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Educating the next generation of Computational Physicists

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Abstract

Many “senior” Computational Physics researchers began their careers perched on of the other vertices of the Landau triangle as either theorists or experimentalists. It is now 25 plus years since the first textbooks on Simulational or Computational Physics appeared. Has the phase transition into the reality where Computational Physics is an integrated part of Physics Education occurred? Results from surveys of student knowledge at the start of the courses and from final course projects in Israel from 1994 to 2013 will be presented.

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1. Introduction

David Landau has proposed a much quoted (eqilateral) “triangle” with vertices for simulation, theory and experiment, see Figure 1. A few of us began our research careers on the Computational/Simulational vertex from the start - even if we did not call it that. Others began as experimentalists or theorists, and many researchers who use Computational Physics today still prefer not to be named as such. This retinence is not unique to physics, but it is less entrenched among engineers. In fact many good computational physicists have made their homes in engineering faculties. Of course the situation varies country to country and university to university.

It is at least twenty five years since the Simulational/Computational Physics community began to organise itself. DCOMP of the American Physical Society was founded in 1986. Since 1989 there have been joint APS-EPS “Physics Computing” conferences, although the formal organization of the C20 Commission of IUPAP came ten years later. The 26 workshops on Computer Simulation Studies in Condensed Matter Physics at UGA span this period admirably. It is also some 25 years since a large number of influential Computational/Simulational Physics textbooks were published and many universities began to provide at least one Computational Physics class to physics students. A delightful account of an early Computational Physics class was provided by Peter Borcherds (see Figure 2) in an article published in 1986 [1]. At the recent CCP2012 in Kobe, Steve Gottlieb presented a paper on “From many students per VAX to many cores per student”[2]. Indeed, in this quarter century there have been dramatic changes in computer power, and there has been an evolution of the student level, not always in a positive direction from the High Performance Computing viewpoint. I will not emphasize hardware aspects, except where directly relevant to educational issues, but the move from batch computing to personal computers and its implications cannot be avioded in any discussion of Computational Physics education.

Is Computational/Simulational Physics substantially closer to recognition as an “equal” corner of the equilateral triangle? Do other science and engineering disciplines share these concerns?

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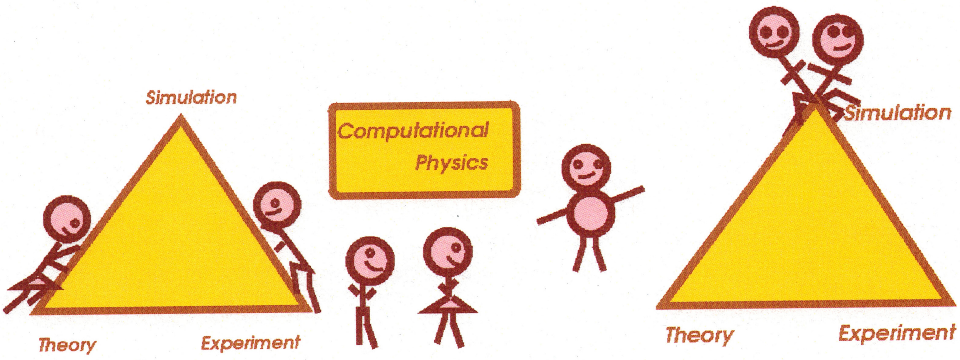

Figure 1: Left, some researchers began as experimentalists or theorists, center, today some are taught computational physics early in undergraduate studies and then, right, start research directly in computer simulations.

Figure 2: Left, students trained already in Computational Physics can train the next generation. Center, early Computational Physics class, taught by Peter Borcherds in Manchester[1] and right some of the early computing equipment, clockwise - computer tape of my Ph.d. codes, undergraduate sliderule, paper tape and computer cards.

2. What is a good Computational Physics course?

The best situation would be that all undergraduate courses would be given in the same computer oriented framework, e.g. University of Oslo[3]. Quite good, is a numerical methods/computational class near the begining of undergraduate study, then active computer related homework with proper support throughout undergraduate education. Better than nothing is an optional numerical methods/computational class near the end of undergraduate or in early graduate school. Passive computer use with support - websites, automated homework etc that most universities provide today is not computational physics. Far worse is active computer related homework without proper support - very frustrating for students. I think that selecting one program, e.g. MATHEMATICA or MATLAB for all (or all physics) undergraduate courses is also bad, because student usually do not learn algorithmic aspects and are unable to function when such code is not accessible later on.

In the physics department at the Technion, we have today the "better than nothing option" with a single optional graduate/senior undergraduate course that spans basic numerical analysis to elementary parallel coding. This course is based on a synthesis of the Gould and Tobochnik (GT)[4] and Koonin and Meredith (KOONIN) [5] texts, with some original material and FORTRAN/PGPLOT adaptions of all codes used. It is not all that different from either Borcherds' or Gottlieb's courses in principle, and covers all areas of Computational Physics, not just a course limited to Statistical Physics based topics as is often given. The students conclude with a project. I wrote about selected projects last year [6]: they are either based on a computational aspect of their research (graduate students), or prepare