Longbow – lowering technological barriers in advanced computing

CoSeC
Computational Science Centre
for Research Communities

Scientists and academics need to run computer simulations designed to imitate a real-life situation – such as exploring how a new drug will attack a cancer cell – using the advanced capability and power of supercomputers. This can be a daunting task as these very high-speed, high-tech computers are expensive to run and can be both difficult and very time consuming to use. Each machine is likely to have a different interface – so the user would have to spend time learning about each system and then write separate configuration files for each one before they could run a simulation.

Additionally, users will need to write a submission file for each simulation, so if an experienced user is running 1,000 simulations they will usually need 1,000 submission files. This manual preparation not only takes a lot of time but also increases the risk of errors being made.

Enter Longbow…

Longbow is a tool that runs simulations on supercomputers whilst giving the impression that they are running on your own desktop or laptop computer. Developed by the High End Computing consortia for Biosimulation (HEC-Biosim*), Longbow will:

- Automatically create the configuration files required to run high-end simulations, lowering technological barriers to make complicated computing infrastructure simple. Users no longer need to spend time reading documentation before sending a simulation; they can just submit it and forget it. Longbow is pre-programmed with defaults for different systems, so it will learn the new system and adapt to the individual computer's configuration.

- Write the submission files for each simulation, so what might have taken several weeks to prepare manually now takes less than a second. Longbow will create the files and perform checks – and it doesn't make mistakes.

- Mimic the software the user is familiar with; so there is a very low learning curve from what they are already doing to having the power of a supercomputer at their fingertips.

- Provide seamless file transfers to bring data back to the user – so although the simulation could be running on millions of processors a thousand miles away, it appears to be running on their own laptop or desktop.

- Save vast amounts of time and money, which in turn enhances the value of the research grant or other funding stream.

Computer-aided drug design

At Edinburgh University, Dr Julien Michel's group uses Longbow in computational projects that feature a large number of protein and protein-ligand molecular dynamic (MD) simulations. (A ligand is a small molecule that is able to bind proteins, and sometimes serves as a signal-triggering molecule.)

One of these projects focuses on understanding loop dynamics – how system process variables behave in response to sudden changes – in a family of proteins called Cyclophilins. These are potential drug targets for a number of conditions, such as Hepatitis C, HIV, cancers and neurodegenerative disorders. Clinical validation requires the development of better and more selective inhibitors so Dr Michel's group is running simulations to help advance this development.

Longbow reduces overheads for running simulations and helps to transfer software across different architectures. This is important to ensure that project partners can reuse the software in their own laboratories without extensive support from the Edinburgh team. Longbow reduces barriers to using High Performance Computing and enables, for example, experimentalists to use simulations in their research, so there are some definitive time and cost savings.

"We are exploring the use of Longbow in prototype software we are currently developing. One project focuses on a virtual-reality user interface for interactive MD simulations. The other project focuses on an adaptive protein MD simulations workflow to discover cryptic pockets in protein surfaces. These pockets may be used to formulate new strategies to discover drugs for treating a wide range of diseases". Dr Julien Michel

Who can use Longbow

Longbow was originally designed for use by researchers and academics working in the field of bio-simulation. Due to its popularity, however, Longbow has been developed into a more generic tool so it is now available for other subject areas and is used in related industries. Users are encouraged to share the knowledge gained from using it with their own communities so that others can benefit.

There are two broad user categories:

- The novice – people new to simulation work, or they come from a non-computing background. Longbow makes it easy for them to use complex machines.

- The experienced experimentalist – highly knowledgeable users with many years' experience and who are likely to run thousands of simulations. Longbow allows them to spend more time doing science rather than unproductive computing set-up tasks.

An added bonus is that researchers working in the field of bio-simulation can also apply to HEC-Biosim for time on ARCHER, the UK's national supercomputing service.

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Researchers can now spend more time doing advanced science and less time doing basic computing."

James Gebbie, Scientific Computing Department, Science and Technology Facilities Council

Longbow is already being used to help experiments dealing with:

- New drug discovery and design

- DNA superstructures - understanding the mechanisms of how DNA forms supercoils and ultimately how it creates chromosomes

- Protein folding (where protein structure assumes its functional shape) - important for understanding some diseases

- Developing more environmentally -friendly engines

Career boost

Developing the Longbow code for HEC Biosim helped Dr Gareth Shannon to advance his scientific career internationally.

He was a Postdoctoral researcher in software development for Biomolecular Simulation at Nottingham University, writing modeling tools to facilitate research.

The recognition of his work in developing Longbow enabled Gareth to obtain a 'green card', allowing him to live and work in the USA. As a result, he joined the NASA Ames Research Center in California as a Computational Biology Research Scientist.

How can you get Longbow?

Longbow is available via public repositories so you can download it from:

- github https://github.com/HECBioSim/Longbow

- pypi https://pypi.python.org/pypi/Longbow/

Or if you don't have access to those you can download the Longbow tool and get support from the HEC-Biosim website: http://www.hecbiosim.ac.uk/

www.scd.stfc.ac.uk

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