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The role of projects in (Computational) Physics Education

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Abstract

Projects are an essential part of any Computational Physics class. They are important for the student who carries them out and, if the project topic is carefully selected by instructor and student, can also assist in the education of other students. In a few cases they can be sufficiently original to make a useful contribution to a research area. Some general ideas and two specific examples are given in this paper.

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1. Introduction

Computational Science, the third corner of the (David) Landau triangle with theory and experiment, requires mastery of both the topic and of the computer. While theory is taught slowly, in traditional sequences and guidance in experimental techniques is often provided by laboratory support staff computational expertise is often neglected in student education. There have been quite a few initiatives to remedy this situation - my favourites being a really special Computational Physics program by Rubin Landau of Oregon State and the material prepared by Harvey Gould and Jan Tobochnik. Some experiments where certain proprietary codes whose names start with the letter M have taught physics to a generation, prepare students who flounder if they need to integrate a function and their package is not at hand. However in large universities where funding is short and physicists conservative, especially those where two or three elementary physics courses are taught, syllabi have hardly changed in many decades - sometimes the only change is a nod to whether the neutrino now has a mass and how many quarks have been found. In this time computational approaches have advanced rapidly and student computational background is varied and constantly changing. Engineering students often have learned quite sophisticated programming and we should be exploiting this to ease the assimilation of physical concepts: one possible approach will be described below. Our graduate students generally learn to compute rather well - the situation where a graduating student takes some aspect of the group's computational expertise with them being well known. We should be using their skills extensively in undergraduate education.

One may ask - how, in an environment of minimal funding and maximal student numbers can new material with a computational slant be introduced such that it also enhances basic physical understanding. Course projects, presented in websites with carefully documented codes are helpful both for the student doing the project and for the following

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generations. After a discussion of general requirements for such projects in computational physics class in the next section and a summary of some recent projects in the following one we present two specific examples in depth. We conclude with a discussion of extending project options to large service teaching physics classes.

Dedication: Kurt Binder, both in his own research and writing and thru the large number of students and junior researchers he has mentored is a giant of our field. His example of concern for his graduates and his efforts towards communicating concepts and applications have had enormous influence on us all. One concept he has encouraged is for the graduate students to maintain the group cluster. This has worked well for all. It is a pleasure to present this paper at the workshop honoring Professor Binder.

2. Project requirements

A good project is one where both the student creating it and other students (both cohorts and successors) can benefit. At the Technion, projects in Computational Physics are given to senior undergraduates (Physics and dual degree students) and to students in the Graduate Computational Physics class, many of whom are from engineering departments. In recent years, projects have been presented as websites where background, algorithms, downloadable code, sets of default or example parameters and typical results are included. Since the first website presented project was submitted in 1998 [1] some hundred more have been prepared. Not all still exist, since unless the project was exceptional, no effort to retain it past the student's graduation was made. Some of the best codes from earlier projects, presented first on diskette and later on an ftp server have been collected into websites, for example, [2]. Others have been incorporated into the webpages for my Computational Physics class, [3].

The methods of preparation of the websites vary from sourcecode html, which is recommended, thru to practically every other possibility with weaker students often presenting their results largely as pdf files. Except for students from the Science Education Department whose sites are aimed at school children, sites must be in the universal language of science, bad English. This issue of website preparation will be discussed further in an appendix.

The Computational Physics project topics vary from parallel algorithms at one extreme, via implementations of algorithms for Computational Physics with clear explanations and examples thru to interactive routines for introductory courses. Students whose research is experimental are allowed to use Matlab for the project, others are expected to use a compilied language. The code must run either on the LINUX machines in our classroom or on the Technion's parallel cluster. Additional windows binaries are encouraged but not mandatory. Visualization is a requirement for all but a very few algorithmically complex projects. Early codes included visualisation with PGPLOT [5] or GL [1]. Later OpenGL/Mesa were used and more recently atomistic simulations have been presented with the Technion's AViz code [6]. One of the main "offlabel" AViz implementations, colored smoke mode (using the AViz dot option), was developed by J. Fox for a project of hydrogen atom electronic density [7] for use in the Modern Physics class. The recent additions to AViz [8, 9] in Version 6.0 have also been invoked with one such example discussed in detail below. For continuum models visualization in Matlab is commonly used, an early example being [10].

