Developing a project-based computational physics course grounded in expert practice

Christopher Burke and Timothy J. Atherton

Department of Physics and Astronomy, Tufts University, 574 Boston Avenue, Medford, MA 02155

We describe a project-based computational physics course developed using a backwards course design approach. From an initial competency-based model of problem solving in computational physics, we interviewed faculty who use these tools in their own research to determine indicators of expert practice. From these, a rubric was formulated that enabled us to design a course intended to allow students to learn these skills. We also report an initial implementation of the course and, by having the interviewees regrade student work, show that students acquired many of the expert practices identified.

I. INTRODUCTION

Computers have been used to solve physics problems since they were first created[1], and with their ever increasing ubiquity, computing has become a fundamental scientific practice in Physics. Some brief examples[2]: in High Energy Physics, computers automatically select detected events for recording, store them and allow processing of the results on large-scale compute Grids; moreover, theoretical predictions are made by simulations. In Astronomy, formation processes are simulated at multiple length scales from star formation to galaxy evolution. In Condensed Matter Physics, many-body quantum mechanics simulations predict the electronic structure of crystals and molecules, bulk properties from molecular dynamics and continuum behavior by solving PDEs. Moreover, almost since they became available, computers have been used in Physics Education for visualization and simulation[3], and their immense potential as educational tools was recognized early on[4 5]. This tradition is continued today in projects such as the PhET[6] simulations, designed for classroom use.

Given the central importance of computation to physics research, and hence the need for appropriately trained students and professionals to perform it, it is perhaps surprising that computing is often only weakly integrated into the physics curriculum. Several approaches have been tried to remedy this[7]. At the largest scale, whole majors on Computational Science have been created[8]; courses[9] or sequences of courses[10][11] have been created within departments; computational projects and homework problems have also been integrated into existing courses and laboratories, both for majors[12] and at the introductory level[13][14]. Encouragingly, a large-scale survey performed about a decade ago[15], showed widespread support for these efforts. A valuable starting point for those seeking to implement one of these approaches is a special double volume[16] of the American Journal of Physics on Computation published in 2008 and including several of the articles cited above. Of particular practical help is the extensive Resource Letter[17], an updated version of[18].

In this work, we discuss a Computational Physics class recently created at Tufts University. Central to our vision was a desire to ground the course in actual professional practice, following a movement to refocus science education around real scientific practices[19]. We therefore conducted interviews of scientists, mathematicians and computer scientists to determine these practices. The results of these interviews were distilled into a rubric that aims to describe indicators of expert practice in computational physics. From the rubric, we used a backwards course design approach to create a sequence of projects that allow students to acquire these practices in a structured manner. We gave the course for the first time in the Spring 2015 semester, and conducted an after-delivery assessment exercise to determine whether student work did indeed contain evidence of expert practice. We report in detail the design process in the hope it might be of use to others planning project-based courses with other subject matter.

The structure of the paper follows our design and assessment exercise: the rubric and its development is described in section II, the course design process is explained in section III, brief comments on the initial implementation are given in section IV, our a posteriori analysis of the success is presented in section V. We finish with discussion and conclusions in section VI.

II. RUBRIC DEVELOPMENT

The initial phase of our design process was to develop a rubric for the course, capturing in a single document indicators of expert practice in Computational Physics. The purpose of this was threefold: First, and most obviously, the rubric would be a tool to help assess the quality of student work submitted in the course. Second, by making this document available to students during the course, we wished to convey these excellent practices as a norm and engender a climate of professionalism in the classroom. Finally, we anticipated that by distilling the practices into a rubric, the resulting document would be a powerful tool to assist in the design of the course, ensuring that the content and assessment would be mutually aligned, and that both would prepare students to solve computational problems in actual physics research.
We began by determining the typical content of Computational Physics courses. We examined course syllabi from a range of institutions, Boston University, University of Connecticut, East Tennessee State University, Northeastern University and Oregon State University. From these syllabi, and our own experiences as professionals, we proposed an initial set of competencies that seem essential to the practice of computational physics: Physical transcription, the formulation of the physical system of interest into a mathematical problem and creation or selection of algorithm(s) to solve it; Planning, organizing the overall program into modules and selecting appropriate data structures; Programming, implementation of the approach; Visualization, post-processing of the results and selection of the appropriate representations to interpret them; Numerical analysis, assessing error and stability of the program; Physical analysis, relating the results of the program back to the initial problem and determining whether the approach has provided the required insight.

