ROBERT ARBON

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SUMMARY

I am a computational chemist and data scientist, with experience in both statistical consulting for life sciences and humanities, as well as analysis of biomolecular simulations. I have contributed to open-source projects as well as building a custom (and proprietary) package for analysis of large-scale simulation data. I am interested in developing software for scientific applications.

PROFESSIONAL EXPERIENCE

Aug. 2022 – Jul. 2023
Redesign Science, New York, USA
SENIOR SCIENTIST

Aug. 2021 – Aug. 2022
Redesign Science, New York, USA
SENIOR SCIENTIST (PART-TIME)

Aug. 2021 – Aug. 2022
Antonia Mey research group, University of Edinburgh, UK
POST-DOCTORAL RESEARCH FELLOW (PART-TIME)

Feb. 2021 – Jul. 2021
John Chodera Research Group, MSKCC, New York, USA
SOFTWARE SCIENTIST

Jun. 2018 – Jan. 2021
Bristol, UK
FREELANCE DATA SCIENTIST

Apr. 2012 – Sep. 2015
London, UK
PRIVATE 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

Aug. 2021
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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SKILLS

Programming languages:

- Python (9 years' experience)
- R (6 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
- Simulation analysis: PyMol, VMD, Deeptime and PyEmma, mdtraj.
- Fluency in all the major data analysis packages in Python, including: SciPy, Scikit-learn, Pandas, Matplotlib, PyMC3, Plotly, PyTorch, Dask.
- Good working knowledge of statistical computing in R, including Tidyverse (ggplot, dplyr etc.), Shiny, BRMS (probabilistic programming) and RMS (multivariable regression modelling)
- running software on multi-node CPU and GPU computational clusters using, MPI for Fortran;
- Slurm PBS/Torque; and Prefect 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.

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.

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PUBLICATIONS

1. Bell, K.; Hickel, J.; **Arbon, R**.; Zoomkawala, H. *Which Direction for Sustainable Development? A Time Series Comparison of the Impacts of Redistributive versus Market Policies in Bolivia and South Korea*. Sustainable Development **2023**, 1– 20.
2. Matthews, J. C.; Navasumrit, P.; Wright, M. D.; Chaisatra, K.; Chompoobut, C.; **Arbon, R.;** Khan, M. A. H.; Ruchirawat, M.; Shallcross, D. E. *Aerosol Mass and Size-Resolved Metal Content in Urban Bangkok, Thailand.* Environmental Science and Pollution Research **2022**, 29 (52), 79025–79040.
3. Matheson, E. L.; Smith, H. G.; Lewis-Smith, H.; **Arbon, R. E.;** Diedrichs, P. C. *Game on! A Randomised Controlled Trial Evaluation of Playable Technology in Improving Body Satisfaction and Negative Affect among Adolescents*. New Media & Society **2022**, 24 (12), 2635–2658.
4. **Arbon, R. E**. *Markov Models of Biomolecular Systems*. PhD, University of Bristol, **2021**.
5. Schubert, H.; Morley, K.; Puddy, E. F.; **Arbon, R.**; Findlay, J.; Mounsey, O.; Gould, V. C.; Vass, L.; Evans, M.; Rees, G. M.; Barrett, D. C.; Turner, K. M.; Cogan, T. A.; Avison, M. B.; Reyher, K. K. *Reduced Antibacterial Drug Resistance and BlaCTX-M β-Lactamase Gene Carriage in Cattle-Associated Escherichia Coli at Low Temperatures, at Sites Dominated by Older Animals and on Pastureland: Implications for Surveillance.* Applied and Environmental Microbiology **2021,** 87 (6), e01468-20.
6. Consortium, C. M.; Achdout, H.; Aimon, A.; Alonzi, D. S.; **Arbon, R.**; Bar-David, E.; Barr, H.; Ben-Shmuel, A.; Bennett, J.; Bilenko, V. A.; others. *Open Science Discovery of Potent Non-Covalent SARS-CoV-2 Main Protease Inhibitors*. BioRxiv **2020**, 2020–10.
7. Song, Y.-C., Ingram, S., **Arbon, R.E**., Topping, D.O., Glowacki, D.R., Reid, J.P.,. *Transient cavity dynamics and divergence from the Stokes–Einstein equation in organic aerosol*. Chem. Sci. **2020**, 11, 2999–3006.
8. **Robert E Arbon**, Alex J Jones, Lars A. Bratholm, Tom Mitchell, David R. Glowacki. *Sonifying stochastic walks on biomolecular energy landscapes***.** Proceedings of the International Conference on Audio Display, **2018**.
9. Christopher M. Timperley, **Robert E. Arbon**, Sally A. Saunders, Matthew J. Waters. *Fluorinated phosphorus compounds: Part 6. The synthesis of bis(fluoroalkyl) phosphites and bis(fluoroalkyl) phosphorohalidates***.** Journal of Fluorine Chemistry, **2002** 113 (1), 65-78 .
10. Christopher M. Timperley, **Robert E. Arbon**, Michael Bird, Stuart A. Brewer, Malcolm W. Parry, David J. Sellers, Colin R. Willis *Bis(fluoroalkyl)acrylic and methacrylic phosphate monomers, their polymers and some of their properties***.** Journal of Fluorine Chemistry. **2003**, 121 (1), 23-31.

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.