Banff International Research Station

for Mathematical Innovation and Discovery

Quantum Technology
Computational Models for Quantum Device Design

8th to 13th of January 2012

Meals

- Breakfast (Buffet): 7:00–9:30 am, Sally Borden Building, Monday–Friday
- Lunch (Buffet): 11:30 am–1:30 pm, Sally Borden Building, Monday–Friday
- Dinner (Buffet): 5:30–7:30 pm, Sally Borden Building, Sunday–Thursday
- Coffee Breaks: As per daily schedule, in the foyer of the TransCanada Pipeline Pavilion (TCPL)

Please remember to scan your meal card at the host/hostess station in the dining room for each meal.

Meeting Rooms

All lectures will be held in the new lecture theater in the TransCanada Pipelines Pavilion (TCPL201). LCD projector, overhead projectors and blackboards are available for presentations.

TCPL 201, 202, 107, 5310 (Reading Room), 5210 are available for the scheduled group discussions. TCPL 101, 102, 105, 106 are also available for smaller group discussions, parallel sessions, etc. as required.

Schedule

The workshop consists of surveys, talks, group discussions and feedback sessions. The surveys are 1 hour long and should allow 10 to 15 minutes for questions and discussions. The talks are 30 minutes long and should allow 5 to 10 minutes questions and discussions.

The group discussion sessions are about 1 hour long and the attendees will be split into four groups. Each group has a moderator as listed in the schedule below. Typically the moderator will report back to everyone in the 1 hour feedback session afterwards on the topic discussed in the groups. The speakers on the day (who are often assigned to be moderators for the group discussions or the feedback session) should consider suitable topics for the following group discussion when preparing their talks and raise these during their talk. The surveys should raise the more general questions while talks can focus on more specific issues.

Chairs for the various sessions are listed in the schedule below. The coordinator of a group discussion is repsonsible for grouping the attendees and guiding them to the rooms.

There is also the option to attend evening discussions after dinner. Each of these discussions has a coordinator to arrange a meeting place and be available. The evening discussions are informal and not moderated.

Contacts for the excursion, concert, fitness centre and library are also listed. Please contact them if you are interested to attend any of these events or venues for further information.

BIRS Workshop - Quantum Technology: Computational Models for Quantum Device Design (12w5061) - Timetable 1.6