Our initial model of how these competencies were used by experts to solve problems in physics research is shown in figure 1. We anticipated a formulation phase, in which the physical system and research questions of interest were transcribed into a math problem and then an algorithm developed or selected to solve the problem. Following this, the program is implemented. Having run the program, the results are evaluated both to assess whether the results were numerically meaningful, i.e. whether the program gave stable, repeatable results, and physically meaningful, i.e. whether they answered the original research questions. We envisioned that these activities would be repeated iteratively several times, as the initial product may not fully address the original questions, or the results may lead to new questions. This sequence mirrors famous work on problem solving[20], as well as physics-specific research[21]. We particularly note the parallel with the Integrated Problem-Solving model[22, 23], which divides the problem-solving process into framing, implementation and evaluation, and was recently adapted to assess student learning in Computational Materials Science[24].

From our initial list of competencies and problem solving model, we devised interview questions (listed in Appendix[1]) to determine actual professional practices associated with these competencies. We selected five faculty and postdocs from Physics, Computer Science and Mathematics who actively use computation in their research and have published refereed papers involving computation. These five were interviewed by one of the authors (CJB) and these interviews transcribed. The two authors then coded the transcripts separately according to the prompt “identifiable items we could look for in student work”. Following this step, the coded items were compared and only common items retained. We then categorized the coded items according to our initial competency model.

In performing this exercise, we identified additional competencies that we had not proposed in our initial model: Running, incorporating the ability to create scripts and file structures to execute the program and collect the data, and Testing, incorporating comparison of the output of the program against known solutions as well as profiling the program to assess performance. We renamed the competency Programming in the initial model to Implementation to reflect our inclusion of important non-programming practices associated with implementation, e.g. creation of external documentation and use of version control.

Furthermore, the evidence of the interviews forced us to abandon our initial cyclic model of how Computational Physics programs are created and instead create a more highly connected and iterative model, depicted in fig. 2. Of particular note, we found evidence that ideas from numerical analysis inform almost every as-
pect of computational physics problem solving, and that experts typically use these ideas as a sub-step in each of the Physical Transcription, Planning, Implementing, Testing and Visualization steps. The Numerical analysis, Visualization and Physical Analysis steps of evaluating the program output are also highly interconnected and mutually inform the selection of representations to plot and how to interpret the results. Perhaps our most surprising result is that Visualization was shown not to be limited to assessing the program output, but also a key tool to plan and implement effective programs. Overall, the evidence suggests that while experts do indeed solve Computational Physics problems iteratively, the execution of their strategy does not involve a clearly defined sequence of steps but rather invocation of different competencies as required. While the number of interviewees in this study is small, their nonlinear approach to problem solving parallels that seen in other domains.\cite{25}

A draft rubric was prepared from the coded items, organized along the new competency model, which seeks to define expert practice through the indicators identified from the interviews. The participants interviewed were invited to give feedback on the rubric draft at a panel, together with representatives from the Tufts Center for the Enhancement of Learning and Teaching (CELT) and Tufts Technology Services Educational Technology group who both possessed relevant expertise in computing education. Following the recommendations of the group, we constructed the final version of the rubric shown in table II.

### III. COURSE DESIGN

Having created the rubric described in section II, we set out to design a course in which students could learn the expert practices identified in a structured manner. Following other studies\cite{9}, we decided to adopt a project-based approach. Our overall vision for the course was that students would complete a structured sequence of projects to acquire the practices from the rubric in a scaffolded manner. We proposed to spend the majority of the class time—2.5 hours per week—with the students working in groups, guided by the instructor and TA; we would introduce each class with a short “micro lecture” introducing each project and its associated concepts and algorithms. We also anticipated that the students would create a final term project where they would select and formulate the physics problem to be solved themselves.

First, we sought to distill the essence of the rubric further into a small number of overall course goals for students to learn in the course:

1. Develop mathematical and computational models of physical systems.
2. Design, implement and validate a functioning code for such a model.
3. Understand the role of numerical analysis in formulating, designing and interpreting computer models.
4. Use visualization and physical analysis to test hypotheses.
5. Connect theory, experiment and simulation.

To identify possible projects, we surveyed 17 faculty from the Astronomy, High Energy Physics, Cosmology and Condensed Matter Physics research groups in the Tufts Physics and Astronomy department. For each of the proposed projects—which we supplemented with some of our own—we selected practices from the rubric that might be particularly important. While good programming is a ubiquitous requirement, for example, the Ising model is a suitable problem to study random numbers and issues of repeatability. We then ordered this collection of projects to determine those that could be completed with little specialist knowledge to those requiring more, and identified dependencies between projects.

