Dylan Counsell

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Education

University of Cambridge *Sep 2025 – Present*
PhD in Theoretical Chemistry

- Method development in stochastic and non-orthogonal quantum chemistry, including NOCI, stochastic NOCI, and perutrbative NOCI methods.

University of Cambridge *Sep 2024 – Sep 2025*
MPhil in Scientific Computing

- Grade: Distinction (75%).
- Thesis: *Improved Convergence to the Thermodynamic Limit in Periodic Systems with Full Configuration Interaction and Coupled Cluster Quantum Monte Carlo Methods.*
- Distinction in Thesis, Electronic Structure and Introduction to Topological Materials.
- Additional training in Advanced Atomistic Simulation, Quantum Algorithms, C++, Advanced Research Computing, OpenMP, MPI and CUDA.

University of Leeds *Sep 2020 – Jul 2023*
BSc in Chemistry

- First-Class Honours; Firsts in Dissertation, Quantum Mechanics, and Machine Learning modules.
- Dissertation: *An Ab-Initio Study into the Fundamentals of Physical Aromatic Chemistry.*

Research Projects

Stochastic Non-orthogonal Coupled Cluster & Configuration Interaction *Sep 2025 – Present*
PhD Research, University of Cambridge

- Developed noci-rs, a high-performance Rust package for stochastic and perturbative non-orthogonal quantum chemistry using hybrid Rayon and MPI parallelism.
- Implemented stochastic Non-orthogonal Configuration Interaction (NOCIQMC) methods that recover a larger proportion of the FCI correlation energy than competing approaches.
- Applied matrix-free NOCI-PT2 to ethene torsion, repeatedly evaluating a candidate-space operator with 96.9 billion unique elements per geometry.
- Optimised performance-critical non-orthogonal matrix-element evaluation using hand-written AVX2 and AVX-512 kernels with FMA and runtime CPU-feature dispatch.

Finite-Size Error Correction in Stochastic Determinant-Based Methods *Mar 2025 – Sep 2025*
MPhil Thesis, University of Cambridge

- Extended a finite-size error-correction method to stochastic determinant-based electronic-structure methods, including Full Configuration Interaction Quantum Monte Carlo (FCIQMC) and Coupled Cluster Monte Carlo (CCMC).
- Achieved up to a 78% reduction in finite-size errors in the Uniform Electron Gas and real periodic systems.

Imaginary-Time Evolution on Quantum Circuits *Jan 2025 – Mar 2025*
MPhil Coursework, University of Cambridge

- Implemented probabilistic imaginary-time evolution in Qiskit for the transverse-field Ising and Hubbard models, reproducing published benchmark results.

Experience

Laboratory Technician *Leeds, UK*
AETC — Precision Casting Facility *Jun 2023 – Jun 2024*

- Monitored physical and chemical parameters of 11 production investment-casting slurries.
- Conducted experiments assessing the feasibility of new slurry formulations before production use.
- Updated Standard Practice Instructions and managed controlled documentation using SAP.

Technologies

Languages: Rust, Python, C++, Fortran, Bash
Scientific Computing: PySCF, libcint, OpenBLAS/LAPACK, HDF5, Qiskit
High-Performance Computing: Rayon, OpenMP, MPI, Slurm
Development: Linux, Git, Cargo