Lee James O'Riordan

BSc (Hons), PhD

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Education

2012–2017   **PhD in Science (Physics)**, *Okinawa Institute of Science and Technology* , Japan.
Thesis: *"Non-equilibrium vortex dynamics in rapidly rotating Bose–Einstein condensates"*

2006–2010   **BSc (Hons) in Physics with Computing**, *Waterford Institute of Technology*, Ireland.
Thesis: *"Evaluating magnetic susceptibility in Heisenberg chains using OpenCL implementations of Monte Carlo methods."*

Work experience

2020–Current   **Research Fellow**, National University of Ireland Galway (NUIG), Ireland.

Senior computational scientist, Irish Center for High End Computing (ICHEC), Ireland.

2019–2020   **Postdoctoral Researcher**, NUIG.

Research computational scientist, ICHEC.

Current quantum activity lead at centre. Team lead for 4 researchers, and collaborator with 4 others across activities from HPC, quantum simulation and data analytics. Projects include:

○ **QNLP**: Designed, led and published demonstration of hybrid classical HPC-quantum NLP tasks on a quantum simulator, using **Python**, **C++**, **PyBind11**, **Catch2**, **Docker**, **OpenMP**, **MPI** and backed by Intel's Quantum Simulator (**Intel-QS**).

○ **NEASQC**: Guiding ICHEC's technical contributions to the EU funded NEASQC project for extensions to the QNLP work under WP6 UC2 framework agreement. Public details available at neasqc.eu.

○ **QuantEx**: Currently developing a modular quantum circuit translation framework for composing and mapping quantum use-cases to tensor-network operations using **Julia** for exascale systems. Suite to be released Q2 2021, with alpha versions available at Github:ICHEC/QuantExQASM.jl and Github:ICHEC/PicoQuant.jl.

2018   **Visiting researcher**, Okinawa Institute of Science and Technology Graduate University, Japan.

Collaborated on a study of chaotic dynamics in quantum superfluid systems. Developed C++, Python, MATLAB and CUDA generalisations to the GPU-enabled quantum solver suite, GPUE. Both works published in international journals.

2017–2018   **Postdoctoral Fellow**, Lawrence Berkeley National Lab, United States.

Researched real-time computational analysis of X-ray free electron laser crystallographic data. Extended CCTBX and DIALS software suites to better scale with Intel Xeon Phi processors on NERSC's Cori supercomputer. Work available at GH:ExaFEL. Achievements during this time:

○ **DIALS**: Enabled the study of a previously intractable big data set resulting in publication Acta Cryst. (2018). D74, 877-894, by reducing complexity for a given analysis algorithm from $O(n^2)$ to $O(n \log n)$, in addition to porting the methods from **Python** to **C++**.

○ **LCLS**: Enabled approx. **3x** speed-up of a time critical data analysis pipeline during live use by migration from on-premise system to NERSC's Cori supercomputer, allowing for **sub 10 minute** data quality checks. This prevented a 12 month delay in data collection during a SLAC LCLS experiment, and has led to the publication of the manuscript PNAS (2020) 117 (1) 300-307.

○ **NERSC Cori**: Developed and deployed a portable and more scalable analysis software pipeline through containerisation with Docker, reducing start-up overhead to approx. **25%** of original duration. This was by targeting optimisations supported for the **AVX2** & **AVX512** instruction set architectures of NERSC's Cori supercomputer, and selective pre-caching and pipelining of the environment.

○ **STRUMPACK**: Integrated the **STRUMPACK** sparse matrix package for distributed solution of nonlinear least squares problems into the CCTBX suite, intended to replace **Eigen**. Performance evaluation testing (available here) showed far greater performance using Eigen's solvers than was available using STRUMPACK, indicating efforts better spent elsewhere, and reducing future project workload.

2011–2012   **Research assistant**, University College Cork, Cork, Ireland.

Researching theory of ultracold quantum systems. Ported existing MPI-enabled simulation tool to C-CUDA.

2010–2011	**Software developer**, IBM Ireland, Dublin, Ireland.

Developed server-side applications for use with WebSphere Portal platform. Developed solutions using Java, XML, XSLT, Ant, Shell scripting, JDBC, Python, C. Deployed and managed WebSphere Portal, Lotus Sametime, and Lotus Connections software stacks.

