ROBERT ARBON

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PROFESSIONAL EXPERIENCE

Apr. 2012 – Present
London and Bristol, UK
FREELANCE DATA SCIENTIST & TUTOR

Apr. 2008 – Jan. 2012
Economic Consulting Associates Ltd., London, UK
ECONOMICS ANALYST

Sep. 2007 – Mar. 2008
Campbell Carr Ltd., Bucks., UK
ANALYST

Mar. 2007 – Aug. 2007
London Borough of Havering Council, Essex, UK
POLICY ANALYST

Sep. 2000 - Jul. 2001
DSTL (formerly DERA), MoD, Wilts., UK
RESEARCH ASSISTANT, Organic Chemistry Laboratory

EDUCATION

Dec. 2020
UNIVERSITY OF BRISTOL, UK
PhD in computational Chemistry, title: *Markov models of biochemical systems*

Mar. 2007
HARVARD UNIVERSITY, USA
SM[1] in Applied Physics

Jul. 2005
OXFORD UNIVERSITY, UK
MChem in Chemistry (First Class).
Dissertation title: *Quantum mechanical effects in liquid He-4*

[1] Equivalent to a UK MSc

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RESEARCH SUMMARY

My research is focused on three areas:

1. Statistical modelling of molecular dynamics simulation data to understand the dynamics of biochemical systems, enzymes in particular. I have used Bayesian statistics, response surface methods and Bayesian optimization to improve Markov state models of conformational dynamics.
2. Novel display of scientific data through sonification, data inspired composition (both in collaboration with musicians) and 'deep-art'. I created parameter mappings to sonify hidden Markov models as well as using style transfer to create the multimedia performance *Metastable Impressions* with the composer George Holloway, performed by the Ligeti Quartet.
3. Reproducibility. Co-created and ran an international reproducibility experiment, MAPS (Mapping the Analytic Paths of a Crowd Sourced Data Analysis). The goal was to understand the diverse pathways taken to arrive at an answer given the same question and data. In addition, with my colleagues at the Jean Golding Institute co-created the course *Robust and Open Analysis in R*, currently being converted to a 'Carpentries' course.

PUBLICATIONS

1. Song, Y.-C., Ingram, S., **Arbon, R.E**., Topping, D.O., Glowacki, D.R., Reid, J.P., 2020. *Transient cavity dynamics and divergence from the Stokes–Einstein equation in organic aerosol*. Chem. Sci. 11, 2999–3006. https://doi.org/10.1039/C9SC06228A
2. **Robert E Arbon**, Alex J Jones, Lars A. Bratholm, Tom Mitchell, David R. Glowacki, 2018. *Sonifying stochastic walks on biomolecular energy landscapes***.** Proceedings of the International Conference on Audio Display, 2018. http://doi.org/10.21785/icad2018.032
3. Hannah Schubert, Jacqueline Findlay, Katy Morley, Emma F. Puddy, **Robert Arbon**, Virginia C. Gould, Oliver Mounsey, Madeleine Evans, Gwen M. Rees, David C. Barrett, Katy M. Turner, Tristan A. Cogan, Matthew B. Avison, Kristen K. Reyher, 2019. *Evidence for reduced CTX-M carriage in cattle-associated Escherichia coli at low temperatures and on publicly accessible farmland: implications for surveillance and potential for farm-to-human transmission***.** bioRxiv: 778407
4. Christopher M. Timperley, **Robert E. Arbon**, Sally A. Saunders, Matthew J. Waters, 2002. *Fluorinated phosphorus compounds: Part 6. The synthesis of bis(fluoroalkyl) phosphites and bis(fluoroalkyl) phosphorohalidates***.** Journal of Fluorine Chemistry. Vol 113.
5. Christopher M. Timperley, **Robert E. Arbon**, Michael Bird, Stuart A. Brewer, Malcolm W. Parry, David J. Sellers, Colin R. Willis. 2003. *Bis(fluoroalkyl)acrylic and methacrylic phosphate monomers, their polymers and some of their properties***.** Journal of Fluorine Chemistry. Vol 121.

OTHER OUTPUT

1. **Robert E. Arbon**, George Holloway, Alex J. Jones, Peter Bennett, The Ligeti Quartet, 2019. *Metastable impressions: Artistic representations of Molecular Dynamics*. https://www.youtube.com/watch?v=zmXO6AZMOYU
2. **Arbon, R**., Drax, K., Thurlby, N., Timpson, N. J., Northstone, K., Brown, K. R., … Munafo, M. R*. (2019, February 27). MAPS: Mapping the Analytical Paths of a Crowdsourced Data Analysis.* Retrieved from osf.io/7vq3b. Experimental preregistration.

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TEACHING EXPERIENCE

1. *Private tutor* 2012 – 2019. I have tutored GCSE and A-level students professionally full-time for four years and part time for three years.
2. *Robust and Open Analysis in R*. 2018 – 2020. Co-designed with Natalie Thurlby a 1-day course on reproducible workflows in R which has been delivered four times in Bristol and was scheduled to be delivered in March 2020 (now pending). Supported by UK Reproducibility Network and Cancer Research UK.
3. *Style Transfer for Biochemists.* 2020. Designed a half-day course on using deep learning techniques for novel visualization of biochemical structures. Supported by CCPBiosim.
4. *Thermodynamics*. 2006 – 2007. Teaching assistant for 1 semester course on third year thermodynamics at Harvard university.

SKILLS

Programming languages:

- Python (6 years' experience)
- R (3 years' experience)
- Visual Basic for Applications (VBA) (7 years' experience)
- Fortran (4 years' experience)
- Lua (< 1 year's experience)
- Matlab (< 1 year's experience)
- C (< 1 year's experience)

Scientific computing:

- Molecular dynamics: AMBER, OpenMM and CHARMM
- Fluency in all the major data analysis packages in Python, including: SciPy, Scikit-learn, Pandas, Matplotlib, PyMC3 (Probabilistic programming).
- Good working knowledge of statistical computing in R, including Tidyverse (ggplot, dplyr etc.), Shiny, BRMS (probabilistic programming) and RMS (multivariable regression modelling)

High performance computing:

Good working knowledge of:

- MPI for Fortran;
- running software on multi-node CPU and GPU computational clusters using both Slurm and PBS/Torque work schedulers.

Software contributions:

- New features and bug fixes for **Osprey** (github.com/msmbuilder/osprey). Osprey is a Python library for hyper-parameter optimisation.
- New feature for **CHARMM** (charmm.org). CHARMM is a Fortran code for running molecular dynamics simulations on multi-node CPU and GPU computational clusters.
- Bug fixes for **PyEMMA** (github.com/markovmodel/PyEMMA). PyEMMA is a Python/C library of Markov model algorithms
- Bug fixes for **MSMBuilder** (github.com/msmbuilder/msmbuilder). MSBuilder is a Python/C library of Markov model algorithms.