Following the backward course design approach\cite{20}, we selected a subset of projects that allowed us to span the full list of practices and constructed the course plan shown in table IV. Reading column-wise for each project is an estimate of the time required—one or two weeks—the practices we intended to focus on in the project, the project title, the content of the project as viewed from a traditional course, and any additional skills that may be required for successful completion of the project. From this overall plan, we developed project descriptions, available as supplementary material\cite{27}, as well as brief “micro-lectures” to communicate both the content (i.e. algorithms and concepts) and the Learning Objectives (i.e. the professional practices). The problems themselves will be described in more detail in the following section concerning our initial implementation.

### IV. IMPLEMENTATION

#### A. Student backgrounds

1. Demographics

An initial implementation of the course ran in the Spring semester of 2015 and was ultimately completed by \( n = 22 \) students out of 23 registrants. The course contained 7 women and 14 men. Some 13 were Physics or Astronomy majors, 8 were Computer Science majors with some double majoring in both Physics and Computer Science, 3 were graduate students in Physics and Education.
### Competency | Indicators
--- | ---
Physical Transcription | Analytical methods are first employed to understand the problem to the greatest extent possible, including identification of symmetries, length scales and timescales. An appropriate mathematical model and computational representation are chosen including choice of algorithm and discretization. Multiple methods are considered and their strengths, limitations and complexity are evaluated using literature where appropriate. Important physical constraints and conserved quantities are identified, and the approximations made are clearly stated. The purpose of the calculation and desired results are clearly articulated.
Planning | The program to be written is broken into modules and functions that can be designed, tested and debugged independently. A suitable and efficient representation of the data, such as classes and data structures, is chosen appropriately for the algorithm. Relevant libraries, software packages and existing code are identified. The need for parallelization is considered and incorporated into the design if necessary. An appropriate language is chosen based on needs of the problem, ease of implementation, maintainability and performance.
Implementation | The code can be easily understood and convinces the reader it works through careful commenting, descriptive variable and function names and validation of input. Coding standards are developed and obeyed amongst the implementation team. Comments document the physics, are in proportion to the complexity of the section, and identify input and output to functions. Outside documentation thoroughly describes how the program works and how to run it such that future users and maintainers can easily work with the program. The code is efficient but not at the expense of readability and maintainability. Professional programming tools, e.g. version control and debuggers are used where available.
Testing | Each element of the program is carefully tested separately and together at each step. The program is verified on test cases with known solutions identified in the planning process. Appropriate metrics are used to analyze performance and identify need for optimization. Visualization is used to provide insight into whether the algorithm is working.
Running | Initial conditions are chosen judiciously. Output is organized and labeled and input parameters used in each run are recorded. Multiple runs, if necessary, are automated efficiently through scripts.
Visualization | Visualization is used to gain intuition regarding the output and to present final results in a compelling way. Important results are visualized so that they require little effort to decipher and are appropriate for the given data. Relevant tools are used to make the visualization. Strengths and limitations of the choice of representation and alternatives are discussed. Visualization, including physical objects, may also be used to display program and data structures if necessary.
Numerical Analysis | The source and nature of all approximations made are identified and their impact on the result discussed. The most significant sources of error are carefully analyzed and estimates of the error are given; ideally these are used to guide the algorithm, e.g. in refining the discrete representation. Conditions for stability are identified and quoted. The scaling of computational time with problem size is understood. Reproducibility is verified for non-deterministic algorithms. Floating point arithmetic is used carefully.
Physical Analysis | Results are compared to hypotheses. Adherence to physical constraints (e.g. energy conservation) is verified. Possible improvements or alternate implementations are identified. The results are cross checked with alternative simulation strategies.

2. **Prior experience**

In this section, we discuss the prior experience of students in the class. We first address the issue of programming language. The course design presented above is intentionally language independent because evidence from our interviews indicates that good programming practices are largely independent of the language chosen. Moreover, language selection for a given problem is an important skill. The language chosen should be one used by professional physicists; within the general family of languages familiar to the students; have good quality development tools and have libraries or intrinsic functions to support useful algorithms and visualization.

