

# Paddy Ó Conbhuí

poconbhui@gmail.com

## SOFTWARE DEVELOPMENT

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I specialize in high performance computing (HPC), and computational physics. I have extensive experience in using co-processors, primarily Nvidia GPUs, and have a keen interest to further explore the accelerator landscape.

I have a strong interest in writing high quality software: using modern tools, techniques, and design patterns. I'm particularly interested in writing high-performance tools and libraries which address bottlenecks in existing systems, and enable novel avenues of research & development, enabling the development of high-quality software for others.

I have a strong background in C++, and consider it my “goto” language. However, I have developed and worked on libraries and applications in a wide number of languages, most significantly in Fortran, C, and Python. The following is a more extensive (but not exhaustive!) list of languages, libraries and tools I've used significantly in projects

**Languages:** C++, C, Fortran 90, Python, Bash, JavaScript, Ruby, Haskell

**Parallel Programming:** MPI, MPI-IO, OpenMP, CUDA C/C++, CUDA Fortran, OpenACC, UPC, Coarray Fortran

**Build Tooling:** CMake, Autotools, GCC, Clang, nvcc, MSVC, PGI, MinGW, Cygwin, Linux & macOS toolchains, Docker, Singularity, Spack, Travis-CI, Bitbicket Pipelines, Gitlab-CI

**Scientific Software:** SWIG, FEniCS, CGAL, VTK, ParaView, Mathematica, MATLAB, Zemax, Gnuplot, LaTeX

**Audio Stacks:** PulseAudio, GStreamer, SBC, Bluetooth

**Web Development:** HTML/CSS, PHP, Ruby On Rails, Node.js, jQuery

**Databases:** SQL, CouchDB, MongoDB, Redis, Neo4j

## EXPERIENCE

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### Irish Centre for High-End Computing (ICHEC)

Dublin, Ireland

*Acting Oil & Gas Programme Manager*

*2018 - Present*

Leading a research software engineering team of 9 postdocs with 1 PhD student with a focus on the oil & gas domain, leading a consultancy oil & gas team of 5, and founded & leading a consultancy financial software optimization team of 3. Led and executed several bespoke AI performance optimization projects for Irish SMEs.

- Managed the smooth transition of the duties and consultancy development work of departing Oil & Gas Programme Manager to myself and the current consultancy oil & gas team with limited disruption to our clients. Expanded our capability and capacity to service oil & gas clients.
- Founded a consultancy financial software optimization team. Won a highly competitive contract (competing with 4 other UK-based HPC consultancy firms) with a large financial software company for a (now completed) proof-of-concept consultancy GPU optimization project. Further work with the client expected to begin in Q4 2019.
- Overseeing and contributing to the transition of the ExSeisDat project to its second phase focusing on hardware-level I/O optimization and exascale storage systems, securing ICHEC's partnerships with LERO and DDN to the end of the current funding cycle. Leveraging the learning outcomes of the project to boot-strap a research performance engineering team in the centre.
- Led and contributed to an AI optimization & predictive performance modelling project in the Machine Translation domain for United Language Group using Nvidia GPUs on Microsoft Azure.
- Providing mentorship to postdocs and PhDs in the centre, along with undergraduates through internship programmes.
- Assessing and implementing internal policies and procedures to foster and develop critical skills and experience in our computational scientists. Contributing to development of scalable organizational structures in the centre to allow for future expansion.
- Contributing to technical work needed by the Project Management Organization, ensuring the smooth operation of our project management software.
- Developing best-practice guidelines, FAQs, and teaching material for software development within the centre.
- Developing capability within ICHEC to develop and present Nvidia GPU training material and workshops. Mentoring in Nvidia-sponsored OpenACC hackathons.

## Irish Centre for High-End Computing (ICHEC)

*Computational Scientist*

Dublin, Ireland

2017 - 2018

Contributed to the development of academic and enterprise software, primarily in the context of oil & gas. Ported and optimized software for clients to leverage GPU accelerators, primarily for AI applications.

