

# QCC2015 Book of Abstracts

## Tutorials

**Steffen Glaser**

**TU München**

---

### *Optimal control of spin dynamics and beyond*

The field of Optimal Control Theory offers powerful analytical and numerical tools to explore the ultimate performance limits of pulse sequences. In the last decade, these tools not only provided pulse sequences of unprecedented quality and capabilities, but also new analytical and geometrical insight [1,3,7,10,11] and a deeper understanding of pulse optimization problems. Efficient numerical algorithms, such as the GRAPE algorithm [2,4,5], make it possible to develop robust time-optimal or relaxation-optimized pulse sequences, taking into account experimental limitations and imperfections, such as maximum pulse amplitudes, maximum pulse power, pulse inhomogeneity as well as transient effects associated with the switching of pulse amplitudes and phases. In this tutorial, important concepts of Optimal Control Theory will be discussed and applications of uncoupled and coupled spin systems will be presented. Examples will be shown for applications in NMR spectroscopy of small molecules and of large biomolecules, as well as electron spin resonance spectroscopy [6] and magnetic resonance imaging [7,8]. These include broadband [9] and band-selective pulses, coherence transfer experiments [2,3] and novel ultra-broadband decoupling sequences [12]. In addition to individually optimized pulses, simultaneously optimized pulses provide significant performance gains by exploiting cooperative effects [13].

[1] N Khaneja, R Brockett, SJ Glaser, Time Optimal Control in Spin Systems, Phys. Rev. A 63, 032308 (2001).

[2] N Khaneja, T Reiss, C Kehlet, T Schulte-Herbrüggen, SJ Glaser, Optimal Control of Coupled Spin Dynamics: Design of NMR Pulse Sequences by Gradient Ascent Algorithms, J. Magn. Reson. 172, 296-305 (2005).

[3] NC Nielsen, C Kehlet, SJ Glaser, N Khaneja, Optimal Control Methods in NMR Spectroscopy", Encyclopedia of Nuclear Magnetic Resonance (2010).

[4] P de Fouquières, SG Schirmer, SJ Glaser, I Kuprov, Second Order Gradient Ascent Pulse Engineering, J. Magn. Reson. 212, 412-417 (2011).

[5] S Machnes, U Sander, SJ Glaser, P de Fouquières, A Gruslys, S Schirmer, T Schulte-Herbrüggen, Comparing, Optimizing and Benchmarking Quantum Control Algorithms in a Unifying Programming Framework, Phys. Rev. A 84, 022305 (2011).

[6] PE Spindler, Y Zhang, B Endeward, N Gershenson, TE Skinner, SJ Glaser, TF Prisner, Optimal Control Pulses for Increased Excitation Bandwidth in EPR, J. Magn. Reson. 218, 49-58 (2012).

[7] B Bonnard, SJ Glaser, D Sugny, A Review of Geometric Optimal Control for Quantum Systems in Nuclear Magnetic Resonance, Adv. Math. Phys. 2012, 857493 (2012).

[8] M Lapert, Y Zhang, MA. Janich, SJ Glaser, D Sugny, Exploring the Physical Limits of Saturation Contrast in Magnetic Resonance Imaging, Sci. Rep. 2, 589 (2012).

[9] K Kobzar, S Ehni, TE Skinner, SJ Glaser, B Luy, Exploring the Limits of Broadband 90° and 180° Universal Rotation Pulses, J. Magn. Reson. 225, 142-160 (2012).

[10] M Lapert, E Assémat, SJ. Glaser, D Sugny, Understanding the Global Structure of Two-Level Quantum Systems with Relaxation: Vector Fields, Magic Plane and Steady-State Ellipsoid, PRA 88, 033407 (2013).

[11] M Lapert, E Assémat, SJ Glaser, D Sugny, Optimal Control of the Signal-to-Noise Ratio per Unit Time for a Spin-1/2 Particle, Phys. Rev. A 90, 023411 (2014).

[12] F Schilling, LR. Warner, NI Gershenson, TE Skinner, M Sattler, SJ Glaser, Next-Generation Heteronuclear Decoupling for High-Field Biomolecular NMR Spectroscopy, Angew. Chem. Int. Ed. 53, 4475-4479 (2014).

[13] M Braun, SJ Glaser, Concurrently optimized cooperative pulses in robust quantum control: Application to broadband Ramsey-type pulse sequence elements, New J. Phys. 16 (2014) 115002.

---

**Christiane Koch**

**Universität Kassel**

### *Quantum optimal control using Krotov's method*

A quantum control problem is characterized by the optimization target including constraints and by the equations of motion. Krotov's method derives an optimization algorithm from these ingredients using the variational principle. It leads to a set of coupled non-linear equations for the control and the state which need to be solved iteratively. The essence of Krotov's method consists in ensuring monotonic convergence of the iterative solution by separating the dependences of the optimization functional on control and state. For quantum dynamics, Krotov's existence proof of monotonically convergent algorithms can be turned into a

constructive one, providing algorithms to tackle practically any quantum control problem. In particular, it allows to freely construct the optimization functional, with the only mathematical requirement being analytically known first order derivatives with respect to control and state. With this set of tools, we can test the fundamental limits of quantum control but also explore new opportunities arising in open quantum systems or electron dynamics.

**Ilya Kuprov**

**University of Southampton**

---

*Quadratically converging control sequence optimization algorithms*

Most current algorithms for control sequence optimization either use non-gradient methods with no asymptotic convergence rate guarantees, or gradient descent and quasi-Newton methods, which provide linear or superlinear asymptotic convergence. In this communication we report an efficient algorithm for computing the full Hessian of the optimal control objective function in a large class of practically relevant cases, and use it to analyze the convergence properties of Newton-Raphson, trust-region and rational function optimization methods using the full Hessian matrix.

**Seth Lloyd**

**Massachusetts Institute of Technology**

---

*Quantum metrology*

Quantum mechanics provides the ultimate limits to measurement. This tutorial reviews those limits and shows how they can be attained. Effects such as entanglement and squeezing allow semi-classical bounds such as the standard quantum limit -- standard, quantum, but not a limit -- to be surpassed.

**Karoline Wiesner**

**Bristol University**

---

*What is a complex system?*

Complex systems research is becoming ever more important in both the natural and social sciences. It is commonly implied that there is such a thing as a complex system, different examples of which are studied across many disciplines. However, there is no concise definition of a complex system, let alone a definition on which all scientists agree. We review various attempts to characterize a complex system, and consider a core set of features that are widely associated with complex systems in the literature and by those in the field. We argue that some of these features are neither necessary nor sufficient for complexity, and that some of them are too vague or confused to be of any analytical use. In order to bring mathematical rigour to the issue we then review some standard measures of complexity. We will comment on complexity in quantum and classical systems.

## Talks

**Christian Arenz**

**Aberystwyth University**

---

*Local noise yielding full control*

Typically the interaction of a quantum system with the environment is considered to be detrimental for quantum information processing. Quantum gates one wants to perform become noisy. Based on the Zeno effect it was recently argued [1] that a strong dissipative process described by an amplitude damping channel applied locally on parts of the considered quantum system can have a beneficial effect. Quantum operations that could not be implemented without the dissipative process become now achievable.

Here we study the ability to perform quantum gates on a qubit coupled to another qubit that is subject to a strong dissipative process. For certain control operations we show that the qubit becomes fully controllable only in the presence of the dissipative process. Using optimal control theory we numerically calculate the control pulses that lead to a desired target gate and identify a parameter regime in which the gates become achievable with high fidelity.