To aid this decision, and generally guide our preparation, we circulated a brief survey before the course to assess student course preparation in physics, computer science and math as well as programming language familiarity and confidence in programming. The questions are listed in Appendix II. From the 14 responses, we coded student preparation in each subject as Introductory, Intermediate, Advanced or Graduate depending on the highest level course taken by the student. The courses General Physics 1 and 2, Calculus 2, Multivariable Calculus and Introduction to Programming were classified as Introductory. Modern Physics, Linear Algebra, Differential Equations and Data Structures were classified as Intermediate. Any courses with higher numbers were classified as Advanced.
| Week | Learning Objectives | Assignments | Content | Additional skills |
|------|---------------------|-------------|---------|-------------------|
| 1-2  | Documenting code   | Double pendulum | Discretization — ODEs — Integration | Group work |
|      | Testing each component separately | | | |
|      | Version control | | | |
| 3-4  | Dividing code into functions | ID quantum mechanics | Eigensystems — Root finding — Shooting | Reading papers |
|      | Identifying sources of error | | | |
| 5    | Selecting a model or algorithm | Model fitting | Optimization — Statistics | Consulting textbook/internet resources |
|      | Identifying improvements | | | |
| 6    | Identifying sources of approximation | Linear combination of atomic orbitals | Linear Algebra | |
|      | Using visualization to analyze results | | | |
| 7-8  | Scripting | Ising model of magnetism | Monte Carlo — Random Numbers | |
|      | Reproducibility | | | |
| 9-10 | Identify symmetries / conserved quantities | Time dependent Schrödinger equation | PDEs | |
|      | Test physical acceptability of sol’n | | | |
| 11-12| Identify existing packages | Laplace’s equation | Relaxation — Interpolation/Extrapolation | Finite Differences |
|      | Choose representation of data structures | Analyze and optimize performance | Finite Elements | |
|      | Analyze stability/scaling | | | |
|      | Choose language | | | |
|      | Use visualization to present a compelling case | | | |
| ongoing | Develop a hypothesis | Final project | | |

Table IV. Course plan

| None Intro. | Inter. | Adv. | Grad. |
|-------------|--------|------|-------|
| Physics     | 0      | 1    | 7     | 4     | 2     |
| CS          | 4      | 6    | 3     | 1     | 0     |
| Math        | 0      | 3    | 7     | 4     | 0     |

Table V. Subject preparation.

| Language | None Intro. | Inter. | Adv. | Confident |
|----------|-------------|--------|------|-----------|
| C++      | 10          | 8      |      |           |
| Mathematica | 9      | 4      |      |           |
| Python   | 9          | 4      |      |           |
| Java     | 6          | 3      |      |           |
| MATLAB   | 5          | 3      |      |           |
| FORTRAN  | 1          | 0      |      |           |

Table VII. Language familiarity.

The results for subject preparation are shown in table [V]. Most obviously, students were best prepared in Physics, but only slightly less well prepared in Math. While most students had some familiarity with Computer Science, it is very clear that preparation in this subject was weaker than the other two subjects. A table of student numbers sorted by both Physics and Computer Science preparation, displayed in table [VI] shows that the majority of students had an intermediate or better preparation in both subjects. No students had taken advanced or graduate classes in both subjects.

Languages with which students expressed familiarity or confidence are shown in table [VII]. The list is somewhat abbreviated: exactly one student each expressed familiarity with Javascript, Lua, Objective-C, Ruby, Scheme, SQL, Swift and Visual Basic. All respondents self-assessed their own experience with programming as familiar or better. Interestingly, all students provided concrete examples of programming tasks they had completed outside Introductory Computer Science classes, referring to data analysis, simulations and programs written for research purposes.

With this information, we decided to use both Mathematica and Python for the course as these were both near the top of languages students were already familiar with. Both of these languages are high level, easy to
In this section, we describe our approach to organizational matters. The class met twice a week for 1 1/2 hour sessions. As noted above, the typical class structure involved short presentations by the instructor on the project physics background, a numerical analysis topic, or one of the competencies identified in the rubric. *Numerical Recipes* [28] was recommended as a textbook, and was used by students as a reference for standard algorithms. Support was provided through portions of class time dedicated to student group work during which the instructor and TA were available to help troubleshoot issues, as well as traditional office hours. A *Piazza* forum was also provided for the course which received 2-3 posts per week. Questions on the forum were typically answered quickly, on average within half an hour. Students tended to use the forum to share links to helpful resources, organize groups for the final project, and pose syntax questions.