	Su, 8/1/2012	Mo, 9/1/2012	Device Modelling	Tu, 10/1/2012	Bio and Spin Systems	We, 11/1/2012	System Identification	Th, 12/1/2012	Control	Fr, 13/1/2012	
7:00		Breakfast		Breakfast		Breakfast	**Frank Langbein, Jonathan Quinn**	Breakfast		Breakfast	
8:45		BIRS	**Introduction by Station Manager**			Survey, 8am	Bayesian Learning and Optimisation				
09:00		Introduction	**Schirmer, Langbein, Hollenberg**	Survey	**Martin Plenio**	Survey	**Steffen Glaser**	Survey	**Sophie Schirmer**	Survey	**Thomas Schulte-Herbruggen**
09:15		chair: Sophie Schirmer	**Plenio, Bandrauk, Glaser, Sanders, Schulte-Herbruggen**	chair: Thomas Schulte-Herbruggen	Quantum Coherence and Biological Systems	chair: Mark Balas	Spectroscopy, Tomography & Beyond / Optimal Control of Uncoupled and Coupled Spins	chair: Frank Langbein	Coherent Control and Closing the Modelling-Simulation-Control-Identification Loop	chair: Lloyd Hollenberg	Symmetry Principles in Quantum Systems Theory
09:30		Survey	**Richard Muller**								
09:45		chair: Sophie Schirmer	Development of Few-Electron Si Quantum Dots for Use as Qubits								
10:00				Bio and Spin Systems	**Stephan Hoyer**	Coffee		Control	**Matthew James**	Coffee	
10:15				chair: Barry Sanders	Quantum Control of Light-Harvesting Systems	System Identification	**Daniel Oi**	chair: Tomasso Calarco	Quantum Feedback Networks	Group discussion	**Group 1 - Steffen Glaser**
10:30		Coffee		Coffee		chair: T Schulte-Herbruggen	Maximum Likelihood Hamiltonian and Decoherence Estimation	Coffee		Conclusions and Next Steps	**Group 2 - Andre Bandrauk**
11:00		Device Modelling	**Jim Fonseca**		**Paul Rees**		**Daniel Burgarth**		**Ian Peterson**	coordinator: Lloyd Hollenberg	**Group 3 - Tomasso Calarco**
11:15		chair: Lloyd Hollenberg	NanoHUB and NEMO5		Mathematical Techniques for Cell Cycle Analysis		Quantum System Identification with Limited Resources		Robust Stability of Uncertain Quantum Systems	Feedback	**Sophie Schirmer, Frank Langbein, Lloyd Hollenberg**
11:30		Lunch			**Jianming Cai**		**Clemens Muller**		**Giulia Gualdi**	Conclusions and Next Steps	
11:45					Diamond Based Single Molecule Magnetic Resonance Spectroscopy		Characterizing Defects in Superconducting Phase Qubits		Approx.Open Quantum Sys.Dyn.in a Controlled and Efficient Way		Check-out by 12:00
12:00	Informal meeting possible			Lunch		Lunch		Lunch		Lunch	
13:00	contact: Frank Langbein	BIRS	**Guided tour of Banff Centre**								
13:30			Meet at BIRS 2nd floor lounge of Corbett Hall		**Ilya Kuprov**		**Edmond Jonckheere**	chair: Edmond Jonckheere	**Tomasso Calarco**	Open session	
13:45			**Group Photo: meet at front steps of Corbett Hall**		Alg.and Software for Large-Scale Quantum Spin Dyn.Simulations		Differential Topology of Adiabatic Gap		Quantum Technology Taken to its (Speed) Limit	Emerging topics, arising opportunities, collaborations, grants, etc	
14:00			**Erik Nielsen**	Survey	**Andre Bandrauk**	Group discussion	**Group 1 - Mark Balas**	Survey	**Barry Sanders**		
14:15			The QCAD Framework for Quantum Device Simulation	chair: Sophie Schirmer	Modelling Molecules in Intense Laser Pulses and Attosecond Simulations	Topics on System Identification	**Group 2 - Daniel Burgarth**	chair: Edmond Jonckheere	Efficient Quantum Algorithms for Simulating Hamiltonian Evolution on a Quantum Computer / Optimal Phase Estimation Using Particle Swarm Optimisation		
14:30			**Suzey Gao**				**Group 3 - Celmens Muller**				
14:45			Semiclassical Poisson and Poisson-Schrodinger Solvers in QCAD			coordinator: Sophie Schirmer	**Group 4 - Daniel Oi**			coordinator: Frank Langbein	Tea and cofee items available in tea lounge
15:00		Coffee		Coffee		Coffee	Excursion to upper hot springs (open 10:00 - 22:00, bus: http://www.banff.ca/locals-residents/public-transit-buses.htm, taxi: tel. 403 762 4444, 403 762 0000)	Coffee			Informal meetings possible
15:30			**Rajib Rahman**	chair: Sophie Schirmer	**Lloyd Hollenberg**			Group discussion	**Group 1 - Ian Peterson**		contact: Frank Langbein
15:45			High Prec. Quantum Dev. Simulations with Atomistic TB		Quantum Sensing Technology and Modelling			Topics on Control	**Group 2 - Matthew James**		
16:00	BIRS	Group discussion	**Group 1 - Suzey Gao, Erik Nielsen**	Group discussion Topics on	**Group 1 - Stephan Hoyer**		contact: Sophie Schirmer		**Group 3 - Barry Sanders**		
16:15	Check-in	Topics on Device Modelling, Simulation, Control	**Group 2 - Rajib Rahman**	Modelling, Simulation, Control of Bio and Spin Systems	**Group 2 - Paul Rees**			coordinator: Jon Quinn	**Group 4 - Edmond Jonckheere**		
16:30			**Group 3 - Jim Fonseca**		**Group 3 - Ilya Kuprov**			Feedback	**Andre Bandrauk**		
16:45		coordinator: Lloyd Hollenberg	**Group 4 - Thomas Schulte-Herbruggen**	coordinator: Frank Langbein	**Group 4 - Tomasso Calarco**			Control			
17:00		Feedback	**Richard Muller**	Feedback	**Martin Plenio**						
17:15		Device Modelling, Simulation, Control		Modelling, Simulation, Control of Bio and Spin Systems							
17:30	Buffet Dinner										
17:45											
18:00		Dinner		Dinner		Dinner		Dinner			
19:30									Dala at The Club, Theatre Complex ($22, Doors 19:30)		
20:00	Informal gathering: at TCPL Pavilion	Discussions	Meet at Corbet Hall Lounge on second floor	Discussions	Meet at Corbet Hall Lounge on second floor	Feedback	**Steffen Glaser**	Discussions	contact: Frank Langbein		
	coordinator: Frank Langbein	coordinator: Sophie Schirmer		coordinator: Lloyd Hollenberg		System Identification	in TCPL 201	coordinator: Sophie Schirmer	Meet at Corbet Hall Lounge on second floor		

All meetings in TCPL 201 unless otherwise stated	TCPL 101, 102, 105, 106 for discussions, open sessions, possibly parallel sessions as needed (small groups)	Group discussion	1h with moderator as listed, coordinator to arrange grouping	~10 people/ group, extra	Survey: 1h incl. 10-15mins questions/discussion	Sally Borden Fitness Centre contact: Jonathan Quinn	Paul D. Fleck Library & Archives at Kinnear Centre, open 9:00 - 17:00 contact: Frank Langbein
TCPL 201,202,107, 5310 (Reading Room), 5210 for group discussions		Feedback	1h, everyone with moderator as listed		Talk: 30min incl. 5-10mins questions/discussions		

