The Chicken or the Egg?
NAG provides an essential ingredient to help researchers find the answer

November 2010 - When researchers at the University of Warwick and the University of Sheffield decided to use the UK's national academic supercomputer HECToR to study a problem in egg shell formation, they made use of NAG HPC software engineering expertise (http://www.nag.com/hpc/index.asp). The results they obtained may also give a partial answer to the age old question "which came first - the chicken or the egg?" The answer to the question seems to be 'chicken' - at least for one particular protein.

Researchers knew that a chicken eggshell protein called ovocledidin-17 (OC-17) must play some role in egg shell formation. The protein is found only in the mineral region of the egg (the hard part of the shell) and laboratory results showed that it appeared to influence the transformation of calcium carbonate into calcite crystals. How this process could be used to form an actual eggshell remained unclear.

University of Warwick researchers Mark Rodger and David Quigley, in collaboration with colleagues at the University of Sheffield, used molecular dynamics simulation and the HECToR supercomputer (a 12,000 core Cray XT4), to solve the problem. The researchers created a model to show how the protein bound to a calcium carbonate surface. However the early performance of the simulation software on HECToR would have kept the validation of this model beyond reach.

Luckily, as well as the Cray supercomputers managed by the University of Edinburgh, the Research Councils' HECToR service includes a comprehensive Computational Science and Engineering (CSE) support service provided by NAG. One of NAG's HPC experts identified input and especially output (I/O) as the bottleneck for the simulation software, known as DL_POLY_3 - originating from Daresbury Laboratories. A solution was provided for this research and NAG has gone on to optimize all the I/O routines, to help other users of DL_POLY_3. This was done by reordering data to take

advantage of modern file systems, and then further improved by performing the I/O in parallel. This 6 months of work resulted in the I/O for DL_POLY_3 being, on average, around 50 times faster.

With the performance improvement, use of the specific model to investigate the eggshell formation became tractable. Results of the simulation now show how the protein binds using two clusters of amino acid residues on two loops of the protein. This creates a chemical clamp to nano-sized particles of calcium carbonate which encourages calcite crystallites to form. Once the crystallites are large enough to grow on their own, the protein drops off. This frees up the OC-17 to promote yet more crystallization, facilitating the overnight creation of an eggshell – started, first, by this chicken protein.

Dr David Quigley from the Department of Physics and Centre for Scientific Computing, University of Warwick, said*: "Prior to the I/O improvements, DL_POLY_3 was unable to make effective use of the parallel file system on HECToR, severely crippling the performance of our simulations. The new code has reduced the time taken to write a single snapshot from 3 minutes to less than half a second, resulting in an overall factor of 20 improvement in our net performance. Without this development, HECToR would have been effectively useless for our purposes."*

The researchers believe that this insight into the elegant and highly efficient methods of promoting and controlling crystallization in nature will be of great benefit to anyone exploring how to promote and control artificial forms of crystallization.

For more details of the research please refer to: Freeman et al, "Structural Control of Crystal Nuclei by an Eggshell Protein" Angew. Chem. Int. Ed. 49 (30) pp 5135-5137 (2010)

About NAG

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