A key issue in designing the class was the choice of group size. Following generic advice, the first two projects listed below were executed in teams of 4 or 5; project 3 was performed in pairs; project 4 was performed in teams of 4. At this point in the semester, we circulated a mid-semester survey with one question that asked students what they thought the optimal group size was based on their experiences. We had 12 responses, which are summarized in table VIII. Students were also asked to explain the reasons for their selection, which revealed two opposing effects: logistics, such as finding convenient times to meet physically and synchronizing efforts favor smaller group sizes while division of labor tends to favor larger group sizes. However, students reported that in larger groups, there tended to be people who didn’t contribute significantly. We therefore concluded that groups of 3 were preferable for this course and used this size for the remainder of the semester with occasional groups of 4 where required to accommodate the whole class.

![Table VIII](image)

| Preferred group size | No. respondents |
|----------------------|-----------------|
| 2                    | 4               |
| 3                    | 6               |
| 4                    | 2               |
| 5                    | 0               |

Table VIII. Preferred group size.

Another important matter is the issue of grading in a team-based class. As described above in section III, the instructors gradually scaffolded the competencies during the course and this was reflected in the grading. For example, the first project was graded primarily on the quality of the code as well as successful completion of the project. A key mechanism we established to provide accountability was to require short individual self-assessments to be completed after each project online through Tufts’ Course Management System (Sakai). The questions asked are listed in appendix III. These submissions allowed the instructors to understand who had done what as well as where students felt their own work stood in comparison to the grading criteria. Project submissions were graded as a team, but each student received an individual grade and feedback form—collated and emailed automatically by a *Mathematica* script—including their own self-assessment as a component. The instructor occasionally modified grades if there were sufficient evidence that an individual had failed to contribute meaningfully to a project, though this was used very sparingly.

An overview of the projects, as well as the project descriptions themselves, is provided in supplementary material [27]. A final project, performed in parallel with the last third of the course, was intended as the summative assessment, allowing students to attempt a problem of their own choosing and replacing the final exam of a typical class. A list of project ideas was provided, largely connecting with TJA’s research in Condensed Matter Physics, but included the option to formulate a problem that connected with student’s research field. Some students chose to work individually, others in teams of up to four. The class concluded with a mini research symposium where each group gave a short five minute presentation showcasing their findings. Each student was required to fill out a self-assessment different from the other projects, asking instead how the project demonstrated their professional practice in each competency.

C. Student work

We present two brief case studies of student work that illustrate some of the ways groups creatively engaged with the projects and used visualization to analyze the performance of their program. The first example comes from project 1, the Double Pendulum. In this project, each group implemented a different algorithm, and the project was performed in two stages: first, students used their assigned algorithm to solve the simple harmonic oscillator equations and presented their findings to the class, afterwards they extended their code to solve the double pendulum. The numerical analysis concepts of Error, Order and Stability were introduced in
class, but only the performance of the Euler algorithm was discussed in detail. The group that used the Runge-Kutta algorithm spontaneously conducted an analysis of the discrepancy between their numerical solution and the analytical solution as a function of time-step. They presented the graph shown in fig. 3(a) to the class after the first part of the project, and used the FindFit function of Mathematica to verify that the error was \( \propto (\Delta t)^4 \) as expected. In the second part of the project, they created a similar plot [fig. 3(b)], comparing the solution at a specified \( \Delta t \) to that with much smaller \( \Delta t = 0.0005 \). The graph was annotated in their notebook by the comment,

“show max error and the convergence fit for small \( dt \), which is actually of order 5 in this case. Note that the error is considerably larger, even at small \( dt \), than the more well-behaved single pendulum, and also that the chaos in the system is very evident at larger \( dt \)”

indicating that this group had appreciated that the Runge-Kutta algorithm was performing as expected in some regime of \( \Delta t \), but failing in others, and that the highly nonlinear double pendulum equations were more challenging to solve.

The second example comes from project 6, the Time Dependent Schrödinger Equation, in which students solved a number of classic 1D problems. For their report, most groups presented snapshots of the wavefunctions at different times. One group, however, utilized a kymograph representation to show both spatial and temporal evolution. Two examples taken from their report are shown in fig. 3(c) and (d), both showing the propagation of a gaussian wavepacket as a function of time. Periodic boundary conditions are enforced, so the wavepacket exits from the right and re-enters from the left during the simulation. The two figures represent different algorithms, fig. 3(c) is a non-unitary cell-centered finite difference scheme; fig. 3(d) is a unitary scheme. Paired with these figures was the text,

“By applying periodic boundary conditions, we see the particle exit the frame on the right and reappear on the left, as expected. The results from the two different algorithms are shown in Figure X. Notice how the first algorithm gives undesirable results, such as dissipation and a non-constant velocity of the wavepacket. The second algorithm, however, gives the expected results.”

showing that the students selected this representation to make such comparisons straightforward. The wavepacket in fig. 3(c) clearly changes velocity as the slope of the line changes. The students went on to use this representation to verify time-invariant behavior, i.e. eigenfunctions, as well as reflection from a barrier and crystal.

