3.7	Reading Data from a File
Section	3.8	On-line Help
Section	3.9	M-Files
Section	3.10	Eigenvalues and Eigenvectors
Section	3.11	Graphing Scalar Functions of One Variable
Section	3.12	Making Hard Copy
Section	3.13	Graphing Scalar Functions of Two Variables
Section	3.14	Graphing Scalar Functions of Three Variables
Section	3.15	Graphing Vector Fields
Section	3.16	Animation
Section	3.17	Advanced Graphing Features
Section	3.18	Miscellaneous Occasionally Useful Tidbits
Section	3.19	References
Section	3.20	Exercises

Table 5.2: Sections in the Chapter on MATLAB.

benefits from exploitation of the computational technique with which the chapter deals. Subsequent sections—here Sections 11.2–11.4—describe how one might use a *symbolic* tool in application to some of the problems set in the first section, then—here Section 11.5—describe appropriate numerical algorithms generically, and finally—here Sections 11.6–11.12—illustrate how those algorithms can be implemented with a variety of tools. Each chapter concludes—here Section 11.13—with numerous exercises that students can use to hone their skills. Listings of programs developed in the chapter are included as appendices to the *chapter* rather than to the *book* as a whole. The generic sections—here Sections 11.1, 11.5, and 11.13—would be included in all versions of the chapter; each individual instructor would select which of the remaining sections are appropriate to that instructor's site and only those sections would be included in a version for that site.

Yet one level further down in the overall structure, Table 5.4 shows the present list of sample problems for Chapter 11. They range over several subareas of physics and reveal that evaluation of integrals, perhaps as functions of one or more parameters, plays an important role in many areas of physics.

5.3 Potential Uses

As illustrated by our uses at Lawrence, *CPSUP* is suitable for a sophomore course aimed at introducing physics majors to computational approaches to problems in physics. Through selection of sections and choice of the examples in mechanics or in electromagnetic theory or ..., the text would also function well as a supplement to support introduction of computational approaches in the standard courses in the intermediate-level program of a typical physics major. Since it is in many places structured as a tutorial, *CPSUP* could also support self-studies, independent studies, or tutorials by individual students interested in learning how to apply computation to physics—and occasional students at Lawrence have used the materials in that mode. Finally, especially after a student has

Section	11.1	Sample Problems
Section	11.2	Evaluating Integrals Symbolically with MACSYMA
Section	11.3	Evaluating Integrals Symbolically with MAPLE
Section	11.4	Evaluating Integrals Symbolically with *Mathematica*
Section	11.5	Algorithms for Numerical Integration
Section	11.6	Evaluating Integrals Numerically with IDL
Section	11.7	Evaluating Integrals Numerically with MATLAB
Section	11.8	Evaluating Integrals Numerically with MACSYMA
Section	11.9	Evaluating Integrals Numerically with MAPLE
Section	11.10	Evaluating Integrals Numerically with *Mathematica*
Section	11.11	Evaluating Integrals Numerically with FORTRAN
Section	11.12	Evaluating Integrals Numerically with C
Section	11.13	Exercises
Appendix	11.A	Listing of `trapezoidal.f`
Appendix	11.B	Listing of `trapezoidal.c`

Table 5.3: Sections in the Chapter on Integration.

11.1.1.	One-Dimensional Trajectories
11.1.2.	Center of Mass
11.1.3.	Moment of Inertia
11.1.4.	Large-Amplitude Pendulum (Elliptic Integrals)
11.1.5.	The Error Function
11.1.6.	The Cornu Spiral
11.1.7.	Electric/Magnetic Fields and Potentials
11.1.8.	Quantum Probabilities

Table 5.4: Sample Problems in Section 11.1.

spent some time with some of the chapters, *CPSUP* should be a useful reference work to have in one's library. Broadly, *CPSUP* is a flexible text that can be used in a variety of ways—including as the text for stand-alone courses, as a supplement to existing courses, and as the text for tutorials and self-study—to support introduction of computational approaches to problems in physics alongside the more traditional analytic approaches.

While the motivation throughout *CPSUP* lies in and all examples are drawn from physical contexts, the ultimate objective is for students to develop a sound understanding of the capabilities of a spectrum of computational tools, of a variety of computational techniques, strategies, and algorithms, and of the ways in which those capabilities and techniques can be productively exploited to address serious and substantial problems in physics. Students cannot profitably attempt to run in this arena, however, before they have learned to walk. While *CPSUP* draws its examples from physical contexts and students working their way through the book will learn physics, the book assumes that the student has completed at least an introductory calculus-based survey course in physics to justify placing the greater emphasis on the computational tools and techniques. That focus also leads to a two-fold organization based on the most important capabilities of the tools and on generally useful computational techniques rather than on the standard subdisciplines of physics. The typical user will jump around in *CPSUP* to study only those sections that relate to available software packages, only those illustrative exercises that apply to the particular subdiscipline of physics of concern. Though some of the later sections in the book depend on some earlier sections, the linkages are not particularly tight. Thus, the order of presentation *in the book* does not compel any particular order of treatment *in a course or program of self-study.*

5.4 Workshops

For purposes of both evaluation and dissemination, the 2000 NSF grant and its 2003 supplement supported four week-long summer workshops at Lawrence. In each workshop, participants raced through exercises that familiarized them with the Lawrence computational environment, with the primary features of IDL or MATLAB (1 day), and of MAPLE or MATHEMATICA (1 day), and then with applications of these programs to address problems in physics involving ordinary differential equations (1 day), evaluation of integrals as functions of parameters (1 day), and finding roots (1 day). A total of seventy faculty members representing sixty-six distinct physics departments from around the country participated in these workshops and provided feedback on the growing manuscript. A few served more formally as beta testers, and several are among those who have continued to use *CPSUP* in the years after its completion. Dissemination also occurred as a consequence of talks and posters—see a full listing in Appendix A.6—presented at national meetings and occasional announcements emailed and/or US-mailed to the chairs of departments offering the bachelor's degree in physics and others on a growing locally maintained mailing list.

5.5 Addressing the Publishing Challenge

Present-day customizable and print-on-demand publishing is not yet capable of providing the microscopic section by section customization that *CPSUP* requires, especially when the number of copies ordered of any particular version is likely to be small (5–20). Until an on-going search for a commercial publisher meets with success, the book is being self-published by the author.[3] With the assistance of TeX, LaTeX, and an assortment of associated pieces of software, the process of producing a PostScript file containing the generic components and the selected software-specific components for any particular version is almost trivially easy. Once all the appropriate LaTeX source files containing the text of the various components (with embedded formatting and indexing commands) have been created and, in addition, a buyer-specific file containing true/false values for the flags that select the components to be included is available, the process involves

- running LaTeX,
- running LaTeX a second time to set the internal cross references and table of contents correctly,
- running LaTeX a third time, especially if insertion of the proper internal references in the second pass causes the pagination to change,[4]
- running `makeindex` to generate the file from which the index will be produced,
- running LaTeX one last time (third or fourth time) to produce an output file that contains the proper index, and
- running `dvips`.

After about five minutes of processor time on a contemporary desktop computer, the PostScript file for a 400–900 page book is in hand!!! That file is then sent electronically to a nearby commercial print shop, whose staff members provide it as input to a fascinating machine that digests the file and produces bound copies as output, all without human intervention. That commercial establishment

[3]Self-publishing has its drawbacks, but one advantage of the approach and the associated on-demand printing is that typos, grammatical infelicities, and unclear passages discovered now and then can be corrected immediately and be right in all subsequent printings.

[4]The system prints a warning during the second pass if a third pass is necessary.

Version	# Institutions	# copies
Class-sized Adoptions		
Maverick versions	4	43
IDL-MAPLE+other components	5	38
IDL-*Mathematica*+other components	5	92
MATLAB-MAPLE+other components	5	39
MATLAB-*Mathematica*+other components	11	106
TOTAL	30	318
Single Examination Copies Sent		
Full	10	10
IDL-MAPLE+other components	7	7
IDL-*Mathematica*+other components	11	11
MATLAB-MAPLE+other components	16	16
MATLAB-*Mathematica*+other components	29	29
TOTAL	73	73

Table 5.5: Summary of Distribution of Self-Published Copies of *CPSUP* from 1 August 2003 to 1 August 2006. Versions contain IDL-MAPLE, IDL-*Mathematica*, MATLAB-MAPLE, or MATLAB-*Mathematica* and various selections from the other options. The few versions containing more than one of IDL and MATLAB and/or more than one of MACSYMA, MAPLE, and *Mathematica* are identified as "maverick versions". In the column labeled '# institutions', institutions to which copies were sent in more than one year are tallied once for each year. Beyond the above-enumerated distribution, seventy copies of the full version (as it existed at the time of each workshop) are in the hands of those who participated in the workshops, and four different institutions have purchased a total of seven copies, mostly of the full version, as library acquisitions.

then ships the completed books to the buyer. The process is economical even for as few as half a dozen copies. Copies can be produced and delivered in about three weeks. Since its essential completion in the summer of 2003, one or another version—see Table 5.5—of *CPSUP* has been adopted for class use at thirty institutions and examination copies, again of one or another version, have been requested by seventy-five individual physics teachers.

5.6 The Future of *CPSUP*

The first edition of *CPSUP* has been essentially complete since late 2003. The search continues for a commercial publisher with the capacity to provide customization economically for small orders. In the meantime, self-publication by the author will continue.

As with most large projects, as deadlines loom the scope is scaled back. *CPSUP* was originally to include chapters on statistical data analysis and curve fitting, partial differential equations, Fourier analysis, and image processing. Chapters on Monte Carlo techniques and examples from thermal and optical physics are candidates for inclusion. Other software packages (particularly OCTAVE, which is a shareware version of MATLAB, MAXIMA, which is a shareware version of the now unavailable MACSYMA, and MathCAD) could defensibly be incorporated as options by including chapters specifically on these packages and by adding sections illustrating the use of these packages in other chapters. And other languages like Java, publishing packages beyond LaTeX, and drawing programs beyond Tgif should perhaps be made available as options.

Beyond the flexibility easily to accommodate a variety of choices of hardware and software, the structure adopted has also the convenient—perhaps even fortuitous—capability of easy expansion. With support from the 2001 W. M. Keck Foundation grant, a step in the direction of a second edition has already been taken with the drafting of at least parts of the chapters that support the course *Computational Physics*. Chapter 13 on finite difference and finite element approaches to partial differential equations, Chapter 14 on the package MUDPACK, which contains FORTRAN solvers that use multigrid techniques to address elliptic partial differential equations in two and three dimensions, and Chapter 15 on MARC/MENTAT, which is a commercial pair of programs for setting up and solving partial differential equations by finite element techniques are well along. As of December, 2006, the generic parts of these chapters are complete, but the software-specific parts exist only for the software packages in use at Lawrence.

As the author moves towards retirement from full-time teaching, he expects to devote more of his efforts to filling in these gaps. Chapters on many other computational topics and on other software packages may well come into being. Further, once the publishing wrinkles have been satisfactorily worked out and the structure of the files has been refined and documented, other authors may be attracted to contributing components on their favorite topics or software packages, so the book may expand to offer as options a wider and wider spectrum of hardware and software and to include topics not originally incorporated and, more particularly, topics that go beyond the knowledge, skill, and/or energy of the initial author. Periodically, reports of progress on these fronts will be posted on the project website at the URL `http://www.lawrence.edu/dept/physics/ccli`.

Appendix A

Computational Physics Laboratory

A.1 A Brief History

In 1987, convinced that the scientific careers of its majors would be significantly enhanced by a broad exposure to computational approaches to problems in physics, the Department of Physics at Lawrence successfully sought support amounting to about $400,000 from the W. M. Keck Foundation, the National Science Foundation, and several vendors to conduct a pilot project designed to nurture both the personal initiative and the individual skills to use sophisticated computational tools intelligently and independently. To this end, we have created the Lawrence Computational Physics Laboratory (CPL), which gives 45 or so physics majors each year (typically 12 seniors, 13 juniors, 20 sophomores) and five faculty members exclusive 24-hour per day access to an impressive collection of computational hardware and software as well as a library of pertinent manuals, text books, and locally prepared documents. In addition, we have engaged in faculty development, and—most importantly—we have embedded numerous computer-based classroom demonstrations and homework exercises in many of our upper-level offerings, thereby encouraging and supporting continued independent use both in our junior/senior courses and in senior-level independent studies. This pilot project has received national attention, being described in several published papers and invited talks (see later section). Its existence served as the basis for convening a small national conference (Summer, 1990) at Lawrence (supported by the Sloan Foundation), and it has stimulated several individual visits to the Lawrence campus.

In 1993, additional funds amounting to about $150,000 were received from the National Science Foundation and the W. M. Keck Foundation to permit addition of 3D graphics capabilities and color printing capabilities to the Computational Physics Laboratory initially equipped by the grants received in 1987 and 1988.

In 1998, grants from Lawrence University allowed us to begin replacing the oldest SGI equipment with up-to-date SGI equipment. This process will be ongoing, two or three older units being replaced each year with state-of-the-art equipment.