Sunday, 8/1/2012

12:00	Informal meetings possible (contact: Frank Langbein)
16:00	Check-in begins (Front Desk - Professional Development Centre - open 24 hours)
17:30–19:30	Buffet Dinner, Sally Borden Building
20:00	Informal gathering in 2nd floor lounge, Corbett Hall Beverages and a small assortment of snacks are available on a cash honor system. (coordinator: Frank Langbein)

Monday, 9/1/2012 — Device Modelling

7:00	Breakfast
8:45	Introduction and Welcome by BIRS Station Manager, TCPL
9:00	Introduction to Workshop Sohie Schirmer, Frank Langbein, Lloyd Hollenberg
	Introduction of survey talk speakers Richard Muller, Martin Plenio, André Brandrauk, Steffen Glaser, Thomas Schulte-Herbruggen
	Survey Talk (chair: Sophie Schirmer)
9:30	Richard Muller, Sandia National Laboratories Development of Few-Electron Si Quantum Dots for Use as Qubits
10:30	Coffee break
	Session: Device Modelling (chair: Lloyd Hollenberg)
11:00	Jim Fonseca, Purdue University NanoHub and Nemo5
11:30	Lunch
13:00	Guided Tour of Banff Centre Meet at BIRS 2nd floor lounge of Corbett Hall
13:45	Group Photo Meet at front steps of Corbett Hall
	Session: Device Modelling cont.
14:00	Erik Nielsen, Sandia National Laboratories The QCAD Framework for Quantum Device Simulation
14:30	Suzey Gao, Sandia National Laboratories Semiclassical Poisson and Poisson-Schrodinger Solvers in QCAD
15:00	Coffee break
15:30	Rajib Rahman, Sandia National Laboratories High Precision Quantum Device Simulations with Atomistic Tight Binding
16:00	**Group Discussion: Topics on Device Modelling, Simulation, Control** (coordinator: Lloyd Hollenberg) Group 1 – Suzey Gao, Erik Nielsen Group 2 – Rajib Rahman Group 3 – Jim Fonseca Group 4 – Thomas Schulte-Herbruggen
17:00	**Feedback: Device Modelling, Simulation, Control** (moderator: Richard Muller)
18:00–19:30	Dinner
20:00	Evening discussions Meet at Corbet Hall Lounge, can use TCPL Pavilion Foyer, etc (coordinator: Sophie Schirmer)

Tuesday, 10/1/2012 — Biological and Spin Systems

7:00	Breakfast
9:00	**Survey Talk** (chair: Thomas Schulte-Herbruggen) Martin Plenio, University of Ulm Quantum Coherence and Biological Systems
10:00	**Session: Bio and Spin Systems** (chair: Barry Sanders) Stephan Hoyer, University of California, Berkeley Quantum Control of Light-Harvesting Systems
10:30	Coffee break
11:00	Paul Rees, Swansea University Mathematical Techniques for Cell Cycle Analysis
11:30	Jianming Cai, University of Ulm Diamond Based Single Molecule Magnetic Resonance Spectroscopy
12:00	Lunch
13:30	Ilya Kuprov, University of Oxford Algorithms and Software for Large-Scale Quantum Spin Dynamics Simulations
14:00	**Survey Talk** (chair: Sophie Schirmer) André Bandrauk, Université de Sherbrooke Modelling Molecules in Intense Laser Pulses and Attosecond Simulations
15:00	Coffee break
15:30	Lloyd Hollenberg, University of Melbourne Quantum Sensing Technology and Modelling
16:00	**Group discussion: Topics on Modelling, Simulation, Control of Bio and Spin Systems** (coordinator: Frank Langbein) Group 1 – Stephan Hoyer Group 2 – Paul Rees Group 3 – Ilya Kuprov Group 4 – Tomasso Calarco
17:00	**Feedback: Modelling, Simulation, Control of Bio and Spin Systems** (moderator: Martin Plenio)
18:00–19:30	Dinner
20:00	Evening discussions Meet at Corbet Hall Lounge, can use TCPL Pavilion Foyer, etc (coordinator: Lloyd Hollenberg)

Wednesday, 11/1/2012 — System Identification

7:00 Breakfast

Survey Talk (chair: Sophie Schirmer)
8:00 Frank Langbein, Jonathan Quinn, Cardiff University
Bayesian Learning and Optimisation

Survey Talk (chair: Mark Balas)
9:00 Steffen Glaser, Technical University Munich
Spectroscopy, Tomography & Beyond / Optimal Control of Uncoupled and Coupled Spins

10:00 Coffee break

Session: System Identification (chair: Thomas Schulte-Herbruggen)
10:30 Daniel Oi, Strathclyde University
Maximum Likelihood Hamiltonian and Decoherence Estimation
11:00 Daniel Burgarth, Imperial College
Quantum System Identification with Limited Resources
11:30 Clemens Muller, Université de Sherbrooke
Characterizing Defects in Superconducting Phase Qubits

12:00 Lunch

13:30 Edmond Jonckheere, USC
Differential Topology of Adiabatic Gap

14:00 **Group discussion: Topics on System Identification**
(coordinator: Sophie Schirmer)
Group 1 - Mark Balas
Group 2 - Daniel Burgarth
Group 3 - Celmens Muller
Group 4 - Daniel Oi

