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Computational Physics : An Introduction

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Abstract : Computers are playing an increasingly important role in the lives and education of physicists. Several areas in physics have problems which cannot be treated exactly or analytically and must be solved numerically. Computational physics allows developing models of physical phenomena and understanding things at depths greater than possible otherwise. It enables learning physics with computers. This paper provides a brief introduction to computational physics.

Keywords: **Computational Physics, Computer Experiment, Numerical Experiment**

I. INTRODUCTION

Since the beginning of the computer era, physicists have been at the forefront of computational science. They used computers to solve a practical problem important at that moment: to develop thermonuclear weapons. The work was implemented on the MANIAC 1 mainframe computer in Los Alamos [1].

Computational physics (CP) is part the general area of computational science. It deals with applying numerical methods in solving physical problems. It supplements theoretical physics and experimental physics, the three common ways of solving problems in physics. Since most physics problems are difficult to solve exactly or may be nonlinear in nature, CP involves computer simulation and is often regarded as "computer experiments." It is possible to find a computational branch for every field in physics, e.g. computational mechanics, computational electromagnetics, computational electrodynamics, computational fluid dynamics, computational statistical physics, computational particle physics, computational astrophysics, and computational solid state [2,3]. Topics covered in a regular course on CP include differentiation, integration, Fourier analysis, data fitting, nonlinear least-squares fitting, Monte Carlo methods, and Runge-Kutta method [4].

II. ROLES OF COMPUTATION PHYSICS

Besides its application to studying physical phenomena, computational physics plays other key roles [5]:

• It develops our understanding of the basic physics and clarifies the importance of physical effects
• It allows developing models of physical phenomena and understanding things at depths greater than possible otherwise.
• It solves actual physical small-scale or bigger problems
• It helps us to learn to compute better and ask more penetrating, relevant questions

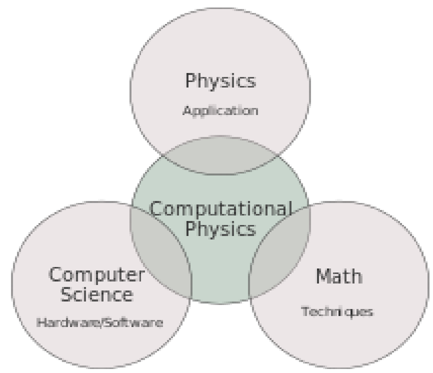

Figure 1 – Relationship between CP and other related disciplines [2].

III. APPLICATIONS

Computational physics provides solution to linear and nonlinear systems of equations, ordinary and partial differential equations, Fourier transforms, stochastic processes, and Monte Carlo methods. Depending on whether the researcher is a born digital or digital immigrant, programming languages used in computational physics include FOTRAN, C, C++, and Python. The researcher develops self-contained programs in any of these high-level scientific languages. One could also use a mathematical software package, such as MATHEMATICA, MAPLE, EXCEL, or MATLAB. A thorough discussion on these languages and software packages can be found in [6].

IV. CHALLENGES

In spite of the several CP textbooks available in the market, developing a curriculum including computational physics in a meaningful way is not straightforward. One may be compelled to teach topics that should normally be covered in mathematics and computer science since students may not be prepared on those topics. Figure 1 shows the relationship between CP and other disciples [2].

Another problem is deciding whether the student should program themselves or use existing software. One may assume that commercially available software packages would the best method for student efforts because they would prevent the students from becoming bogged down with direct programming.

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However, experience shows that some of the packages may be difficult to use and will distract students from learning [7]. It is hereby recommended that students should be allowed to use advanced products of computational tools for investigation of only complex physical phenomena appropriate for building virtual laboratories. Simulation in virtual laboratory helps in understanding complicated processes [8].

V. CONCLUSION

Physicists have realized the power of computation in both physics and education. They have integrated CP in physics curricula and written CP textbooks [9]. Some universities even offer a four-year curriculum leading to a bachelor's degree in computational physics [10]. Although only time will judge the viability of programs such as this, a carefully developed course on CP can contribute to the goals of a liberal arts curriculum in a unique manner.

Computational knowledge from one researcher to another is transmitted through conferences and journal. The *Journal of Computational Physics* publishes research works on all aspects of numerical solution of physical problems.

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