[1] D. Burgarth et. al., Nature communications 5 (2014).

**Rami Barends**

**Google**

---

*Exploring fault tolerance in a superconducting quantum circuit with repetition code error correction*

Arguably one of the most challenging tasks in quantum information is preserving a quantum state. A viable quantum error correction scheme must be able to protect a state from bit and phase flips with modest physical requirements. Superconducting quantum devices have recently reached the fidelity requirements for surface code error correction. The surface code is the preferred scheme for superconducting circuits, as it requires nearest neighbour coupling only, and has lenient fidelity requirements.

I will discuss ongoing work at Santa Barbara, where we are attempting to enhance the lifetime of a quantum state by implementing the repetition code in a nine qubit device. The repetition code protects against bit flips, and can be seen as a one-dimensional primitive of the surface code, as the qubits are aligned in a chain, and error correction is achieved in a rapidly-cycled scheme with logic gates and measurements which is derived from the surface code.

**Jonathan Baugh**

**IQC, University of Waterloo**

---

*Quantum control in a hyperfine coupled electron-nuclear system: algorithmic cooling*

The hyperfine interaction enables the indirect manipulation and readout of nuclear spins through an electron spin interface. I will present recent electron spin resonance experiments on the stable radical in single crystal malonic acid that demonstrate quantum control of multiple nuclear spins via the electron. We explore the crystalline orientations and possible isotopic labelings of the molecule and find the most suitable systems and control schemes for quantum information testbed experiments. In particular, we are interested in implementing algorithmic cooling, which takes advantage of the higher polarization and shorter relaxation time of the electron in order to obtain non-equilibrium polarizations of the nuclear spins. Algorithmic cooling can be thought of as a way to remove entropy and purify ancilla qubits for quantum error correction.

**Hendrik Bluhm**

**RWTH Aachen University**

---

*Optimized gates for GaAs spin qubits*

Experiments on GaAs based spin qubits have shown that all the fundamental requirements for quantum computing can be fulfilled by these devices. However, demonstrated gate fidelities are much lower than what should be possible based on coherence times. Part of the difficulty lies in the inapplicability of standard Rabi control techniques and highly nonlinear control. By simulation and numerical optimization, we find control pulses resulting in a gate fidelity well above 99 %, taking realistic constraints imposed by the experimental hardware into account. Systematic errors in these gates can be eliminated using a self-consistent calibration protocol based on experimental feedback [1]. A subset of these gates are dynamically corrected gates that are to first order insensitive to both electric and nuclear hyperfine field noise, the two dominant dephasing channels. I will also discuss experimental progress in the implementation of these gates and may touch on an idea to test experimentally whether a classical noise model can describe a given bath acting on a qubit.

[1] 1. P. Cerfontaine, T. Botzem, D. P. DiVincenzo, H. Bluhm, Phys. Rev. Lett. 113, 150501 (2014).

**Alfio Borzi**

**University of Wuerzburg**

---

*Advances in the numerical solution of quantum control problems*

Recent developments in nanotechnology are boosting intensive investigation in quantum control problems. This fact explains the increasing number of research works in the field of quantum control theory and related quantum modeling and numerical simulation and optimization. From the physical and application point of view, quantum control theory is largely involved in nuclear magnetic resonance spectroscopy, magnetic resonance imaging, quantum optics, electronic engineering, and in the control of photochemical processes. Mathematically, many topics are involved in quantum control as exact controllability, optimal control theory, stabilisation, and the development of sophisticated algorithms for simulation and optimisation.

In this talk, efficient and robust computational schemes are discussed, that solve large classes of optimal control and exact-controllability problems. The focus is on matrix-free reduced-Hessian semismooth Krylov-Newton schemes and appropriate modified Crank-Nicholson schemes. Theoretical estimates and results of numerical experiments illustrate the computational ability of the proposed framework to solve challenging quantum control problems.

**Tommaso Calarco**

**University of Ulm**

---

*Steering many-body quantum dynamics*

Quantum technologies are based on the manipulation of individual degrees of freedom of quantum systems with exquisite precision. Achieving this in a real environment requires pushing to the limits the ability to control the dynamics of quantum systems of increasing complexity. Optimal control techniques are known to enable steering the dynamics of few-body systems in order to prepare a desired state or perform a desired unitary transformation. I will present a recently developed optimal control method that allows doing so for a many-body quantum system undergoing e.g. a quantum phase transition in the non-adiabatic regime. This opens the way to a range of applications, from the suppression of defects in a superfluid-Mott-insulator transition with ultra-cold atoms in an optical lattice to the achievement of various quantum gates at the quantum speed limit. I will present detailed calculations we performed for different experimental scenarios, together with the corresponding results obtained by experimental groups in different fields, from cold atoms to spin squeezing in atomic ensembles and diamond NV centers. Our control method also allows for exploring more general questions like the complexity of reversing quantum many-body dynamics, steering it back to its initial state even without the ability to revert the sign of the whole Hamiltonian. I will conclude by showing some recent results we obtained in this context, as well as further questions opened by our investigations.

**Giuseppe Florio**

**Centro Fermi & Università di Bari, Italy**

---

*Optimization and quantum metrology with identical particles*

We explore the quantum metrology exploiting the bosonic correlations among identical particles. We recast the problem of determining the parameters of a quantum Hamiltonian through a scattering process in the framework of classical probability. We evaluate the Quantum Fisher Information (QFI) for several physical situations, namely fixed number of scattering particles, fixed average of the number and fixed variance. Finally, we combine the results in order to optimize the QFI.

**Nicolai Friis**

**Institute for Quantum Optics and Quantum Information, Innsbruck**

---

*Quantum-enhanced deliberation of learning agents using trapped ions*

A scheme that successfully employs quantum mechanics in the design of autonomous learning agents has recently been reported in the context of the projective simulation (PS) model for artificial intelligence. In that approach, the key feature of a PS agent, a specific type of memory which is explored via random walks, was shown to be amenable to quantization, allowing for a speed-up. In this work we propose an implementation of such classical and quantum agents in systems of trapped ions. We employ a generic construction by which the classical agents are 'upgraded' to their quantum counterparts by a nested process of adding coherent control, and we outline how this construction can be realized in ion traps. Our results provide a flexible modular architecture for the design of PS agents. Furthermore, we present numerical simulations of simple PS agents which analyze the robustness of our proposal under certain noise models.

**John Edward Gough**

**Aberystwyth University**

---

*Quantum Coherent Feedback*

We discuss the modelling issues behind quantum coherent feedback control, and compare it measurement-based feedback. In particular, we shall show the network rule for forming interconnected open quantum systems where the coherent signals are propagated by quantum field channels. Current applications to Quantum technology will be given.

