High End Computing Terascale Resource Capability Challenge

Introduction

The UK's newest national supercomputing facility, HECToR (High-End Computing Terascale Resource) is a public project, which is funded through Research Councils of UK. To accompany its official launch in October 2007, the Engineering and Physical Sciences Research Council (EPSRC) provided an opportunity for UK investigators who require access to supercomputer facilities to apply for resources through the HECToR Capability Challenge project. This would provide successful applicants with the means to explore the capabilities of HECToR and deliver high quality scientific output.

Fifteen proposals were submitted to the panel for review after the 25th October deadline. Six were identified as the most computationally intensive, large-scale research projects that could make high-impact scientific advances through the use of HECToR resources. The allocated compute resources were available strictly from 1st January 2008 until 30th June 2008.

Scientific achievements

The successful projects were lead by researchers in the areas of Geosciences, Materials Chemistry, Materials Engineering, Laser Physics and Fluid Dynamics. The outcomes clearly demonstrate how new avenues of research may be opened by utilising the capabilities of massively parallel computing architectures. In particular, how the use of supercomputing facilitates performing existing problems at higher resolutions and a significant increase in the current size of systems modelled. Individual summaries of the aims and achievements of the projects will now follow:

- To understand the generation of the Earth's magnetic field which shields us from the solar wind, and plate tectonics which are responsible for earthquakes and volcanic eruptions, Geoscientists are trying to determine the temperature of the earth's core. Knowing this would enable a much better understanding of the earth's thermal structure. However, it is impossible to determine the exact temperature, instead we have to consider the melting temperature of the molten iron which surrounds the core. To investigate this, a large molecular simulation code based on quantum physics was run on HECToR over many processors. On completion, a successful result was obtained for this temperature which has subsequently enabled us to move significantly closer to understanding the thermal properties of the earth's core.

- For designing new man-made materials the theory of Chemistry is often used to help us to understand crystal nucleation and growth. The crystallization process of birds' eggshells are of particular interest in this area as they form very quickly and their features are extremely complicated. To investigate this, a large computational simulation of their molecular behaviour was performed using HECToR. The results from these calculations provided useful information needed by experimental groups to aid in the design of new molecules for crystal types. Without the use of a supercomputing resource such as HECToR this would not have been possible.

- Another area of interest in material modelling is the prediction of the bulk properties of materials with complex architectures, such as composites and foams. Computational models exist which can predict their behaviour, but the input data required by these models has to be created by extracting information from high resolution images obtained through micro-imaging. This results in over a billion unknowns which require several Terabytes of data storage. To calculate these would take 15 years on a desktop PC but takes less than a day on HECToR. They are not far from being the largest in the world of their kind and the results obtained from using HECToR resources have enabled the investigators to assess new modelling approaches in collaboration with other world-wide researchers.

- On a more theoretical level, the fundamental behaviour of atom-laser and manybody interactions can be revealed by the laws of quantum mechanics. Simulations to study laser-driven two-electron atoms were carried out using numerical integration of the time-dependent Schroedinger equation. These calculations used almost all of HECToR's processing capabilities. The results were both surprising and new and have very recently been confirmed by laboratory experiment. This particular theoretical model has made a significant advance in helping us to demonstrate some of the fundamental theories in laser physics.

- The theory of Fluid dynamics enables us to understand turbulent motion in fluid flows for many varieties of application. But when modelling more than one fluid a very large amount of data is required in order to obtain meaningful results. In such cases, terascale sized simulations are necessary. In particular, to investigate the properties of liquid mixtures and liquid crystals such as those used in LCD displays, a supercomputing resource is required. A computational fluid dynamics model was run on HECToR using system sizes that were generally eight times larger than any previous simulations. This used almost all of HECToR's processing capabilities running for over 50 hours and resulted in world-class results that will be extremely useful for designers of new LCD display devices.

- Simulations in fluid dynamics often require the use of a large supercomputer, especially when the total volume of the flow concerns a very large spatial region but the features of the flow occur within relatively small volumes. For this type of direct numerical simulation, the length scale is very large and a very high resolution grid is required in order to capture the features of the flow. Simulations for such a model were performed using 1/10th of HECToR's processing power for a total of 2000 hours using more than five billion unknowns. This would not have been possible without the exceptional computational resources provided by HECToR. The work provided the investigators with an unprecedented insight into turbulence behaviour.

Users' experience of HECToR

The expectations of the researchers were exceeded by the supercomputing capabilities of HECToR. Through the use of HECToR's resources, they were successfully able to explore new and exciting areas of research covering a broad range of science. Several comments made by the investigators are noted below:

On the performance and general use of HECToR:

- *“The machine is very good, fast, and easy to use.“*

- *“Experience was very positive. After a relatively short learning period, the system was found to be easy to use and the system response was very responsive.”*

- *“The performance of the system is very good, both in computational speed and I/O for large problem sizes. The system is easy to use, and response time of the helpdesk is good.”*

- *“System (hardware and software) was a pleasure to use. We are happy to report that support was outstanding, comparable to the best we have ever observed.”*

On the computational science and engineering user support (CSE) and distributed (in depth) (dCSE) support provided by NAG Ltd:

- *“The project was helped significantly by the HECToR user support, and by the NAG dCSE support, which with some rewrite of the code used for the calculations allowed us to overcome memory limitations, and to run on very large systems, effectively making the project a success. The responses by the user support were always fast and competent.“*

- *“I cannot find any fault with the service provided and know of no problems experienced by my team. In fact, the NAG team have been very helpful, positive and professional in their dealings with the researchers involved in this project.“*

To conclude, the HECToR Capability Challenge project enabled investigators with the means to research scientific areas which would not have been possible without the capabilities of a supercomputer. The project also demonstrates the potential of HECToR to advance the frontiers of UK based research.