

A Multi-Discipline Discipline

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You may have heard the term “computational science and engineering” bandied about recently. It is growing in use as a convenient way to describe the collective term for much of the multi-disciplinary work that has its roots in work with computing. **Computational Science and Engineering** is being widely used to refer to those aspects of scientific and engineering work that are critically dependent on the use of computations.

The area of computer simulation and associated model development is one key element of this. Other areas involving the processing of very large scale scientific data sets and especially when data feeds from different instruments such as particle physics experiments or remote sensors such as satellites are involved. Simulation itself is often called the third branch of science after “experiment” and “theory”, and often a large scale numerical simulation is formulated to test a particular aspect of a theory and may well produce output synthetic data that must be analysed in a similar manner to real experimental data.

Computational engineering often involves the use of simulations or design tools that support inquiry into “what-if” questions about large or complex systems that would otherwise be infeasible with the use of computational methods.

In some sense computational science is now almost a tautology with the present high levels of involvement of computers in so many aspects of scientific inquiry. The term “computational science” is therefore best reserved for only those aspects where the computations are a fundamental part of the work, rather than just being standard IT aids such as word processors, databases or spreadsheets.

There has been growing recognition of the role of “computation and “simulation” as parts of science and engineering that are now critical to economies and the human endeavour in general. The high-performance computing community has long been a particular proponent of this recognition and many of the so-called grand challenge problems such as weather forecasting, climate change prediction and the study of large scale complex systems such as economies and social phenomena are major users of high-performance computational approaches.

Two recent visionary documents support the role of computational science and engineering in broad terms. Firstly the 2005 report of the USA President’s Information Technology Advisory Committee (PITAC) on “Computational science: Ensuring America’s Competitiveness” [PITAC] presents a large set of application examples of where computation is already having an impact on America’s economy. It also points out the problems in producing enough “computational scientists” if it is not recognised as an actual discipline in American educational institutions. A more recent (2006) document from a multi-disciplinary group of experts assembled at Microsoft’s Cambridge Research Laboratories presents views on the role on computational science as part of the vision for what science and engineering will be occupied with in the year 2020 [2020].

Other documents that make reference to Computational science are the SIAM Report on Graduate Education [SIAM] which discusses the role of formal education programmes in the new discipline, and also the Atkins report on Cyber-infrastructure [CYBER] which describes (USA-centric) views on the roles of the Cyber-Infrastructure for computational science and engineering.

There have been some regular publications in the field already. The excellent practitioner magazine “Computing in Science and Engineering” grew out of a previous IEEE publication called “Computers in Physics.” It has some very good cross-disciplinary and applied articles on techniques and software such as the systems our IIMS authors have described in this newsletter in recent months. Some textbooks with titles like “Introduction to Computational Science” are now appearing – surely a sign that the discipline is gaining credence.

It is not clear whether Computational Science and Engineering should be recognized as an **undergraduate discipline**. It may be hard to achieve sufficient depth and breadth in an undergraduate degree programme. I do believe however that we will see some excellent **postgraduate programmes** spiring up globally under this label. These will provide a postgraduate route for graduates from all sort of numerate science or engineering based undergraduate degree programmes. I am not sure what individuals graduating from such programmes will want to call themselves however.

IIMS is well-positioned to take advantage of the growing global interest and recognition of computational science. Our programmes already provide a good undergraduate grounding in the area. They also offer a powerful springboard to postgraduate study in computational science and engineering.

References:

- [PITAC] **Computational Science: Ensuring America’s Competitiveness** – Report to the President, June 2005, President’s Information Technology Advisory Committee(PITAC) www.nitrd.gov/pitac & www.ostp.gov/PCAST/pcast.html

- [2020] **Towards 2020 Science**, 2005, a background report & special Issue of “Nature.” research.microsoft.com/towards2020science/background_overview.htm

- [SIAM] SIAM Report on **Graduate Education for Computational Science and Engineering**, <http://www.siam.org/students/resources/report.php>

- [CYBER] NSF **Atkins Report on Cyber infrastructure**
www.communitytechnolog.org/nsf_ci_report/report.pdf