**Arne Grimsmo**

**Université de Sherbrooke**

---

*Delayed coherent quantum feedback*

Feedback is a key concept in both classical and quantum control. In this talk I consider the problem of a quantum system subject to coherent feedback, mediated by a travelling quantum field. This type of feedback can be implemented in a variety of physical platforms, where individual quantum systems are efficiently coupled together over long distances via waveguides (optical fibers, microwave transmission lines, nanowire photonic crystal waveguides, etc.). The conventional theoretical treatment of this type of feedback is to assume that the length of the feedback waveguide is effectively zero. I will try to argue that going beyond this limit opens up a new, and potentially very rich, regime of quantum feedback control. An enormous amount of

information can be stored in the correlations between the system and the travelling field, which, at least in principle, could be exploited for control purposes. However, this potentially powerful feature, is also the main obstacle to developing a theory that allows for efficient modelling of such systems, since the total system+field Hilbert space is huge. To deal with this problem, I borrow ideas from the intersection of the condensed matter and quantum information community: I show that a formal dynamical solution can be found as the continuum limit of a so-called “tensor network”. This leads to an essentially Markovian evolution in an extended system space, from which the true system state can be computed efficiently. All in all, this constitutes a practical means to model an arbitrary quantum system subject to delayed coherent quantum feedback.

**Martin Hürlimann**

**Schlumberger - Doll Research**

---

*Application of optimal control to NMR well logging*

Magnetic resonance well logging is conducted with specialized NMR sensors that are lowered into boreholes. The technique is used to quantify and characterize the properties of the fluids filling the pore space of earth formations. Over the last decade, it has become an important tool in the commercial exploration of hydrocarbon bearing reservoirs. Such NMR well logging measurements are particularly challenging because the sample is located outside the sensor. This makes it difficult to generate signals with adequate signal-to-noise ratio. Furthermore, the static and rf magnetic fields applied to the samples are necessarily grossly inhomogeneous. As a consequence, off-resonant effects play a key role in the spin dynamics governing the relaxation and diffusion measurements in NMR well logging applications. I will discuss the role of optimal control theory in the development of new pulse sequences consisting of phase modulated excitation and refocusing pulses and demonstrate improvements in the resulting signal-to-noise ratio by over a factor of 4.

**Christiane Koch**

**Universität Kassel**

---

*Learning how to control open quantum systems using optimal control theory*

Quantum control is an important prerequisite for quantum devices. A major obstacle is the fact that a quantum system can never completely be isolated from its environment. The interaction with the environment causes decoherence. Optimal control theory is a tool that can be used to identify control strategies in the presence of decoherence. I will show how to adapt optimal control theory to quantum information tasks for open quantum systems and present examples for cold atoms and superconducting qubits. The perspective on decoherence only as the adversary of quantum control is nevertheless too narrow. There exist a number of control tasks, such as cooling and measurement, that can only be achieved by an interplay of control and dissipation. I will show how to utilize optimal control theory to derive efficient cooling strategies for molecular vibrations where the timescales of coherent dynamics and dissipation are very different. Another opportunity for open system control, less obvious than cooling, arises from a coupling to the environment that results in non-Markovian dynamics. I will discuss how non-Markovianity of the open system time evolution can be exploited for control, using a superconducting phase circuit as example.

**Seth Lloyd**

**Massachusetts Institute of Technology**

---

*Quantum machine learning*

Machine-learning tasks frequently involve problems of manipulating and classifying large numbers of vectors in high-dimensional spaces. Quantum computers are good at manipulating high-dimensional vectors in large tensor product spaces. This talk shows how quantum computers can provide an exponential speed-up over their classical counterparts for a variety of problems in machine learning and big data analysis.

**Easwar Magesan**

**IBM**

---

*Detecting arbitrary single-qubit errors in a planar array of superconducting qubits*

Superconducting systems are a promising architecture for building towards fault-tolerant quantum computation using the surface code. An important problem in these systems is to detect whether errors have occurred in large networks of qubits. I will discuss recent experimental results that demonstrate the ability to detect arbitrary single-qubit errors in a four qubit sub-lattice of the surface code. High-fidelity syndrome measurements of the stabilizers of an error-detection code are used to detect the errors and the method is demonstrated for a variety of different errors. We also verify the non-demolition nature of the protocol by reconstructing the expected output state after the stabilizer measurements. These results combine various techniques and operations required for building towards larger networks of superconducting qubits.

**T S Mahesh**

**IISER Pune**

---

*Quantum control techniques in NMR and their applications in Quantum Computing*

NMR has long been a convenient playground for designing, testing, and improving quantum control techniques. Well defined Hamiltonians, long coherence times of ensembles of nuclear spin-systems at room temperature coupled with highly sophisticated hardware developed over five decades enable us to precisely control the dynamics of small spin systems using cleverly designed RF pulses. Shaped pulses, composite pulses, adiabatic pulses, and more recently, GRAPE pulses are being used in routine NMR experiments. Controlling large spin systems remains a challenge and various optical control techniques are being explored. I will overview the issues in the NMR quantum control and discuss a few possible solutions. Examples from NMR quantum computing will be used for illustrations.

**Sabrina Maniscalco**

**University of Turku**

---

*Non-Markovianity hinders Quantum Darwinism*

We investigate Quantum Darwinism and the emergence of a classical world from the quantum one in connection with the spectral properties of the environment. We use a microscopic model of quantum environment in which, by changing a simple system parameter, we can modify the information back flow from environment into the system, and therefore its non-Markovian character. We show that the presence of memory effects hinders the emergence of classical objective reality. We conjecture that this phenomenon is connected to the absence of a measurement-scheme interpretation for quantum trajectories in the non-Markovian regime.

**Charles Marcus**

**University of Copenhagen**

---

*The noise environment for spin qubits*

This talk discusses the use of electron spin as a holder of quantum information, how the environment decoheres spin, and methods for preserving coherence using dynamical decoupling and screening, based on Refs. [1,2]. The noise environment in several spin-based qubits are compared, and a simple relationship between the scaling of coherence time ( $T_2$ ) with the number of echo pulses and the spectral density of the noise environment is presented. Feedback control of the decohering environment, pioneered by the Yacoby group at Harvard, will also be discussed.

[1] J. Medford et al., Scaling of Dynamical Decoupling for Spin Qubits. Phys Rev Lett 108, 086802 (2012).

[2] A. P. Higginbotham et al., Coherent Operations and Screening in Multielectron Spin Qubits. Phys Rev Lett 112, 026801 (2014).

**John Morton**

**University College London**

---

*Quantum control of spins in silicon from clock transitions to electric fields*

Electron and nuclear spins of donor atoms in silicon are promising candidates for representing quantum bits. Understanding and overcoming spin decoherence mechanisms in these materials and finding optimal methods to manipulate the spins are key steps in developing silicon-based quantum computers. We have studied donor electron spins decoherence at so-called 'clock-transitions' where the ESR transition frequency has zero-first order magnetic field dependence ( $df/dB=0$ ). At such transitions, in isotopically engineered silicon, we measure electron spin coherence times up to about 3 seconds at 5 K [1]. Studying such dynamics in natural silicon (with 5%  $^{29}\text{Si}$ ) gives insights into the quantum nature of the nuclear spin bath. Turning to spin manipulation, we investigate how DC electric fields could be used to generate a Stark shift and study its magnitude for all four Group V donors. This can be used to tune spins in and out of resonance with a globally applied microwave magnetic field, enabling conditional spin control. We further show how a combination of applied RF and DC electric fields allows for X- and Z- rotations of the spin. Finally, we suggest that AC electric fields could be used to resonantly drive certain donor spin transitions directly, enabling the possibility of entirely local quantum control of donor spins.

