The Future of UK Supercomputing

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The nature of research in science and engineering has changed over the past two decades – from an activity based almost entirely on theory and experiment, to one based on theory, experiment and computation in comparable measure. Computational simulations are now indispensable for the numerically oriented fields of research, such as climatology, earth sciences, particle physics, cosmology, astrophysics, chemistry, materials, fluid dynamics, atomic and molecular physics, plasma physics, nanoscience and biomolecular sciences. The increasing sophistication of mathematical models and complexity of simulations, along with continuing improvement in computing power, has made it possible to address new scientific questions, which in turn increases the demand for greater computational resources.

The fundamental principle of the UK's long-standing strategy, as re-stated in the Strategic Framework for High End Computing issued by the High End Computing Strategy Committee (HSC) in June 2003, is to provide national general purpose high performance computing systems at a world-class level, with more specialised systems to address particular scientific questions. This strategy has evolved with time reflecting the changing requirements of the scientific community, the development of the technology and the need to ensure value for money. Greater emphasis is now placed on capability rather than capacity computing and on the establishment of a service, which includes not only the system itself but the facilities management of that system and the provision of Computational Science and Engineering (CSE) support.

There has been much debate on the definition of capacity and capability computing! My own attempt to articulate the difference is as follows. Capacity computing is sufficient for the high throughput of a large number of simulations, each of which addresses a relatively small problem size. It can be provided using the distributed computer infrastructure at departmental and university level, access to which will be enabled by the emerging e-Infrastructure. Capability computing on the other hand is needed for simulations that address much larger problem sizes. Such simulations, which require high communication bandwidth and low latency times, can only be achieved in a viable timescale by a high performance system and not by using a distributed computing architecture.

Of crucial importance is not the theoretical peak performance of a system or its sustained performance according to Linpack, but the sustained performance of scientific codes. CSE support is therefore vital, and accordingly its level was increased for the HPCx service, with a further increase planned for the proposed HECToR service. For HECToR there will also be much greater use of a suite of scientific codes to evaluate the performance of the system, supplemented with industry standard benchmarks from the HPC Challenge benchmark suite. A personal aspiration is not to run the Linpack benchmark at all, as I consider it to be a very poor indicator of the performance of scientific codes and hence highly misleading, but I suspect that it will be politic to do so in order to provide an assessment of HECToR's ranking within the world.

The procurement process for HECToR is proceeding well, but because of financial constraints the planned start date of the 6-year service has been delayed until April 2007. A decision on a partnership with the Met Office will be made in July 2005 and the OJEU notice issued at the beginning of November 2005.

Because of its integrated strategy, the CSAR and HPCx services, and plans for the HECToR service, the UK is recognised within Europe as being a key player in High End Computing. EPSRC, representing the UK, has been involved in discussions with initially the French and Germans, but with the intention of including other countries as well, about the establishment of a European petascale high performance computing infrastructure during the timescale of the 7th Framework Programme of the European Commission. Clearly, these are early days for this initiative, but if it is successful then Europe should have a high performance computing capability that enables it to compete scientifically world-wide.