15:00-15:30 Coffee break

18:00–19:30 Dinner

19:30–20:30 **Feedback: System Identification**
(in TCPL 201, moderator: Steffen Glaser)
20:30 Evening discussions
Meet at Corbet Hall Lounge, can use TCPL Pavilion Foyer, etc
(coordinator: Sophie Schirmer)

15:00 Excursion to upper hot springs
Open 10:00–22:00, bus: http://www.banff.ca/locals-residents/public-transit-buses.htm, taxi: tel. 403 762 4444, 403 762 0000
(contact: Sophie Schirmer)

Thursday, 12/1/2012 — Control

7:00	Breakfast
9:00	**Survey Talk** (chair: Frank Langbein) Sophie Schirmer, Swansea University Coherent Control and Closing the Modelling-Simulation-Control-Identification Loop
10:00	**Session: Control** (chair: Tomasso Calarco) Matthew James, Australian National University Quantum Feedback Networks
10:30	Coffee break
11:00	Ian Peterson, UNSW Robust Stability of Uncertain Quantum Systems
11:30	Giulia Gualdi, University of Kassel Approximating Open Quantum System Dynamics in a Controlled and Efficient Way: A Microscopic Approach to Decoherence
12:00	Lunch
13:30	**Session: Control** cont. (chair: Edmond Jonckheere) Tomasso Calarco, University of Ulm Quantum Technology Taken to its (Speed) Limit
14:00	**Survey Talk** (chair: Edmond Jocnkheere) Barry Sanders, University of Calgary Efficient Quantum Algorithms for Simulating Hamiltonian Evolution on a Quantum Computer / Optimal Phase Estimation Using Particle Swarm Optimisation
15:00	Coffee break
15:30	**Group discussion: Topics on Control** (coordinator: Jon Quinn) Group 1 - Ian Peterson Group 2 - Matthew James Group 3 - Barry Sanders Group 4 - Edmond Jonckheere
16:30–17:30	**Feedback: Control** (moderator: André Bandrauk)
18:00–19:30	Dinner
20:00	Evening discussions Meet at Corbet Hall Lounge, can use TCPL Pavilion Foyer, etc (coordinator: Sophie Schirmer)
20:00	Concert - Dala at The Club, Theatre Complex Ticket $22, doors 19:30 (contact: Frank Langbein)

Friday, 13/1/2012

7:00	Breakfast
9:00	**Survey Talk** (chair: Lloyd Hollenberg) Thomas Schulte-Herbruggen, Technical University Munich Symmetry Principles in Quantum Systems Theory
10:30	Coffee break
10:00	**Group discussion: Conclusions and Next Steps** (coordinator: Lloyd Hollenberg) Group 1 - Steffen Glaser Group 2 - André Bandrauk Group 3 - Tomasso Calarco
11:00	**Feedback: Conclusions and Next Steps** (moderator: Sophie Schirmer, Frank Langbein, Lloyd Hollenberg)
	Checkout by 12 noon, unless you have an extension
12:00	Lunch
13:30-15:00	**Open Session** (coordinator: Frank Langbein) Emerging topics, arising opportunities, collaborations, grants, etc Tea and cofee items available in tea lounge
15:00	Informal meetings possible (contact: Frank Langbein)

5-day workshop participants are welcome to use BIRS facilities (BIRS Coffee Lounge, TCPL and Reading Room) until 3 pm on Friday, although participants are still required to checkout of the guest rooms by 12 noon.

Quantum Technology
Computational Models for Quantum Device Design

8th to 13th of January 2012

Abstracts

(in alphabetic order by speaker surname)

Modelling Molecules in Intense Laser Pulses and Attosecond Simulations

Bandrauk, André D
Université de Sherbrooke

The description and simulation of the nonlinear nonperturbative interaction of molecules with intense laser pulses requires the numerical solution of multidimensional partial differential equations, pde's such as the time-dependent Schroedinger equation, TDSE for fs-asec electron-nuclear movement beyond traditional Born-Oppenheimer approximations and for the zps time scale, TimeDependent Dirac Equations, TDDE's for relativistic effects such as the increase of spin-orbit coupling with increasing nuclear charge and pulse intensity. The complete description of the nonlinear nonperturbative response of intense molecule-laser interactions requires finally the coupling of Maxwell's (laser, photon) equations to include collective effects via propagation in a medium. The main goal of the FAZSST large scale computation project is to use advanced numerical algorithms on large memory machines to advance the development of the new Attosecond Science via numerical solutions of multidimensional TDSE and TDDE's coupled to appropriate Maxwell equations.

Quantum System Identification with Limited Resources

Burgarth, Daniel
Imperial College

The aim of quantum system identification is to estimate the ingredients inside a black box, in which some quantum-mechanical unitary process takes place, by just looking at its input-output behavior. Here we establish a basic and general framework for quantum system identification, that allows us to classify how much knowledge about the quantum system is attainable, in principle, from a given experimental setup. Unlike usual quantum metrology, our theory applies to cases where the set of observables are not topographically complete, and where knowledge about the system can only be retrieved indirectly. When the topology of the system is known, the framework enables us to establish a general criterion for the estimability of the coupling constants in its Hamiltonian.