**Felix Motzoi**

**University of California, Berkeley**

---

*Optimality of feedback-based generation and stabilisation of entanglement between distant superconducting qubits*

We consider the problem of using measurement combined with feedback to deterministically entangle remote

qubits. This can be achieved in the dispersive and near-resonant regimes of circuit and cavity QED using simple protocols that require only a single-frequency drive that interacts sequentially with each cavity-qubit system. The protocols work by combining correlated environmental interactions with symmetry breaking. We derive entanglement generation conditions that optimise for speed and maximal concurrence and discuss the optimality of the technique. Moreover, we show that even when there is high photon loss in the transmission channel (and therefore much ongoing dephasing) it is experimentally feasible to achieve significant concurrence. Finally, we discuss combatting such loss to stabilise and provide on-demand entanglement.

**Giuseppe Davide Paparo**

**Universidad Complutense de Madrid**

---

### *Quantum PageRank for Complex Networks*

In this talk I will present the recently proposed Quantum PageRank algorithm and describe its behavior in large complex networks. We find that the algorithm is able to univocally reveal the underlying topology of the network and to identify and order the most relevant nodes. Furthermore, it is capable to clearly highlight the structure of secondary hubs and to resolve the degeneracy in importance of the low lying part of the list of rankings. The quantum algorithm displays an increased stability with respect to a variation of the damping parameter, present in the Google algorithm, and a more clearly pronounced power-law behaviour in the distribution of importance, as compared to the classical algorithm. We test the performance and confirm the listed features by applying it to real world examples from the WWW. Finally, we raise and partially address whether the increased sensitivity of the quantum algorithm persists under coordinated attacks in scale-free and random networks.

**Chandrasekhar Ramanathan**

**Dartmouth College**

---

### *Engineering the dynamics of electron and nuclear spins in solids*

Electron and nuclear spin system are excellent platforms for the study of coherent quantum dynamics, as spin degrees of freedom are typically well isolated from the other degrees of freedom of the system. In this talk I will describe two examples of how we controllably engineer spin dynamics in solids. Firstly I will describe how we are using coherent averaging techniques based on Average Hamiltonian Theory to manipulate the many-body dynamics of nuclear spins in a lattice. Secondly I will describe our on-going efforts to enhance the efficiency of dynamic nuclear polarization schemes through improved control of the electron spins using millimeter-wave modulation techniques.

**Tony Reinsperger**

**Karlsruhe Institute of Technology (KIT)**

---

### *The BROCODE of NMR: BROadband COoperative DEcoupling of Nuclear Spins*

In Nuclear Magnetic Resonance (NMR) spectroscopy, heteronuclear decoupling sequences are a key element in every correlation experiment where resolution or spectral dispersion and sensitivity are of higher importance than the information provided by resonance lines that are split due to couplings between spins. Pulse sequences are needed which provide high signal intensity paired with low artifact levels for a wide range of resonance offsets. Up to recently it was best-practice to pursue these goals in three steps:

- 1) Find a robust inversion pulse (since this is the fundamental building block in order to coherently decouple spins);
- 2) Expand this inversion pulse by phase cycling;
- 3) Dynamically alter the mode of execution (e.g. the timing) of the sequence in order to achieve cancellation of artifacts.

Maybe the best standard implementation addressing artifacts originating from the three-step approach is adiabatic bilevel decoupling. It relies on adiabatic frequency sweeps as inversion elements and a temporal variation at the beginning of the sequence for each of the successive scans of an NMR experiment that ultimately cancels the most spurious artifacts that are introduced by the repetitive sweeping scheme. Recently, methods based on Optimal Tracking have been introduced that tackle all of the three above-mentioned tasks simultaneously. By combining the Optimal Tracking algorithm with multi-scan cooperativity, it is possible to derive a complete set of decoupling sequences that compensate each other's imperfections *de novo*. In this work, we compare the results of the Optimal Control approach with the adiabatic bilevel technique in cases where the radio frequency power levels are high enough as well as too low to fulfill the adiabatic condition.

**Ludovic Santos**

**Université Libre de Bruxelles**

---

*Quantum dynamics simulator with the motional states of an ion in an anharmonic trap*

Following a recent proposal [1], we theoretically illustrate the possibility of using the motional states of a Cd<sup>+</sup> ion trapped in an anharmonic potential to realize a quantum dynamics simulator of a single-particle Schrödinger equation. The anharmonicity renders the states energetically non equidistant and allows the control of population transfer between states with an electromagnetic field. The simulated dynamics is discretized on spatial and temporal grids. The gate associated to an elementary evolution is estimated by the Split Operator formalism [2]. The radio-frequency field able to drive the corresponding unitary transformation among the qubit states encoded into the ion motional states is obtained by optimal control theory [3]. The field is unique for a given simulated potential. We also perform the computation of the field for the preparation of the initial simulated wave packet. This one needs to be adapted. The stability of the optimal electric fields driving the elementary evolution is checked by performing dissipative Lindblad dynamics [4,5] in order to consider fluctuations in the trap potential due to external fields [6].

[1] L. Wang and D. Babikov, "Feasibility of encoding Shor's algorithm into the motional states of an ion in the anharmonic trap", J. Chem. Phys. 137, 064301 (2012).

[2] M. D. Feit, Jr J. A. Fleck, and A. Steiger, "Solution of the Schrödinger equation by a spectral method", J. Comput. Phys. 47, 412 (1982).

[3] W. Zhu, J. Botina and H. Rabitz, "Rapidly convergent iteration methods for quantum optimal control of population", J. Chem. Phys. 108, 1953 (1997).

[4] G. Lindblad, "On the generators of quantum dynamical semigroups", Commun. Math. Phys. 48, 119 (1976).

[5] W. Zhu and H. Rabitz, "Closed loop learning control to suppress the effects of quantum decoherence", J. Chem. Phys. 118, 6751 (2003).

[6] S. Schneider and G. J. Milburn, "Decoherence and fidelity in ion traps with fluctuating trap parameters", Phys. Rev. A 59, 3766 (1999).

**Thomas Schulte-Herbrüggen**

**Technical University of Munich (TUM)**

---

*Good News for Controlling Open Quantum Systems*

Exploiting symmetries provides a systematic way of dissipative state engineering as will be illustrated by a plethora of examples. We present the geometry of control design in terms of a unified Lie picture. It elucidates demarkation lines between Markovian and non-Markovian quantum maps. Moreover, the picture helps to understand limits of open-loop versus closed-loop control.

**Dominique Sugny**

**Laboratoire Interdisciplinaire Carnot de Bourgogne**

---

*Recent advances in the control of spin systems*

In this talk, I will present some recent results about the optimal control of spin systems in Nuclear Magnetic Resonance and Magnetic Resonance Imaging. This work has been done in collaboration with the group of S. J. Glaser in Munich. A geometric analysis is performed to investigate simple systems. We will discuss in particular the optimization of the signal to noise ratio of a spin 1/2 particle. A numerical approach based on the GRAPE algorithm is used to solve control problems with an ensemble of spins. In this case, we will show how a robust control field can be designed efficiently.

**Vlatko Vedral**

**University of Oxford**

---

*Quantifying complexity with quantum epsilon machines*

While we have intuitive notions of structure and complexity, the formalization of this intuition is non-trivial. The statistical complexity is a popular candidate. It is based on the idea that the complexity of a process can be quantified by the complexity of its simplest mathematical model - the model that requires the least past information for optimal future prediction. I would like to review how such models, known as  $\epsilon$ -machines, can be further simplified through quantum logic, and explore the resulting consequences for understanding complexity. In particular, I will present a new measure of complexity based on quantum  $\epsilon$ -machines. I will then apply this to a simple system undergoing thermalization. The resulting quantum measure of complexity aligns more closely with our intuition of how complexity should behave.