- Contributed to the ExSeisDat library, focusing on parallel I/O and I/O optimization for oil & gas data formats and workflows. Introduced a number of common best-practices, including but not limited to: configuring with CMake, fixing the root-causes of *every* compiler warning, static analysis, automatic code formatting, and continuous integration using multiple compilers and dependency versions / implementations.
- Contributed to the development of consultancy oil & gas software.
- Ported an oil & gas code (Kirchhoff Depth Migration) to run on Microsoft Azure cloud platform, leveraging Nvidia GPU acceleration for a multi-national oil & gas company.
- Analyzed and ported AI software stack in the Natural Language Processing domain to leverage GPU acceleration for Opening.io.
- Participated in numerous workshops (primarily with PRACE), further developing skills in high performance C++, parallel I/O, seismic data processing, FPGA programming, performance analysis tools, and modern parallel programming models for exascale systems.
- Achieved professional certification as Certified Scrum Master (CSM) from Scrum Alliance.

## University Of Edinburgh

*PhD Student*

Edinburgh, Scotland

2013 - 2017

Investigated numerical techniques for understanding how rocks record changes in the earth's magnetic field. This was done primarily through the lens of micromagnetic modelling, using high-performance finite element analysis, C++ and Fortran.

- Developed theory and computational techniques for including magnetostrictive and multi-phase effects in non-uniformly-magnetized 3D finite-element micromagnetic models with free boundaries. This was implemented in our group's Fortran-based micromagnetics code, MERRILL, with results presented at conferences, and published in a thesis.
- Developed a meshing application in C++, MESHRRILL, leveraging the CGAL library to generate unstructured meshes for micromagnetic simulations. The application generates meshes for a number of pre-defined shapes, typical for ferromagnetic crystals, but also generates surface reconstructions of geometries from coarse tomography images. Data generated by this software has been used in publications.
- Developed software, HoloMag, written in C++ and Python to produce simulated electron holography data from micromagnetic models. This is provided as a ParaView plugin and has been optimized to produce holography results in near real-time, allowing researchers to develop an intuition for how 3D magnetizations effect the 2D holography images. Data generated by this software has been used in publications.
- Developed workflows for compiling software for reliable distribution. This included building as-static-as-possible versions of programs like MERRILL, along with shared-library version of MESHRRILL with all dependencies installed in a subdirectory and RPATHs set appropriately, so it could easily be used and linked as a C++ library to mesh complex user-defined geometries. HoloMag was also compiled to be ABI-compatible with ParaView binaries downloaded from the ParaView website.

## Dublin Web Summit Limited

*Technical Analyst*

Dublin, Ireland

Summer 2012

Evaluated new technologies for use in projects. Built and maintained applications for internal and external use. Analyzed and modified applications to handle higher user loads as necessary.

- Developed browser-based apps leveraging Facebook's JavaScript API and FBQL API.
- Identified and eliminated bottlenecks in Ruby-on-Rails ticketing system for large events with many users.
- Implemented caching and distribution of content through a CDN for events sites to handle high traffic.
- Researched and evaluated IaaS platforms, deployments in cloud environments and NoSQL database systems.

## LULI, École Polytechnique

*Intern*

Palaiseau, France

Summer 2011

Identified sources of alignment errors encountered by prior experiments using ellipsoidal plasma mirrors (EPM) for focusing lasers, by developing a twinned numerical and physical experiment. Identified which classes of misalignment the system was sensitive to, informing future alignment procedures.

## University Of Edinburgh

*PhD, Geophysics*

Edinburgh, Scotland

2013 to 2017

Trained as a researcher in Geophysics, primarily in computational paleomagnetism.

### **Thesis:** *Micromagnetic Modelling of Imperfect Crystals*

Developed the theory needed to simulate non-uniformly-magnetized, multi-phase, ferromagnetic crystals including magnetostriction and crystal defects, with free boundary conditions. Presented implementations and results.

## University Of Edinburgh

*MSc, High Performance Computing – With Distinction*

Edinburgh, Scotland

2012 to 2013

The course centred around building high performance applications, primarily through parallelism, and through deep understanding of the underlying architecture of a given system and language.