In early 2000, a grant of $177,026 (supplemented in 2003 with an additional $3781) from the Educational Materials and Development (EMD) track of the Course, Curriculum and Laboratory Improvement (CCLI) Program of the National Science Foundation provided support for the collection of numerous local instructional documents into a text and the conduct at Lawrence of four week-long summer workshops for physics faculty members from around the United States. The resulting book, titled *Computation and Problem Solving in Undergraduate Physics* (*CPSUP*), is flexible in design. Through the inclusion of components using the selected software packages, the book can be adapted to respect the particular hardware and software available at specific institutions. Details can be found at the project website at the URL `http://www.lawrence.edu/dept/physics/ccli`.

In December, 2001, the Department received a third grant from the W. M. Keck Foundation. Of the $400,000 total grant, $106,853 was allocated to further development of the CPL. The primary objectives of this infusion were to introduce a *required* sophomore course in computation and mechanics, to introduce an elective junior/senior course in computational physics, and to increase the extent to which computational resources are used throughout the physics curriculum at Lawrence. In anticipation of increased use generated by those changes in our curriculum, the grant supported an expansion of the total number of workstations in the laboratory and an upgrading of the server, the existing workstations, and the printers.

In the remainder of this appendix, we enumerate the current spectrum of hardware and the most frequently used pieces of software and list the several papers and presentations that have arisen in the context of developing this resource and writing the text already mentioned.

A.2 Hardware

The first computational physics laboratory, which was constructed in 1988, was equipped with Digital Equipment Corporation (DEC) VAXstations and a VAXserver running VMS. By the early 1990s, VMS was fading and UNIX was ascending as the operating system of choice for scientific workstations and, with outside grant support from the NSF and the W. M. Keck Foundation, we reequipped the CPL with Silicon Graphics (SGI) Indigo workstations and a Challenge S server, all running IRIX, SGI's implementation of the UNIX operating system. Subsequently, these workstations in turn were replaced by SGI O2 and O2+ workstations and an SGI Origin200 server. In January, 2006, we officially replaced the SGI hardware with Hewlett-Packard hardware running the LINUX operating system. Currently, hardware in the CPL includes

- eleven Hewlett-Packard xw9300 workstations, each with a single AMD Opteron 248/2.2GHz 64-bit processor, 1 GB of memory, one 80 GB hard drive, an NVIDIA Quadro FX3400 video card, and 17" flat-screen monitor and running the Fedora Core 4 implementation of the LINUX operating system. Two of these machines are in faculty offices; the remaining nine are in the Computational Physics Laboratory, to which about 50 sophomore, junior, and senior majors each term have 24/7 access.
- a Hewlett-Packard ProLiant DL380 file server with a single Intel XEON 3.20GHz/1MB 32-bit processor, 1GB of memory, four 72GB harddrives (two of which mirror the other two), and one DAT tape drive for backup purposes and running the Red Hat Enterprise 3.x implementation of the LINUX operating system. This server is housed in the server closet that is maintained by personnel in Lawrence's Center for Information Technology (IT), where it is on an uninterruptable power supply.
- a Hewlett-Packard 4200dtn monochrome network PostScript printer with two paper trays and a capability for duplex printing when requested.
- a Tektronix Phaser 350 color network PostScript printer.
- nine SGI O2 or O2+ workstations and an SGI Origin200 server, which have officially been replaced but will remain in use as long as they continue to function. Service contracts are no longer maintained.

The CPL is housed in a single, attractively decorated, quiet, well lighted, and inviting room of about 1200 square feet, to which, because we issue keys, upper-division physics majors have 24-hour access.

Personnel in Lawrence's Department of Instructional Technology Services regularly assist with overall system maintenance, in particular changing the backup tapes and monitoring the overall health of the server, but the bulk of the responsibility for maintenance (installing software upgrades, trouble shooting when system malfunctions occur, ...) lies with the faculty member in the Department who oversees the facility.

A.3 Software

Available software in the Computational Physics Laboratory reflects not only the spectrum of capabilities enumerated in Section 1.1 but also a deliberate focus on professionally-developed, generally useful packages. In addition to operating systems [UNIX, Linux, Windows-XP), windowing systems (X, Windows), system utilities, language compilers (C, C++, FORTRAN), graphics support (IDL, MAPLE, *Kaleidagraph*), spreadsheet (EXCEL), and text editors (xemacs, nedit, notepad), available software includes

- MAPLE (from Waterloo MAPLE Software, Inc.)—for doing algebra and calculus symbolically.
- IDL (Interactive Data Language, from ITT Industries, Inc.)—for processing arrays, producing graphical displays (including animated displays), and processing and displaying images.
- NUMERICAL RECIPES (from Numerical Recipes Software)—FORTRAN and C subroutines for doing numerical analyses.
- ODEPACK (from the Lawrence Livermore library of public-domain software)—FORTRAN subroutines for solving a wide variety of ordinary differential equations, both single equations and (possibly large) systems of equations.
- MUDPACK (from the University Corporation for Atmospheric Research)—FORTRAN subroutines for solving elliptic partial differential equations by multigrid methods.
- SPICE (from the University of California Berkeley)—for designing and analyzing electronic circuits.
- MARC/MENTAT (from MSC Software, Inc.)—for setting up and solving problems in heat flow, structures, elasticity, and electromagnetics with finite element methods.
- TeX and LaTeX (from Stanford University)—for preparing technical manuscripts.

We also have single licenses for MATLAB (from the MathWorks, Inc.) and *Mathematica* (from Wolfram Associates, Inc.).

A.4 The CPL Library

Beyond the hardware and software in the CPL, students have access to a small library of printed materials, including an assortment of software manuals, a selection of books on computational approaches to problems in physics, and notebooks containing about 60 student-written 5–25 page documents detailing computationally based studies undertaken by students at Lawrence. While these documents are still available, many have been superceded by the book *CPSUP* already mentioned.

A.5 Network Connections

All workstations in the CPL are connected to the University network and, through a firewall, have access to the world wide web.

A.6 Publications about the Project

A.6.1 Published Books and Papers

- D. M. Cook, *Solutions to Selected Exercises* to accompany *Computation and Problem Solving in Undergraduate Physics* (Lawrence University Press, Appleton, WI 2004). These solutions have been published electronically and are available to users of the book from a password-protected website.
- D. M. Cook, *Computation and Problem Solving in Undergraduate Physics* (Lawrence University Press, Appleton, WI 2004). Information about this book and details regarding examination copies and orders can be found at the URL `http://www.lawrence.edu/dept/physics/ccli`.
- D. M. Cook, "Computers in the Lawrence Physics Curriculum: Part I", *Computers in Physics* **11** (3; May/Jun), 240–245 (1997); "..., Part II", *Computers in Physics* **11** (4; Jul/Aug), 331–335 (1997).
- D. M. Cook, R. Dubisch, G. Sowell, P. Tam, and D. Donnelly, "A Comparison of Several Symbol Manipulating Programs: Part I", *Computers in Physics* **6**(4; Jul/Aug), 411–420 (1992); "..., Part II", *Computers in Physics* **6**(5; Sep/Oct), 530–540 (1992).
- D. M. Cook (editor), *Computing in Advanced Undergraduate Physics*, the proceedings of a conference held 13–14 June 1990, at Lawrence University. Published in November, 1990, these proceedings contain 19 papers on uses of computers in undergraduate curricula around the country and record also the discussions following each paper. The proceedings were widely distributed to institutions offering bachelors degrees in physics and continue to be occasionally requested.
- D. M. Cook, "Incorporating Uses of Computational Tools in the Undergraduate Physics Curriculum" (lead paper in the above proceedings).
- D. M. Cook, "Computational Exercises for the Upper-Division Undergraduate Physics Curriculum", Comput. Phys. **4**(3; May/June), 308–313 (1990)
- D. M. Cook, "Introducing Computational Tools in the Upper-Division Undergraduate Physics Curriculum", Comput. Phys. **4**(2; Mar/Apr), 197–201 (1990)

A.6.2 Invited Talks and Posters

Professor Cook has presented physics colloquia, invited talks, or invited posters at

- the winter meeting of the AAPT, Seattle, WA (January, 2007);
- (poster) the summer meeting of the AAPT, Syracuse, NY (July, 2006);
- the March meeting of the APS, Montreal, QB (March, 2004);
- the International Conference on Computer Science, San Francisco, CA (May, 2001);
- the Washington meeting of the APS, Washington, DC (April, 2001);

- the winter meeting of the AAPT, San Diego, CA (January, 2001);
- the *Physics Revitalization Conference: Building Undergraduate Physics Programs for the 21st Century*, Arlington, VA (October, 1998);
- the summer meeting of the AAPT, College Park, MD (August, 1996);
- the summer meeting of the AAPT, Boise, ID, (August, 1993);
- the summer meeting of the AAPT, Orono, ME, (August, 1992);
- the Davidson College (NC) Conference on Computational Physics, (October, 1991);
- the spring meeting of the Pacific Northwest Association for College Physics, University of Puget Sound (April, 1991);
- the summer meeting of the AAPT, San Luis Obispo, CA (June, 1989);
- Michigan Technological University (September, 1991);
- University of Wisconsin–Eau Claire (October, 1990);
- Hope College (November, 1989);
- Kansas State University (September, 1989); and
- University of Nebraska (September, 1989).

A.6.3 Contributed Talks and Posters

Professor Cook has presented contributed talks and posters at

- (poster) the summer meeting of the AAPT, Salt Lake City, UT (August, 2005);
- (poster) the summer meeting of the AAPT, Sacramento, CA (July-August, 2004);
- the summer meeting of the AAPT, Sacramento, CA (July-August, 2004);
- the summer meeting of the AAPT, Rochester, NY (July, 2001); and
- the summer meeting of the AAPT, Guelph, ON (July, 2000); and
- the summer meeting of the AAPT, Spokane, WA (July, 1995).

Appendix B

Problems from Assignments in Computational Mechanics

B.1 Problems from Assignment 1

Assignment 1 involves a review and embellishment of kinematics and dynamics of translation and rotation; Newton's laws; impulse, momentum, work, energy, and power; gravitational and electromagnetic forces and friction; and force diagrams. The assignment also includes a tutorial introduction to the Computational Physics Laboratory (CPL) but no computationally based problems are assigned.

•• **Sample 1.1:** Work your way through the "whirlwind tutorial" contained in Section 2 of the *Lawrence Local Guide*. This tutorial helps you determine your user name and initial password, leads you through the login process, helps you change your password, and then guides you through a few exercises designed to familiarize you with the rudimentary capabilities of software available in the CPL. There is nothing to *hand in* for this "problem", but it must be done by the due date for this assignment, since subsequent assignments will assume that you are already familiar with the contents of this tutorial. Note also the schedule when a consultant will be in the CPL to offer assistance.

•• **Sample 1.2:** A hemisphere of radius a and total mass M uniformly distributed throughout its volume with density $\rho = M/(\frac{2}{3}\pi a^3)$ is located with its center at the origin and its flat surface in the xy plane. (a) Find the position of the center of mass of this hemisphere. (b) Calculate the moment of inertia tensor with respect to the x, y, and z axes. *Hint*: Use spherical coordinates, in which $x' = r' \sin\theta' \cos\phi'$, $y' = r' \sin\theta' \sin\phi'$, $z' = r' \cos\theta'$, and $dm' = \rho\, dv' = \rho\, r'^2 \sin\theta'\, dr'\, d\theta'\, d\phi'$.

•• **Sample 1.3:** The position vector $\mathbf{r}(\mathrm{t})$ of a particle or mass m moving in a circle is given by

$$\mathbf{r} = R\cos\omega t\,\hat{\mathbf{i}} + R\sin\omega t\,\hat{\mathbf{j}}$$

where R and ω are constants. If the particle has mass m, find as functions of time (a) the angular momentum L about the point $\mathbf{r}(0)$, (b) the force F, and (c) the torque N about the point $\mathbf{r}(0)$. Then, (d) verify that the angular momentum theorem $dL/dt = N$ is satisfied.

•• **Sample 1.4:** Consider the spool of mass M, inner radius r_i, outer radius r_o, and moment of inertia I about its axis. As shown in Fig. B.1, a force F is applied by pulling on a string wound on the spool. (a) Assuming that the spool rolls without slipping across the floor, show that the

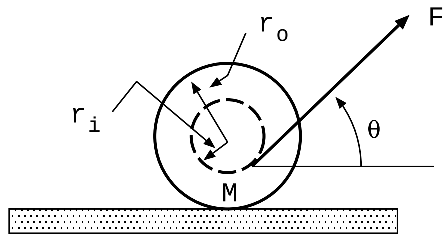


Figure B.1: Systems for Sample Problem 1.4.

acceleration a —measured positive to the right—of this spool and, in terms of that acceleration, the frictional force f are given by

$$a = \frac{T(r_o \cos\theta - r_i)}{Mr_o(1 + I/(Mr_o^2))} \quad ; \quad f = T\cos\theta - Ma$$

(b) Determine and defend conditions on θ such that the spool will move to the left. ... to the right. (c) Show that there is an angle θ for which the spool remains at rest. (d) At this critical angle, find the maximum T for equilibrium to be maintained. Assume a coefficient of static friction μ_s and remember that the static frictional force is constrained by $f \leq \mu_s N$.

