

Dr Adam Luke Baskerville

CURRICULUM VITAE

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Summary

- Postdoctoral research fellow with over 6 years' experience in scientific research.
- Expertise in quantum chemical physics, theoretical physics and scientific programming.
- Lecturer, teacher and mentor.
- Lab manager and lead computer program developer for the research group.
- Publications in peer-reviewed journals.
- Presented research at national and international conferences.

Skills

Languages: Python, C++, Bash, CUDA, Maple, Julia, HTML, \LaTeX .

Tools: PyTorch, TensorFlow, NumPy, SciPy, rdkit, OpenCV, Pandas, Eigen, qd, Arb, Git, Psi4, Gaussian09, ORCA

Operating Systems: Linux, Mac, Windows.

Experience

Postdoctoral Research Fellow

DEPARTMENT OF CHEMISTRY, SCHOOL OF LIFE SCIENCES, UNIVERSITY OF SUSSEX

Brighton, UK

May. 2018 - Current

Projects:

- **3Body Library:**
 - Developed extensive library of high accuracy programs applicable to solving the Schrödinger equation for any three-particle system, exploring new quantum chemical physics using their wavefunctions. All programs thoroughly documented for use by students.
 - Utilizes C++, Python, CUDA and Maple with Bash orchestrating to allow operations between each language. Non-linear parameter, NLP, optimisation was extensively used and all programs designed to use double, quadruple, octuple and ball arithmetic precision.
- **Density-Energy Space:**
 - Developed new physical framework which has shown a direct relationship between radial electron density and the total energy for quantum mechanical systems; a realisation of the Hohenberg and Kohn theorem. *Submitted for publication in Nature.*
 - Utilised communication between Maple and C++ which conducted numerical integration in parallel over a unit hypercube using quadruple precision.
- **Electron Correlation in Electronic Structure Theory:**
 - Calculated the current best electron correlation data for two-electron atoms through the Fully Correlated (FC) and Hartree Fock (HF) programs I developed in the 3Body library.
 - Developed highly optimized, vectorized and parallelized C program to rapidly calculate millions of two-electron integrals using 200-digit precision with rigorous error bounds for each integral.
 - Collaborators at Bristol University using this data to develop functional for use in Density Functional Theory (DFT).
- **Density Functional Theory Investigation:**
 - Implemented work of Colle and Salvetti (CS), Lee, Yang and Parr (LYP) and other DFT functionals to interface with my high accuracy FC and HF wavefunctions.
 - Showed that the CS and popular LYP functional work because of inaccurate function fit conducted by CS; questioning the physical basis behind the most popular functional used in DFT. *Submitted for publication in Royal Society Open Science.*
 - Currently developing functional for weakly bound systems which DFT struggles to calculate. *In preparation for publication in Physical Chemistry Chemical Physics.*

- **Weakly Bound and Excited States:**

- Implemented theoretical methodologies to analyse asymmetric behaviour of fermions in two-electron systems. This has been used to show quasi-bound behaviour in atoms near electron detachment, and to calculate highly excited Rydberg states. *In preparation for publication.*
- Developed a deep-learning inspired GPU technique using PyTorch to successfully circumvent computational difficulties owing to ill-conditioned matrices.

Roles and Responsibilities:

- Lead programmer in the research group requiring knowledge across wide variety of scientific problems.
- Lab manager responsible for maintaining computational resources in the research group.
- Teacher and mentor to numerous MChem and PhD students.
- Write papers for publication and present research in the form of oral presentations and posters at national and international conferences.
- Helped develop 'Quantum Leap', an interactive game to explain quantization at outreach events.
- **Lecturer:**
 - Created and taught my own scientific Python programming course for staff and students.
 - Lectured maths and data analysis for undergraduate students in the chemistry department.
- **Associate Tutor:**
 - Assisted in teaching mathematics, data analysis, point group symmetry, bonding, spectroscopy, and computational chemistry across multiple year groups from foundation to final year students in bioscience and chemistry departments. This involved problem-based workshops and marking.

Education

Ph.D. in Quantum Chemical Physics

DEPARTMENT OF CHEMISTRY, SCHOOL OF LIFE SCIENCES, UNIVERSITY OF SUSSEX

Thesis: The Quantum Chemical Physics of Few-Particle Atoms and Molecules.

Brighton, UK

Sep. 2014 - Jun. 2018

MPhys in Physics and Astrophysics, First-class honours

DEPARTMENT OF PHYSICS, SCHOOL OF PHYSICAL SCIENCES, UNIVERSITY OF KENT

Thesis: Magnetic Monopoles in Spin Ice.

Canterbury, UK

Sep. 2010 - Sep. 2014

Awards

- 2019 **NVIDIA GPU grant award**, NVIDIA. Awarded a Titan V GPU from NVIDIA as part of their *Accelerated Data Science* program.
- 2017 **Young Modellers Forum (YMF) talk prize**, *Young Modellers Forum (YMF), Greenwich*. Awarded for my presentation: "Going beyond standard approximations in quantum chemistry."
- 2016 **Doctoral overseas grant award**, *School of Life Sciences, University of Sussex*. Awarded £1000 to attend the IX Congress of the International Society for Theoretical Chemical Physics (ISTCP) which took place in North Dakota USA.
- 2016 **Institute of Physics funding award**, *Institute of Physics (IOP)*. Awarded £300 to attend the IX Congress of the International Society for Theoretical Chemical Physics (ISTCP).
- 2014 **MPhys final year research prize**, *School of Physical Sciences, The University of Kent*. Awarded for the best final year research project.
- 2012 **Second year student prize**, *School of Physical Sciences, The University of Kent*. Awarded for the highest total mark in second year.

Interests

I combined my passion for computation and astrophotography by building a specialised astrophotography camera using a Raspberry Pi and developing a GUI program called AstroPitography to control it. I also enjoy strongman and powerlifting training and oil painting.

I run a blog called Textbook to Terminal, T>T, (<https://adambaskerville.github.io>) which discusses how to program interesting science and mathematical related problems along with useful tools and ideas for researchers.