Dr Tom McAuliffe

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EDUCATION

Imperial College London, PhD - *Unsupervised ML for electron microscopy* — Sep 2017 – Nov 2020

University of Cambridge, 1st Class BA & MSci - *Natural sciences* — Oct 2013 – Jul 2017

EXPERIENCE

Arabesque AI: *Machine learning research* — Nov 2020 – Feb 2021

- Unsupervised ML to inform timeseries classification. Variational, convolutional, self-attention encoders built and integrated with GCP. Timeseries transformed to images and computer vision approaches employed.
- SVM model development and deployment including implementing a 10x speedup.

Imperial College London: *PhD research* — Sep 2017 – Present

- Unsupervised ML and statistical inference for electron microscopy feature extraction and physical insight. Emphasis on deriving physically meaningful latent features [1-3].
- Fourier space cross-correlation employed for comparison of latents to simulated templates. This permits efficient determination of crystalline structure and orientation [1-3].
- Hyperparameter numerical optimisation for improved fidelity of diffraction simulations [2].

Imperial College London: *Undergraduate teaching* — Oct 2018 – May 2019

- Tutored maths (including linear algebra, statistics, calculus) to undergraduates.
- Led experimental practicals (one weekly lab and one longer, full-term project).
- Co-supervised MSc student projects in alloy development and microscopy data analysis.

Rolls-Royce PLC: *External material surveillance* — Jul 2016 – Oct 2016

- Quality control on outsourced forging and machining. New statistical process control template developed and implemented.

SKILLS

- **Python** - NumPy, Pandas, PyTorch, Multiprocessing, SKLearn, Matplotlib, SciPy packages *etc*.
- **MATLAB** - Experienced with Machine Learning, Statistics, Parallel Computing toolboxes, *etc*.
- **DevOps** - Experienced with Unix/Linux, shell scripting, Git. Development with VS code, Jupyter, Vim.
- **Presentation** - Visualisation with Matplotlib. Very experienced with generating publication-quality figures with Adobe Illustrator, Photoshop, Inkscape.
- **Teamwork** - Collaborated on many projects, both leading and providing analytical support. Have assisted in use of pipelines that I have developed, and co-developed pipelines with other researchers.
- **Time management** - Five substantive papers, three software packages over course of PhD.

ACHIEVEMENTS

- Student Academic Choice Award Nominee, Imperial College — 2018 – 2019
  For undergraduate maths tutoring and supervision.
- Armourers & Brasiers' Guild Prize, City of London — Jan 2019
  Funding awarded to present internationally on electron microscopy and applied data science.
- Institute of Materials, Minerals & Mining Prize — Jul 2017
  Awarded to University of Cambridge undergraduate with the most impressive research project.
- Scholar of Jesus College, Cambridge — Jul 2017
  Elected as scholar of Jesus College for outstanding performance in Natural Sciences tripos.
- CREST Gold Award & Nuffield Foundation 'Best use of Maths' Prize — Oct 2012
  Awarded by British Science Association for nanotube property MATLAB modelling internship.

PUBLICATIONS

[1] **"Advancing characterisation with statistics from correlative electron diffraction and X-ray spectroscopy, in the scanning electron microscope,"** - McAuliffe *et al* - *Ultramicroscopy*, 2020 - *Clustering and classification of hyperdimensional (and multimodal) electron microscopy datasets.*

[2] **"Spherical-angular dark field imaging and sensitive microstructural phase clustering with unsupervised machine learning"** - McAuliffe *et al* - *Ultramicroscopy*, 2020 - *PCA, NMF, autoencoder neueral network comparison for latent feature extraction in electron backscatter diffraction.*

[3] **"The Use of Scanning Electron Beam-based Phase Classification as a Crucial Tool in Alloy Development for Gas Turbine Engine Applications,"** - McAuliffe *et al* - *Microscopy & Microanalysis*, 2019 - *Combination of multimodal data for material analysis*.

[4] **"Quantitative precipitate classification and grain boundary property control in Co/Ni-base superalloys"** - McAuliffe *et al* - *ArXiv*, 2020 (under review) - *Applying unsupervised ML to understand and improve aersoapce materials' high temperature capability.*

[5] **"4D-STEM elastic stress state characterisation of a TWIP steel nanotwin"** - McAuliffe *et al* - *ArXiv*, 2020 (under review) - *Measurement of crystal lattice stress and strain tensors over a highly resolved spatial domain.*

[6] **"On the prediction and the formation of the sigma phase in CrMnCoFeNix high entropy alloys,"** - Christofidou, McAuliffe *et al* - *Journal of Alloys & Compounds*, 2018 - *Measurement and modelling of modern aerospace alloys.*

[7] **"Interface characteristics in an alpha + beta titanium alloy,"** - Ackerman *et al* - *Physical Review Materials*, 2020 - *Measurement and modelling of atomic coherence.*

SOFTWARE

ebspy: *Python analysis of electron backscatter diffraciton data* - [8]

- Created and fully developed by me for loading, handling, and cleaning microscopy data. Provides normalisation, background correction, and pipelines to interface with SKLearn for ML characterisation.
- Used within my research group and others' in the UK and abroad.

AstroEBSD: *Crystallographic analysis of electron microscopy data* - [9].

- Orientation determination, signal clustering, and structure classification with template matching in MATLAB.
- Initially developed in the group for Hough transforms and geometrical analysis of diffraction data.
- Recently updated with my contributions: an open-source PCA pipeline for analysis of correlative multimodal datasets, including Fourier cross-correlation of simulated templates for orientation ID.

crosspy: *Fourier image registration and subset tracking in Python* - [10].

- Co-created and developed for loading, handling, and analysing digital images for displacement tracking.
- Code for cross-correlation, displacement tracking, and data loading developed by me. Includes least-squares fitted polynomial plane for correcting out-of-image displacement. This massively improves fidelity of calculable displacements upon a second pass.
- Collaborated with co-creator for calculation of strain tensor components given the displacements.