Guest Editor's Introduction

Computational Science and Engineering Education

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***Abstract*—This special issue presents experience reports on computational education in various subjects of science and engineering. They include descriptions of early and current general courses at undergraduate and early graduate levels, as well as some computational exercises for specific courses. General computer science courses were intentionally excluded, because our emphasis is on applications of computers to science and engineering subjects.**

OVERVIEW

Despite the enormous impact of computers in our lives, and their frequent use in the administrative side of education, most university course syllabi have barely changed over the years to reflect this. These days, most students have a required computing course, but it rarely is placed in context of their other courses or teaches relevant numerical algorithms for their field. Faculties around the world justify the lack of computational aspects in their courses with excuses like: it is too time-consuming and disruptive; we do not have funding; this is how it has always been. Such explanations could be due to lack of knowledge and therefore confidence on the part of the lecturers. Good faculty development and availability of support materials can help overcome this. It is also a good idea to bring the students' knowledge into class content; e.g., by giving them a challenge in advance to answer a specific question.

This issue's articles highlight courses in computational science and engineering, within traditional degree programs. A type of course covered in CiSE before is the introduction to high-performance computing (HPC).[1] Less emphasis is placed here on computer science courses, or degrees and certificates in computational science and engineering. Providing students with computing expertise in one or two courses is the challenge we choose to address here.

A 2006 special issue of CISE[2] addressed Computational Physics education, either via the additional course or two, or an entire degree; one example of the latter is long-time CiSE editor Rubin Landau's article in that issue. The present issue has a more general coverage, but the context is similar.

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PAST AND PRESENT COMPUTATIONAL SCIENCE AND ENGINEERING COURSES

This list cannot be all-inclusive and apologies to authors of work not mentioned here. Several well-funded initiatives exist aimed at course development with integration of science and engineering material with computational support, for example, a national initiative in Norway.[3]

Computational physics courses going back to the 1980 s have been described in the archival literature. Steve Koonin wrote an article about his courses in several languages with the first in BASIC dating from 1983 at Caltech.[7] Peter Bocherds taught a laboratory-format course in computational physics since about 1984,[4] and CiSE Associate Editor-in-Chief Steven Gottlieb taught his class since 1987.[5] I have been teaching a similar course since 1988, which I described in a 2014 article.[6] Although developed independently, these courses have similar features, such as hands-on experiences in class. Many such courses have been developed, in some cases leading to the writing of a textbook. Notable examples include: the early book in True BASIC by Gould and Tobochnik;[8] a 1997 tome by Giordano,[9] and Joaquin Marro's material in Spanish.[10] In more recent years, Titus Beu[11] published an excellent book with Python and C/C++ code.

Many of the older courses and books have an implicit orientation toward end-use of HPC, as indeed do I. Today, new educational efforts emphasize programming ease, relying on open-source environments and tools such as Jupyter,[13] with diverse examples in science and engineering; many of these have less of a physics orientation than the texts mentioned above.

IN THIS ISSUE

The articles in this special issue cover a wide range of subject areas. The issue had an open call for papers, and was advertised in CiSE and at several computational physics meetings, plus via few personal letters from the guest editor. The response was wider than expected and several good manuscripts had to be declined.

One of the most exciting aspects for me is the number of female authors, and another pleasing observation is the range both of countries (USA, Chile, Russia, and Northern Ireland), and of fields, which ranged from engineering, physics, chemistry, to video game development. Authors came from academic and industrial research centers and a range of universities of different types.

Articles include "Preparing a Computationally Literate Workforce" by Scott Lathrop, Katherine Cahill, Steven Gordon, Jennifer Houchins, Robert Panoff, and Aaron Weeden, from several universities and the Shodor Education Foundation. This is a general article with an HPC orientation, and discusses virtual shared courses. A more specific topic is discussed in "Artificial Intelligence and Mobile Programming Courses for a Video Game Development Program in Chile," by Nicolas A. Barriga and Felipe Besoain from Chile, presenting curriculum design for two third-year undergraduate courses. Another undergraduate course for noncomputer-science students is Lorena Barba's (CiSE Editor-in-Chief starting this year) "Engineers Code: Reusable Open Learning Modules for Engineering Computations," which uses Python and Jupyter and includes modules for first-time programmers.

At the graduate level, there is Cathryn Peoples from Northern Ireland's "Research-Based Education on a Master of Science Degree in Professional Software Development." Research-based education describes the application of the results of research to facilitate and complement student learning.

Finally, there are two articles concerning natural science computational education. Polina Pine of Loyola University in Chicago (based on a pedagogical method from Russia by Liudmila Ivanovna Paina) wrote "Computational Methods in Chemistry and Biochemistry Education: Visualization of Proteins." This article gives an introduction to the use of VMD with clear instructions to give students. Amy Lisa Graves of Swarthmore College and Adam Light of Colorado College present "Hitting the Ground Running: Computational Physics Education to Prepare Students for Computational Physics Research." This article discusses which computational skills might be best learned in the curriculum (prior to research) versus during research.

Please read and enjoy the special issue and keep CiSE in mind for future articles about your own courses and material. CiSE has an Education Department to host such articles on an ongoing basis.

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