### V. ANALYSIS

In this section, we present feedback on the initial implementation of the course from several sources. An informal feedback session was held during class and students completed the usual course evaluation required by the university. Furthermore, we asked the experts interviewed to develop the rubric in section \( \square \) to regrade student work to determine whether it aligned with their conception of professional practice.
A. Informal feedback

Students in the final class were asked to collaboratively construct ideas for things to do differently in future classes. First among these were the course requirements, which were kept deliberately minimal in the first iteration. Students thought that the requirements should be Modern Physics due to the presence of Quantum Mechanics projects, an intermediate math class such as Linear Algebra and the second Computer Science class, i.e. Data Structures. We note that many, but not all, students would have met these requirements given the backgrounds presented in section IVA. A second important issue was the level of course credit and class time. The course was initially offered as a Special Topics class worth 1 course credit (equivalent to 3 Semester Credit Hours); students felt that $1\frac{1}{2}$ or $1\frac{2}{3}$ might be more appropriate given the workload, similar to a lab course, and that additional class time e.g. through an associated recitation would be valuable. When prompted by the instructor, students preferred to increase the course credit rather than delete projects. It was felt that an opportunity to cross-examine other groups work would be helpful, first by having students upload their work to a repository, and second by incorporating an after project de-brief. Finally, students requested more structure and scaffolding in the initial projects, including internal deadlines and clearer stages. Following the class, several students noted that they had continued to work on projects initiated in the class; we are aware of at least one project that resulted in a journal publication.

B. Course evaluations

The course evaluation was completed by 15 students. Tufts course evaluation questions use a 5 point scale (Very poor—Less than satisfactory—Satisfactory—Very good—Excellent). Students’ overall evaluation of the course was a mean of 4.47 corresponding to Excellent and compared to a departmental average for undergraduate major courses of 4.1, weighted by enrollment. The mean response to the question “How would you rate the success of the course in accomplishing its objectives as stated on the course syllabus” was 4.40 and “How would you rate the use of out-of-class activities to promote your learning” yielded a mean of 4.20, indicating that the project-based approach was well received. Of mild concern is that students’ responses to a question on the use of in-class time received a lower mean score of 3.73, suggesting that some reorganization of this aspect might be necessary.

Written response questions provided more detail to these views. In response to the question, “In what ways has this course made you think differently or more deeply?”, most students commented on the subject matter, for example,

“this class gave me a glimpse of many different types of interesting physics problems. The range of problems tackled during the class gave me a sense of the range of applications of computation in physics”

“The projects were felt ‘real’. They were non-trivial and felt like the kinds of problems a real computational physicist might work on”

or the problem-solving aspects,

“It was really amazing to get to learn about this approach to solving problems—how to approximate solutions, how to tell how accurate the approximation is, and how to make physics so much more accessible with computers”

“The class made me think more deeply about computation. Instead of being content to write code that gets something done, I think about how the code is getting something done and what methods will be best to reduce error, runtime, etc. This is an extremely useful and marketable class. I could have used this ages ago.”

but also group work,

“Combining coding skills with communication skills was a new and different task for me.”

“I am better at working in groups and I now have an idea of what it is like to do computational physics as a profession.”

In response to “What aspects of this course worked best to facilitate your learning?”, students universally mentioned the projects, which were “super interesting and well thought out”. However, positive experiences with group work was also a theme, in spite of the challenges,

“Group work was great. I say this in spite of my complaints about certain group members. Students were forced, in these projects, to go out and discover how to make a certain approach work. This led to strong engagement and lasting impression.”

“Different groups worked together in different ways, and not all of them were great. But I feel like I really know and like a ton of the people in the class because we were together through the hardest of times. I also feel like I was able to learn a lot of different things from everyone I worked with.”

The final question on how to improve the course provoked a great deal of responses. The vast majority of these repeated topics in the in-class discussion, including the need for prerequisite courses, additional class time and managing group size. Many of the remainder touched on more delicate themes about group work. Challenges
identified included that “there was a TON of variance in ability” as well as others referring to differing levels of effort put in by some students. One student felt that,

“The instructor should more clearly adjust grades of students who don’t participate equally in groups. I have a sense that it was 2-3 students who were consistently bad group members, but it was a definite problem. Without the grade incentive, I honestly think that there’s a portion of students who will just not do the work and coast along.”