•• **Sample 1.5:** Suppose the total mass M of a planet of radius R is uniformly distributed throughout the volume of the planet so that the density (mass per unit volume) of the planet is $\rho = M/(\frac{4}{3}\pi R^3)$. Show that the force of attraction of this planet for a point particle of mass m located *outside* the planet at a distance z from the center of the planet is directed toward the center of the planet and has magnitude GMm/z^2, i.e., show that the force exerted on the particle in these circumstances can be computed by supposing that the planet is a point particle of mass M located at the center of the planet. *Hint*: Choose a coordinate system whose origin is at the center of the planet and whose z axis is directed from the center of the planet towards the particle so that $\mathbf{r} = z\,\hat{\mathbf{k}}$. In that coordinate system, a mass element would be located at $\mathbf{r}' = r'\sin\theta'\cos\phi'\,\hat{\mathbf{i}} + r'\sin\theta'\sin\phi'\,\hat{\mathbf{j}} + r'\cos\theta'\,\hat{\mathbf{k}}$ and have mass $dm' = \rho\,dv' = \rho\,r'^2\sin\theta'\,dr'\,d\theta'\,d\phi'$. With an element of shrewdness, the resulting integral over the planet doable. *Optional*: Redo the calculation assuming that the observation point is *inside* the planet, i.e., that $z < R$.

B.2 Problems from Assignment 2

In doing Assignment 2, students spend much of their time at the computer learning the basic capabilities of IDL and Tgif and doing exercises that involve, particularly, graphical visualization of assorted functions. They also learn that Newton's laws generate differential equations and deduce those differential equations for several physical systems.

•• **Sample 2.1:** Consider two circular disks, each of radius R, located with their centers on the z axis such that their planes are parallel to the xy plane. Let the first disk have its center at the point $(0, 0, b/2)$ and the second at the point $(0, 0, -b/2)$. If the top disk carries a uniform, constant charge density σ and the bottom disk carries a uniform, constant charge density $-\sigma$, the electrostatic potential at the point $(0, 0, z)$ is given by

$$V(z) = \frac{\sigma}{2\epsilon_0}\left[\sqrt{R^2 + \left(z - \frac{b}{2}\right)^2} - \left|z - \frac{b}{2}\right| - \sqrt{R^2 + \left(z + \frac{b}{2}\right)^2} + \left|z + \frac{b}{2}\right|\right]$$

Obtain graphs of $V(z)/(\sigma R/2\epsilon_0)$ versus z/R for various values of b/R and write a paragraph describing these graphs. *Hint*: Remember the IDL function `abs`.

•• **Sample 2.2:** The Planck radiation law gives the expression

$$u(\lambda, T) = \frac{8\pi ch}{\lambda^5} \frac{1}{e^{ch/(\lambda kT)} - 1}$$

for the distribution of energy in the radiation emitted by a black body. Here, c is the speed of light, h is Planck's constant, k is Boltzmann's constant, λ is the wavelength of the radiation, and T is the absolute temperature. *Using appropriate dimensionless units*, plot this function (a) as a function of λ for several T and (b) as a surface over the λT-plane. Write a paragraph about the way the peak changes in position, height, and width as T changes. *Hint*: Choose a reference wavelength λ_0 arbitrarily and recast the expression in terms of the dimensionless variable $\overline{\lambda} = \lambda/\lambda_0$. Then, note that $T_0 = ch/(\lambda_0 k)$ has the dimensions of temperature and re-express the temperature T in terms of the dimensionless quantity $\overline{T} = T/T_0$. (You might find it informative to evaluate T_0 for $\lambda_0 = 550$ nm.)

B.3 Problems from Assignment 3

Assignment 3 is particularly long and extends over two weeks. It covers the topics identified for weeks 3 and 4 in Table 4.1 and has only limited incorporation of the computer. It is followed by the first hour examination. (See Appendix C.)

•• **Sample 3.1:** Find the minimum velocity of impact of a projectile on the surface of the moon and the speed with which the projectile must be launched upward from the earth if it is to arrive at the moon with this minimum velocity. *Hint*: Sketch a graph of the potential energy of the projectile along a line from the earth to the moon, perhaps even use IDL to generate a careful graph of that function.

•• **Sample 3.2:** The Lennard-Jones potential energy $U_{LJ}(x)$ is important in chemical bonding theory and is given by

$$U_{LJ} = 4\epsilon\left(\frac{\sigma^{12}}{x^{12}} - \frac{\sigma^6}{x^6}\right) \quad \text{or} \quad \frac{U_{LJ}}{\epsilon} = 4\left(\frac{1}{\bar{x}^{12}} - \frac{1}{\bar{x}^6}\right)$$

where ϵ and σ are constants and $\bar{r} = r/\sigma$. (a) Sketch a graph of this potential energy. (b) Use IDL to obtain a careful graph of $U_{LJ}(x)/\epsilon$ versus x/σ. (c) Locate any equilibrium points, (d) determine which ones are stable, and (e) find the frequency of small oscillations about about any equilibrium point that is stable.

•• **Sample 3.3:** The equations of motion for a projectile moving in the xz plane in air under the downward gravitational attraction of the earth and subject to a linear viscous damping force are

$$m\frac{d^2x}{dt^2} = -b\frac{dx}{dt} \qquad ; \qquad m\frac{d^2z}{dt^2} = -mg - b\frac{dz}{dt}$$

(a) Show that

$$x(t) = \frac{mv_{x0}}{b}\left(1 - e^{-bt/m}\right) \qquad ; \qquad z(t) = \left(\frac{m^2g}{b^2} + \frac{mv_{z0}}{b}\right)\left(1 - e^{-bt/m}\right) - \frac{mg}{b}t$$

if the projectile starts at the origin at $t = 0$ with an initial velocity $\mathbf{v}(0) = v_{x0}\,\hat{\mathbf{i}} + v_{z0}\,\hat{\mathbf{k}}$. (b) Show that the highest altitude reached by this projectile is given by

$$z_{\max} = \frac{mv_{z0}}{b} - \frac{m^2g}{b^2}\ln\left(1 + \frac{bv_{z0}}{mg}\right)$$

Hint: The highest point occurs when $v_z(t) = 0$. (c) Expand this result for $z_{\rm max}$ in a power series in b, keeping terms up to first order in b, and verify that the zeroth order term gives the correct result in the absence of damping. Note the expansion $\ln(1+x) = x - x^2/2 + x^3/3 + \cdots$, which is valid when $x \ll 1$.

•• **Sample 3.4:** A object of mass m passes through $x = 0$ at $t = 0$ with a positive velocity v_0. From that point, the object experiences only a velocity-dependent force that is given either by (a) $F = -b\dot{x}$ or (b) by $F = -c\dot{x}^2$. For each case, find $v(x)$, $v(t)$, and $x(t)$ and then comment on the limits of each of these expressions as t becomes large.

•• **Sample 3.5:** Consider a system of two identical blocks of mass m moving along a straight line on a horizontal frictionless surface. Let each block be connected to the wall at its end of the line by a spring of constant k and let the blocks be connected to each other with a spring of constant k'. (a) Find the normal modes of oscillation, the natural frequencies of those modes, and the normal coordinates for the system; (b) draw graphs of the two natural frequencies (in units of $\omega_0 = \sqrt{k/m}$ versus the strength of the coupling spring (in units of k'/k; (c) find $x_1(t)$ and $x_2(t)$ explicitly if $x_1(0) = x_{10}$ and $x_2(0) = 0$, and (d) use IDL to draw graphs of x_1/x_{10} and x_2/x_{10} versus $\omega_0 t$ for several different values of k'/k, carrying your graphs far enough in time to embrace 20 or 30 cycles of motion at the frequency ω_0.

B.4 Problems from Assignment 4

Assignment 4 is devoted to a study of central forces and the planetary problem. This assignment also introduces students to LaTeX, and students are expected to use LaTeX to prepare their solutions to a couple of the problems on this and all subsequent assignments.

•• **Sample 4.1:** Consider a particle moving in a circular orbit under the inverse square gravitational force, for which $f(\rho) = -GMm/\rho^2$. (a) Show that the period of this motion is given by $T = 2\pi\sqrt{\rho_{\rm eq}^3/GM}$. (b) Show that the the speed of the particle in its orbit is given by $v_{\rm tan} = \sqrt{GM/\rho_{\rm eq}}$. (c) Suppose the particle is orbiting the earth, whose radius is R_e. Show that these relationships reduce to

$$T = 2\pi\sqrt{\frac{R_e}{g}}\left(\frac{\rho_{\rm eq}}{R_e}\right)^{3/2} \quad ; \quad v_{\rm tan} = \sqrt{gR_e}\sqrt{\frac{R_e}{\rho_{\rm eq}}}$$

where g is the acceleration of gravity on the earth. (d) Find expressions for the period $T^{\rm graze}$ and the orbital speed $v_{\rm tan}^{\rm graze}$ for a particle whose orbit grazes the surface of the earth, and then determine these quantities numerically, expressing the period both in seconds and in hours and the speed both in meters per second and in miles per hour. (e) Find the radius of the orbit whose period is 24 hours and the speed of the particle in that orbit, expressing the first as a numerical multiple of R_e and the second as a numerical multiple of $v_{\rm tan}^{\rm graze}$. (f) Use IDL to obtain careful graphs of $T/T^{\rm graze}$ and $v_{\rm tan}/v_{\rm tan}^{\rm graze}$ versus $\rho_{\rm eq}/R_e$.

•• **Sample 4.2:** Explore the motion of a particle of mass m when it moves under the influence of the potential energy $U(\rho) = K\rho^4$, where K is a positive constant. Determine (a) the energy and angular momentum of a circular orbit of radius a; (b) the period of that special orbit; (c) and the period of small radial oscillations about that special orbit.

•• **Sample 4.3:** Using the orbital equation, find the central force necessary to produce an elliptical orbit with the force center at the center of the ellipse. *Hints*: In Cartesian coordinates, the equation of an ellipse with its center at the origin is $(x/a)^2+(y/b)^2 = 1$. Recognizing that $x = \rho\cos\phi$

and $y = \rho \sin\phi$, begin by showing that this ellipse is described by the equation $u^2 = A\cos^2\phi + B\sin^2\phi$ in polar coordinates. Here, $A = 1/a^2$, $B = 1/b^2$, and $u = 1/\rho$. Answer: $f(\rho) = K\rho$, where K is a constant.

•• **Sample 4.4:** Show that the eccentricity ϵ, the square of the angular momentum L, and the energy E for an elliptical orbit in an inverse square force $F = -\alpha/\rho^2$ are given in terms of the perigee ρ_p and apogee ρ_a by

$$\epsilon = \frac{\rho_a - \rho_p}{\rho_a + \rho_p} \quad ; \quad L^2 = 2m\alpha\frac{\rho_a\rho_p}{\rho_a + \rho_p} \quad ; \quad E = -\frac{\alpha}{\rho_a + \rho_p}$$

B.5 Problems from Assignment 5

Assignment 5 provides an introduction to the general capabilities of MAPLE and then addresses the use of MAPLE to solve ordinary differential equations.

•• **Sample 5.1:** The Legendre polynomials $P_n(x)$, which are valid and useful over the interval $-1 \le x \le 1$, can be defined in many ways. They emerge as the coefficients in the Taylor expansion of the generating function

$$g(x,t) = \frac{1}{\sqrt{1 - 2xt + t^2}} = \sum_{n=0}^{\infty} P_n(x)\, t^n$$

Alternatively, they can be determined from the recursion relationship

$$(2n+1)\, x\, P_n(x) = (n+1)\, P_{n+1}(x) + n\, P_{n-1}(x)$$

provided we include the first two $P_0(x) = 1$ and $P_1(x) = x$ to get started. Yet again, they can be found from application of multiple differentiation as implied by Rodrigues' formula

$$P_n(x) = \frac{1}{2^n\, n!}\frac{d^n}{dx^n}\Big((x^2 - 1)^n\Big)$$

a. Use the generating function and MAPLE's capabilities for evaluating Taylor series to find the first half-dozen Legendre polynomials, extracting each as an expression bound to a variable.

b. Start by binding the value 1 to P[0] and the value x to P[1]. Then, using the recursion relationship, find the next several Legendre polynomials.

c. Find the first half-dozen Legendre polynomials by using the command `diff` to evaluate Rodrigues' formula. *Hint*: You might find that using a loop would simplify your approach.

d. Be clever and, using either matrices or loops constructed in MAPLE, find the values of *all* of the integrals

$$\int_{-1}^{1} P_n(x)\, P_m(x)\, dx$$

where n and m take on independently the values 0, 1, 2, 3, 4, 5. (There are 36 integrals to be evaluated. Try to be efficient in your coding, and remember the command `map`, which will be useful in constructing a single statement that evaluates the integral of each element in a multi-element structure.)

e. Within MAPLE, obtain graphs of the first six Legendre polynomials over the interval $-1 \le x \le 1$.

f. It is known that a function $f(x)$ defined over the interval $-1 \leq x \leq 1$ can be expanded in a series of Legendre polynomials of the form $f(x) = \sum a_n P_n(x)$ where the coefficients a_n are given by

$$a_n = \frac{2n+1}{2} \int_{-1}^{1} f(x) P_n(x) \, dx$$

Find the first six coefficients for the expansion of the function $f(x) = 0$ when $-1 < x < 0$ and $f(x) = 1$ when $0 < x < 1$. Then, construct the (partial) series representing this function and obtain a graph of that approximation to compare with the graph of the original function.

g. MAPLE actually knows quite a bit about many of the important special functions of mathematical physics. In particular, the package `orthopoly` can be loaded with the command `with(orthopoly)` and is described fully in the MAPLE manuals. Take a look at that documentation and then use the function `P` in that package to determine the first several Legendre polynomials.