Diamond Based Single Molecule Magnetic Resonance Spectroscopy

Cai, Jianming
University of Ulm

We demonstrate that a single nitrogen-vacancy (NV) center in diamond can be used to construct a nanoscale single molecule spectrometer. The proposed device may find applications in single molecule spectroscopy in chemistry and biology, such as in determining protein structure or monitoring macromolecular motions and can thus provide a tool to help unravelling the microscopic mechanisms underlying biomolecular function.

Quantum Technology Taken to its (Speed) Limit

Calarco, Tomasso
University of Ulm

Quantum effects form the basis of most present-day information technologies. However, the full power of quantum coherence has not yet been tapped for everyday technological applications. The exquisite level of control of current atomic physics experiments may enable this, for instance in the field of quantum communication and quantum computing - but scalable quantum information processing requires extremely precise operations. Quantum optimal control theory allows to design the evolution of realistic systems in order to attain the best possible performance that is allowed by the laws of quantum mechanics. I will present a range of its applications to a variety of quantum technologies, and discuss its use in probing the ultimate limits to the speed of the corresponding quantum processes.

NanoHUB and NEMO5: a Science Cyberinfrastructure and a Nanoelectronic Modeling Tool

Fonseca, Jim
Purdue University

The NanoHUB is a cyberinfrastructure for the development, deployment, and use of scientific software. Students, teachers, developers, and researchers are able to collaborate in an online environment. A web browser provides the user with access to available tools that are run on high performance parallel computers. One tool that is under construction for nanoelectronic modeling is NEMO5. The core capabilities of NEMO5 lie in the atomic-resolution calculation of nanostructure properties: a multimillion-atom strain calculation, bulk electron and phonon band structures, a 1-D Schrödinger-Poisson simulation, a multiphysics simulation of a resonant tunneling diode, and quantum transport through a nanowire transistor.

Semiclassical Poisson and Poisson-Schrodinger Solvers in QCAD

Gao, Suzey
Sandia National Laboratories

We discuss the technical details of the semiclassical Poisson and the self-consistent quantum Poisson-Schrodinger solvers in the Quantum Computer Aided Design (QCAD) LDRD project at Sandia. We have developed as a first step a nonlinear Poisson solver, including Boltzmann or Fermi-Dirac statistics and incomplete ionization of dopants, which provides a good first-order description of the electrostatics in quantum devices. We have also developed a self-consistent Poisson-Schrodinger (P-S) solver to capture the unique quantum effects. This description includes the exchange-correlation potential within the local density approximation. Efficient convergence of the self-consistent solution is achieved using a predictor-corrector iteration scheme. Applications of the QCAD framework to 1-, 2-, and 3-D quantum systems demonstrate high accuracy and robustness of the solvers.

Optimal Control of Uncoupled and Coupled Spins

Glaser, Steffen
Technical University Munich

Based on principles of optimal control theory, the physical limits of quantum control can be explored and time-optimal and relaxation-optimized pulse sequences can be designed to control the dynamics of spin systems. Furthermore, robust pulse sequences, compensating experimental imperfections and taking into account experimental limitations can be optimized. Recent advances include time-optimal pulses for saturation and for maximizing contrast in magnetic resonance imaging (MRI), robust pulses that effect point-to-point transfers and/or desired unitary transformations that tolerate a large range of rf scaling, e.g. a factor of six in toroid NMR probes. As demonstrated experimentally, these pulses make it possible to perform sophisticated 2D NMR experiments on this hardware platform. The design of cooperative pulses opens new avenues for improved performance of multi-pulse experiments. Finally, the application of optimal control methods to the problem of spin decoupling yields not only significantly improved performance but also unprecedented flexibility in the design of tailored decoupling sequences.

Approximating Open Quantum System Dynamics in a Controlled and Efficient Way: A Microscopic Approach to Decoherence

Gualdi, Giulia
University of Kassel

We demonstrate that the dynamics of an open quantum system can be calculated efficiently and with predefined error, provided that a basis exists in which the system-environment interactions are local and hence obey the Lieb-Robinson bound. We show that this assumption can generally be made. Defining a dynamical renormalization group transformation, an effective Hamiltonian for the full system plus environment is obtained that comprises only those environmental degrees of freedom that are within the effective light cone of the system. The reduced system dynamics can therefore be simulated with a computational effort that scales at most polynomially in the interaction time and the size of the effective light cone. Our results hold for generic environments consisting of either discrete or continuous degrees of freedom.

Quantum Sensing Technology and Modelling

Hollenberg, Lloyd
University of Melbourne

Quantum Control of Light-Harvesting Systems

Hoyer, Stephan
University of California, Berkeley

I will review the evidence for the relevance of quantum coherence to photosynthetic energy transfer, and discuss our theoretical progress towards controlling these dynamics using shaped ultra-fast laser pulses. I will also present a scheme for experimental validation in a pump-probe spectroscopy setup.