3. Examples

One set of projects [3] from the mid-late nineties involved PGPLOT visualizations many of the example routines from the Koonin and Meredith [11] book. Some of these were made into videos and later copied to mpgs. The sourcecode/LINUX orientation has ensured that codes and sites from the nineties remain useful; and there are quite a few series of projects where each extends an earlier one. One such series starts with an extension of the 2D Xtoy Ising simulations of Mike Creutz [12] to the case of an external field and a different ensemble, by A. Geminterm [3]. 3D Ising simulations were then made, and described on the project website with a fortran code with 3D data output to AViz for depth perception with the dot style visualization, [13]. Recently, an MPI parallel C version has been prepared.

Several earlier projects have been presented alone or in combination in proceedings of this workshop or of other conferences, [14, 15, 16, 17, 18, 19, 20]. In Ref. [17] a site used for Modern Physics teaching is described, and the others mainly relate to either algorithms such as simulated annealing or visualization issues. All are planned to appeal to students who will be taking the course in the future and are designed for self-learning. A notable one not presented in the archival literature, but used in Technion laboratory courses is [21]. Two exceptional projects from the most recent Computational Physics class are presented below in detail.

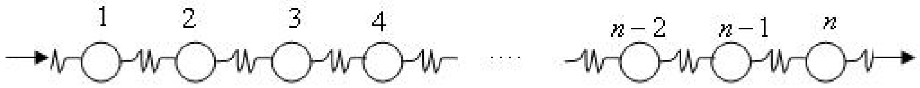

Figure 1: The system of springs.

Figure 2: A snapshot of the system, showing the shorter bonds with a greater thickness.

3.1. System of one dimensional masses with linear springs

This project had dual aims of providing a complete guide to molecular dynamics simulation of masses connected by springs and of exploiting and further exploring the variable bond width feature of AViz 6.0. The system is a one dimensional row of masses, connected by linear springs with given parameters and periodic boundary conditions and is shown in Figure1. A still image snapshot of a simulation of 30 masses is shown in Figure2.

On this project's website [22] in addition to a careful comparison between Verlet and predictor-corrector algorithms there is a routine to turn the output from the simulation programs presented on the site into .xyz input files. for AViz. Animations of the system oscillations are presented on the site, and the AViz 6.0 feature which draws shorter bonds with larger width indded assists in the viewing.

3.2. Nanotube generation

During research for a project that was presented in part at this meeting last year [23] concerning the similarities between nanotubes and certain rolled-up configurations of polymers, we discovered that the standard Dresselhaus picture of nanotubes as rolled up sheets of graphene requires modification for narrow tubes. In particular, the curvature is not correctly described in the standard model.

We soon realised this was not an original discovery and that a detailed study had recently been made by an Australian group in a series of papers [24, 25, 26, 27, 28]. This study, however had failed to achieve substantial recognition in the nano-community where many continued to build initial nanotube samples from the popular websites (mainly for carbon) not based on the correct polyhedral model. Thus an alternative website was desirable. Such a site has been prepared [29] and we will now describe it in detail. The site does not (at the moment) work interactively on the internet but downloadable files can be quickly installed. Visualization is with our AViz code and the program prepares the input .xyz files. Some examples are given in Figure 3. We still need to work on making the code come up higher in search engines.

The new model is known as the general polyhedral model and provides a mathematical basis to obtain far more precise coordinates and radii. Very briefly bond lengths in nanotubes may vary depending on the direction; this has been shown in molecular dynamics simulations. Of course, if one starts from an initial state that is less accurate, eventually a molecular dynamics code will iterate to the correct configuration, but this can cost substantial computer time that could be put to better use.

4. Projects in physics service teaching

Several of the projects described above were prepared for use in a service teaching Modern Physics course for engineers. So why could these students not prepare projects of a more limited scope themselves? The process of providing ideas and support for individual undergraduate projects, or for a relatively small number of graduate Computational Physics class students is quite distinct from carrying out projects with a several hundred student Modern