•• Sample 5.2: Using MAPLE, find complete (symbolic) solutions to each of the following problems, and use MAPLE also to verify that the solutions you obtain actually *do* satisfy the original ODE and initial conditions.

a. $\dfrac{d^2x}{dt^2} = a$, $x(0) = x_0$, $v(0) = v_0$, where a is constant, i.e., find position as a function of time for a particle moving under the action of a constant force and launched with arbitrary initial conditions.

b. $m\,\dfrac{d^2x}{dt^2} = -eE_0 \cos(\omega t + \theta)$, $x(0) = x_0$, $v(0) = v_0$, i.e., find position as a function of time for a charged particle moving under the action of a sinusoidal force and launched with arbitrary initial conditions.

c. $m\,\dfrac{d^2x}{dt^2} = -mg + b\left(\dfrac{dx}{dt}\right)^2$, $x(0) = 0$, $v(0) = 0$, i.e., find position as a function of time for a particle released from rest at the origin and allowed to fall freely under the action of gravity and a viscous retarding force proportional to the *square* of the speed.

d. the differential equations for $x(t)$ and $z(t)$ in P4.50.[1]

•• Sample 5.3: Consider a system of two objects of different masses m_1 and m_2 connected by a spring of constant k. Suppose the blocks are constrained to move along a straight line. Measuring from an arbitrarily selected origin on that line, let the coordinates of the particles be x_1 and x_2, respectively. The equations of motion for this system are

$$m_1 \frac{d^2x_1}{dt^2} = k(x_2 - x_1) \quad ; \quad m_2 \frac{d^2x_2}{dt^2} = -k(x_2 - x_1)$$

Let the system be put into motion with arbitrary initial conditions

$$x_1(0) = x_{10} \quad ; \quad x_2(0) = x_{20} \quad ; \quad \frac{dx_1(0)}{dt} = v_{10} \quad ; \quad \frac{dx_2(0)}{dt} = v_{20}$$

Using MAPLE, solve this initial-value problem for $x_1(t)$ and $x_2(t)$ and then examine the behavior of the particular quantities

$$X(t) = \frac{m_1 x_1(t) + m_2 x_2(t)}{m_1 + m_2} \qquad \text{and} \qquad Y(t) = x_2(t) - x_1(t)$$

which are, respectively, the position of the center of mass of the system and the position of the second block relative to the first block.

[1] P4.50 is the problem presented in this appendix as Sample 3.3.

B.6 Problems from Assignment 6

Assignment 6 deals with the numerical solution of the ordinary differential equations that appear in classical mechanics.

•• **Sample 6.1:** In a previous problem,[2] we found that the potential

$$U(x) = -U_0 \frac{a^2(a^2+x^2)}{8a^4+x^4} \qquad \text{or} \qquad \frac{U(x)}{U_0} = -\frac{1+\overline{x}^2}{8+\overline{x}^4}$$

where $\overline{x} = x/a$ admits a variety of motions (bound motion in either the left or the right well when $-\frac{1}{4} \leq E/V_0 \leq -\frac{1}{8}$; bound motion over the whole well when $-\frac{1}{8} \leq E/V_0 \leq 0$; unbound motion when $E/V_0 > 0$). Find the equation of motion for a particle in this well, cast it in a suitable dimensionless form, and then explore each of the different types of motion possible. Be sure to look both at graphs of x and $v = dx/dt$ versus t *and*—especially for the periodic motions—at the phase plane plots, v versus x—all in suitable dimensionless units. It might be interesting to examine period as a function of energy for this oscillator. Write several paragraphs describing and presenting evidence for your discoveries. *Hint*: Perhaps a suitable dimensionless time would be $\bar{t} = \omega_0 t$, where ω_0 is the frequency of small amplitude oscillations when the particle is confined to one side of the well.

•• **Sample 6.2:** Explore the behavior of the Van der Pol oscillator described in dimensionless form by the equation

$$\frac{d^2\overline{x}}{d\bar{t}^2} = \frac{d\overline{x}}{d\bar{t}}(1-\overline{x}^2) - \overline{x}$$

obtaining graphs of position versus time, velocity versus time, and velocity versus position (the phase-plane trajectory), each for several different initial conditions. Convince yourself that the final, steady-state path in the phase plane is independent of the initial conditions.

B.7 Problems from Assignment 7

Assignment 7 introduces the use of MAPLE for symbolic and IDL for numerical evaluation of integrals and then applies those capabilities to several physical contexts, not all of them originating in classical mechanics.

•• **Sample 7.1:** Consider a surface in the xy plane having uniform mass density σ and having the shape of a cardioid given in polar coordinates by the function $r(\phi) = a(1-\cos\phi)$. Using symbolic integration, find (a) the center of mass of this object, (b) the moment of inertia tensor of this object about the x, y, and z axes, and (c) the radius of gyration about the z axis. *Hints*: The (vector) position $\mathbf{R}_{cm}$ of the center of mass and the ij element of the 3×3 moment of inertia tensor I are defined by

$$\mathbf{R}_{cm} = \frac{\int \mathbf{r}\,dm}{\int dm} \quad ; \quad I_{ij} = \int \left[(x_1^2+x_2^2+x_3^2)\delta_{ij} - x_i x_j\right] dm$$

where x_1, x_2, and x_3 symbolize x, y, and z, respectively; δ_{ij} is the Kronecker delta, which has the value 1 when $i = j$ and the value 0 otherwise; and the radius of gyration is defined in the text.

•• **Sample 7.2:** The n-th order Bessel function can be defined by the integral

$$J_n(x) = \frac{1}{\pi}\int_0^\pi \cos(n\theta - x\sin\theta)\,d\theta$$

[2] This problem is not included in this appendix.

By evaluating this integral numerically as a function of x for different values of n, obtain graphs of $J_0(x)$, $J_1(x)$, and $J_2(x)$ over the range $0 \leq x \leq 10$.

•• Sample 7.3: A circular current loop of radius a lies in the xy-plane with its center at the origin and carries a current I' counterclockwise as viewed from a point on the positive z axis. The magnetic field at a point in the xz plane is given by

$$\frac{\mathbf{B}(x,z)}{\mu_0 I'/2\pi a} = a^2 \int_0^\pi \frac{z\cos\phi'\,\hat{\mathbf{i}} + (a - x\cos\phi')\,\hat{\mathbf{k}}}{[x^2+z^2+a^2-2ax\cos\phi']^{3/2}}\,d\phi'$$

Explore both components of this magnetic field numerically as functions of x/a for various values of z/a, including $z/a = 0.0$ (which will require some creativity for dealing with the point $x/a = 1.0$, at which the integrand diverges at one point in the range of the integration variable).

Appendix C

Examinations from Computational Mechanics

C.1 Hour Examination #1 – 1 February 2006

Physics 225: Computational Mechanics **Hour Examination 1** 1 February 2006

This examination is a closed book examination, but calculators, integral tables, and *CPSUP* are allowed. Answer all questions, and *be sure to include enough narrative with each solution so that I can understand easily what you were thinking as you solved the problem.* The examination is to be completed by the end of the class period. Each of the three questions will receive the same weight in the grading. The following information may—or may not—be useful.

$$U(\mathbf{r}) = U(\mathbf{r}_{\text{ref}}) - \int_{\mathbf{r}_{\text{ref}}}^{\mathbf{r}} \mathbf{F}(\mathbf{r}') \bullet d\mathbf{r}' \quad ; \quad v_{\tan} = \omega r \quad ; \quad N = F_{\tan} r$$

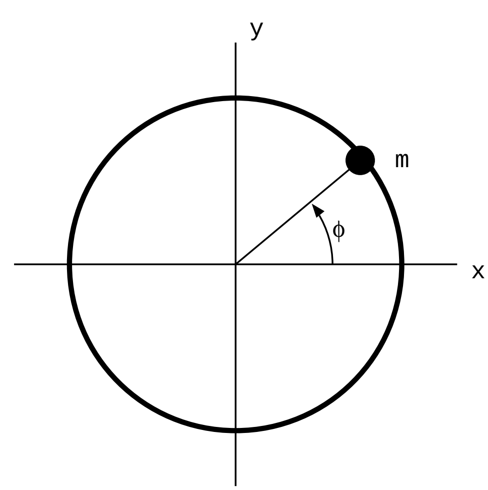
$$I\alpha = \frac{dL}{dt} = N \quad ; \quad \alpha = \frac{d\omega}{dt} = \frac{d^2\phi}{dt^2} \quad ; \quad \omega = \frac{d\phi}{dt} \quad ; \quad L = I\omega \quad ; \quad K_{\text{rot}} = \frac{1}{2} I\omega^2$$

QUESTION 1. Torque Depending Only on Time

An object of mass m moves in a circular path of radius d lying in the xy plane and centered at the origin. The object experiences a sinusoidally varying torque given by $N(t) = N_0 \sin \omega_0 t$. Thus, with $\phi(t)$ being the angular position of the object at time t, the equation of motion is

$$I \frac{d^2\phi}{dt^2} = N_0 \sin \omega_0 t$$

where $I = md^2$ is the moment of inertia of the object about the z axis. Suppose that, at $t = 0$, the object is at rest $[\omega(0) = d\phi/dt|_{t=0} = 0]$ at the angular position for which $\phi(0) = 0$, i.e., at rest at the point $\mathbf{r} = d\,\hat{\mathbf{i}}$ on the positive x axis.



(a) By solving the above differential equation subject to the given initial conditions, show that

i. $\omega(t) = \dfrac{d\phi}{dt} = \dfrac{N_0}{I\omega_0}\Big(1 - \cos\omega_0 t\Big)$ and ii. $\phi(t) = \dfrac{N_0}{I\omega_0^2}\Big(\omega_0 t - \sin\omega_0 t\Big)$

(b) Show that the power input $P(t)$ to this object by the applied torque is given by

$$P(t) = \frac{N_0^2}{I\omega_0}\sin\omega_0 t\Big(1 - \cos\omega_0 t\Big)$$

Hint: Convert the expression $P(t) = \mathbf{F} \bullet \mathbf{v} = F_{\tan}(t)\, v_{\tan}(t)$ into the descriptive terms appropriate to rotation.

(c) Show that the result in part (b) is dimensionally correct, i.e., that the quantity $N_0^2/(I\omega_0)$ has the units J/s (Joules/second).

QUESTION 2. Conservation of Energy

Suppose a particle of mass m moves along the *positive* x axis under the action of an *attractive* force that varies inversely as the *fourth* power of its position from the origin, i.e.,

$$\mathbf{F} = -F_0 \frac{a^4}{x^4}\,\hat{\mathbf{i}}$$

where a—a length—and F_0—a force—are *positive* constants. Suppose that, initially, the particle is projected toward increasing x with speed v_0 from the point $x = a$.

(a) Declaring that the potential energy shall be zero at $x = \infty$, show that the potential energy associated with this force is given by

$$U(x) = -\frac{F_0 a^4}{3x^3}$$

(b) Write out the IDL coding that will generate the graph in Fig. C.1 showing $U(x)/(F_0 a)$ versus x/a. Pay attention not only to the curve but also to the labels, ranges on the axes, etc. *Note*: I am asking only for coding that will produce the graph on the screen, not for coding to produce printed hard copy of the graph.

(c) With what minimum speed should the particle be projected from $x = \frac{1}{2}a$ if it is to escape altogether from the influence of the force? *Hint*: Apply conservation of energy.