Quantum Feedback Networks

James, Matthew
Australian National University

Background: Systems and control theory is concerned with ensuring that systems behave in a desired way. At the most basic level, the system should operate in a stable manner, and beyond this, systems and control theory endeavours to assess, and where possible, optimise, performance. For example, in the 18th century James Watt designed a governor system to ensure that his steam engines maintained a constant speed, (and as is well known, the steam engine powered the industrial revolution). The steam engine governor is a classic example of a feedback control system. A feedback system is a network: an interconnection of the system being controlled (e.g. steam engine or atom) and the system facilitating the control (e.g. governor or another atom). Networks are ubiquitous in science and technology, e.g. electronic circuits, the internet, etc, etc.

Over many years, many methods have been developed for modeling and design. Models and design techniques have been developed for particular purposes, at different levels of abstraction and detail. For example, detailed transport equations could be used to describe the flow of electrons and holes in a transistor within a standard operational amplifier chip, or a simple model could be used when the opamp is included in a negative feedback circuit. Widely used abstractions include Gaussian and white noise models (e.g. for the movement of particles in a fluid, or to describe sensor noise) and Boolean algebra (used to describe classical logic). Methodologies that have been developed at these levels of abstraction include probability and stochastic processes, information theory, and computational complexity.

At the present time, quantum technology is developing rapidly, spurred on by the significant potential of key application areas, notably, quantum computation, information, and metrology. The qbit is now omnipresent, and fundamental to the conceptual and experimental developments in quantum technology in recent decades. The qbit, of course, is a quantum generalization of the classical bit from classical logic, and indeed quantum generalizations of information theory and computation have been developed. Gaussian states are very common, particularly in quantum optics, and a theory of quantum stochastic processes has been available now for several decades. However, this later theory has yet to be fully exploited in quantum technology.

This talk will discuss ideas concerning quantum feedback networks (QFN). These ideas go back to Yurke-Denker in the 1980's, Wiseman-Milburn, Gardiner and Carmichael in the 1990's, and Yanagisawa and others in the 2000's. QFNs consist of components modeled as open quantum systems, interconnected by free fields and/or by direct physical couplings (it is worth thinking about how electronic amplifiers are cascaded together, and how a steam engine is connected to a governor). An important feature of the developing theory of QFNs are the simple symbolic rules for describing interconnections, based on underlying quantum stochastic models. The talk will discuss this theory, as well as some recent applications in quantum optics and quantum information.

Differential Topology of Adiabatic Gap

Jonckheere, Edmond
USC

In this talk, we provide a new interpretation of the adiabatic theorem in quantum computation with special attention to the gap problem and the crossing avoidance of the various energy levels. It is indeed argued that the mere plotting of the various energy levels versus the time spent in the adiabatic process hides some deeper issues as to how the energy levels are intertwined. Central in this new interpretation is the numerical range of a matrix constructed with the initial and terminal Hamiltonians. The fundamental fact is that the various energy levels encountered along the time through the adiabatic process are the various critical value curves of the numerical range viewed at an angle that parameterizes the time spent in the process. The boundary of the numerical range represents the ground state, while that curve closest to the boundary is the first excitation level. Generically, the boundary curve is smooth, but all other energy level curves are highly singular with cusps. With this interpretation, the known scaling of the gap is easily recovered and new results are derived from topological consideration on the numerical range. But probably most importantly, this approach explains how the various energy levels are intertwined by a two-stage unraveling process: (i) by going from the classical energy level plots to the highly singular critical value curves in the numerical range, and (ii) by lifting the critical value curves to (smooth) Legendrian knots in a contact space. The smooth curves in the contact space are possibly knotted, possibly linked, which provides the ultimate explanation of the non-crossing phenomena observed "down" at the most elementary level of the classical energy level plots.

Algorithms and Software for Large-Scale Quantum Spin Dynamics Simulations

Hogben, HJ[1], Edwards, LJ[2], Krzystyniak, M[2], Charnock, GTP[2], Hore1, PJ[1], Kuprov, Ilya[2]
[1] Chemistry Department, University of Oxford, South Parks Road, Oxford, UK.
[2] Oxford e-Research Centre, University of Oxford, 7 Keble Road, Oxford, UK.

We introduce a software library incorporating our recent research into efficient time-domain simulation algorithms for large spin systems. Liouville space simulations (including symmetry, relaxation and chemical kinetics) of most liquid state NMR experiments on 40+ spin systems can now be performed without effort on a desktop workstation. Much progress has also been made with improving the efficiency of ESR, solid state NMR and Spin Chemistry simulations. The functionality available at the time of writing includes:

- Low-dimensional matrix representations for spin operators in large spin systems that enable the simulation of magnetic resonance experiments on systems previously considered too big for any practical simulations.
- Generalized symmetry module (any number of groups of equivalent spins of any quantum number).
- Krylov subspace based time propagation routines that avoid matrix exponentiation.
- Generalized rotation module and a Lebedev powder integrator.
- Generalized relaxation theory module, supporting all types of magnetic resonance spectroscopy (NMR, ESR, DNP, Spin Chemistry, etc.). Anisotropic rotational diffusion tensors are supported in full generality.
- Optimal Control waveform design module using BFGS-GRAPE algorithm with exact gradients. Optimization of broadband pulses, selective pulses and universal rotations is implemented in both Cartesian and phase-amplitude coordinates.
- Functions for multi-grid parallel soft pulses and (algebraic) decoupling.
- Functions for the simulation of magnetochemical experiments.
- Functions for the simulation of common NMR experiments (COSY, DQF-COSY, NOESY, HSQC, HMQC, HETCOR, etc.), basic ESR experiments (ESEEM, ENDOR, etc.) as well as building blocks for the writing of user-specified experiment simulations.

Spinach is an open-source Matlab library available at http://spindynamics.org.

Bayesian Learning and Optimisation

Langbein, Frank C, Quinn, Jonathan A
Cardiff University

Machine learning aims to construct a model for an unknown or only partially known environment. This is directly related to identifying quantum systems. We give an overview of various machine learning techniques, the underlying models and efficient algorithmic techniques, especially focused on Bayesian learning techniques. In the second part we overview core search and optimisation methods, useful for model fitting, parameter identification and control.

Development of Few-Electron Si Quantum Dots for Use as Qubits

Muller, Richard P, Bielejec, ES, Bishop, N, Ezra Bussman, E, Carroll, MS, Gao, S, Landahl, A, Lilly, MP, Lu, TM, Nielsen, E, Pluym, T, Rahman, R, Shirkhorshidian, A, Stalford, HL, Tracy, LA, Witzel, WM, Young, RW
Sandia National Laboratories, Albuquerque, NM

This talk will describe a modeler's perspective on existing experimental efforts to create a Si qubit, the challenges to overcome, and the opportunities for modeling to have an impact on the experimental direction. The talk will review options we?ve considered for the materials stack and the gate layout, and will discuss how issues like spin- and charge disorder, valley splitting, and gate design impact the development of few-electron quantum dots. I will conclude with observations on how computer simulation can help accelerate this development.

This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

Characterizing Defects in Superconducting Phase Qubits

Müller, Clemens
Université de Sherbrooke

Spectroscopy of superconducting phase qubits often shows characteristic anti-crossings, indicating the presence of additional coherent and strongly coupled quantum systems. The origin of these two-level defects is not yet fully understood, although a variety of models have been proposed. I will show a summary of our joint theory-experiment efforts to determine the parameters of possible microscopic models of the defects in order to determine their physical nature. I will also talk about the possibility of applying Hamiltonian tomography on this system and present the specific challenges we face there.

The QCAD Framework for Quantum Device Simulation

Nielsen, Erik
Sandia National Laboratories

The Quantum Computer Aided Design (QCAD) LDRD project at Sandia National Labs is developing an integrated tool designed for the simulation of few-electron quantum devices. We discuss the software framework and capabilities of this tool, and compare these with existing tools. We emphasize the close relationship with our experimental effort, and discuss how QCAD has been utilized for rapid design guidance. This work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories.

Maximum Likelihood Hamiltonian and Decoherence Estimation

Oi, Daniel
Strathclyde University

Advances in quantum systems engineering and control are leading to the ability to fabricate and manipulate large scale devices operating in the coherent regime. However, precision operation requires knowledge of the behaviour of the system, both in response to control fields and to environmental noise and decoherence. The traditional approach to system behaviour, process tomography, presupposes the ability to prepare complete sets of initial states and to be able to measure in many different bases, abilities which may not be initially present without control. A method is required to bootstrap the characterisation process utilising a more restricted set of preparation and measurement primitives. Even for small systems, signal complexity can overwhelm conventional analysis. We have applied maximum likelihood methods to extract model parameters and invert system dynamics. Scaling up and increasing efficiency remain as challenges, these may be possible using adaptive experiment design and compressive sensing methods.

Robust Stability of Uncertain Quantum Systems

Petersen, Ian
UNSW

This talk considers the problem of robust stability for a class of uncertain quantum systems subject to unknown perturbations in the system Hamiltonian. Some general stability results are given for different classes of perturbations to the system Hamiltonian. Then, the special case of a nominal linear quantum system is considered with either quadratic or non-quadratic perturbations to the system Hamiltonian. In this case, robust stability conditions are given in terms of strict bounded real conditions.

Quantum Coherence and Biological Systems

Plenio, Martin
University of Ulm

The interplay between coherence and the vibrational environment is of key interest for the quantum dynamics of bio-molecular systems. In this talk I will present some fundamental ideas in this regard, then I will discuss briefly methods to simulate the dynamics in the relevant regime of intermediate strength coupling between system and environment. Finally, if time allows I may discuss some aspects concerning measurement techniques in these systems.