**Paola Verrucchi**

**ISC-CNR and Physics Department University of Florence**

---

*Getting information via a quantum measurement: the role of decoherence*

In this work we investigate the relation between quantum measurements and decoherence, in order to formally express the necessity of the latter for obtaining an informative output from the former. To this aim, referring to the Von Neumann scheme for ideal quantum measurements, we first look for the minimal structure that the interaction between principal system and measurement apparatus must have for properly describing the process, beyond the quantum measurement limit, and then analyze the dynamical evolution induced by one such interaction. The analysis is developed by means of a recently introduced method for studying open quantum systems, namely the parametric representation with environmental coherent states, that allows us to determine a necessary condition that the quantum state of the apparatus must fulfill in order to give information on the observable being measured. We find that this condition strictly implies decoherence in the principal system, with respect to the eigenstates of the hermitian operator that represents the measured observable, thus establishing that there cannot be information flux from a quantum system towards a readable analyser unless decoherence occurs. The relevance of dynamical entanglement generation is highlighted, and consequences of the possible macroscopic structure of the measurement apparatus are also commented upon.

**Mattia Walschaers**

**University of Freiburg**

---

*The Statistical Signature of BosonSampling*

A long standing endeavor in the field of quantum computation, is to challenge and even falsify the extended Church-Turing thesis, which states that any efficient computation performed by a physical device can be performed in polynomial time by a classical computer. Much as quantum information science has progressed, for an actual falsification, an actual physical device is required. As universal quantum computers still are out of reach, the BosonSampler, an optical setup that can efficiently probe many-boson interferences, has attracted much attention as a candidate for such a device. One huge problem, however, is certification of the process, after all, how could one verify whether a device works the way it should work, if its outputs are by definition unfeasible to simulate on a classical computer? In this contribution, we show that a careful statistical assessment, based on the theory of complex systems, can provide a solution.

**Frank Wilhelm-Mauch**

**Saarland University**

---

*Optimal control for superconducting quantum processors: From few to many qubits*

Superconducting quantum processors present a powerful paradigm for the realization of a scalable quantum processor and are also a testbed for optimal quantum control. While good control has been achieved recently based on manual pulse design, optimal control, and closed loop tuneup, the next challenge lies in multiplexing control to a larger processor. This poses several challenges including wiring and filtering, frequency crowding, and limitations in readout. These can be addressed as follows: First of all, I will discuss a novel way to generate control pulses on chip using ultrafast classical digital superconducting logics. These pulses only have a one bit amplitude resolution but offer very high time resolution. Optimizing these all-digital pulses can be accomplished using learning control and leads to composite rotation-style pulses. Secondly, I will describe an analytical method based on average Hamiltonian theory that allows to drive quantum gates in frequency-crowded system, i.e., that select certain wanted transitions in the proximity of unwanted ones. Thirdly, I will outline how optimal control of open systems can help to optimize measurement contrast, which is an example of quantum control towards a non unitary target.

**Jörg Wrachtrup**

**3rd Institute of Physics, University of Stuttgart**

---

*Quantum control of few spin systems: application in quantum information and sensing*

Engineering few spin systems from a single spin to spin arrays is a challenging experimental task. In addition the control of even a few interacting spins in a solid environment, i.e. including heterogeneities required dedicated efforts. In my talk I will describe how we use optimal control to achieve high fidelity entanglement between electron spin pairs and nuclear spins in a nanostructured spin array. In addition I will detail our efforts to use optimized dynamic decoupling to sense the NMR signal of a few nuclear spins outside diamond. I will discuss what future role quantum control will have in improving performance of this method.

*Minimal model for synchronization*

Spontaneous synchronization is one of the paradigmatic phenomena in the study of complex systems. It has been explored theoretically and experimentally mostly to understand natural phenomena, but also in view of technological applications [1] and more recently it started to be explored in the quantum regime [2]. The quest for the simplest scenario to observe synchronization has actually been fundamental in showing the possibility to have spontaneous synchronization even in linear systems, under suitable dissipation conditions [3]. Synchronous dynamics has been reported in complex networks or in motifs, in presence of dissipation acting locally or in a common environment [3], but not under pure dephasing [4]. Beyond the classical regime, synchronization between (even unlinked) nodes has been shown to witness the presence of quantum correlations and entanglement. Continuing in the quest for the simplest model for spontaneous synchronization, we consider finite harmonic networks (in absence of external losses), where part of the network constitutes a sink for the dynamics of two probes. Synchronization of these probes is explored considering different network configurations [5].

[1] A. Pikovsky, M. Rosenblum, and J. Kurths, *Synchronization: A Universal Concept in Nonlinear Sciences*, (Cambridge University Press, 2003).

[2] G. Heinrich, M. Ludwig, J. Qian, B. Kubala and F. Marquardt, *Phys. Rev. Lett.* 107 043603 (2011); G-L. Giorgi, F. Galve, G. Manzano, P. Colet, and R. Zambrini, *Phys. Rev. A* 85, 052101 (2012); A. Mari, A. Farace, N. Didier, V. Giovannetti, and R. Fazio, *Phys. Rev. Lett.* 111, 103605 (2013)

[3] G. Manzano, F. Galve, E. Hernandez-Gracia, G. L. Giorgi, and R. Zambrini, *Sci. Rep.* 3, 1439 (2013)

[4] G-L. Giorgi, F. Plastina, G. Francica, R. Zambrini, *Phys. Rev. A* 88, 042115 (2013)

[5] R. Vasile, F. Galve, R. Zambrini, *Phys. Rev. A* 89, 022109 (2014); C. Benedetti, A. Mandarino, F. Galve, M.A. Paris, R. Zambrini, in preparation.

## Posters

*What we talk about when we talk about non-Markovianity*

We present a detailed critical study of several recently proposed non-Markovianity measures. We analyse their properties for single qubit and two-qubit systems in both pure-dephasing and dissipative scenarios. More specifically we investigate and compare their computability, their physical meaning, their Markovian to non-Markovian crossover, and their additivity properties with respect to the number of qubits. The bottom-up approach that we pursue is aimed at identifying similarities and differences in the behavior of non-Markovianity indicators in several paradigmatic open system models. This in turn allows us to infer the leading traits of the variegated phenomenon known as non-Markovian dynamics and, possibly, to grasp its physical essence.

*Measuring general quantum correlations in NMR multipartite systems*

The quantum properties of physical systems can be exploited to enable advances in information and communication technologies. Entanglement certainly implies an important role in this context, but many important results were also obtained using separable states (nonentangled), some of them based upon General Quantum Correlations (GQCs). We have shown how to implement the set of Bell diagonal quantum states (two qubits) based on two spins  $\frac{1}{2}$  coupled by  $J$  scalar coupling and a spin  $\frac{3}{2}$  quadrupolar nucleus as well as to monitor the behavior of the aforementioned GQCs quantifiers under decoherence using Nuclear Magnetic Resonance (NMR) techniques. With this, we experimentally investigated the influence of the initial state in the decoherence behavior, presenting the first experimental observation of freezing and double sudden-changes in GQCs time evolution. We also investigated the presence and behavior of GQCs in more general systems (with three qubits), where the sudden-change phenomena could also be observed.