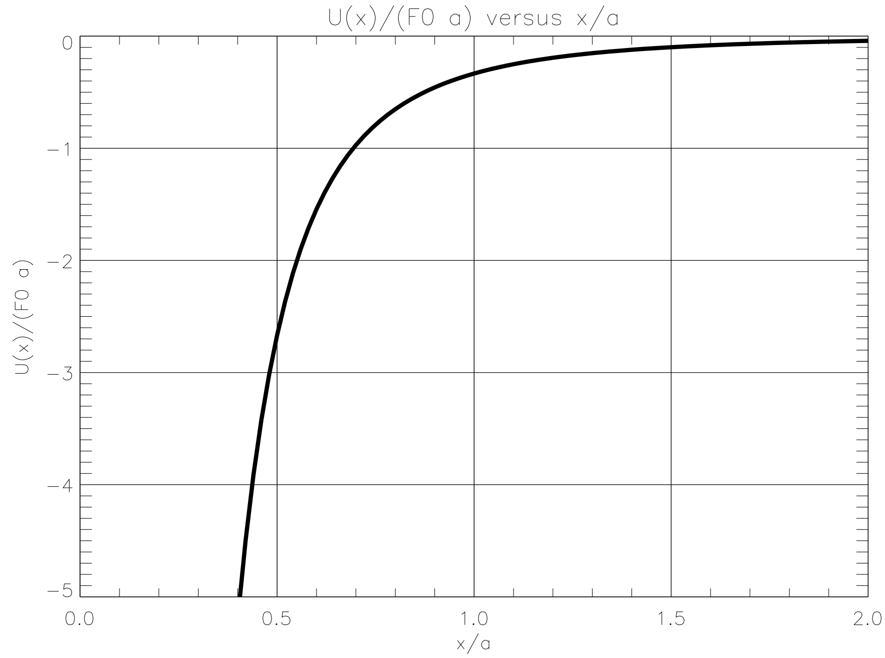
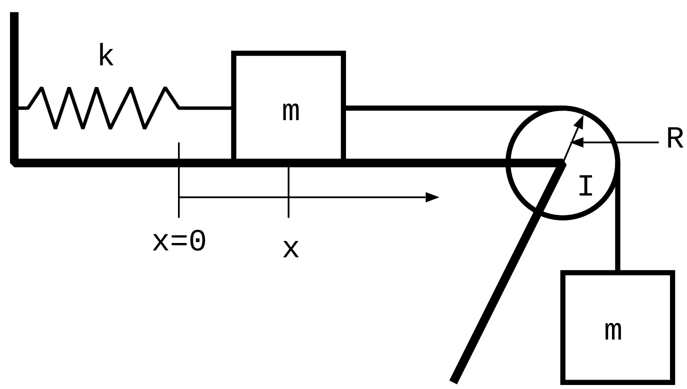


Figure C.1: Figure for Question 2, Part (b).

QUESTION 3. Dynamics of a Non-trivial System



A system consists of a spring of constant k and two blocks, each of mass m. One end of the spring is attached to a wall and the other end is attached to one of the blocks, which slides without friction on a horizontal table. A massless, inextensible, and perfectly flexible rope runs from the other side of this first block, over a pulley of radius R and moment of inertia I about its axis of rotation, and to the second block, which hangs from the rope over the pulley and edge of the table. Let the position of the block on the table be measured from its location when the spring is neither stretched nor compressed, ignore friction in the bearings of the pulley, and assume the rope and pulley move together without slipping.

(a) Draw and label a complete force diagram for each of the three main objects in this system (each block and the pulley).

(b) Describe *briefly* in words each force to which you give a symbol on the diagram.

Given sufficient time, you could write down the consequences of Newton's second law, identify all necessary auxiliary conditions, and manipulate them to conclude that the primary equation of motion for this system is

$$m_{\text{eff}} \frac{d^2x}{dt^2} + kx = mg \tag{C.1}$$

where $m_{\text{eff}} = 2m + I/R^2$. (*Note*: I did *not* ask you to deduce this equation.)

(c) Starting with Eq. (C.1), and assuming that $x(0) = x_0$ and $v(0) = v_0$, show that the quantity

$$\frac{1}{2} m_{\text{eff}} v^2 + \frac{1}{2} kx^2 - mgx$$

is conserved. *Hint*: Remember that $d^2x/dt^2 = v\, dv/dx$.

REMINDER: Pledge.

C.2 Hour Examination #2 – 1 March 2006

Physics 225: Computational Mechanics **Hour Examination 2** 1 March 2006

This examination has two parts. Part I is closed book, but calculators and integral tables are allowed; it is to be completed by the end of the class period. Part II, which will be given to you when you turn in Part I, is open book but closed classmate (and closed other physics majors). To complete Part II, you will need to use the facilities of the CPL. Part II is to be turned in no later than 5:00 PM on Friday, 3 March.

Answer all questions, and—both in Part I and in Part II—*be sure to include enough narrative with each solution so that I can understand easily what you were thinking as you solved the problem.* The weight to be given each question in the grading is shown with the question. In total, the in-class portion, which contains two questions, will count 40% and the out-of-class portion, which also contains two questions, will count 60%.

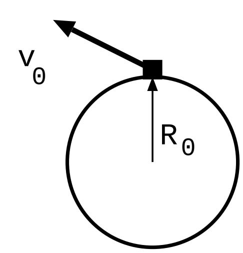
PART I: IN-CLASS CLOSED-BOOK PORTION

Possibly useful information:

$$U = -\frac{Gm_1m_2}{|\mathbf{r}_2 - \mathbf{r}_1|} \quad ; \quad |\mathbf{F}| = \frac{Gm_1m_2}{|\mathbf{r}_2 - \mathbf{r}_1|^2}$$

QUESTION 1: Motion near an Asteroid (weight=20%)

Suppose an astronaut of mass m is located initially at the surface of a spherically symmetric asteroid of mass M and radius R_0. Suppose, further, that she is capable of launching herself from a point on the surface of the asteroid with a velocity of magnitude v_0 in any direction.



(a) Apply conservation of energy to show that the escape velocity from this asteroid is given by $v_{\text{esc}} = \sqrt{2GM/R_0}$.

(b) By matching centripetal to gravitational forces, show that, if the astronaut launches herself along a tangent to the surface of the asteroid, the particular value of v_0 that will launch her into a *circular* orbit of radius R_0—i.e., a grazing orbit—is given by $v_{\text{circle}} = v_{\text{esc}}/\sqrt{2}$.

(c) Suppose now that the astronaut's launch speed satisfies $v_{\text{circle}} < v_0 < v_{\text{esc}}$, so that she can launch herself into an elliptical orbit by "jumping" at speed v_0 along a path that is tangent to the asteroid's surface at the point of launch. Find an expression for the eccentricity ϵ of the astronaut's orbit. Your answer may involve v_0, v_{circle}, and R_0 but not G, m, and M. *Hints*: (1) Remember that the orbit in an inverse-square gravitational force is given by

$$r(\phi) = R_0 \frac{v_0^2/v_{\text{circle}}^2}{1 + \epsilon \cos\phi}$$

where ϕ is measured from the line from the center of the asteroid to the perigee, and (2) the astronaut's initial point is at the perigee of the orbit.

QUESTION 2: Orbits in Inverse Cube Force (weight=20%)

Consider a particle of mass m moving in the xy plane with position and velocity given in Cartesian coordinates by

$$\mathbf{r} = x\,\hat{\mathbf{i}} + y\,\hat{\mathbf{j}} \quad ; \quad \mathbf{v} = v_x\,\hat{\mathbf{i}} + v_y\,\hat{\mathbf{j}}$$

Suppose that the particle moves under the influence of an attractive inverse cube force so the equation of motion—Newton's second law— is given by

$$m\frac{d\mathbf{v}}{dt} = m\frac{d^2\mathbf{r}}{dt^2} = \mathbf{F} = -\frac{K}{\rho^3}\,\hat{\mathbf{r}} = -\frac{K}{(x^2+y^2)^{3/2}}\,\hat{\mathbf{r}}$$

In these expressions, K is a positive constant. In a coordinate system whose origin coincides with the force center, whose x axis runs from the force center through the initial position of the particle, and whose y axis lies in the plane of the orbit, the initial position of the particle has only an x component but the initial velocity may have both x and y components. To set a notation, take

$$\mathbf{r}(0) = a\,\hat{\mathbf{i}} \quad ; \quad \mathbf{v}(0) = \frac{d\mathbf{r}}{dt}(0) = v_{x0}\,\hat{\mathbf{i}} + v_{y0}\,\hat{\mathbf{j}}$$

where a, v_{x0} and v_{y0} are (known) constants.

(a) Show that the angular momentum $\mathbf{L}$ of this particle about the origin is conserved. *Hint*: Evaluate $d\mathbf{L}/dt$ where $\mathbf{L} = \mathbf{r} \times m\mathbf{v}$.

(b) Find the x and y components of the equation of motion and then, introducing the dimensionless coordinates $\overline{x} = x/a$ and $\overline{y} = y/a$, show that

$$\frac{d^2\overline{x}}{d\overline{t}^2} = -\frac{\overline{x}}{(\overline{x}^2+\overline{y}^2)^2} \quad ; \quad \frac{d^2\overline{y}}{d\overline{t}^2} = -\frac{\overline{y}}{(\overline{x}^2+\overline{y}^2)^2}$$

Along the way, of course, you will have to deduce the relationship between t and $\overline{t}$.

REMINDER: Pledge.

PART II: OUT-OF-CLASS OPEN-BOOK PORTION

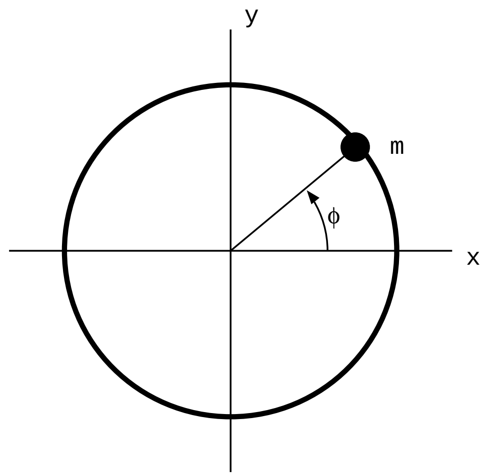
In this portion of the examination, you may consult any printed or on-line materials that are available to you but consultations with your classmates and other physics majors are off-limits. This portion is to be completed and handed in by 5:00 PM on Friday, 3 March.

QUESTION 3: Symbolic Approach with MAPLE (weight=30%)

An object of mass m moves in a circular path of radius d lying in the xy plane and centered at the origin. The object experiences a sinusoidally varying torque given by $N(t) = N_0(1-\cos\omega_0 t)$. Thus, with $\phi(t)$ being the angular position of the object at time t, the equation of motion is

$$I\frac{d^2\phi}{dt^2} = N_0(1-\cos\omega_0 t)$$

where $I = md^2$ is the moment of inertia of the object about the z axis. Suppose that, at $t = 0$, the object is at the angle $\phi(0) = 0$ and is at rest, i.e., it has angular velocity $\omega(0) = d\phi/dt|_{t=0} = 0$.



Using MAPLE,

(a) Solve this equation subject to the given initial conditions to find $\phi(t)$ and $\omega(t) = d\phi(t)/dt$.

(b) Verify that the solution you have obtained indeed satisfies *both* the original differential equation *and* the initial conditions imposed on it.

(c) Remembering that the power input to this system is given by $P(t) = N(t)\,\omega(t)$, find an expression for $P(t)$ and plot a graph of $P(t)/(N_0^2/I\omega_0)$ versus $\omega_0 t$.

Submit your solution to this question by printing the MAPLE notebook in which you work the solution out. Be sure in your submitted output that your argument moves directly and smoothly from the starting point to the desired end results, that your notebook reads linearly down the page, and that each step in the solution is carefully motivated/explained/defended. Do not include all the statements that you try before finding the ones that work. I want to read a clear presentation of your approach, unencumbered by false starts and error messages.

QUESTION 4: Numerical Approach with IDL (weight = 30%)

In the closed-book portion of this examination, you convinced yourself that, in Cartesian coordinates, the orbit of a particle under an inverse cube central force was described in dimensionless form by the equations

$$\frac{d^2\overline{x}}{dt^2} = -\frac{\overline{x}}{(\overline{x}^2+\overline{y}^2)^2} \quad ; \quad \frac{d^2\overline{y}}{dt^2} = -\frac{\overline{y}}{(\overline{x}^2+\overline{y}^2)^2}$$

Use `ludiffeq_23` and/or `ludiffeq_45` to examine the behavior of this system when the initial conditions are given by

$$\overline{x}(0) = 1 \quad ; \quad \overline{v}_x(0) = 0 \quad ; \quad \overline{y}(0) = 0 \quad ; \quad \overline{v}_y(0) = \overline{v}_{y0}$$

You will need to give attention to

- Creating the appropriate pro-file to define these equations for `ludiffeq_23` or `ludiffeq_45`.
- Using (`ludiffeq_23` and/or `ludiffeq_45`) and `plot` to generate the solution and a graph of the orbit for $\overline{v}_{y0} = 1$ (which should produce a circular orbit) and for two other values of this velocity, one *slightly* larger than 1 and the other slightly smaller than 1. In each case, choose the time interval over which you generate the solution wisely to show enough of the orbit to reveal its full character.
- Verifying that the solutions you ultimately accept are accurate at least to the resolution of the graphs—and presenting evidence to support your contentions in this regard. Remember that you have both `ludiffeq_23` and `ludiffeq_45` at your disposal, that each of these routines has a keyword `tol`, and that energy and angular momentum given in dimensionless form by

$$\overline{E} = \overline{v}_x^2 + \overline{v}_y^2 - \frac{1}{\overline{x}^2 + \overline{y}^2} \quad ; \quad \overline{L} = \overline{x}\,\overline{v}_y - \overline{y}\,\overline{v}_x$$

  are—or should be—conserved.

