Alastair Marshall

Researcher

Education

2018–2022 **PhD**, *Ulm University*, Ulm, *Pending*

Working in a start-up I am finishing my PhD in quantum optimal control (QOC) as part of the European project QuSCo. During this time I have work on applying QOC to a variety of different experimental systems, from NVs in diamond to organic crystals to liquid state NMR systems. I have also worked on developing open source QOC packages in both Julia and Python in my free time.

2013–2018 **MPhys**, *University of St Andrews*, St Andrews, *First Class Honours*

I completed an integrated Masters in Physics in St Andrews, Scotland. During this time I took classes on quantum mechanics and on monte carlo simulations.

PhD Thesis

title *Quantum Optimal Control for Sensing and Hyperpolarization - (in prep.)*

supervisors Fedor Jelezko, Philipp Neumann

description Quantum optimal control (QOC) is a method for controlling quantum systems to guide them from some initial state to some final state. As interest in quantum technologies increases it will become increasnigly important to get even small increases in performance, QOC is perfect for this task. In my thesis we show how QOC can be applied to enable the first sensing scheme that uses the full spin 1 of an NV centre in diamond. We then show that closed-loop QOC can be beneficial for hyperpolarization applications where we optimize a pulse that reduces the time to polarize a crystal by a factor of 3. Finally, we explore para-hydrogen induced polarization and show that while working at ultra-low fields radio frequency pulses are an incredibly efficient method for transferring polarization.

Master's Thesis

title *Probing the Optical Event Horizon with Pulsed Light*

supervisors Friedrich Koenig

Publications

Scalable and Tunable Diamond Nanostructuring Process for Nanoscale NMR Applications

Authors Martin Gierse, Alastair Marshall (joint 1st author)

Year 2022

✱ *8 March 1995*

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Description Nanostructuring of a bulk material is used to change its mechanical, optical, and electronic properties and to enable many new applications. We present a scalable fabrication technique that enables the creation of densely packed diamond nanopillars for quantum technology applications. The process yields tunable feature sizes without the employment of lithographic techniques. High-aspect-ratio pillars are created through oxygen-plasma etching of diamond with a dewetted palladium film as an etch mask. We demonstrate an iterative renewal of the palladium etch mask, by which the initial mask thickness is not the limiting factor for the etch depth. Following the process, 300–400 million densely packed 100 nm wide and 1 m tall diamond pillars were created on a 3 × 3 mm2 diamond sample. The fabrication technique is tailored specifically to enable applications and research involving quantum coherent defect center spins in diamond, such as nitrogen-vacancy (NV) centers, which are widely used in quantum science and engineering. To demonstrate the compatibility of our technique with quantum sensing, NV centers are created in the nanopillar sidewalls and are used to sense 1H nuclei in liquid wetting the nanostructured surface. This nanostructuring process is an important element for enabling the wide-scale implementation of NV-driven magnetic resonance imaging or NV-driven NMR.

Radio Frequency Sweeps at µT Fields for PHIP of Biomolecules

Authors Alastair Marshall (1st author), et al.

Year 2022

Description Magnetic resonance imaging of ^{13}C-labeled metabolites enhanced by parahydrogen-induced polarization (PHIP) can enable real-time monitoring of processes within the body. We introduce a robust, easily implementable technique for transferring parahydrogen-derived singlet order into ^{13}C magnetization using adiabatic radio-frequency sweeps at μT fields. We experimentally demonstrate the applicability of this technique to several molecules, including some molecules relevant for metabolic imaging, where we show significant improvements in the achievable polarization, in some cases reaching above 60%. Furthermore, we introduce a site-selective deuteration scheme, where deuterium is included in the coupling network of a pyruvate ester to enhance the efficiency of the polarization transfer. These improvements are enabled by the fact that the transfer protocol avoids relaxation induced by strongly coupled quadrupolar nuclei.

Macroscopic Hyperpolarization Enhanced with Quantum Optimal Control

Authors Alastair Marshall (joint 1st author), Thomas Reisser, Phila Rembold, et al.

Year 2022

Description I prepared our experiment for interfacing with optimal control algorithms. We then use the optimal control software suite known as redCRAB to optimize hyperpolarization sequences. We introduce a general optimal control framework, ARISE, for these types of problems. We optimize the hyperpolarization sequence the company uses and achieve a 28% increase in signal with a 15% faster buildup, allowing the polarization of multiple crystals per day

Hyperpolarized solution-state NMR spectroscopy with optically polarized crystals

Authors Company Publication (12th author)

✱ 8 March 1995
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Year 2021

Description Using hyperpolarized pentacene-naphthalene crystals we successfully transferred polarization to external molecules. The hyperpolarization sequence in use was something that I optimized.