**Elie Assémat**

**Universität des Saarlandes**

---

*Phase space approach to strong field multielectron dynamics*

We present a method of simulating the dynamics of a quantum system which has the advantage of requiring memory and a time-complexity which is only dependent on the volume of phase-space which is actively occupied by the system. By utilizing a basis which is bi-orthogonal to phase-space localized Gaussians, we derive a sparse representation of the state, allowing for huge savings in both storage and computation. The proper use of bi-orthogonal basis produces an extremely accurate and stable simulation. This approach allows, for example, the simulation of ionization of Helium-like atoms controlled by strong atto-second fields. Moreover, it is extendible to eigenstate calculations, and directly parallelizable to cluster-scale computation.

**Tobias Chasseur**

**Universität des Saarlandes**

---

*Detours to diabaticity*

This poster presents a way to keep a Landau-Zener (LZ) crossing fully diabatic at finite crossing velocity based on an ansatz of an oscillation augmented sweep. Several pulse shapes will be explained by a model of separated photon-assisted linear LZ-transitions as well as through numerical methods of optimal control. Furthermore there is a discussion of their mutual advantages and an examination of robustness.

**Gabriele Ciaramella**

**Universität Würzburg - Institut für Mathematik**

---

*Non-smooth optimal control of quantum systems*

Optimal control and exact-controllability of quantum systems are largely investigated topics. In most cases, the corresponding optimization problem is smooth, thus allowing the use of classical optimization techniques. On the other hand, much less is known in the case of nonsmooth optimization of quantum systems, as for instance, when the objective functional has non-differentiable components. We present a non-smooth optimization framework for the control of spin systems, that is characterized by  $L^1$ -components in the cost functional. The non-smoothness of such a problem results in control functions having a useful sparsity structure. Specifically, we obtain control solutions that are zero in open subsets of the time-domain. In particular, in the case of bang-bang solutions, the control does not jump directly between the lower and upper bound. These properties can be advantageous for an adequate implementation of the control functions in laboratory machines and laser pulse shapers. We discuss a semi-smooth Newton method for the solution of our non-smooth control problems and present theoretical results characterizing the sparsity of the optimal controls. Results of numerical experiments demonstrate the validity of our framework for controlling quantum spin systems.

**Luis A. Correa**

**Universitat Autònoma de Barcelona**

---

*Nanoscale autonomous refrigerators for quantum technologies*

Cooling quantum systems down to ultra-cold temperatures is essential for various technological applications ranging from quantum error correction to high precision thermometry or feedback control. In this poster, I review the recent progress in quantum absorption refrigeration, that is, the realization of cooling cycles solely driven by heat on a single finite-dimensional quantum system. The focus is placed on the finite-time thermodynamics of these nanoscale autonomous refrigerators and, in particular, on the ultimate limitations on their coefficient of performance at maximum cooling load. The scaling of the performance of these devices with their size when combined in multi-stage configurations, and the possible enhancement of their cooling load using suitable reservoir-engineering techniques are also discussed.

**Sara Di Martino**

**Università di Bari**

---

*Entanglement: Monogamous or not?*

Understanding the structure of entanglement distributed among many parties is central to diverse aspects of quantum information theory. In 2000 Coffman et al found that the entanglement that can be shared among three parties (A, B, C) is constrained by the so-called monogamy inequalities. After some years Osborne et al found that a set of similar inequalities holds for systems of  $n$  qubits: the sum of the entanglement that one qubit shares with each one of the other qubits of the system is bounded from above by the entanglement that this qubit shares with the rest of the system. We investigate the generalization of these inequalities for four-qubit pure states where all the possible bipartition of the system are taken into account. In particular we prove

that some classes of states, as the one composed by states that are superpositions of four-partite GHZ and W states, satisfy a strong monogamy inequality, by constructing a lower bound on the measure of entanglement. We also show numerical evidence that the inequality holds for arbitrary pure states of four qubits.

**Esteban Goetz**

**University of Kassel**

---

*Optimization of Photoelectron Spectra*

Motivated by previous work in the field of photoionization, in particular on charge transfer and decoherence of hole states and in the field of coherent quantum optimal control, we present for the first time an implementation of Krotov's algorithm within the time-dependent configuration-interaction singles [TDCIS] formalism for the optimization of photoelectron angular distributions. The optimized ionization pulse is supposed to steer a given initial quantum state, to a given final state whose photoelectron spectrum fulfills specific desired properties. We construct the corresponding target functional and optimization algorithm.

**David Goodwin**

**University of Southampton**

---

*Efficient calculation of the fidelity functional Hessian in Optimal Control problems*

We report an investigation into the possibility of efficient calculation of second derivatives of the fidelity functionals encountered in Optimal Control of quantum systems. The rationale is that, while the calculation of the Hessian matrix would take some effort, the rapid convergence of Newton-Raphson methods (compared to quasi-Newton methods as well) are desirable for complicated systems. Using multiple time and commutation symmetries found in the Hessian as well as the augmented matrix technique for the calculation of matrix exponential integrals, we were able to substantially reduce the computational effort. Structure within the Hessian matrix is analysed and the convergence is compared to that of quasi-Newton methods in trust-region and line-search methods.

**Jukka Kiukas**

**University of Nottingham**

---

*Local asymptotic normality in system identification for quantum Markov chains*

We consider the problem of identifying and estimating dynamical parameters of an ergodic quantum Markov chain, when only the stationary output is accessible for measurements. Assuming that the dynamics depends on an unknown parameter, we show that parameters can be estimated at the 'standard' rate  $n^{-1/2}$ , and give an explicit expression of the (asymptotic) quantum Fisher information of the output, which is proportional to the Markov variance of a certain 'generator'. More generally, we show that the output is locally asymptotically normal, i.e. it can be approximated by a simple quantum Gaussian model consisting of a coherent state whose mean is related to the unknown parameter.

**Frank Langbein**

**Cardiff University**

---

*Efficient system identification for non-ensemble quantum systems*

For quantum systems, system identification often refers to quantum state and later quantum gate estimation, where it is also known as quantum state or operator tomography. Quantum processes, however, are usually practically realized by dynamically changing certain controllable parameters to effect a particular desired evolution of the system. We present an approach to identifying the underlying dynamical generators of the processes and their dependence on the control parameters. For a single quantum system such as a particular quantum dot or an ion in a trap, a single measurement usually yields a discrete outcome; in the simplest case this is a binary result. Hence, we assume the system can be initialised in a set of discrete states and we measure if the system is in a particular state after time  $t$ , yielding a true or false result only. We consider what information can be obtained from such experiments about the system Hamiltonian  $H$  and how to design experiments to efficiently obtain this information.

**Burkhard Luy**

**Karlsruhe Institute of Technology (KIT)**

---

*Excitation with variable flip angle: RADFA (rf amplitude dependent flip angle) pulses*

Using optimal control based algorithms, the limits of broadband excitation with rf-dependent effective flip angle is explored. Clearly certain pulse families are favored and will be discussed in the contribution.

