Beitrag ID: **36** Typ: **nicht angegeben**

FitBenchmarking: an open source tool for comparing data analysis software

Donnerstag, 27. Oktober 2022 09:00 (45 Minuten)

STFC's Computational Mathematics Group provides support and mathematical software for the UK's large scale facilities, such as the ISIS Neutron and Muon source, the Diamond Light Source, the Central Laser Facility, and the Culham Centre for Fusion Energy. These facilities are visited by thousands of researchers each year, and they produce increasingly large amounts of data that needs to be processed. Furthermore, as the scale of data increases, it is more likely to need to be analysed without human intervention. Therefore it is more important than ever that scientists use the most robust and most efficient numerical algorithms.

Much of the data analysis that is carried out takes the form of fitting parameters to models, usually by formulating the problem as a nonlinear least-squares problem. Recently we have developed RALFit, a tensor-Newton nonlinear least-squares solver, and GOFit, a global nonlinear least-squares algorithm. Alongside these we have developed FitBenchmarking: an open source python package which interfaces scientfic data analysis software with a range of fitting back ends.

FitBenchmarking has been designed to help:

- Scientists, who want to know the best algorithm for fitting their data to a given model using specific hardware.
- Scientific software developers, who want to identify the best fitting algorithms and implementations. This allows them to recommend a default solver, to see if it is worth adding a new minimizer, and to test their implementation.
- Mathematicians and numerical software developers, who want to understand the types of problems on which current algorithms do not perform well, and to have a route to expose newly developed methods to users.

Representatives of each of these communities are involved in the design and implementation of FitBenchmarking.

The FitBenchmarking project embodies the FAIR principles, not only in terms of curated datasets we supply from a range of applications from across the UK's National Facilities, but also in terms of assisting scientists in finding cutting edge algorithms (and new implementations of algorithms). The tool has helped to foster fruitful
interactions and collaborations across the disciplines and we plan to grow its reach further in the coming years.

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Sitzung Einordnung: Invited Talks