**Subjects:** Message Passing Programming, Threaded Programming, Parallel Numerical Algorithms, Parallel Programming Languages, HPC Architectures, HPC Ecosystems, Performance Programming, Software Development, Advanced Parallel Programming, Parallel Design Patterns.

### **Dissertation:** *Towards Exascale Molecular Dynamics*

Compared replicated data and systolic loop schemes for molecular dynamics simulations, and presented a novel hybrid replicated systolic scheme with impressive scaling properties.

## Trinity College, Dublin

*BA Mod, Theoretical Physics – II-1*

Dublin, Ireland

2008 to 2012

The course taught practical problem solving skills and analytical thinking in the fields of Mathematics and Physics.

**Subjects:** Computer Simulation, GPU Programming, Experimental Labs, Classical Mechanics, Quantum Mechanics, Classical Field Theory, Quantum Field Theory, Special Relativity, General Relativity, Classical Statistical Mechanics, Quantum Statistical Mechanics, Condensed Matter Physics, Spectroscopy, Optics, Electromagnetism, Magnetism, Thermodynamics, Electronics, Chaos and Complexity, Linear Algebra, Analysis, Topology.

### **Dissertation:** *Computing Two Point Correlators For A Lattice QCD Theory On Graphics Processing Units*

Wrote complex-valued matrix multiplications routines in CUDA C which beat cuBLAS (at the time) by 20%. Re-cast the full set of matrix multiply-traces needed to compute the correlator matrix into a large matrix-matrix multiplication, providing up to 20x performance improvement over independent multiply-trace operations.

## PUBLICATIONS

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Fisher, M. A., Conbhuí, P. Ó., ... & Short, R. (2018). ExSeisDat: A set of parallel I/O and workflow libraries for petroleum seismology. *Oil & Gas Science and Technology–Revue d'IFP Energies nouvelles*, 73, 74.

Conbhuí, P. Ó. (2018). Micromagnetic modelling of imperfect crystals, PhD Thesis, University of Edinburgh.

Conbhuí, P. Ó., Williams, W., Fabian, K., Ridley, P., Nagy, L., & Muxworthy, A. R. (2018). MERRILL: Micromagnetic earth related robust interpreted language laboratory. *Geochemistry, Geophysics, Geosystems*, 19(4), 1080-1106.

Valdez-Grijalva, M. A., Muxworthy, A. R., Williams, W., Conbhuí, P. Ó., Nagy, L., Roberts, A. P., & Heslop, D. (2018). Magnetic vortex effects on first-order reversal curve (FORC) diagrams for greigite dispersions. *Earth and Planetary Science Letters*, 501, 103-111.

Nagy, L., Williams, W., Muxworthy, A. R., Fabian, K., Almeida, T. P., Conbhuí, P. Ó., & Shcherbakov, V. P. (2017). Stability of equidimensional pseudo-single-domain magnetite over billion-year timescales. *Proceedings of the National Academy of Sciences*, 114(39), 10356-10360.

Almeida, T. P., Muxworthy, A. R., Kovács, A., Williams, W., Nagy, L., Conbhuí, P. Ó., ... & Dunin-Borkowski, R. E. (2016). Direct observation of the thermal demagnetization of magnetic vortex structures in nonideal magnetite recorders. *Geophysical Research Letters*, 43(16), 8426-8434.

Einsle, J. F., Harrison, R. J., Kasama, T., Conbhuí, P. Ó., Fabian, K., Williams, W., ... & Midgley, P. A. (2016). Multi-scale three-dimensional characterization of iron particles in dusty olivine: Implications for paleomagnetism of chondritic meteorites. *American Mineralogist*, 101(9), 2070-2084.

Einsle, J. F., Fu, R. R., Weiss, B. P., Kasama, T., Fabian, K., Conbhuí, P. Ó., ... & Harrison, R. J. (2015). Focused ion beam nanotomography of chondritic meteorites: Closing the mesoscale length gap in paleomagnetic studies. *Microscopy and Microanalysis*, 21(S3), 2261-2262.