Another student suggested additional structure for group work,

“[People] need to be taught time management if they are going to be working in groups. In order to do this, I think that you should have intermediate deadlines for the first few projects (not just the first one), and you should require that students turn in a work plan (including internal deadlines) before they do anything else for each project. Without an authority endorsing this sort of behavior, responsible group members are unlikely to be able to hold other group members accountable.”

Several students also mentioned the need for additional supporting resources,

“I would make sure those of us with less experience have clear resources for information. It seemed like I had no way of figuring out what to do or where to turn sometimes.”

“[I’d like to see] Reading recommendations to get necessary mathematical background”

“I would provide some more background information for people who may not have extensive math or programming background. The Mathematica and python tutorials that were posted were really helpful, so more online resources or ‘crash course’ type things for some of the computational and mathematical methods we used would have been great to get everyone on the same page.”

Overall, feedback from students in both formal and informal contexts suggests that the course was a success, that this form of pedagogy is effective, if intensive, but needs additional support to accommodate students with different course backgrounds as well as more structure in managing group dynamics.

C. Post course grading study

From the initial implementation of the course, we wished to determine whether student work produced in the class satisfied the views on professional practice held by the experts whom we interviewed to create the rubric. Moreover, we wished to establish whether there was evidence that these were acquired during the class itself.

To test inter-grader consistency, we selected two submissions from project 5 that the we felt displayed a large difference in quality, receiving a C grade and an A grade respectively. We asked the experts to grade these two projects, for each competency assigning a label from the categorizations Good—Fair—Poor as well as Insufficient Evidence. The results are shown in table IX. Submissions A and B were clearly distinguished from one another in quality by the graders, but the degree of consistency is different between the two. To find out why, we held a panel with four of the experts in attendance and invited them to discuss their rationale where there seemed to be discrepancies. In discussion, it seemed that most of the difference between graders could be attributed to whether or not they looked at the code to make their distinction or just looked at the report. For example, grader 4 felt that the quality of the implementation for submission A was good, having looked at the code and noted extensive commenting. The other graders had given more weight to the quality of the report. The experts all agreed that submission B represented work of a high quality. In the panel, we asked all the graders whether they felt that submission B accorded with their own vision of expert practice and they answered affirmatively. We therefore established that at least some students displayed evidence of expert practice as articulated by our rubric, and determined additional guidance necessary to promote inter-grader consistency.

To track the work longitudinally, we amended our grading instructions to require examination of the code and asked the graders to grade other projects from the course. Project 3 involving data fitting was not graded because it was substantially shorter and more prescriptive than the other projects. The projects were stripped of information that identified their ordering, and randomly assigned to different graders; each submission was graded by a single grader, and each competency was graded on the same Good—Fair—Poor scale above. In total, 24 submissions from possible total of 49 were regraded.

From these, a mean grade was calculated for each

| Phys. Trans. | Submission A | Submission B |
|-------------|--------------|--------------|
| Planning    | 2            | 5            |
| Implementation | 2            | 5            |
| Testing     | 2            | 5            |
| Running     | F            | F            |
| Visualization | F            | F            |
| Num. Ana.   | P            | P            |
| Phy. Ana.   | P            | P            |

Table IX. Comparison of expert grading of two projects.
project that is displayed in the visualization in fig. 4. This is intended to provide a snapshot of how well students acquired the competencies during the class. Some trends are immediately clear: happily, it appears that after the initial project, the quality of work rapidly improved, and continued to improve up to the last class project (Laplace’s equation). The very swift improvement after the first project suggests that the students already possessed relevant abilities—whatever they were—to do this kind of work, but needed to find out how to apply them. It is possible that the presence of the rubric helped this.

There are differences between the skills: some such as Planning, Implementation and Running seem to have been picked up without trouble. Visualization improved substantially later in the class. Two skills, however, Testing and Numerical Analysis seem to have presented more difficulty. It is important to be careful in interpreting this: it is not necessarily the case that students failed to test their code adequately, though this may be true, but rather that the evidence of testing was insufficiently detailed to the graders. Physical transcription and Physical analysis were also somewhat inconsistent, suggesting that the more abstract competencies are more challenging to students to acquire. In future iterations of the class, additional scaffolding and emphasis should be introduced to address these competencies. It is also clear that the final projects were substantially weaker, in the eyes of the graders, than most of the class projects. In part, this is because the write-ups for these projects were kept very short; it is also inevitable that formulating and executing a project is a much more complex task than solving a prescribed problem. While the instructors were very pleased with the results of the final projects, it appears that in future classes additional time, support and reporting requirements should be introduced to improve the final projects.

