So supercomputers are mega-powerful, but what can they actually do?

April 1 2014, by Alan Simpson

Engineer on the prowl between the big black boxes. Credit: University of Edinburgh, CC BY-NC-ND

A new supercomputer, called ARCHER, has recently been launched. ARCHER is a Cray XC30, funded by EPSRC and NERC. It is more than three times more powerful than its predecessor, HECToR, and is hosted by the University of Edinburgh. But what can you actually do with a supercomputer?

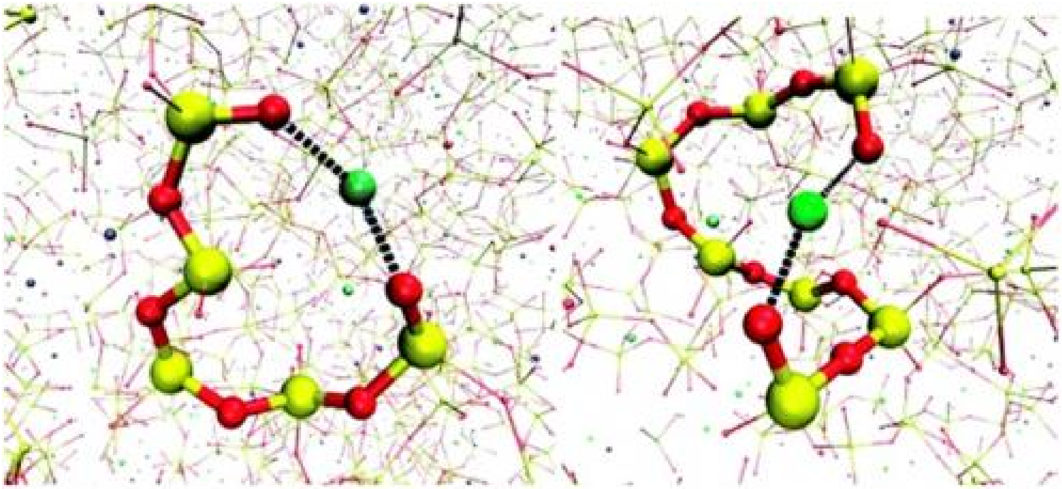
Supercomputers allow researchers to carry out experiments that would otherwise be impossible because they are too small or too large, too fast or too slow, or simply too expensive. Coupling supercomputers to large data repositories also allows researchers to solve problems by analysing Big Data and so opening doors to even more new areas.

The most exciting developments in computational science are the significant growth in the range of scientific and engineering problems that can be solved and the corresponding increase in the impact on the lives of all of us. Supercomputers can solve important problems for the environment, transport, health and energy.

ARCHER's research power

The single largest area of science that ARCHER will be used for is the realm of chemistry and materials science. The larger computing power available is enabling researchers in this area to actually explore the chemical properties of materials in physically realistic environments rather than making approximations and using idealised systems. This step-change in modelling ability allows the scientific research to have a direct impact on our day-to-day lives much more quickly than was possible previously.

Bioactive silicate glasses are key materials used to help restore, regenerate and repair bones and other tissues in the body. A key mechanism in their function is the fast dissolution of their surface in the biological environment – this releases key ions and promotes the repair process.



Atomic structures from simulations of a bioglass. Tilocca, Phys. Chem. Chem. Phys., 2014, 16, 3874-3880, DOI: 10.1039/C3CP54913E

Using ARCHER, researchers are able to investigate this process in a realistic biological environment at the quantum scale. This has simply not been possible using previous generations of supercomputers. Understanding these processes at the quantum level is driving the design of new, improved bioactive glasses.

Also of great importance in the medical arena, ARCHER is being used to understand the resistance of many bacteria to modern antibiotics. This is one of the most important problems in contemporary public health: it limits our ability to combat infection both through the reduced efficacy of the drugs and though the constraints placed on prescription of the drugs.

Researchers are using a combination of experiment and large molecular simulations to understand how, at a molecular level, mutations enable resistance to antibiotics in the causes of, among others, bacterial meningitis. Simulating these systems in realistic biological environments for the long timescales required to understand the mechanism of resistance has not previously been possible. The additional speed and capacity of ARCHER allows the researchers to gain a more detailed understanding through realistic simulations, allowing them to shorten the time between research and real impacts for everyone.