**Katarzyna Macieszczak**

**University of Nottingham**

---

*Magnet field sensing in the quantum Zeno effect regime*

We discuss magnet field sensing with  $N$  two-level atoms in the presence of decoherence. In the case of unitary evolution of the atoms, the precision of the optimal sensing protocol is given by Heisenberg scaling  $\sim N^{-2}$ , which is a result of entangled preparation of the atoms. The presence of noise lowers the precision of estimating magnetic field and changes its scaling with  $N$ . For typical examples of local Markovian noise, the scaling becomes standard  $\sim N^{-1}$  and there is no quantum enhancement when using entangled atoms. For local non-Markovian noise, however, in the quantum Zeno effect regime, we argue that the precision of the optimal sensing protocol obeys the new Zeno scaling  $\sim N^{-3/2}$ , which has been reported for non-Markovian dephasing noise and the atoms prepared in the GHZ state [2,3].

[1] K. Macieszczak, The Zeno limit in frequency estimation with non-Markovian environments, ArXiv e-Prints (2014), arXiv:1403.1333 [quant-ph].

[2] Y. Matsuzaki, S. C. Benjamin, J. Fitzsimons, Magnet field sensing beyond the standard quantum limit under the effect of decoherence, Phys. Rev. A 84, 012103 (2011).

[3] A. W. Chin, S. F. Huelga, M. B. Plenio, Quantum Metrology in Non-Markovian Environments, Phys. Rev. Lett. 109, 233601 (2012).

**Federico Maiolini**

**University of Camerino**

---

*Quantum stabilizer codes embedding qubits into qudits*

We study, by means of the stabilizer formalism, a quantum error correcting code which is alternative to the standard block codes since it embeds a qubit into a qudit. The code exploits the noncommutative geometry of discrete phase space to protect the qubit against both amplitude and phase errors. The performance of this code is evaluated on Weyl channels by means of the entanglement fidelity as a function of the error probability. A comparison with standard block codes, like 5- and 7-qubit stabilizer codes, shows its superiority.

**Riccardo Mengoni**

**University of Camerino**

---

*Entanglement from dissipative dynamics into overlapping environments*

We consider two ensembles of qubit dissipating into two overlapping environments, that is with a certain number of qubit in common that dissipate into both environments. We then study the dynamics of bipartite entanglement between the two ensembles by excluding the common qubit. To get analytical solutions for an arbitrary number of qubit we consider initial states with a single excitation and show that the largest amount of entanglement can be created when excitations are initially located among side (non-common) qubit. Moreover, the stationary entanglement exhibits a monotonic (resp. non-monotonic) scaling versus the number of common (resp. side) qubit.

**Davide Nuzzi**

**Università degli Studi di Firenze**

---

*Generating solitons on discrete Heisenberg chains and how to possibly use them*

Solitons are non-linear excitations with specific space and time localization; they propagate along one-dimensional media with constant shape and velocity, and are further characterised by a robust stability against noise and perturbations. These features make them particularly suitable for some practical applications, such as the transmission of signals between distant parties. Classical spin chains, in the limit of continuous support, are known to own solitons among their dynamical excitations. However, when discrete support or quantum nature of spins are introduced, it is not completely clear whether solitons keep being present in the spectrum or not; moreover it is not clear how to possibly inject this kind of excitations in systems known to support them. In this work we propose a theoretical scheme in order to practically achieve the generation of soliton-like excitations on discrete classical Heisenberg chain by applying a time-dependent magnetic field to one of the chain ends. We present numerical results for the dynamics of an Heisenberg chain, showing the effective injection of solitons under the proposed scheme and their robustness against thermal disorder. Moreover, we propose a setup where the generated solitons are used as magnetic signals travelling along the chain so as to reach a distant qubit coupled to the chain. Numerical results confirm that solitons are indeed suitable for this task, showing the effective possibility to control the qubit state by choosing the proper excitation.

**Alexander Pitchford**

**Aberystwyth University**

---

*Control pulse optimisation of coupled oscillators using High Performance Computing*

An open source Python library was developed for the optimisation of control pulses for quantum systems, supporting unitary, Lindbladian and symplectic dynamics. The library is currently being incorporated into QuTiP, which is open-source software for simulating the dynamics of open quantum systems [1]. The library was used to determine control pulses to synthesise gates on many-bodied systems. Using the new library, the results of previous work [2] on the spin-star system (a model of a central spin coupled to a number of bath spins, where the system is controlled through time varying fields on the central spin) were reproduced and extended. Building on the theoretical work proving the controllability of coupled oscillators [3], the control of a chain of oscillators through the control of a single oscillator is simulated. The dynamics are described using symplectic matrices, and Frechet derivatives are used to calculate the fidelity gradients, as it is important to use exact gradients in efficient use of quasi-second order multi-dimensional optimisation algorithms. The focus of the simulations is to determine the minimum time required control the system. Many simulations, with different initial starting conditions, are required to determine maximal fidelity for a given total evolution time, and a range total times are used to determine to fidelity relationship. With larger dimensional systems, the processing demands are very high. Therefore the HPC Wales cluster was used to produce results from modelling larger systems within a reasonable time scale.

[1] J. R. Johansson, P. D. Nation, & F. Nori (2013) *Comp. Phys. Comm.*

[2] C. Arenz, G. Gualdi, & D. Burgarth. (2014) *New Journal of Physics*

[3] M. Genoni, A. Serafini, M. Kim, & Burgarth, D. (2012). *Phys. Rev. Lett.*

**Benjamin Russell**

**University of York**

---

*Applications of Finsler geometry to quantum control and the limitations of quantum technologies*

We use a geometric method to determine speed limits for the implementation of quantum gates in controlled quantum systems that have a specific class of constrained control functions. We achieve this by applying a recent theorem of Shen, which provides a connection between time optimal navigation on Riemannian manifolds and the geodesics of a certain Finsler metric of Randers type. This result is then used to assess some small quantum systems and specific gates.

**Carlos Sabin**

**University of Nottingham**

---

*A quantum thermometer for an ultracold BEC*

In this talk, we introduce a primary thermometer which measures the temperature of a Bose-Einstein Condensate in the sub-nK regime. We show, using quantum Fisher information, that the precision of our technique improves the state-of-the-art in thermometry in the sub-nK regime. The temperature of the condensate is mapped onto the quantum phase of an atomic dot that interacts with the system for short times. We show that the highest precision is achieved when the phase is dynamical rather than geometric and when it is detected through Ramsey interferometry. Standard techniques to determine the temperature of a condensate involve an indirect estimation through mean particle velocities made after releasing the condensate. In contrast to these destructive measurements, our method involves a negligible disturbance of the system.

Reference: C. Sabin, A. White. L. Hackermuller, I. Fuentes, *Scientific Reports* 4, 6346 (2014).

**Rebecca Schmidt**

**University of Nottingham**

---

*What is quantum cybernetics?*

“Cybernetics is the scientific study of control and communication in the animal and the machine.” (Norbert Wiener, 1948). In other words, cybernetics is the information theoretic formulation of the control of open systems, with focus on the rich interplay between disturbance, regulation and system-of-interest. What changes fundamentally, if the involved systems are quantum? Which role do Quantum correlations between the subsystems play? We illustrate the concept by focusing on Ashby's law of requisite variety.