2009 **Product engineer (intern)**, Analog Devices BV, Limerick, Ireland.

Member of semiconductor device yield improvement team. Analysed and implemented strategies for device failure analysis. Developed software for die yield analysis and characterisation.

Relevant project & technical experience

Toolbox: C, C++, Python, CUDA, OpenCL, MATLAB, Mathematica, Julia, Bash, SQL, Linux (RedHat, CentOS, Ubuntu, Arch), MacOS, Windows+WSL, PowerPC, x86, ARM, GCC, LLVM, GDB, LLDB, Intel Compiler, MKL, OpenMP, MPI, Numpy/Scipy, FFTW, CMake, Dask, Pandas, PyBind11, Intel VTune, Docker, Travis CI, Gitlab, Github, Catch2 Unit Testing, Nvidia Visual Profiler, SLURM, Spack, Eigen, STRUMPACK.

Project: Researcher developing software for composition and simulation of quantum computing algorithms
QuantEx using tensor network methods. Team size: 6. Languages & technologies: Julia, Python, C++, Quantum computing. Open source project components available at GH:ICHEC/QuantExQASM.jl and GH:ICHEC/PicoQuant.jl.

Project: Developed hybrid classical (HPC) & quantum algorithms for natural language processing. Partnership
QNLP with Intel and Enterprise Ireland. Team size: 4+. Languages & technologies: C++, MPI, Python, Quantum computing. Source code available at GH:ICHEC/QNLP, and paper at DOI:10.1088/2632-2153/abbd2e.

Project: Architect & developer of GPUE: GPU-enabled Gross–Pitaevskii equation solver; a 1/2/3D parallel
GPUE pseudospectral linear and nonlinear quantum (Schrodinger equation) partial differential equation solver and simulation tool. Team size: 3+. Languages: CUDA, C/C++, Python, MATLAB, Shell. Source available at GH:gpue-group/gpue with documentation at GH:gpue-group.

Project: Exascale Free Electron Laser project: exascale capable extensions to CCTBX (Computational crystal-
ExaFEL lographic toolbox) and DIALS X-ray diffraction analysis software projects. Team sizes: 5-10+. Technologies: Python, C++, Boost.Python, MPI, OpenMP, Eigen, Bash, Docker. Available at GH:ExaFEL, GH:cctbx-project/cctbx, and GH:dials/dials.

Professional certifications

2020 **Certified ScrumMaster**, *Scrum Alliance*, Credential ID: 1196787.
Issue Date: 27/02/2020, Expiration Date: 27/02/2022.

2020–Current **IBM Data Science Professional Certificate**, IBM, through Coursera.
In progress. Estimated completion: Feb 2021

Publications

2020 **A hybrid classical-quantum workflow for natural language processing**, L. J. O'Riordan, *et al.*, IOP Mach. Learn.: Sci. Technol. (2020). DOI: 10.1088/2632-2153/abbd2e

2019 **Photoreversible interconversion of a phytochrome photosensory module in the crystalline state**, E. Sethe Burgie, *et al.*, Proceedings of the National Academy of Sciences, 117 (1) 300-307 (2019). DOI: 10.1073/pnas.1912041116

Chaotic few-body vortex dynamics in rotating Bose-Einstein condensates, T. Zhang, J. Schloss, A. Thomasen, L. J. O'Riordan, T. Busch, A. White, Physical Review Fluids, (**4**) 5, 054701 (2019). DOI: 10.1103/PhysRevFluids.4.054701

2018 **GPUE: Graphics Processing Unit Gross-Pitaevskii Equation solver**, J. R. Schloss, L. J. O'Riordan, Journal of Open Source Software, (**3**) 32, 1037 (2018). DOI: 10.21105/joss.01037

Improving signal strength in serial crystallography with DIALS geometry refinement, A. S. Brewster, D. G. Waterman, J. M. Parkhurst, R. J. Gildea, I. D. Young, L. J. O'Riordan, J. Yano, G. Winter, G. Evans, N. K. Sauter, Acta Cryst. D., **74**, 877-894. DOI: 10.1107/S2059798318009191