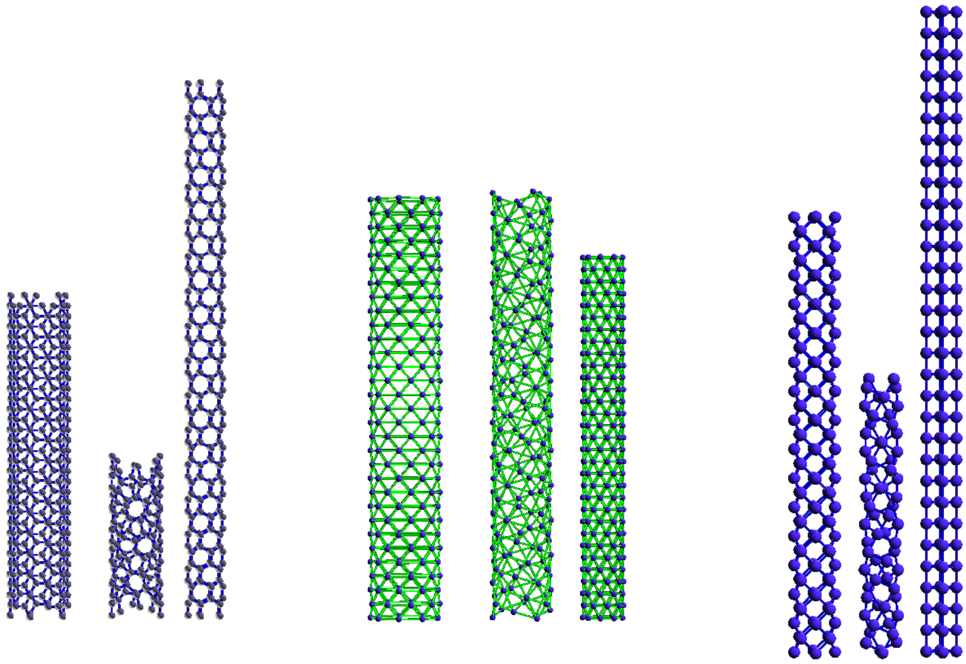

Figure 3: Left to right: Carbon, boron and silicon nanotubes.

Physics class that has a single teaching assistant. However the potential gain, both in student enthusiasm and the possibility to create useful material in Hebrew is considerable.

Offering these service course students the opportunity to prepare projects is a worthy goal. A first attempt at this was amusing (mainly in retrospecct and to others). Only a small fraction of 300 hundred extremely apathetic students in a Modern Physics bothered to attend lectures about superposition of waves, in preparation for group velocity and wave packets. Adding to functions is well within their mathematical/computational skills but several years of suggesting they do this failed to meet with any response. Hence a new tack. An announcement midway thru class of bonus points for the first 3 students who send a code (by email) for superposition of waves, was expected to yield a few over the next week. Several of the best students must have left early, because immediately after class there was a flood of emails arriving at an alarming rate. An announcement that no more would be accepted was immediately sent, but those which had come in did have to be considered for bonus points. Fortunately the announcement that group projects would get the points divided among the students slightly minimised the number of responses.

There were many different approaches. Our undergraduate's favourite excel spreadsheet, all the M packages, but also compiled codes and my favorites, links to webpages which enable interactive use of gnuplot. A website listing these has proved useful to later students.

To be fair to those who did not think of leaving class early to get in first, a different project was offered a few weeks later where all who submitted by a certain date would get a smaller number of points. To encourage lecture participation names were collected at one class to determine how many to prepare and a few weeks later cards with the projects we handed out - only to those present in class - (in the first year mainly about Nobel prize winners mentioned in Modern Physics) at random. This went better and is continuing with a variety of themes (this year we had application of Modern Physics concepts and the research of people who had units named after them). The process seems to both generate useful material and motivate the students to attend class.

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to place it on record.

5. Appendix - website preparation technicalities

The Computational Physics undergraduate or course projects are required to be placed on websites; students are given accounts on the Computational Physics (Linux) webserver or may use another of their choice. While a fair amount of freedom is given in site preparation, sourcecode html is strongly recommended. A template is provided and help is given as required to implement it. We initially began this in part as a way to train our graduate students (who are also teaching assistants) to work with websites. Since the project as website began in the late nineties, The Technion Physics Department has gone thru WebCT, our own locally programmed homework system and several versions of Moodle. Only the sourcecode material is still accessible beyond the current Moodle, and it is the only one that has ever been accessible from beyond our firewall.

Although the undergraduates may also use html, the logistics of 40 odd undergraduate student websites submitted in a few days are such that pdf submission via email is encouraged. Note that the undergraduates mainly present in Hebrew and Hebrew websites have a whole additional spectrum of problems both with bidirectional requirements and Hebrew fonts that distract from the science.

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