Submit your solution to this question by creating a LaTeX document that includes (1) sufficient narrative and sufficient sample IDL code to explain your approach and (2) the graphs associated with your presentation of your solution.

C.3 Final Examination – 15 March 2006

Physics 225: Computational Mechanics **FINAL EXAMINATION** 15 March 2006

This examination is a closed book examination, but reference to *CPSUP* is permitted and, unless otherwise noted, calculators and integral tables are allowed. The examination is designed to take no more than three hours. Each student is to answer Question 1 and any *four* of the remaining *five* questions (Questions 2, 3, 4, 5, and 6). In all cases, *be sure to include enough narrative with each solution so that I can understand easily what you were thinking as you solved each problem.* In the grading, Question 1 will carry weight 3 and each of the remaining questions will carry weight 2.

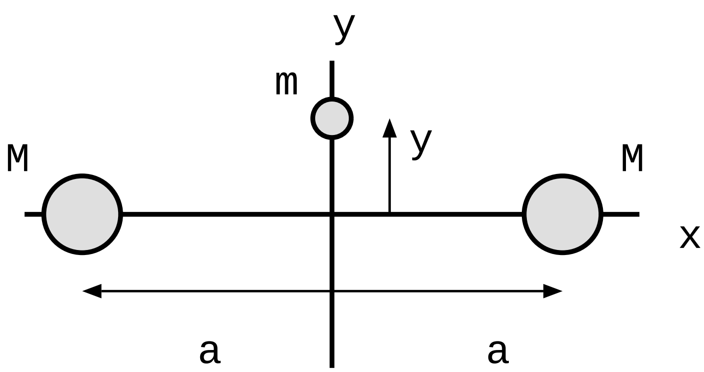
Possibly useful information:

$$U = -\frac{Gm_1m_2}{|\mathbf{r}_2 - \mathbf{r}_1|} \quad ; \quad U = \frac{1}{2}kx^2 \quad ; \quad U = mgz \quad ; \quad K = \frac{1}{2}mv^2 = \frac{1}{2}I\omega^2$$

$$(1+\epsilon)^q = 1 + q\epsilon + \ldots \quad ; \quad M\mathbf{R}_{CM} = \sum_i m_i\mathbf{r}_i \quad ; \quad W = \int \mathbf{F} \bullet d\mathbf{r}$$

REMEMBER: You must answer Question 1.

QUESTION 1: Gravitation; Small Amplitude Oscillations



Two objects, each of mass M, are fixed on the x axis, one at $x = +a$ and the other at $x = -a$. Another object of mass m is constrained to stay on the y axis but is free to move along that axis.

(a) Show that, when m is located at the point $\mathbf{r} = y\,\hat{\mathbf{j}}$, the potential energy of m is given by

$$U(y) = -\frac{2GMm}{[a^2 + y^2]^{1/2}}$$

(Don't work too hard. I am not asking you to evaluate an integral of the force, merely to use the known potential energy of a mass near a second mass to construct the potential energy in the present situation.) Were you to draw a graph of this function, I would hope you would deduce something like the graph at the end of this question. (Note that I did *not* ask you to generate—or even defend—this graph.)

(b) Locate the one equilibrium point and classify it as stable or unstable on the basis of features of the potential energy.

(c) Find the y component of the force on m by evaluating an appropriate component of the gradient of the potential energy, and show that the equation of motion of m is

$$\frac{d^2y}{dt^2} = -\frac{2GMy}{(a^2 + y^2)^{3/2}}$$

(d) Examine the equation to which this equation of motion reduces when $y \ll a$, i.e., when y^2 can be ignored relative to a^2, and determine the frequency of small amplitude oscillations about the equilibrium point.

Now, if you introduce the dimensionless coordinates $\overline{y} = y/a$ and $\overline{t} = \sqrt{2GM/a^3}\,t$, you will find that the equation of motion becomes

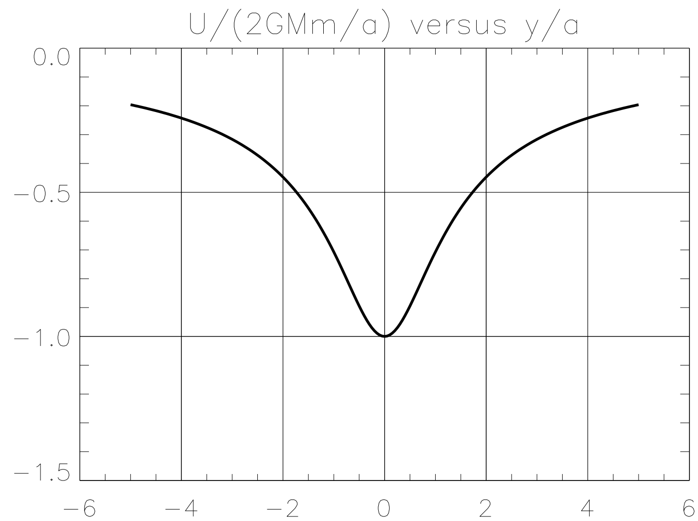
$$\frac{d^2\overline{y}}{d\overline{t}^2} = -\frac{\overline{y}}{(1 + \overline{y}^2)^{3/2}}$$

(Note that I did *not* ask you to deduce this form.)

(e) You wish to draw a graph of the position $\overline{y}$ of this object as a function of time $\overline{t}$ when $\overline{y}(0) = 1.0$ and $\overline{v}_y(0) = 0$. The ODE does not have an analytic solution, so you will have to invoke IDL and use a numerical method. Choose `ludiffeq_23`. Describe what you would do to

- effect that solution,
- obtain the desired graph, and
- assess the accuracy of your solution.

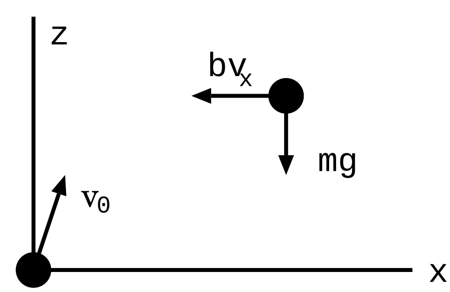
In particular, be specific about the coding that you would use, both to define the ODE for IDL and to generate and plot the solution. *Note*: I am asking only how you would produce a graph on the workstation screen, not how you would produce hard copy of the graph.



<u>*REMEMBER*: You are to answer any four of the remaining five questions.</u>

QUESTION 2: A Projectile in a Strange Atmosphere

A projectile is fired from the origin with an initial velocity $\mathbf{v}_0 = v_{x0}\,\hat{\mathbf{i}} + v_{z0}\,\hat{\mathbf{k}}$ into a strange atmosphere in which air resistance acts only horizontally. The projectile thus experiences the forces shown in the figure to the right. You may assume that the projectile remains in the xz plane.



(a) Apply Newton's second law to determine the equations of motion for this projectile.

(b) State the initial conditions to be imposed on the solution to the equations in part (a).

(c) Solve the equations obtained in part (a) subject to the initial conditions you identified in part (b) to show that

$$x(t) = \frac{mv_{x0}}{b}\left(1 - e^{-bt/m}\right) \qquad ; \qquad z(t) = -\frac{1}{2}gt^2 + v_{z0}t$$

(d) Explain briefly what is meant by the range of a projectile and then find an expression for the range of *this* projectile.

QUESTION 3: Orbits in Inverse Square Forces

In previous work, we have learned that a satellite of mass m orbiting a planet of mass M and radius R is an ellipse characterized by eccentricity ϵ and constant angular momentum L. If we choose a coordinate system in which the force center is at the origin and the angle ϕ is measured from the perigee (point of closest approach), the radial coordinate ρ of the orbit is given as a function of ϕ by the equation

$$\rho(\phi) = \frac{L^2/(m^2GM)}{1 + \epsilon\cos\phi}$$

where $\epsilon = 0$ for a circular orbit and $0 < \epsilon < 1$ for elliptical orbits.

(a) *For a general elliptical orbit*, suppose that *at perigee* the speed of the satellite is v_p and its distance from the force center is ρ_p.

i. Starting with the definition $\mathbf{L} = \mathbf{r} \times m\mathbf{v}$, show for that orbit that $L = mv_p\rho_p$.

ii. Using the result just obtained, show that,

$$\frac{\rho(\phi)}{R} = \frac{\left(\dfrac{v_p}{v_{\text{graze}}}\dfrac{\rho_p}{R}\right)^2}{1 + \epsilon\cos\phi}$$

where, as we have deduced in earlier work, $v_{\text{graze}} = \sqrt{GM/R}$.

(b) Now, suppose a satellite is initially in the *specific circular* orbit of radius $4R$. (*Don't overlook the 4*.

i. By requiring the gravitational force to provide for the requisite centripetal acceleration, show that the speed of *this* satellite is given by $v_s = \frac{1}{2}\,v_{\text{graze}}$.

ii. At a fateful instant, a *very short but powerful* burn of a rocket boosts the speed of this satellite to $\frac{2}{3}\,v_{\text{graze}}$, thus putting the satellite into a new (elliptical) orbit whose perigee is at the point where the boost was applied. Find

- the eccentricity ϵ of this new orbit.
- the radial coordinate of the new orbit at apogee (point of furthest distance from the force center).

The first of these quantities will be a pure number; the second can be left as a multiple of R.

QUESTION 4: Center of Mass; Integration with MAPLE and IDL

A slender rod of length l (assume $l > 0$) lies along the x axis with one end at the origin and the other end at $x = l$. The rod carries a total mass M distributed non-uniformly with mass per unit length $\lambda(x)$ given at coordinate x by $\lambda(x) = Ax^2e^{-x/l}$. Remembering that

$$\mathbf{R}_{\text{cm}} = \frac{1}{M}\int \mathbf{r}\,dm$$

and taking M as a given (i.e., do not trouble to determine how A and M are related[1]),

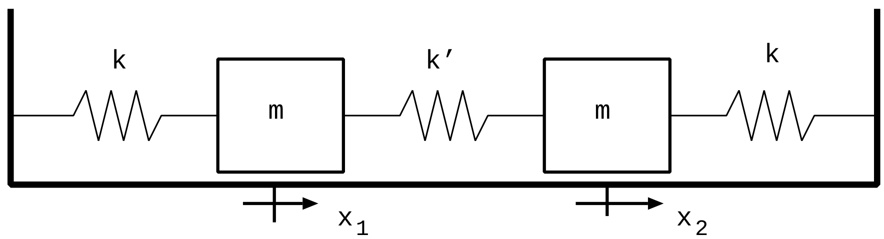
[1] If you *must* know, $A = M/[l^3(2 - 5/e)]$.

(a) Deduce an integral for the x coordinate $X_{\rm cm}$ of the center of mass of this rod.

(b) Describe how you would use MAPLE to evaluate the integral. Be specific about the statement(s) you would submit to MAPLE.

(c) Cast the integral in a dimensionless form and then describe how you would use `luqsimp` in IDL to evaluate it and assess the accuracy of your result. Be specific about the coding you would use, both to define the integrand for IDL and to evaluate the integral once the integrand has been defined.

QUESTION 5: The Lagrangian Approach

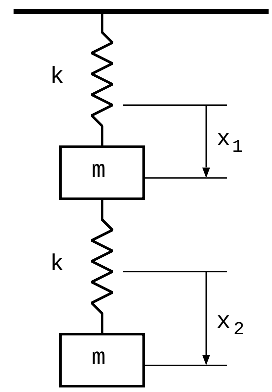


In the text and in class, we found the equations of motion for the illustrated system by examining the forces experienced by the two blocks and invoking Newton's second law. This problem leads you through an alternate, simultaneously mysterious and wondrous, way to deduce these same equations from a starting point that focuses on *energy* rather than on forces. Take the table to be horizontal and frictionless, let the springs be neither stretched nor compressed when the system is in equilibrium, and let the state of the system be described by the coordinates $x_1(t)$ and $x_2(t)$, which measure the positions of the blocks from their equilibrium positions, and the velocities $\dot{x}_1(t)$ and $\dot{x}_2(t)$. Using the symbols x_1, x_2, $\dot{x}_1$ and $\dot{x}_2$,

- write down the kinetic energy K of the system.
- write down the potential energy U of the system.
- evaluate the Lagrangian $\mathcal{L}$ defined by $\mathcal{L} = K - U$ of the system.
- pretending—this is the mysterious part—that x_1, x_2, $\dot{x}_1$ and $\dot{x}_2$ are independent of one another, evaluate the quantities
$$\frac{\partial \mathcal{L}}{\partial \dot{x}_1} \quad \text{and} \quad \frac{\partial \mathcal{L}}{\partial x_1}$$
- finally, admitting that the positions and velocities are time dependent, evaluate
$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}_1}\right) - \frac{\partial \mathcal{L}}{\partial x_1} = 0$$

and marvel at the result. (Done correctly, this process will lead you to the equation of motion for block 1 without the hassle of figuring out the forces and making sure that all of them have been taken into account!)