2017 **Non-equilibrium vortex dynamics in rapidly rotating Bose-Einstein condensates**, L. J. O'Riordan, Okinawa Insitute of Science and Technology Graduate University. DOI: 10.15102/1394.00000165

2016 **Topological defect dynamics of vortex lattices in Bose–Einstein condensates**, L. J. O'Riordan, Th. Busch, Phys. Rev. A 94, 053603. DOI: 10.1103/PhysRevA.94.053603

Moiré superlattice structures in kicked Bose-Einstein condensates, L. J. O'Riordan, A. C. White, Th. Busch, Phys. Rev. A 93, 023609. DOI: 10.1103/PhysRevA.93.023609

2013 **Coherent transport by adiabatic passage on atom chips**, T. Morgan, L. J. O'Riordan, N. Crowley, Th. Busch, Phys. Rev. A 88, 053618. DOI: 10.1103/PhysRevA.88.053618

Recent presentations, talks and tutorials

2019 **QNLP 2019**, *Invited talk*, Oxford, UK.
Title: "*Calculating sentence similarity using a hybrid quantum-classical workflow*"

Intel DevCon @ SC'19, *Talk*, Denver, Colorado, USA.
Title: "*Extensions to Intel® Quantum Simulator for Quantum Natural Language Processing and Beyond*"

National University of Ireland Galway, *Tutorial*, Galway, Ireland.
Title: "*Numerical computing with Julia*"

Dublin Institute for Advanced Studies, *Tutorial*, Dublin, Ireland.
Title: "*Numerical computing with Julia*"

HPCS 2019, *Tutorial*, Dublin, Ireland.
Title: "*Simulating quantum computers on high-end HPC systems*"

ISC 2019, *Talk/technical session*, Frankfurt, Germany.
Title: "*Natural language processing with Intel® Quantum Simulator*"

2018 **DIALS Workshop 2018**, *Talk/tutorial*, Lawrence Berkeley National Lab, USA.
Title: "*Data analysis and development using Jupyter*"

2017 **Waterford Institute of Technology**, *Seminar*, Waterford, Ireland.
Title: "*Ultracold atomic gases*"

Competitions, grants & awards

2017 **Government of Ireland Postdoctoral Fellowship**, *QuSys*, Trinity College Dublin.
Project title: "Advanced computational techniques for steady-state quantum thermodynamics".
Declined award, accepted LBNL postdoc instead.

2014 **Best Customer Interaction**, *Kyued-Up Innovation Event*, Okinawa Institute of Science and Technology Graduate University, Japan.
Project title: "Okinawa Science Discovery Center"

2013 **2nd place**, *Euraxess Links Japan, Science Slam 2013*, Tokyo Institute of Technology, Japan.
Talk title: "Quantum Typhoons"

2010 **Student of the Year**, *School of Science, Waterford Institute of Technology*, Ireland.

2010 **Best undergraduate project**, *Department of Computing, Maths and Physics, Waterford Institute of Technology*, Ireland.
Title: "Evaluating magnetic susceptibility in Heisenberg chains using OpenCL implementations of Monte Carlo methods".

University service

2017-2020 **First alumnus board member**, *Board of Councilors*, OIST, Japan.

2015-2016 **Chair**, *Student Council*, OIST, Japan.
Elected by student body. Facilitated meetings between the student body and faculty. Improved institutional policies and conditions for students. Developed mentoring program for incoming students.

2014-2017 **HPC advanced users group representative**, *Quantum Systems Unit*, OIST, Japan.
Research unit representative to the OIST HPC and scientific computing team. Trained group members on the use of HPC software and advanced programming techniques.

2013-2016 **President**, *Music Club*, OIST, Japan.
Founder of Music club at OIST. Practiced, trained, and performed with many members on a regular basis.

2013-2016 **ITSSC member**, *OIST*.
Member of university task force for updating IT policies and compliance.

2013-2015 **Outreach**, *Quantum Systems Unit*, OIST, Japan.
Delivered talks to local schools on quantum physics. Delivered a team-based Scratch programming language tutorial for children aged 8-16. Mentored several interns and trained them on numerical computing for quantum physics.