High Precision Quantum Device Simulation with Atomistic Tight-Binding Technique Coupled with Semi-Classical Poisson Solver and Many-Electron Configuration Interaction Method

Rahman, Rajib
Sandia National Laboratories

Due to the rapidly shrinking dimensions of semiconductor devices, modeling techniques need to incorporate the underlying atomistic nature of the materials the devices are built from. Widely used continuum models very often fail to capture the subtle quantum properties that govern the operations of modern devices. The semi-empirical tight-binding method offers a promising way to simulate these devices as it treats interactions on an atomic scale and is also scalable to realistic device sizes of millions of atoms. In general, the tight-binding approach captures various features of materials and devices such as hetero-structure properties, inhomogeneous strain distributions, lattice miscuts, surface roughness, full bandstructure, interfaces, electro-magnetic fields - all under a unified framework.

However, tight-binding being essentially a single electron theory misses out important many electron interactions that some quantum devices rely on. Here, we describe two methods to augment the tight-binding method with many electron interactions. The first is based on coupling the tight-binding Hamiltonian with a semi-classical Poisson solution of the device with realistic gate geometries and voltages to describe mean field interactions in terms of the electron density. The second is based on coupling tight-binding to an exact many-electron configuration interaction method, which captures Coulomb, exchange, and correlation effects with accurately. The complete suite of these tools constitutes a powerful package for high precision device simulation.

As applications of these techniques, we show simulations of two important quantum information processing systems in silicon. Simulations of a single donor spin qubit in silicon in a field effect transistor show the subtle electric field tuning of the donor spin and explain experimental measurements. Computations of the many electron levels of a double quantum dot in silicon along with nearby defects reveal complex interplay of valley physics and many electron effects, which are manifested in the nature of the voltage tuned exchange curve of the double quantum dot.

Mathematical Techniques for Cell Cycle Analysis

Rees, Paul
Swansea University

The aim of systems biology is to understand the complex interactions which occur between the components of a biological system. By identifying the relevant components within the complex system a host mathematical tools can be used to attempt to identify the nature of the mechanisms between them. Here we take inspiration from a traditional systems engineering approach which relates the output of a system to the input by a transfer function. This requires a significant simplification of the complex biological system however we will demonstrate that appropriately designed experiments couple with simple mathematic models of the transfer function can accurately elucidate biological function. In casting the problem in this manner we are able to use systems engineering theory to describe and analyze the biological system. We outline this technique by giving examples for the assessment of drug treatments on cancer cell populations and the study of uptake of nanoparticles and the toxic effect on cells.

Efficient Quantum Algorithms for Simulating Hamiltonian Evolution on a Quantum Computer / Optimal Phase Estimation Using Particle Swarm Optimisation

Sanders, Barry

I present efficient quantum algorithms for simulating Hamiltonian evolution on a quantum computer both for an oracle setting for the Hamiltonian and also without the oracle model for the specific case that Hamiltonians are sums of non-commuting tensor products of Pauli operators. For the time-dependent Hamiltonian case, we establish sufficient smoothness criteria to deliver bounded-error quantum simulations of state evolution efficiently. Technically we employ Lie-Trotter-Suzuki approximations for ordered-operator exponentials with strict error bounds for these expansions. For the specific case of Hamiltonians that are sums of non-commuting tensor products of Pauli operators, our efficient classical algorithm delivers circuit designs for efficient quantum simulation, and I show applications to Kitaev's toric-code and honeycomb Hamiltonian systems.

Coherent Control and Closing the Modelling-Simulation-Control-Identification Loop

Schirmer, Sophie
Swansea University

When we talk about quantum devices there is an implied assumption of functionality, i.e., the device is supposed to perform certain tasks as required by an application. Achieving such functionality requires careful device design as well as control to manipulate the behaviour of the system. Effective device and control design is a non-trivial task that requires understanding the intrinsic dynamics of the system as well as its interaction with the control apparatus, sensors and actuators, as well as the effect of the environment. Generally, this means that we require a model not only of an isolated system but its interaction with a controller and environment. In simple cases such models can be constructed directly from first principles, e.g., for a simple quantum system we may be able to write down a Hamiltonian for the intrinsic dynamics of the system and maybe the effect of certain types of coherent control fields. For more complex systems from nano-electronics to biomolecules, however, this approach usually does not suffice, and it is crucial to incorporate data from observations of the actual behaviour of the system to construct effective models. In this talk we will discuss some general requirements for control system models as well as some techniques for constructing and adaptively refining such models.

Symmetry Principles in Quantum Systems Theory

Schulte-Herbruggen, Thomas
Technical University Munich

Elucidating quantum optimal control in terms of symmetry principles has triggered us in a number of recent advances to be elucidated in survey:

(i) it leads to a new and handy controllability criterion,
(ii) it guides the design of universal quantum hardware,
(iii) it governs which quantum system can simulate another one given,
(iv) with little modification it specifies the limit between time-optimal control and relaxation-optimised control of open systems, and
(v) it provides a pattern that may help to understand new coherent pathways in noise-assisted energy transfer in light-harvesting biomolecules.

How principles turn into practice is illustrated in a plethora of examples showing practical applications in solid-state devices and circuit-qed. The algorithmic tools are presented in a unified programming framework.