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Scientific Computing

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Computational software saves time, energy and costs for research experiments

A computational mathematics package is helping beamline scientists and others researching a multitude of areas – from medicines to innovative engineering and cutting-edge technology; and facilitating physics, chemistry, materials science, geology, engineering, and biology experiments.

The rapidly increasing volume of data being generated and analysed in experimental research using large-scale facilities requires a significant amount of compute time and energy – and with it comes an associated carbon cost.

Developed by STFC Scientific Computing, the 'FitBenchmarking' software package is enabling researchers to focus on their scientific research by identifying the "fitting" algorithm that is the best fit for their research data, whilst saving both time and energy costs.

The Challenge

Scientists from many fields can obtain research grants to use large-scale National Facilities such as the Diamond Light Source - the UK's national synchrotron, where they can use a machine that is 10,000 times more powerful than a traditional microscope; and the ISIS Neutron and Muon Source - where non-destructive 'super microscopes' are available for experiments, and which provide results that cannot be achieved by other techniques.

They enable researchers to gain extraordinary insights into how materials will behave in different situations and environments, without having to break or damage them. For example, they can test how the turbine blades of a jet engine will operate under enormous mechanical and thermal stresses, or find the most efficient, safe and cost-effective materials for use in everyday items such as soap or shampoo.

When carrying out these experiments, scientists collect huge quantities of data (typically petabytes) that they subsequently need to analyse.

The scientists have specialist domain expertise coupled with specific technique knowledge on beamline research stations, but they very rarely have training in computational mathematics.

They usually need to spend significant amounts of time researching the different computational algorithms available to them, taking them away from their research.

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Our Approach

The FitBenchmarking package devised by STFC Scientific Computing's Computational Maths Group can be used to understand which software works best for the scientist's particular computer set-up, data requirements and experiment parameters. The differences in data and characteristics between experiments means that the best algorithm for one set of experiments or machine specification might not be the best for another.

The chosen software program can then be used to minimise the difference between the predictions and the data gathered in the experiments.

The Mantid project team from STFC's ISIS Neutron and Muon Source was the earliest user of the FitBenchmarking tool. Mantid has been in operation since 2007 and provides computational tools to support the processing and visualisation of materials-science data. The team was using a well-known minimisation routine for crystal field fitting but hitting a problem with fitting the data, as it was giving scientists completely the wrong answers.

> **"Researchers might get lucky and stumble across a relevant algorithm fairly quickly or have an appropriate one recommended to them by their supervisor – or alternatively they might spend a year researching to find the best one to use. And then they might do all that work to choose an algorithm, and then find out that it doesn't work well on their data."**
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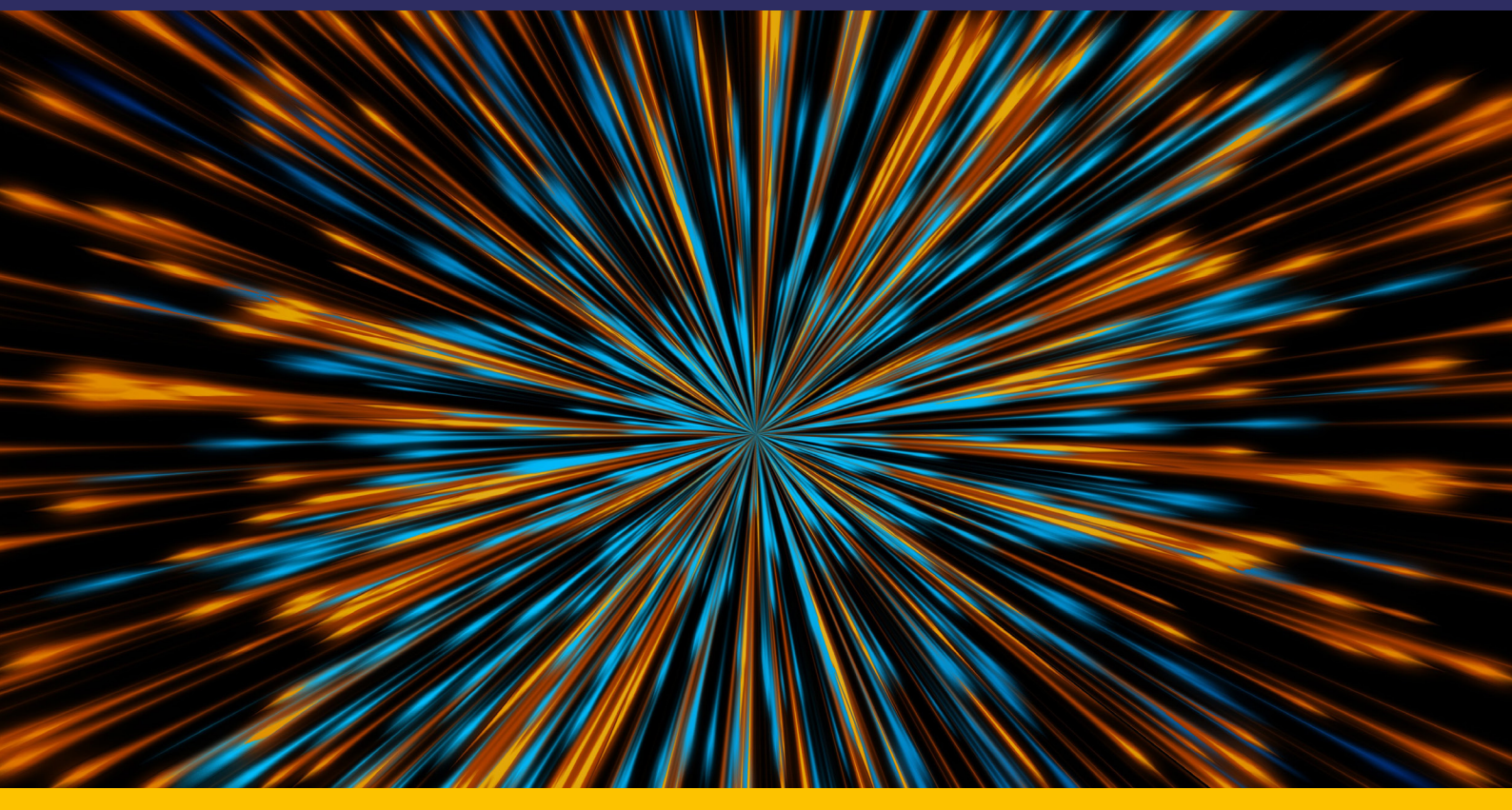
> **Dr Tyrone Rees**
> Computational Maths Theme Leader, STFC Scientific Computing.