QUESTION 6: Natural Frequencies and Normal Modes



Two objects, each of mass m, are suspended as shown from the ceiling with two springs, each of constant k. With x_1 and x_2 measured from the positions of equilibrium under gravity, we can for this system imagine that gravity isn't present at all. A force analysis then leads to the equations of motion

$$m\ddot{x}_1 = -kx_1 + k(x_2 - x_1)$$

and

$$m\ddot{x}_2 = -k(x_2 - x_1)$$

(a) Find the (two) natural frequencies of this system as multiples of $\omega_0 = \sqrt{k/m}$.

(b) Determine how the blocks should be displaced initially so that, when released from rest, the system will oscillate in a mode corresponding to one—your choice—of the frequencies.

Hint: Begin by assuming a solution of the form

$$x_1(t) = x_{10} \cos \omega t \quad ; \quad x_2(t) = x_{20} \cos \omega t$$

Reminders: (1) Pledge. (2) Please make sure you have clearly indicated the question you have elected to omit.

Appendix D

Options for Projects in Computational Physics

Each of Assignment 3 covering finite difference methods and Assignment 6 covering finite element methods in Physics 540 contains a small number of problems to be solved by everyone in the class and one assigned project for each student. Completion of each of these assignments involves

- reading appropriate sections in the text to learn about the method covered in the assignment,
- solving and writing out solutions to one or two exercises common to the entire class,[1]
- with respect to the assigned "big" exercise, putting a special effort into
  - generating a solution and
  - writing a carefully written document that
    - describes in some detail how the problem was set up and solved (including a discussion of any particular wrinkles that had to be addressed),
    - defending the accuracy of the solution,
    - exploring the solution in as many creative ways as possible and, in particular, as a function of any parameters—if any—in the exercise,
    - making any other comments that seem appropriate, and
    - discussing the features of the solution and its dependence on the parameters, and
- preparing a 15-minute oral summary of the solution and its properties and delivering that summary in class.

The problems that are assigned to individual students for each of these two assignments are tabulated in Sections D.1 and D.2, respectively.

Assignment 7 contains only a project, this time of the student's choice but subject to the instructor's approval. Students spend about three weeks working on this project, which can involve any of the techniques addressed during the term but must be substantial and challenging. The handout describing this assignment is presented in Section D.3.

[1] On Assignment 3, the two common exercises involve (a) modifying a template discussed in the text to solve a 1D ODE and (b) adding a convergence test to a program for solving Laplace's equation. On Assignment 6, the one common exercise involves using a commercial finite element program to find the electrostatic potential and charge distributions in an annular region with Dirichlet boundary conditions at both the inner and outer radii.

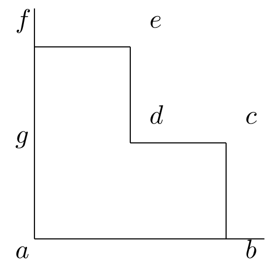


Figure D.1: Diagram for Big Exercise B1.1 and B1.2.

D.1 Big Exercise #1 (Assignment 3)

Each student will be assigned one of the following problems as a component of Assignment 3. Should the course sometime enroll more than six students, additional problems will be found.

B1.1 A two-dimensional plate is made by taking a square of side 1 unit and cutting a square of side 0.5 unit out of one corner as shown in Fig. D.1. Suppose the temperature along sides af and ab is maintained at 0 °C, the temperature increases linearly from 50 °C at e and at c to 100 °C at d, and sides fe and bc are insulated. If the entire plate is initially at 0 °C, use LSODE to study the approach of the temperature to equilibrium and, in particular, determine the equilibrium temperature.

B1.2 Consider a thin membrane stretched over the frame shown in Fig. D.1. Introduce a coordinate system in which the point a defines the origin and the lines ab and af—each of unit length—lie along the x and y axes, respectively. In the chosen coordinates, the point d has coordinates $(\frac{1}{2}, \frac{1}{2})$. Suppose this membrane to be drawn aside from the plane of the paper so that the rectangle $gdcba$ is undisplaced and the square $gdfe$ assumes a shape given by $u(x, y, 0) = 64x(\frac{1}{2} - x)(y - \frac{1}{2})(1 - y)$. Suppose further that this membrane is then released from rest. Use LSODE to study the subsequent motion of the membrane. In particular, obtain surface plots of the shape of the membrane over the xy plane for enough different times to make the character of the motion clear. Remember that, in a dimensionless presentation, the motion of the membrane satisfies the two-dimensional wave equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

B1.3 Suppose a quantum particle of mass m is initially in the state

$$\Psi(x, 0) = \frac{1}{\sqrt{a\sqrt{\pi}}} e^{-(x+5a)^2/2a^2}\, e^{ik_0 x}$$

which represents a particle (1) whose wave function initially is Gaussian with a width on the order of a centered at $x = -5a$ and (2) the expectation value of whose momentum is $\hbar k_0$ and—assuming non-relativistic motion—(3) the expectation value of whose velocity is $v_0 = \hbar k_0/m$. Suppose also that the particle moves under the influence of a static potential energy given by

$$V(x) = \begin{cases} 0 & x < -a \\ \frac{1}{2}V_0\left(1 + \cos\frac{\pi x}{a}\right) & -a \le x \le a \\ 0 & x > a \end{cases}$$

Solve the Schrödinger equation,

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\,\Psi$$

and obtain graphs of $|\Psi(x,t)|^2$ versus x for several values of t, extending your graphs over a time at least as great as $t_{end} = 2x_0/(\hbar k_0/m)$. Time permitting, compare the behavior for different values of k_0. In effect, you are looking at the scattering of a particle of incident energy $E = \hbar^2 k_0/2m$ from a potential hump having the shape of a single hump of the cosine curve. *Hints*: (1) Cast the problem in dimensionless form using a as the unit of length, finding a suitable unit of time, and introducing a dimensionless wave number $k = k_0 a$. (2) Recognize that the quantum wave function is complex, write $\Psi = \Psi_r + i\Psi_i$, and show that the real and imaginary parts of the (dimensionless) Schödinger equation are

$$\frac{\partial\Psi_r}{\partial t} = -\frac{\partial^2\Psi_i}{\partial x^2} + V\Psi_i \quad ; \quad \frac{\partial\Psi_i}{\partial t} = \frac{\partial^2\Psi_r}{\partial x^2} - V\Psi_i$$

(3) Seek a solution over the interval $-10a \le x \le 10a$ and assume that the wave function is and remains zero at the two ends of this region for all time, though you can't then generate the solution for too long, since this assumption will certainly not be valid forever.

B1.4 In (two-dimensional) polar coordinates (ρ,ϕ), the Laplace equation is

$$\nabla^2 u = \frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial u}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2 u}{\partial\phi^2} = 0 \quad\Longrightarrow\quad \rho^2\frac{\partial^2 u}{\partial\rho^2} + \rho\frac{\partial u}{\partial\rho} + \frac{\partial^2 u}{\partial\phi^2} = 0$$

Suppose a solution is sought in the region $0 < a \le \rho \le b$, $0 \le \phi \le 2\pi$ subject to the boundary conditions

$$u(a,\phi) = f(\phi) \qquad ; \qquad u(b,\phi) = g(\phi)$$

and the requirement that the solution be periodic with period 2π in ϕ. Let $\Delta\rho = (b-a)/n$ and $\Delta\phi = 2\pi/m$ and then let $\rho_i = a + i\,\Delta\rho, i = 0,1,2,\ldots,n$ and $\phi_j = j\,\Delta\phi, j = 0,1,2,\ldots,m$. Finally let $u_{i,j} = u)\rho_i,\phi_j)$. Discretize this equation. In particular use a central difference formula to approximate the derivative $\partial u/\partial\rho$. You should find ultimately that

$$u_{i,j} = \frac{u_{i+1,j}\left(\rho_i^2\,\Delta\phi^2 + \frac{1}{2}\rho_i\,\Delta\phi^2\,\Delta\rho\right) + u_{i-1,j}\left(\rho_i^2\,\Delta\phi^2 - \frac{1}{2}\rho_i\,\Delta\phi^2\,\Delta\rho\right) + \left(u_{i,j+1} + u_{i,j-1}\right)\Delta\rho^2}{2\,\rho_i^2\,\Delta\phi^2 + 2\,\Delta\rho^2}$$

Determine how this equation must be modified when $i = 0$, $i = n$ and/or $j = 0$, $j = m$, and then write a program to solve this equation when

$$f(\phi) = 0 \quad ; \quad g(\phi = \begin{cases} -100 & -\pi < \phi < 0 \\ 100 & 0 \le \phi \le \pi \end{cases}$$

Finally, compile, link, and run your program to explore the solution in some detail.

B1.5 Demonstration that the full discretization of the wave equation $\ddot{u} = c^2 u''$ leads to an unstable method unless $c^2\,\Delta t^2/\Delta x^2 \le 1$ is extremely difficult. To illustrate this the instability, recast `fdmwave1d` to solve the wave equation subject to the boundary conditions $u(0,t) = u(l,t) = 0$ and the initial conditions $u(x,0) = 0$, $\partial u(x,0)/\partial x = 0$. The solution should, of course, be zero at all subsequent times, since we have started the string in its equilibrium position with zero velocity. Now, suppose that a computer-roundoff error occurs such that, instead of being zero at all nodes, $u(x,\Delta t) = 0$ everywhere *except at one node near the middle of the string* and, at that node $u(x,\Delta t)$ mistakenly acquires the value 1 (one). Use your program to solve this problem for choices of the parameters that make $\alpha = 0.5$ and other choices that make $\alpha = 1.5$. Look at the solution with print or plot frequency 1 and compare the way in which that one disruption of a value at the end of the first time step propagates forward in time for the two values of α.

B1.6 Demonstration that the full discretization of the diffusion equation $\dot{u} = \alpha^2 u''$ leads to an unstable method unless $\alpha^2\,\Delta t/\Delta x^2 \le 1/2$ is extremely difficult. To illustrate this instability, recast `fdmdiffus1d` to solve the diffusion equation subject to the boundary conditions $u(0,t) = u(l,t) = 0$ and the initial condition $u(x,0) = 0$. The solution should, of course, be zero at all subsequent times, since we have started the temperature distribution with its equilibrium values. Now, suppose that a computer-roundoff error occurs such that, instead of being zero at all nodes, $u(x, \Delta t) = 0$ everywhere *except at one node near the middle of the rod* and, at that node $u(x, \Delta t)$ mistakenly acquires the value 1 (one). Use your program to solve this problem for choices of the parameters that make $\gamma = 0.25$ and other choices that make $\gamma = 1.0$. Look at the solution with print or plot frequency 1 and compare the way in which that one disruption of a value at the end of the first time step propagates forward in time for the two values of γ.

D.2 Big Exercise #2 (Assignment 6)

Each student will be assigned one of the following problems as a component of Assignment 6. Should the course sometime enroll more than six students, additional problems will be found.

