Chapter 20
The State of Development of CSE

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ABSTRACT

Computational Science and Engineering (CSE) is an emerging, rapidly developing, and potentially very significant force in changing scientific practice by offering a "third way" of carrying out research in addition to, or indeed, instead of, theory and experiment. It is unlikely that such a significant change can continue to be accommodated by the organizational structures that were put in place for other established research practices. This chapter will explore how research practices are changing to accommodate CSE and how that in turn may further affect structures designed to organize, co-ordinate, and fund scientific research, the most obvious change being the proliferation of cross-disciplinary collaborative teams. The chapter will end by considering what impact these changes have on ideas of professional and ethical best practice.

INTRODUCTION

'Computational Science and Engineering' (CSE) is an emerging field of scientific activity. We stress the 'emerging' because, as will be seen, whilst there are strong developments producing parallel transformations in the state of scientific practice, these are often independent of each other, are uneven in the pace and level of their development, and are embedded in and distributed across a range of specialized environments. In our view understanding the current state and assessing the prospects of CSE requires attention to organizational issues which surround its practice and influence its form.

CSE is a relative newcomer on the academic scene but is bound to have increasing effects on the way in which science is conducted because of the (still) rapidly increasing power, lowering costs, advancing capacities, and ubiquitous availability of computing resources. Computational science enables a third new means of discovery in the

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natural sciences in addition to experimentation/observation and theory. Computation, through simulation, is increasingly used to explore complex systems that are (relatively) inaccessible to experiment or observation because of scale, cost or technological difficulties. Computational simulations are based on mathematical models embodying theoretical understanding from the scientific discipline and, where possible, results are validated against observational/experimental data. With valid computational models 'virtual experiments' can produce new findings. However, this practice is not consistent across all areas of science, for example in some areas of mathematical simulation such as astrophysical simulations which aim is to explore all possible universes the comparison to our universe through observational data is not always important (Leng, 2006).

Because CSE is pitched at the leading edge of scientific and engineering research and also at advanced levels of computing developments it is, by its nature, necessarily interdisciplinary. In a world of globalised internet access amongst researchers, CSE, from its beginnings, has been a means of inter- and multi-national research collaboration. Equally, by its very nature, CSE involves interdisciplinary collaboration between computational specialists, on the one hand, and specialists from one or more scientific research disciplines on the other in order to produce meaningful results. Other communities (such as vendors or service providers) are stakeholders in these activities and can have influence on them even though not normally active in the scientific part of the collaboration.

This can mean that the development of CSE as a recognizable and distinctive area of work does not yet have a strong institutional identity or organizational coherence. This is reflected in the fact that there is as yet little sound data on the extent to which CSE has developed as a distinct discipline in the UK (EPSRC & DFG, 2005) and there are as yet few degree programs or textbooks dedicated to the field, although there is no question that in the USA and in the UK[1] and Europe the presence of CSE is increasingly felt. Thus, although CSE is catching on, it has not yet become a strongly coordinated development since the exploitation of CSE and the conditions of its development has been very much a distributed process, with CSE researchers being located in existing research structures (university settings most prominently) and therefore tied to either the organization of university IT service arrangements or to IT service arrangements within specific research departments.

Computers are ever more prevalent and powerful so computational science utilizes desktop machines as well as high performance computing (HPC) for more than simulation (e.g., statistical analyses and data-mining). Over time the techniques used in CSE have broadened as more academic disciplines use computers for research purposes. CSE is currently the most accepted term for this type of research, subsuming the terms *computational science* and *scientific computing* while possibly waiting to be replaced by the term *eScience*. While social scientists are still not great users of academic HPC services or CSE there is an adoption pathway from the natural sciences through to the social science, humanities and arts in the Western world, via central government funding for the development of eScience. Equally there is an adoption pathway from the developed world to the developing world. CSE's name will no doubt continue to change as new disciplines take up and advance its practice, producing divergent fields such as the computational humanities, or as it ceases to be a distinguishable element within the research disciplines it has been transforming such as bioinformatics.

Some consider data-mining to be an independent research paradigm, but though there is validity to such a viewpoint, there can be benefits to including it with the CSE research developments as part of a single research paradigm - *computer aided research*. All require computer resources, management of those resources and