

Education for Computational Science and Engineering

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Abstract

Computational science and engineering (CSE) has been misunderstood to advance with the construction of enormous computers. To the contrary, the historical record demonstrates that innovations in CSE come from improvements to the mathematics embodied by computer programs. Whether scientists and engineers become inventors who make these breakthroughs depends on circumstances and the interdisciplinary extent of their educations. The USA currently has the largest CSE professorate, but the data suggest this prominence is ephemeral.

Computational science and engineering (CSE) embodies the challenges in President Obama’s vision of the future, “ours to win” [1]. Wealthy nations with comparable scientific institutions can achieve parity in technical prowess. When countries have similar populations of technical professionals, one way to excel is to make better use of expert talent through computing. Research and development (R&D) proceeds more quickly and with greater certainty by using computers to analyze information and to pursue the implications of scientific theories.

The preceding “elevator speech” has been heard in Washington before.¹ From “NSF Plans Help with Big Computer Problems” [2] in 1985, through “Energy Labs Urged to Boost Supercomputing Capability” [3] in 1997, to “An Endless Frontier Postponed” [4] in 2005, CSE has been used to justify the purchase of massive computers — and is being used again, in President Obama’s budget. To the contrary, the fastest computers are irrelevant to the innovations in CSE that bettered peoples’ lives and transformed how R&D is done.

The breakthroughs in CSE are the mathematical programs of computing, not the machines themselves. President Obama misunderstood the “Sputnik moment” when the People’s Republic of China (PRC) built “the world’s fastest computer.”

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¹For a brief history of CSE, search the text of articles in *Nature* or *Science* for the exact phrase “computational science.” For a more detailed timeline, search for “supercomputer.”

Japan and the USA previously built such machines to little effect because availability of the fastest computers is severely limited by cost [5]. The cost of the absolutely fastest machines remains high even though their composition has changed. The extreme engineering that once made computers fast was overtaken by silicon miniaturization for the mass market. Today's fastest machines are merely huge "clusters" of commodity devices working in parallel [6, 7], which many research groups can acquire in small configurations [8]. These cluster computers were predicted to be difficult to use [9, p. 458], and have proven so.

At present there are two paths to achieving great speed. Either computer programs might be written to excel on clusters, or special chips might be built for one type of calculation. (Examples of specialty chips are in cell phones and game consoles.) Programming skill is also critical for the special-purpose chips because likely programs must be well characterized before building silicon to suit. The scientific literature has examples of both approaches for calculations of molecular dynamics [10, 11, 12]. The flexing motions of large molecules affect their reactivity [13], so these calculations reveal how molecules are biologically active.

The importance of clever programming begins only after there is something to write a program about. The prerequisite mathematical invention often is obscured by the continuing work to keep up with computing practice. For example, at the turn of the 19th century, A. M. Legendre and C. F. Gauss [14, 15] invented what is now called regression analysis, which is used to infer parametric models in diverse fields such as econometrics and epidemiology. Gauss in 1810 [16] also invented a way to calculate regression coefficients by hand that was used for 150 years, with modifications for various types of manual computing [17, 18]. G. H. Golub in 1965 [19] invented a better way for electronic computers. Today, Golub's method is found in libraries of computer programs, where it evolves with programming techniques [20, 21].

The example of regression analysis illustrates that the paramount breakthroughs in CSE are the mathematical inventions that live through generations of computer programs. These advances come from researchers who learn to work with mathematics across disciplinary boundaries [22]. Prominent examples are: (a) a fast method to evaluate convolutions was invented by two polymaths working in statistics and computer science [23]; (b) a method for inferring structures of proteins from x-ray diffraction patterns was invented jointly by a physicist and a mathematician [24, 25, 26]; and (c) a method for identifying the current state of a dynamical system was invented by a control engineer and refined by a programmer for the tiny computers on early space vehicles [27]. Some of these inventions enable scientific

research, while others are ubiquitous in daily life; the importance of the inventions (a, b, c) is discussed in [28, 29, 30], respectively.

Whether scientists and engineers become inventors who make CSE breakthroughs depends on circumstances and their educations. Success in President Obama's challenge is not decided by the fastest computer, but it may be decided by the size and quality of the CSE professorate. To that end, a census was made of educators who are experts about calculations and the mathematics of a science or engineering field. (The census is described in the Appendix.)

The USA currently has the largest CSE professorate (column 1 in **Table 1**), but the data suggest this prominence is likely to decline. The European Union (EU) already has many more CSE educators than the USA and the same number per capita (column 3). European and Asian countries known for exporting manufactured goods have more CSE educators per-capita than the USA; in contrast, the USA exports mostly agricultural commodities. While the People's Republic

Table 1: (Column 1) populations of educators specializing in CSE, (column 2) general populations, (column 3) ratio of CSE to general. Countries are ordered by decreasing ratios. **Bold** are countries with more CSE educators per-capita than the USA. Many of these countries (*) are members of the EU; Hong Kong is an administrative region of the PRC. Ratios for Japan and PRC may be suppressed by undercounting the scientific literature written in non-Latin alphabets.

	POPULATIONS (USA = 100)		
	CSE EDUC.	GEN. POP.	RATIO CSE/GEN
Hong Kong	12.3	2.3	5.4
Israel	13.4	2.5	5.4
Singapore	5.6	1.6	3.5
*Austria	8.4	2.7	3.1
Switzerland	5.0	2.5	2.0
Canada	19.0	11.1	1.7
*Germany	40.8	26.5	1.5
*France	31.3	21.3	1.5
*United Kingdom	26.8	20.1	1.3
USA	100	100	1
Australia	7.3	7.3	1.0
EU combined	165.4	162.3	1.0
*Netherlands	5.6	5.4	1.0
*Italy	15.6	19.6	0.8
*Spain	10.1	14.9	0.7
Japan	12.3	41.3	0.3
PRC	54.2	433.6	0.1

of China (PRC) continues to develop a manufacturing economy, it already has the second largest number of CSE educators of any country.