STFC Scientific Computing's Computational Maths group developed new solvers and algorithms to help address the problems the Mantid team was facing. They tested them with the FitBenchmarking tool, which made them more efficient and sped up development time.

Using the FitBenchmarking tool, scientists are presented with a website-like output with all the options available.

> **"It's a bit like using an insurance price comparison site! You enter and submit your data, and then it can take just minutes or a few hours to produce the options, depending on the complexity of the problem to be solved. On the other hand, it could take days, weeks, or even months to carry out the research manually – or you might never achieve it."**
>
> **Andrew Lister**
> STFC Mathematical Research Software Engineer.

The FitBenchmarking tool will remember the data that has already been submitted, so when a researcher needs to find a new algorithm or minimiser to solve a problem, they just need to enter any additional information and the tool will run a check to find the best options for them.

Much like the price comparison site, it will recommend a list of software tools they could use. It will also include signposts for alternative data analysis software the researchers might not have thought of.

Benefits

Time spent using the large scale facilities is very expensive, so it's critical that scientists use their experiment time as effectively as possible. Using FitBenchmarking can save them large amounts of time by doing early analysis and helping them to choose the right algorithm or software to direct their research most effectively.

It ensures they can spend most of their time analysing the results using their domain knowledge, rather than researching and testing software tools.

It reduces the energy used in compute time and running the machines, so also reduces the carbon footprint of the experiment.

> **"Use the FitBenchmarking tool once and it informs you for the rest of your research career."**
>
> **Dr Tyrone Rees**
> Computational Maths Theme Leader, STFC Scientific Computing.

Get FitBenchmarking for your own research

FitBenchmarking is available as an open source tool for comparing different minimizers/fitting frameworks. It is cross-platform and we support Windows, Linux and Mac OS.

fitbenchmarking.readthedocs.io/en/stable

The Future

The Computational Maths group is aware that FitBenchmarking could have a much wider use so they have expanded its capabilities to make it a more generic tool to be used by scientists from any field, from beamline scientists, to scientific software developers, and mathematical software developers.

They hope to secure additional funding to develop it further, so that academic researchers and businesses will be able to independently use FitBenchmarking to run their data, without having to rely on the help and expertise of the Computational Maths group to run it for them. This will guarantee that commercially sensitive data is completely secure and contained by the business at all times, and will ensure confidence in the FitBenchmarking tool.

FitBenchmarking has been funded through the Ada Lovelace Centre (ALC), a centre of expertise in scientific software, research software engineering and data management with the primary objective of maximising the scientific impact of the STFC national facilities. ALC is one of STFC Scientific Computing's key programmes.

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