**Ravi Shankar**

**Aarhus University**

---

*tba*

**Martin Sprengel**

**University of Würzburg, Germany**

---

*Towards the optimal control of TDDFT models*

To bypass the enormous difficulties of solving the Schrödinger equation of a many-electron system, an equivalent description given by the time-dependent density functional theory (TDDFT) has been proposed. The TDDFT approach allows accurate simulation of interacting multi-electron systems and has been successfully applied to many quantum models. While the TDDFT simulation of quantum systems is well established, much less is known concerning the optimal control of systems governed by the TDDFT model. The purpose of this work is to investigate the extension of optimal control techniques to solve the problem of driving a TDDFT system to reach a desired target configuration in Hilbert space. For this purpose, in this work adjoint methods are considered, thereby the forward and adjoint equations are solved using operator splitting pseudo-spectral techniques. The resulting reduced gradient is used to implement fast numerical solvers to the TDDFT optimal control problem.

**Lukas Theis**

**Universität des Saarlandes**

---

*Engineering adiabaticity with optimal control*

In this work the time evolution of a system modelled by Landau-Zener physics is studied using numerical optimal control methods. A typical application of this work is in quantum computing, where adiabatic population transfer between two bare states, such as a qubit and a resonator is required. The numerical results reveal the possibility to preserve adiabaticity at limiting time, finding a non-uniform quantum speed limit. Additionally, an analytical approach using the Magnus expansion is presented, which explains the observed pulse shapes.

**Leo Van Damme**

**Université de Bourgogne, France**

---

*Optimal control of a chain of three spins with unequal couplings*

We solve a time-optimal control problem in a linear chain of three coupled spins  $1/2$  with unequal couplings. We apply the Pontryagin maximum principle and show that the associated Hamiltonian system is the one of a three-dimensional rigid body. We express the optimal control fields in terms of the components of the classical angular momentum of the rigid body. The optimal trajectories and the minimum control time are given in terms of elliptic functions and elliptic integrals.

**Daniel Wisniewski**

**University of Nottingham**

---

*Use of Dynamic Monte Carlo for large scale Dynamic Nuclear Polarization simulations in the Hilbert space*

Dynamic Nuclear Polarization (DNP) dynamics can be modelled using a Liouville von Neumann master equation acting on a system density operator. Such simulations very effectively reveal information on the underlying mechanism [1], however as with any quantum mechanical simulation, this approach is limited due to the exponential growth of the Liouville space dimension, with respect to an increasing number of spins in the system. Currently the simulations are restricted to approximately 20 nuclear spins [1,2]. Following our large-system solid effect (SE-DNP) simulations, illustrating the polarization transport dynamics in various geometries, a similar approach was derived for CE-DNP. Starting from the full quantum-mechanical master equation, the dynamics were projected into the Zeeman subspace, using adiabatic elimination [3]. As a consequence, dynamics of a diagonal basis are approximated. The effective subspace is reduced from  $4^n$  to  $2^n$ , for 'n' spins, and thus exhibits the same scaling as the Hilbert space. The effective dynamics derived from a quantum mechanical master equation are classical in form, yet accurately reflect polarization dynamics of the full master equation. The effective master equation can be rewritten in Lindblad form. It consists of a sum of Lindblad dissipators with a set of effective system-state-dependent rates. These rates rely on the nuclear Larmor frequency, relaxation rates, microwave field amplitude, temperature, magnetic field strength, and dipolar coupling parameters. The effective rates correspond to 'jump' operations: single spin operations model relaxation processes, two-spin operations model electron cross-relaxation and electron-nuclear flip-flops, and three-spin operations model the three-spin cross effect mechanism. Variable-time Dynamic Monte Carlo

(DMC) [4] was implemented to simulate polarization dynamics in the Hilbert space of theoretical sample – an example is illustrated (fig. 1). Due to the nature of this approach, computer memory is no longer an issue, and simulations involving 1000s of nuclear spins are possible. The tool has proven most useful in revealing polarization dynamics, particularly from the core nuclei to the bulk, where the process of spin diffusion can be seen, analysed for different parameter sets, and also compared for different DNP mechanisms. Our studies of SE-DNP and CE-DNP have revealed an unphysical problem commonly encountered in small-system simulations: the finite boundary of a small system leads to misleading results as polarization upon reaching the boundary reflects back towards the source. This effect can be reduced or eliminated altogether with larger spin systems, thus reflecting dynamics more accurately. The DMC simulations also enable one to study the effect of varying simulation parameters on polarization values during evolution and in the steady-state, thus indicating effectiveness of the parameter choice.

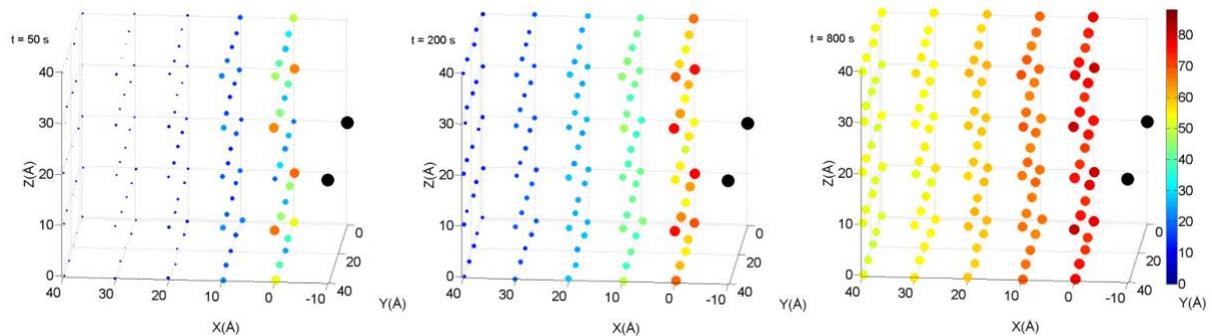


Figure 1: Time evolution of polarization in  $^{125}\text{C}^{13}\text{C}$  nuclei, with an average separation of  $10\text{ \AA}$ . Black dots represent bi-radical electrons ( $40\text{ \AA}$  separation) placed on one cubic surface. Electron  $T_1 = 10\text{ ms}$ ,  $T_2 = 10\text{ }\mu\text{s}$ . Microwave amplitude is  $50\text{ kHz}$ .

- [1] Y. Hovav, A. Feintuch, and S. Vega, 'Theoretical aspects of dynamic nuclear polarization in the solid state- the cross effect', J. Magn. Reson., Vol. 214, pages 29-41 (2012)
- [2] A. Karabanov, A. van der Drift, L.J. Edwards, I. Kuprov, and W. Kockenberger, 'Quantum mechanical simulation of solid effect dynamic nuclear polarization using Krylov-Bogolyubov time averaging and a restricted state-space', Phys. Chem. Chem. Phys., Vol. 14, pages 2658-2668 (2012)
- [4] R. Kühne and G. Reineker, 'Nakajima-Zwanzig's generalized master equation: Evaluation of the kernel of the integro-differential equation', Z. Phys. B Con. Mat., Vol. 31, Iss. 1, pages 105-110 (1978)
- [4] H. Breurer and F. Petruccione, 2007, 'The Theory of Open Quantum Systems', Oxford University Press

**Jonathan Zoller**

**Ulm University**

### *Benchmarking of Quantum Optimal Control Algorithms*

We study a state to state transfer optimal control problem of an atom in a double-well between states located in two different wells, where the control field drives the tilt of the potential. Therefore, we use different optimal control algorithms as the CRAB and Gradient method. These algorithms require initial guess pulses which result in varying final fidelities. We perform a statistical analysis of the fidelity distribution. Furthermore, we apply concepts from classical optimal control that turned out to be effective in that field, to the quantum regime. Vice versa, advances from quantum optimal control theory are being evaluated on classical problems.