Zero- and Low-field Nano-NMR with Nitrogen Vacancy Centers

Authors Philipp Vetter, Alastair Marshall (2nd author), et al.

Year 2021

Description We demonstrate the first experimental verification of double quantum sensing using linearly polarized microwaves. I numerically designed a robust optimal control sensing sequence that our co-author then discovered was part of a family of such sequences

Conference Talks and Posters

Euromar 2022

July 2022

Presenting poster entitled "Radio Frequency Sweeps at μT Fields for PHIP of Biomolecules"

ENC 2022

April 2022

We took existing radio frequency pulses from high-field NMR and brought them to low-field, we then used them to efficiently transfer polarization even in the presence of fast relaxation deuterium.

Quantum Control in Quantum Technologies

October 2022

Gave a talk where I presented our NV Sensing paper and our closed-loop hyperpolarization paper

QuSCo School

September 2021

Presented the initial version of QuantumControl.jl demonstrating how we could use automatic differentiation to easily solve quantum control problems.

DPG Conference

March 2019

Presented initial ideas about applying quantum optimal control for hyperpolarization of NV centres. This eventually became the closed-loop control project.

Experience

Employment

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2018–2022 **Researcher**, *NVision Imaging Technologies*, Ulm

During my PhD I worked for a start-up company based in Ulm that is trying to use hyperpolarization for cancer diagnosis. I was one of two PhD students within the company, mainly composed of senior researchers.
Projects completed:

- NV Sensing
  - Worked with students from Ulm University to develop robust optimal sensing sequence
  - Demonstrated first experimental verifcation of spin 1 sensing with NV centres in diamond
  - Lead project introducing quantum optimal control to our diamond based microscopes
- Organic Crystal Control
  - Lead project to integrate remote dCRAB software directly with experimental setup
  - Interfaced with theoreticians to help develop a model of the system
  - Transferred knowledge to EPR experiments where our findings also improve signal
- Radio Frequency Control
  - Developed and outlined initial idea, provided help simulating quantum system in Julia
  - Built initial experimental setup for performing the control and carried out numerous verification experiments
  - Demonstrated the efficiency of the protocol for polarization transer in the presence of Deuterium relaxation

2017–2018 **EPSRC Summer Research Grant**, *University of St Andrews*, St Andrews

Was award an EPSRC Summer research grant to work in the quantum optics group at St Andrews. My project was focussed on characterising our ultra-fast laser.

Miscellaneous

2016–2017 **Researcher**, *Dukosi Ltd*, Edinburgh

Worked for electric car company Dukosi helping model Li-ion batteries

Languages

English Fluent

German Rudimentary

Programming Experience

	Level	Skill	Years	Comment
Language:	■■■■■	Python	6	*I have been working in Python for years and have used it extensively during my PhD.*
	■■■■■	Julia	2	*I have also picked up, and fallen in love with Julia. My favourite for writing fast quantum mechanical simulations*
	■■■■■	Fortran	6	*I have a lot of experience with writing code in Fortan, including reimplementing Matlab simulations for an order of magnitude speedup.*
	■■■■□	Matlab	1	*I have used Matlab a little but prefer Python or Julia instead.*

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	■■■□□	C++	1	*I have done some programming in C++ and worked with it a little for quantum simulations.*
Libraries	■■■■■	QuantumControl.jl	1	*I developed the initial implementation of QuantumControl.jl and have since helped with the package ecosystem.*
	■■■□□	Zygote.jl	1	*I have used the Zygote automatic differentiation library in Julia for quantum control for the last few years.*
	■■■□□	JAX	1	*I recently started using JAX during some Python based quantum control projects.*
	■■□□□	PyTorch	1	*I have worked with PyTorch a little for some basic machine learning.*

Interests

Reading I am an avid reader, most recently I finished reading Foucault's Pendulum which I thoroughly enjoyed. Hoping to read 60 books this year.

Gaming Ever since I was a child I have loved video games of all kinds. Some of my fondest memories are LAN parties with my little brother, playing Age of Empires. Recently I started reading Games: Agency As Art by C. Thi Nguyen and it has changed how I look at my hobby.

Programming I love programming personal projects, sometimes these also include quantum control projects. I recently started learning Rust because I like developing fast, platform agnostic code.

Running I got really into running during the first lockdown, recently I have not been able to get out as much as I would want

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