Samuel **Jackson**

Data Scientist · Research Software Engineer

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Experience

Scentific Computing Department, STFC

Rutherford Appleton Laboratory, Oxfordshire, UK

Senior Data Scientist — *Feb. 2019 - PRESENT*

- Role: I work to apply machine learning and deep learning techniques to help solve a wide range of complex problems faced by scientific facilities at STFC and the wider UK community.
- Project: Developed an AI ready platform for FAIRly curating historical data from the MAST tokamak. This is a joint project with CCFE.
- Developed the SciML benchmark suite for scientific machine learning as part of the BASE I Excalibur Project. Benchmarks from this work were contributed as part of MLCommons. I am involved in the BASE II project to expand to Exascale capability.
- Project: Pulse shape discrimination and pile-up recovery in organic scintillator detectors which demonstrated a potential 5-10% gain in detector efficiency. This project was joint with ISIS and STFC Technology department.
- Project: Automatically identifying bad particle picks in Cryo-Eletrcon Microscopy data at Diamond Light Source using VAEs and CNNs.
- Project: Predicting damaged optics from diagnostic near field images in high energy laser physics for the Gemini laser at the Central Laser Facility using autoencoders for anomaly detection.

ISIS Neutron & Muon Source, STFC

Rutherford Appleton Laboratory, Oxfordshire, UK

Scientific Software Engineer — *Jun. 2016 - Feb. 2019*

- Role; Worked to develop and maintain code bases for the reduction and analysis of diffraction data from the ISIS facility.
- Led an agile team of 4 people within the Mantid project to develop diffraction analysis tools.
- *Secondment to SCD computational physics group*: Developed code for running & analyzing the results of DFT (CASTEP) & DFTB+ calculations for finding the muon implantation site in organic crystal structures.
- *Secondment to ISIS controls group*: Wrote several new device drivers using EPICS, ported control scripts from an in-house language to Python, and developed test cases & emulators for many devices from temperature gauges to sample stages.

Industrial Placement Student — *Jun. 2013 - Aug. 2014*

- Role: in the scientific computing group on the Mantid project developing the code base for the ISIS molecular spectroscopy instruments. This project was developed using both Python and C++.

Education

University of Aberystwyth

Aberystwyth, Ceredigion, UK

M.Eng. in Software Engineering — *Sept. 2011 - Jun. 2016*

- Achieved a first class honors
- Dissertation: Predicting BIRADs classification of mammograms using classical machine learning approaches using shape, texture, and statistical features derived from breast parenchyma.
- Key modules studied:
  - *Machine Learning*: Covered a wide range of machine learning algorithms, including supervised & unsupervised techniques, with a "hands on" perspective.
  - *Computer Vision*: Covered concepts such as edge detection, motion, segmentation, and 3D data.
  - *Mathematics for Computer Science*: Covered keys ideas in linear algebra, calculus, probability & statistics.
  - *Fundamentals of Intelligent Systems*: Covered key ideas in AI including search and evolutionary optimization.
- Academic Awards:
  - Best Academic Performance, M.Eng Final year award, 2016
  - Best Academic Performance, M.Eng Penultimate year award, 2015
  - Glyn Emery Prize, Best academic performance by a first year student, 2012

Skills

Programming	Python, C++ (incl. C++14 experience), C, R, Fortran
Python Libraries	numpy, scipy, pandas, matplotlib, dask, xarray, hvplot, pytest, ase, mpi4py
C++ Libraries	boost, eigen, pybind11, xtensor, qt, poco, cxxtest, muparser
ML Libraries	pytorch, pytorch-lightning, tensorflow, keras, scikit-Learn, pymc3, horovod, hugging-face
Development	git, jupyter, CMake, LaTeX, docker, singularity, SLURM, LSF, UNIX, jenkins, travis
Web	FastAPI, REST, GraphQL, SQL, S3, GCS, HTML5, CSS

Teaching & Training

SciML Machine Learning Course

Lecturer & Demonstrator — *Jul. 2019 - PRESENT*

- Organised, prepared materials, and presented at machine learning workshops organised by the group.
- Taught up to 50 staff & researchers from across the STFC facilities and the national DiRAC consortium.
- I presented on numerous topics including *classical unsupervised learning*, *autoencoders*, & *scaling ML models on HPC resources*.
- Prepared docker jupyterhub environment and configuration for workshop attendees.

Mantid Software Training Workshops

Lecturer & Demonstrator — *Oct. 2016 - Feb. 2019*

- Led training workshops for ISIS beamline instrument scientists & the wider user community.
- Delivered lectures on "Introduction to Python" and "Extending Mantid with Python".

Aberystwyth University

Student Advisor & Demonstrator — *Sept. 2012 - Jun. 2016*

- Worked as a final year advisor, independently running drop-in workshop sessions for undergraduate students who required help with their coursework or exam revision.
- Worked for the university helping with hands on practical sessions and assessing undergraduate work on variety of courses. This included: *Introduction to Programming*, *C & C++ Programming*, and *Introduction to Robotics*.

Selected Presentations

IEEE NSS-MIC-RTSD

Milan, Italy

Presenter for Neutron Detectors and Gamma Imaging Applications — *Nov. 2022*

- Presented outputs from the PSD detector efficiency project to the wider neutron detector community.

Supercomputing

Denver, Colorado, USA

Presenter and Panel Member for Benchmarking Machine Learning Ecosystem on HPC systems — *Nov. 2020*

- Presented progress of SCD benchmarking efforts and acted as a panel member for a wider discussion of ML benchmarking for science

Publications

2020 — **Philosophical Transactions of the Royal Society A.**, Machine learning and big scientific data, *Hey T., Butler K., Jackson S., Thiyagalingam J.*

2019 — **Journal of Chemical Physics**, Comparison between density functional theory and density functional tight binding approaches for finding the Muon stopping site in organic molecular crystals, *Sturniolo S., Liborio L., Jackson S.*

2014 — **Journal of Physics: Conference Series**, VESUVIO data analysis goes MANTID, *Jackson S., Krzystyniak M., Seel A. G., Gigg M., Richards S. E., Fernandez-Alonso F.*

Peer Review

2021 - 2022, IEEE Transactions on Neural Networks and Learning Systems

2019 - 2020, Concurrency and Computation: Practice and Experience

Professional Activities

Scientific Computing Department, STFC

Computing Graduate & Apprentice Mentor — *2017 - PRESENT*

- I am a volunteer mentor at STFC for both computing graduates and apprentices. The STFC mentorship scheme links senior staff members with junior staff from another department. I help to provide one-on-one support as they progress through their scheme and guide them towards completion of their course.