ARCHER will also play a key role in UK climate modelling research. Understanding the climate and climate change are inherently complex problems that require coupling between many different systems – atmospheric models, ocean models and land models. The complexity (and so realism) of these individual components is limited by the computing power available.

Mission: Earth

Using ARCHER, climate researchers will be able to run full Earth system models with the additional complexity required in, for example, modelling evaporation from land and the associated plant transpiration. These more detailed integrated models will give us a deeper understanding of the drivers of climate change, the consequences arising and what information we require to prepare properly for future changes in climate. The same techniques and models are also being used to understand climate on planets beyond the solar system.

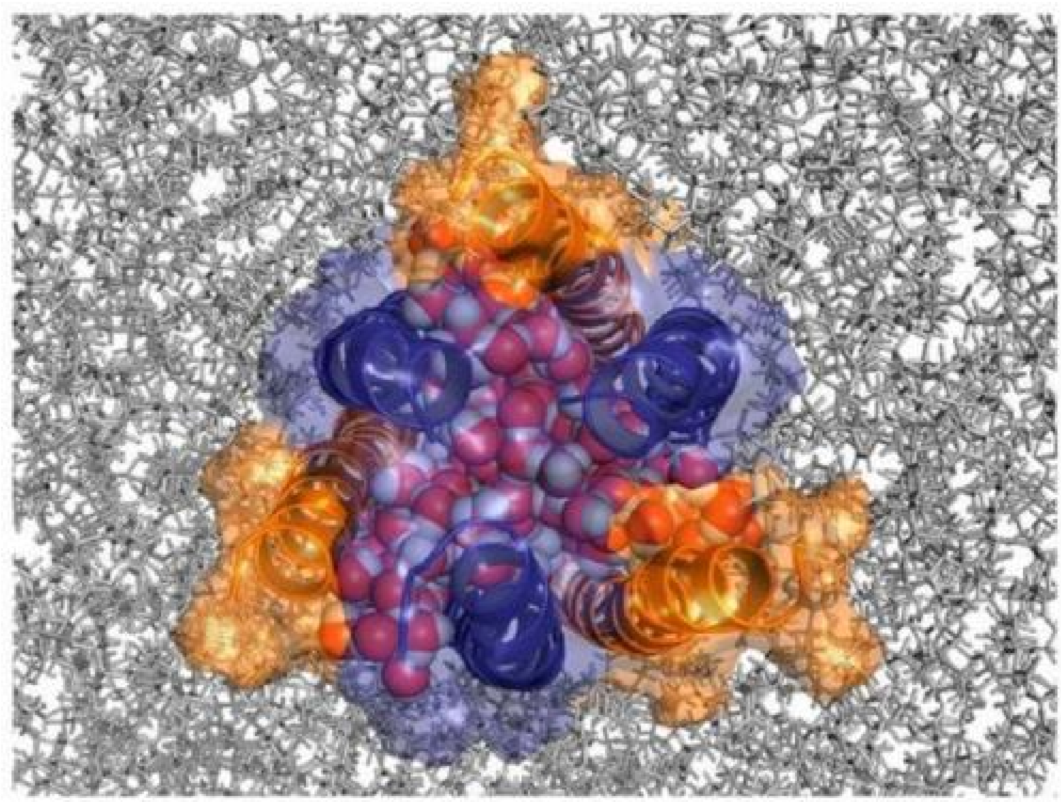


Image from a simulation of a bacterial ion channel that impacts antibiotic effectiveness. Chen Song et al, PNAS (2013), 110:12, 4586–4591, doi: 10.1073/pnas.1214739110

These examples represent only a small sample of the science coming out of supercomputers. Computational science is also using biomechanical models to understand how dinosaurs moved; simulating the energy production of future fusion reactors; exploring new renewable energy technologies such as dye-sensitised solar cells; and designing quieter, more efficient aeroplanes.

Supercomputing continues to grow at an exponential rate. The performance of current systems has allowed exciting progress across many scientific disciplines. Computational research is no longer as limited by computer power to anything like the same extent as 10 years ago. This is allowing creative researchers to address new problems all the time. ARCHER and other similar systems will ensure research breakthroughs in a broad range of important areas with significant socioeconomic benefits for everyone.

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