Improved I/O performance for larger voxel-based simulations (VOX-FE) developed by HECToR dCSE Team

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HPC experts from EPCC, working under NAG's Computational Science and Engineering (CSE) support service for HECToR, the UK's national academic supercomputing facility, have successfully improved the scalability of the voxel-based finite element software, VOX-FE, by parallelising the I/O routines. The VOX-FE bone modelling suite comprises two parts: a GUI for manipulating bone structures and visualizing the results of applying muscle and bite forces, and a parallel Finite Element (FE) solver PARA-BMU which performs the computation required to solve the linear elasticity problem and calculate stresses and strains in the bone. Example applications of VOX-FE include models of a human mandible (jaw bone) undergoing incisor biting, or understanding the stresses in an axially loaded femur. Such calculations require a scalable implementation of PARA-BMU, and before this project, the I/O routines were the main bottleneck. Following this work, I/O time has been reduced by up to a factor of 7, such that good scalability is now possible with PARA-BMU on HECToR, enabling a step-change in capability for new bone modelling simulations.

VOX-FE is a voxel-based finite element bone modelling suite which has been developed by Prof Michael Fagan's Medical & Biological Engineering group at the University of Hull. In VOX-FE, each voxel from the computed tomography scan (CT-voxel) is converted directly into a finite element, which means no loss of detail. Working directly with voxel data simplifies the model creation and it is also advantageous when modelling bony structures. However, due to the large numbers of finite elements involed with the simulations, the use of a scalable version of PARA-BMU together with a large HPC resource is essential.

Commenting on the dCSE project success, *Prof Michael Fagan of the School of Engineering at the University of Hull said: 'Bones have extremely complex geometries with multiscale features that can vary by several orders of magnitude. Capturing that detail is essential to mimic and understand fully the biomechanics of bone, but results in huge FE model files. This dCSE project has been invaluable in providing a way to manage those very large files. It opens up the possibility of modelling whole bones at unprecedented resolution, but also now provides the option of repeated adaptive remodelling simulations to allow the modelling of bone growth and optimisation of the next generation of orthopaedic and dental implants.'*

This dCSE project has enabled VOX-FE users to exploit the capability of HECToR for running large scale voxel-based finite element simulations; this paves the way for bone modelling at unprecedented scale and accuracy.

HECToR

HECToR is managed by EPSRC on behalf of the participating Research Councils with a mission to support capability science and engineering in UK academia. The Cray XE6 supercomputer, located at the University of Edinburgh, is managed by UoE HPCx Ltd. The CSE Support Service is provided by NAG Ltd and ensures users have access to appropriate HPC expertise to effectively exploit advanced supercomputers for their science. A critical feature of the CSE Support Service is the distributed CSE (dCSE) programme which, through lightweight peer review, delivers dedicated performance and scalability projects on specific codes in response to proposals from users. The dCSE programme now consists of over 70 focused projects complementing the traditional HPC user applications support and training also provided by NAG.

The dCSE projects completed so far have delivered outstanding examples of the cost savings and new science that can be enabled through dedicated CSE effort. The VOX-FE project reported here adds to these success stories with a successful performance improvement.

Project Background

VOX-FE has been used successfully on (small-scale) local clusters for several years. However the resource of HECToR will be essential for future large-scale scientific studies and research is ongoing within the EPSRC-funded project "Novel Asynchronous Algorithms and Software for Large Sparse Systems" to replace the existing conjugate gradient solver with a more scalable alternative. The primary aim of this dCSE project was to remove a performance bottleneck in the PARA-BMU (finite element solver) part of the code by parallelising the I/O routines. This would be achieved by converting the files to netCDF-HDF5 formats in order to reduce their overall size and furthermore reduce the file access times by implementing parallel netCDF routines for data input and output.

Michael Fagan of the School of Engineering at the University of Hull was the Principal Investigator for the project. Nick Johnson and Iain Bethune of EPCC carried out the 4 person-month project, in close collaboration with the NAG CSE team.

Project Results

By implementing the netCDF and HDF5 libraries within PARA-BMU, files can now be reduced in size by up to a factor of 190 times their original, leading to a reduction in I/O time by up to a factor of 7. The use of freely available netCDF libraries, with the associated parallel HDF5 backend is an easy way in which to add parallel I/O to any existing application. Furthermore, use of netCDF also allows files to be made self-describing and portable between systems, along with offering good opportunities for compression.

In PARA-BMU the total wall clock time for calculations using the new parallel I/O routines now scales much better than those using the serial I/O routines. A test case was run with 512 MPI processes on HECToR Phase 3, this showed that the speedup over a single core for serial I/O is roughly 22 times and for parallel I/O roughly 90 times. However, the speedup for the solver part of PARA-BMU alone is roughly 180 times indicating that there may still be scope for further optimisation with the parallel I/O.

This development has been submitted to the main trunk of the VOX-FE code on CCPForge so that researchers at the University of Hull may now make use of the work. The impact of this work is that it is now feasible to use HECToR as a platform for running PARA-BMU rather than small-scale local clusters; this paves the way for bone modelling at unprecedented scale and accuracy.

A full technical report on this work can be found at http://www.hector.ac.uk/cse/distributedcse/reports/voxfe/

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