VI. CONCLUSION

We present a project-based Computational Physics Course that was designed around expert practice obtained from interviewing faculty and distilled into a rubric that summarizes identifiable features of this practice. A successful initial implementation of the course, together with extensive post course analysis, was also presented as well as matters to consider in future iterations of the course. By having the expert interviewees grade student work produced in the class, it is clear they found evidence of excellent practices that were acquired by students in the class. It is furthermore clear that the rubric can be used as a tool to separate a strong submission from a weak one.

Our work builds upon previous studies of Computing in Physics Education and proposed course structures by providing an concise version of what constitutes expert practice in this discipline, a tool to measure it and a reference implementation. Due in part to the small size of this study, there are remain numerous avenues for further investigation. For instance, a key limitation is that expert practices were self reported and not directly observed. Even so, our interviews complicate simplistic models of expert problem solving originally formulated for introductory classes. At the very least, such models may simply be inapplicable to complex research-oriented problems such as those attempted by students in this class. There is a clear need for more realistic models, of which that presented in fig. 3 is likely to prove a crude initial sketch. Of course, a scaled-up multi-class multi-university study on project-based approaches to Computational Physics is likely to prove deeply informative, particularly since similar techniques are now being tried in introductory classes. Given the central importance of group dynamics to this strategy, which we have shown to be both challenging and rewarding, micro-level approaches such as video observation and interviews with students might help untangle how students participate in group work in this context. Our work also provides a valuable example of backwards course design that may be applicable in physics to domains other than computation, such as laboratories or graduate classes focussed on preparing students for research.

While our study has shown that students taking a single course on Computational Physics can acquire expert practice, the broader question of the role of Computation in Physics Education remains open. Is it best to have a small number of courses such as the one presented that fo-
cus primarily on Computation, is it better to intersperse Computation into many classes, or is a mixed approach needed? Identifying strategies that produce graduates and PhD students well prepared to perform computational work that meets the needs of future research, industry and other careers is surely of considerable benefit to the community of Physicists.

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I. APPENDIX: EXPERT INTERVIEW QUESTIONS

The following sequence of questions was asked in the expert interviews.

1. Can you think of a problem in your research area that might be suitable for an undergraduate computational physics course?

2. Could you explain the physics of the problem?

3. What are the possible computational approaches to solve this problem?

4. What are the advantages and disadvantages of these approaches?

5. Can you tell me what you see as the issues involved in transforming a physics problem into an algorithm or set of equations to solve?

6. Thinking about the problem from earlier, how would you go about planning a computer program to solve this problem?

7. Could you sketch a flowchart for this program?

8. I’m going to show you a page of code. Tell me what you like about the programming, and what things would you change?

9. What do you think constitutes good programming?

10. What sort of visualization strategies do you think are useful? Which do you use and what challenges do you come across?

11. What sort of visualization might you use for the example problem?

12. Using numerical analysis strategies, for example thinking about error, order, and stability, how would you assess the numerical performance of your algorithm?

13. More generally, what types of numerical analysis do you use to analyze the algorithms you employ in your work?

14. How would you use the results of your hypothetical program to perform a physical analysis of the system you are modeling?

15. What else might you consider while trying to come to physical conclusions from a set of computational results?

II. APPENDIX: STUDENT BACKGROUND SURVEY QUESTIONS

This short survey was circulated before the course.

1. What Physics Courses have you taken?

2. What Computer Science or Applied/Numerical Math courses have you taken?

3. What Computer Languages have you used? Which do you feel confident in?

4. Describe your overall experience and familiarity with programming. Feel free to cite projects you’ve undertaken.

III. APPENDIX: INDIVIDUAL SELF ASSESSMENTS

Self assessments were required after each project.

1. Describe your contribution to the project. Identify things that you yourself did.

2. Overall, what grade would you give to your own contribution to the project? (A—Mastery. I think I did this to a professional level; B—Solid understanding. I got this, though there may be still residual mistakes; C—Progress. I’m still working on learning this.)

3. How well did your team achieve the goals of the project? Explain briefly each member’s contribution. Identify any challenges your team faced and how you overcame them.

4. Overall, what grade to your team’s project submission as a whole? (A—Mastery. I think I did this to a professional level; B—Solid understanding. I got this, though there may be still residual mistakes; C—Progress. I’m still working on learning this.)
5. Did your team do anything over and above that required in the project description?

6. If you have other comments on your group’s project, please write them here.

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