The greatest influence on CSE education is the supply of educators. Whether the USA can sustain the present level of effort is moot because over half the current professorate earned the baccalaureate degree outside the country (**Figure 1**). As enrollments by foreign students fluctuate [31], preeminence in CSE for the USA may depend on extraneous factors such as immigration policy.

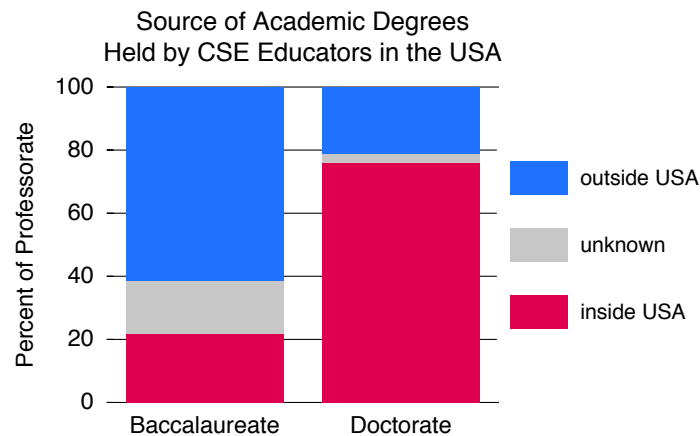


Figure 1: *Country of origin for academic degrees held by CSE educators in the USA. Most CSE educators earned baccalaureate degrees outside the country, which suggests that the immigration of academically talented individuals is critical to the continued prowess of the USA in CSE.*

What universities do control is the content and quality of education. CSE poses a unique combination of difficulties. The first is, knowledge of using computers in a scientific or engineering field does not suffice to extend the methodology. As seen in the prominent examples above, advances in CSE require a combination of mathematics, computer science, and disciplinary (or domain-specific) training. Second is, academic departments for mathematics or computer science do not serve as nuclei for CSE education. Elite mathematics departments in the USA shun interdisciplinary subjects [32, 33, 34]. Computer science departments do have interdisciplinary research interests, but mostly apart from CSE [35, 36]. Mathematics and computer science departments also have declining matriculations [37, 38], which impedes accepting new responsibilities. Third is, interdisciplinary educational programs do not automatically follow from interdisciplinary research programs. University administrators in the USA are adept at encouraging interdisciplinary research [39]. For example, the National Science Foundation built computer centers to support research faculty in the Cold War. However, early in the age of cheap

computers it was foreseen that CSE education would have to be addressed directly [40, 41].

As a consequence of the hurdles to establishing educational programs for CSE, the 108 universities in the USA with very high research activity [42] have a total of just 37 programs for CSE education (**Figure 2**). Illustrating the diversity of administrative structures: a few programs are departments, e.g. [43], while others are interdepartmental institutes with their own degree programs, e.g. [44], and still others are subjects of emphasis for degrees in participating departments, e.g. [45, 46]. These programs are discussed in a small and thinly cited literature [47, 48, 49]. In comparison, the field of bioinformatics is younger than CSE and is already well represented by degree programs and departments in schools of medicine and public health [50]. Considering the historical contributions that CSE has made (which enable all manner of commercial, consumer, medical, military, and scientific devices), the future appears to be the United States' to lose.

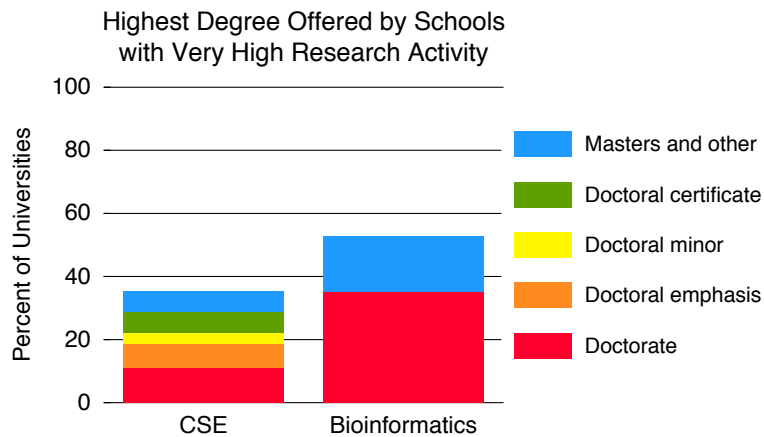


Figure 2: *Highest degrees in CSE and in bioinformatics offered by the 108 universities in the USA with very high research activity. Many more schools have established education programs for bioinformatics than for CSE.*

Appendix

This appendix describes how data were gathered for **Table 1** and **Figure 1**.

Educators are identified from their publications in the database of *Zentralblatt für Mathematik und ihre Grenzgebiete* [51, 52]. The selection criteria are that publications belong to topical classifications 65 or 68 (numerical analysis or computer science) and simultaneously one or more of 60, 62, 70–94 (applied mathematics of

biology, control, information, mechanics, optics, statistics, etc.). Most publications appear outside core mathematics journals as indicated by the database name. Educators are chosen with ten papers in the decade 2000–2009 as evidence of recent, continuing research and to keep the sample manageable. These criteria identify 766 individuals, all of whom are associated with academic institutions.

For perspective on the sample size of 766 CSE educators with ten research publications: (a) the Society for Industrial and Applied Mathematics has a CSE activity group with 936 non-student members, (b) the entire field of probability and statistics (which underlies much research methodology in life sciences) has 2826 authors with ten or more publications, and (c) CSE has 3546 authors with five or more publications.

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