B2.1 Suppose a linear element e is characterized by *three* nodes at $x_1^{(e)}$, $x_2^{(e)}$, and $x_3^{(e)}$. Further, let the solution $\tilde{\varphi}^{(e)}$ on that element be approximated by the quadratic function

$$\tilde{\varphi}^{(e)} = a^{(e)} + b^{(e)}x + c^{(e)}x^2$$

(a) Find the constants $a^{(e)}$, $b^{(e)}$, and $c^{(e)}$ that will make this function match the specific values $\tilde{\varphi}_1^{(e)}$, $\tilde{\varphi}_2^{(e)}$, and $\tilde{\varphi}_3^{(e)}$ at the points $x = x_1^{(e)}$, $x_2^{(e)}$, and $x_3^{(e)}$, respectively. (b) Substituting these values into the above expression and grouping terms appropriately, cast the result in the form

$$\tilde{\varphi}^{(e)} = \sum_{i=1}^{3} \tilde{\varphi}_i^{(e)}\, N_i^{(e)}(x)$$

and show that the shape functions $N_i^{(e)}(x)$ appropriate to this three-noded linear element are

$$N_1^{(e)}(x) = \frac{1}{\Delta}\begin{vmatrix} 1 & x & x^2 \\ 1 & x_2^{(e)} & (x_2^{(e)})^2 \\ 1 & x_3^{(e)} & (x_3^{(e)})^2 \end{vmatrix} = \frac{(x_2^{(e)} - x)(x_3^{(e)} - x)}{(x_2^{(e)} - x_1^{(e)})(x_3^{(e)} - x_1^{(e)})}$$

$$N_2^{(e)}(x) = \frac{1}{\Delta}\begin{vmatrix} 1 & x_1^{(e)} & (x_1^{(e)})^2 \\ 1 & x & x^2 \\ 1 & x_3^{(e)} & (x_3^{(e)})^2 \end{vmatrix} = \frac{(x - x_1^{(e)})(x_3^{(e)} - x)}{(x_2^{(e)} - x_1^{(e)})(x_3^{(e)} - x_2^{(e)})}$$

$$N_3^{(e)}(x) = \frac{1}{\Delta}\begin{vmatrix} 1 & x_1^{(e)} & (x_1^{(e)})^2 \\ 1 & x_2^{(e)} & (x_2^{(e)})^2 \\ 1 & x & x^2 \end{vmatrix} = \frac{(x - x_1^{(e)})(x - x_2^{(e)})}{(x_3^{(e)} - x_1^{(e)})(x_3^{(e)} - x_2^{(e)})}$$

where

$$\Delta = \begin{vmatrix} 1 & x_1^{(e)} & (x_1^{(e)})^2 \\ 1 & x_2^{(e)} & (x_2^{(e)})^2 \\ 1 & x_3^{(e)} & (x_3^{(e)})^2 \end{vmatrix}$$

Finally, (c) show that—with $\xi = (x - x_1^{(e)})/l^{(e)}$—these functions reduce to

$$N_1^{(e)}(x) = 2(\xi - 1)\left(\xi - \frac{1}{2}\right) \quad ; \quad N_2^{(e)}(x) = 4\xi(1-\xi) \quad ; \quad N_3^{(e)}(x) = 2\xi\left(\xi - \frac{1}{2}\right)$$

when $x_2^{(e)}$ is midway between $x_1^{(e)}$ and $x_3^{(e)}$, i.e., when $x_2^{(e)} = x_1^{(e)} + \frac{1}{2}l^{(e)}$ and $x_3^{(e)} = x_1^{(e)} + l^{(e)}$, and (d) obtain graphs of these three shape functions over the interval $0 < \xi < 1$. *Hint*: You may find a symbolic manipulating program to be useful at many points in this problem.

B2.2 Accepting the shape functions $N_i^{(e)}(x, y)$ given in the text when the approximating function $\tilde{\varphi}(x, y) = a + bx + cy$ is applied to a triangular element in two dimensions, (a) verify for each node i that the shape function is zero not only at the two nodes not identified by its index but also along the entire line joining those two nodes, and (b) find the functions to which these functions reduce when $(x_0, y_0) = (-1, 0)$, $(x_1, y_1) = (1, 0)$, $(x_2, y_2) = (0, 1)$ and use IDL to draw a surface plot of each of these three functions under these circumstances.

B2.3 The boundaries of a square region are maintained at zero potential. Centered in this outer square is a second square with edges one-quarter—more or less—the length of the edges of the larger square. The region inside the *smaller* square contains a charge distributed with a constant charge density. Thus, the potential in this region satisfies the Poisson equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\frac{\rho}{\epsilon_0}$$

subject to the boundary conditions that $u(x, y) = 0$ everywhere on the perimeter of the larger square. Further, suppose that the inhomogeniety $-\rho/\epsilon_0$ has some constant nonzero value—what value is merely a matter of scaling—*inside* the smaller square and is zero outside the smaller square.

a. Verify that this equation is elliptic and separable.
b. Find the potential throughout the entire region inside the larger square.
c. Generate a surface graph of the potential over this region.
d. Generate an equipotential map showing contours at judiciously chosen values of the potential.
e. Generate a map showing the field lines in the square.
f. Generate graphs of the charge densities induced on the edges of the square.

Hint: (1) Probably you can calculate electric fields and charge densities most easily within the visualization program you use. Don't try to incorporate those quantities in the output of the program invoking `mud2sp.f`. (2) Remember that $\mathbf{E} = -\nabla V$ and that $\sigma = \epsilon_0 \mathbf{E} \bullet \hat{\mathbf{n}}$.

B2.4 Instead of the inhomogeneity described in the previous exercise, suppose the charge density inside the larger square is nonzero only in *two* square regions having edges one-sixteenth the edge of the larger square, that the charge density is constant and positive in one of these regions and constant (same magnitude) and negative in the other. Further, let these two regions be symmetrically positioned along the diagonal of the larger square. Find the potential in the larger square and obtain the same spectrum of graphs as those identified in the previous exercise.

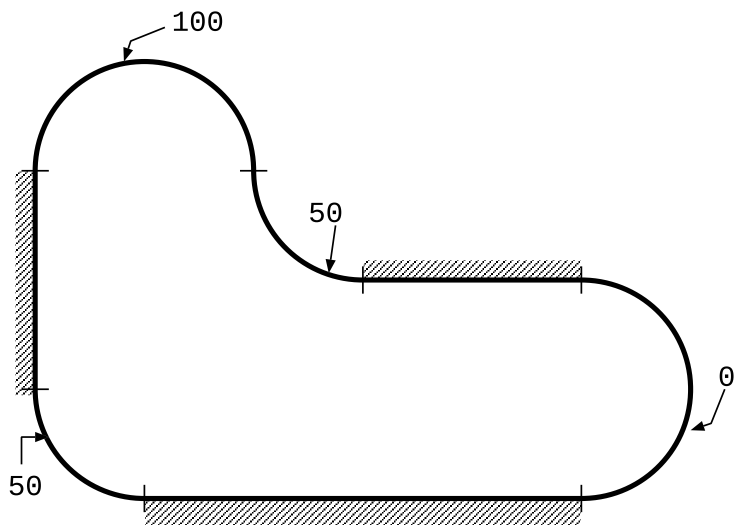


Figure D.2: Geometry for Exercise B2.5.

B2.5 Find the steady state temperature distribution in the geometry shown in Fig. D.2. All arcs are semicircles or quarter-circles of radius 1 unit, and the straight patches are either 2 or 4 units in length. As indicated by the shading, the straight patches are insulated. Each circular arc is maintained at the indicated temperature in degrees Celsius. Assume that the material of which the shape is constructed has uniform thermal conductivity and heat capacity.

B2.6 Find the electrostatic potential in the geometry of Fig. D.3 when the large semicircle and the diameter are maintained at 0 Volts and the region inside the inner circle contains electric charge distributed uniformly with density 1 C/m^2. Note that you will need to mesh the area *inside* the inner circle as well as the area between the inner circle and the outer boundary of the region of interest, but you must do so in a way that preserves the nodes along the inner circle. To specify the charge density, you will have to provide a "boundary condition" on and within that inner circle. I think—but I am not sure—that you want to migrate from the Main menu through the Boundary Conditions menu to the Electrostatic menu from the 'Boundary Condition Class' panel in the Boundary Conditions menu. The 'Face Charge' button in that menu *may* be the one you want in order to apply a distributed charge to a selection of faces.

D.3 Big Exercise #3 (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 at the end of the term. A brief written project proposal is due at the beginning of week 7. I offer the following suggestions to stimulate your thinking about this project. I am, of course, willing to listen to—and to help refine—any other proposals that you might have.

B3.1 The normal modes of oscillation of a square membrane. This problem can be approached by using finite difference methods to generate an equivalent matrix eigenvalue problem and

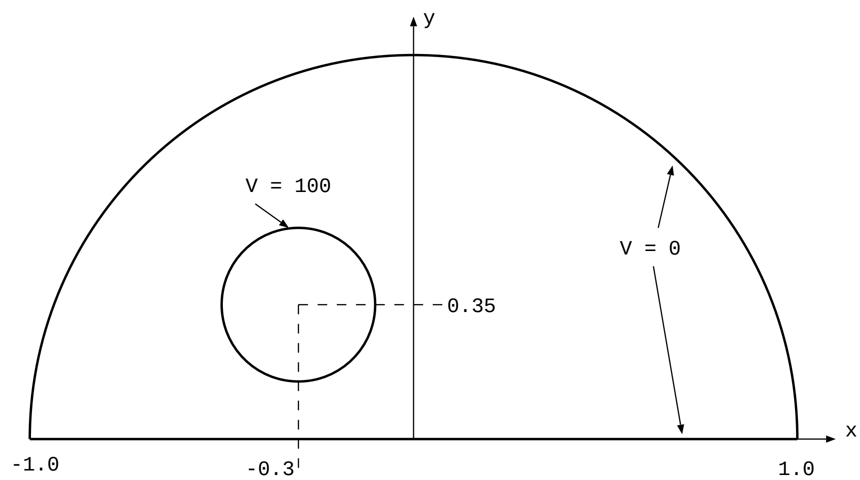


Figure D.3: Geometry for Problem B2.6.

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 have set up the matrix whose eigenvalues and eigenvectors are to be found.

B3.2 A three-dimensional electrostatic problem in Cartesian coordinates whose solution would involve using the multigrid subroutine `mud3sp.f`.

B3.3 The two-dimensional Laplace equation in cylindrical coordinates with some choice (or choices) of boundary conditions. This problem would be approached using the multigrid subroutine `mud2sp.f`, though care would be needed to set up the problem in non-Cartesian coordinates.

B3.4 The temperature distribution inside a three-dimensional region that is cylindrically symmetric. This exercise should be doable with `mud2sp.f`, though care would be needed to set up the problem in non-Cartesian coordinates.

B3.5 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 class.

B3.6 A situation using MARC/MENTAT to set up and solve a problem in a fairly simple three-dimensional geometry.

Bibliography

[1] `NEdit` is a text editor available under a GNU General Public License. Information is available at the website `http://www.nedit.org`.

[2] `XEmacs` is a text editor available under a GNU General Public License. Information is available at the website `http://www.xemacs.org`.

[3] *Excel* is a component of the Microsoft Office suite and is available for purchase from Microsoft Corporation. Information is available at the website `http://office.microsoft.com/en-us`.

[4] IDL is a program for array processing and graphical visualization and is available for purchase from ITT Industries. Information is available at the website `http://www.ittvis.com`.

[5] MATLAB is a program for array processing and graphical visualization and is available for purchase from The MathWorks. Information is available at the website `http://www.mathworks.com`.

[6] OCTAVE is a program for array processing and graphical visualization and is available under a GNU General Public License. Its syntax is similar to that of MATLAB. Information is available at the website `http://www.octave.org`.

[7] MAPLE is a computer algebra system and is available for purchase from Waterloo Software. Information is available at the website `http://www.maplesoft.com`.

[8] *Mathematica* is a computer algebra system and is available for purchase from Wolfram Research. Information is available at the website `http://www.wolfram.com`.

[9] MAXIMA is a computer algebra system and is available under a GNU General Public License. Its syntax is similar to the no-longer-available commercial program MACSYMA. Information is available at `http://maxima.sourceforge.net`.

[10] *Kaleidagraph* is a program for generating publication-quality graphs and is available for purchase from Synergy Software. Information is available at the website `http://www.synergy.com`.

[11] The Numerical Recipes library of FORTRAN and C subroutines is available for purchase from Numerical Recipes Software. Information is available at the website `http://www.nr.com`.

[12] ODEPACK is a package containing numerous FORTRAN solvers for ODEs, of which LSODE (the Livermore Solver for ODEs) is a component. This package is in the public domain. Information is available at the website `www.netlib.org`.

[13] MUDPACK is a package containing numerous FORTRAN solvers for elliptic partial differential equations in two and three dimensions. This package is in the public domain. Information is available at the website `http://www.scd.ucar.edu/css/software/mudpack`.

[14] *Multisim 7* is a program for circuit simulation and is available for purchase from Electronics Workbench Corporation. Information about the product and the appropriate local offices of the company is available at the website `http://www.electronicsworkbench.com`.

[15] SPICE is a program for simulating the behavior of electric circuits and is available for purchase at nominal cost. For information, start at `www.berkeley.edu` and search for SPICE.

[16] *LabView* is a program for designing and executing software to access laboratory equipment for on-line acquisition of data. It is available for purchase from National Instruments Corporation. Information is available from the website `http://www.NI.com/labview`.

[17] LaTeX is freely available for many platforms via `ftp` download from several archives around the world. For information, start at `www.tug.org`.

[18] Tgif is a program for drawing assorted diagrams and writing those descriptions in files of several different types. For information, go to `www.ucla.edu` and search for Tgif.

[19] *PowerPoint* is a component of the Microsoft Office suite and is available for purchase from Microsoft Corporation. Information is available at the website `http://office.microsoft.com/en-us`.

[20] *LoggerPro* is the software that interfaces with *LabPro* hardware to connect a laboratory computer to assorted digital sensors. This software and the associated hardware are available for purchase from Vernier Software and Technology. Information is available at the website `http://www.vernier.com`.

[21] *Praat* is freely available software for Fourier analysis—more broadly phonetics—of digitally recorded sound waves. Information is available at the website `http://www.praat.org`.

[22] *SpaceTime* is software for simulating time dilation, length contraction, and other special relativistic phenomena. It is available for purchase from Physics Academic Software. Information is available at the website `http://www.webassign.net/pas`.

[23] *MARC/MENTAT* is a pair of programs for setting up and solving partial differential equations by finite element techniques and is available for lease from MSC Software. Information is available at the website `http://www.mscsoftware.com`.