The Quantum Times

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Newsletter of the Topical Group on Quantum Information

American Physical Society

Quantum information for chemistry and biology

Alán Aspuru-Guzik

In *Image and Logic: A Material Culture of Microphysics* (1997), Peter Galison, an historian of twentieth-century physics, describes in detail the interaction of experimental and theoretical physicists with engineers working towards the use of early computers for the simulation of experiments in the physical sciences. Perhaps one of the more dramatic consequences of this interaction led to the neutron transport simulations carried out on the MANIAC computer at Los Alamos that were instrumental in the development of the atomic bomb. In *Image and Logic*, Galison defines the concept of a trading zone: In the trading zones, the scientists from different sub-disciplines (and therefore, raised within specific subcultures or traditions) meet to exchange information and advance science. One can imagine such encounters happening in a port in the Mediterranean sea where people from different cultural groups and backgrounds exchanged products. In the case of the Los Alamos scientists and engineers, their products were new ideas that were fundamental for what we now refer to as computer simulation. Of equal importance, these ideas led to advances in the field we now call computer science. Quantum information is a highly relevant example of a modern trading zone in which people from different fields benefit from interactions with each other and develop a new language for the description of reality.

The trading zone encourages the development of new languages or codes through which the people from different communities interact. This is similar to development of the *nuova lingua franca* during the Renaissance in order for the Mediterranean cultures to understand each other. Galison describes this as "the establishment of local languages –pidgins and creoles – that grow and sometimes die in the interstices between cultures."

From time to time, I take the subway to a quantum trading zone. On Mondays, when I can escape from my more mundane duties, I sometimes visit the group meetings of Eddie Farhi at MIT, where computer scientists, physicists, and chemists from my group discuss the current developments in quantum information. Eddie usually begins the weekly ritual with the question, "Is there anything new in the arxiv that we need to learn about?" The arxiv e-print server seems to operate as the new library for this trading zone. At one of these meetings, computer scientist Scott Aaronson (also at MIT) exclaimed (in a rough paraphrase of his words) "I visited UC Berkeley and met some chemists who actually knew what QMA-complete means!" I found the comment amusing since there are many chemists in this field! For example, the speaker at the very first group meeting that I attended, just after landing at UC Berkeley, in 1999, was Daniel Lidar speaking about decoherence free subspaces to the group of William Lester, a quantum Monte Carlo expert. In the same chemistry department, Birgitta Whaley's team in those days included people like Dave Bacon and Ken Brown. And last Monday, Charles Bennett, a renowned former Harvard chemistry graduate student, recently visited his alma mater and spoke to my graduate students about many topics ranging from why bubbles in Guinness float downwards to the quantum Zeno effect in molecular

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systems, and even the quantum mechanics of smell. Chemists are everywhere!

In this column, I would like to mention two examples in which quantum information can be applied to domains of chemistry and biology. For reasons of space, I am leaving out many other fascinating subjects for chemists such as the role of entanglement in chemical bonding.

Quantum simulation of molecular systems

Many quantum chemists incorporate into their Powerpoint slides a famous quotation of Paul Dirac from 1929:

> The fundamental laws necessary for the mathematical treatment of a large part of physics and the whole of chemistry are thus completely known, and the difficulty lies only in the fact that application of these laws leads to equations that are too complex to be solved.[1]

It was not until 2007 that the nature of the complexity was formalized by Schuch and Verstraete who christened the problem "*Interacting Electrons*" and found it to be QMA-hard.[2] This result, for example, prevents finding the magical density functional that would allow for solving the many-body problem in polynomial time using a classical computer.

Richard Feynman, in his celebrated 1982 paper "Simulating physics with computers," proposed the use of quantum systems for simulating other quantum systems, and defined the desired ultimate complexity for the problem. He mused: "The rules of simulation that I would like to have is that the number of computer elements required to simulate a large physical system is only to be proportional to the space-time volume of the system."[3]

Feyman's request was a tall order that wasn't filled until the mid-1990s when quantum simulation pioneers like Seth Lloyd and Chris Zalka defined the algorithms for universal quantum simulation. It was this task that originally attracted me to this field. My postdoctoral work had the goal of developing a quantum algorithm for carrying out what we call in chemistry *full configuration interaction*, what physicists call *exact diagonalization,* and now computer scientists call *Interacting Electrons*. With Peter Love, Tony Dutoi and my advisor Martin Head-Gordon, we put the pieces together and were able to work out a quantum algorithm in which cholesterol – a molecule very dear to my heart – would require about 3000 qubits for its quantum simulation.[4] Our efforts complemented those of Daniel Lidar and Haobin Wang, who published a paper on the simulation of chemical reaction dynamics in 1998. A subfield, that includes such notable researchers as Ken Brown, Sabre Kais, Peter Love, and Franco Nori, had taken off. We are collectively working to develop better quantum algorithms in order to realize Feynman's dream in the context of molecules. Only in 2009 did two different collaborations (Andrew White and our laboratory, followed 3 months later by Jiangfei Du and his co-workers) realize the first quantum chemistry calculations on quantum information processors in quantum optics and NMR respectively.

Understanding biological processes using the language of quantum information

Recent experiments carried out by Greg Engel and his co-workers in the laboratory of Graham Fleming at UC Berkeley showed evidence of long-lived coherences in a photosynthetic complex of green-sulfur bacteria.[5] These coherences last for hundreds of femtoseconds, a relevant timescale for the energy transfer process of this complex, which is of the order of a picosecond. After reading "coherence" and "quantum search" in a single *Nature* publication, many quantum information groups began to study the subject. The list of subsequent publications in this field includes my group's work on connecting the problem to a generalized version of quantum walks that we called environment-assisted quantum walks, or quantum stochastic walks. Others from the quantum information gang that have worked or are working on the subject are Hans Briegel, John Dowling, Seth Lloyd, Gerald Milburn, Ari Mizel, Masoud Mohseni,Alexandra Olaya-Castro, Martin Plenio, Sandu Popescu, Birghita Whaley and Mark Wilde,

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[1] Quantum Mechanics of Many-Electron Systems', *Proceedings of the Royal Society A* **123**, 714-733 (1929).

[2] N. Schuch and Frank Verstraete, "Interacting electrons, Density Functional Theory, and Quantum Merlin Arthur", arXiv:0712.0483v1. Note that QMA in the above paragraph stands for Quantum Merlin Arthur.

[3] R. P. Feynman, "Simulating Physics with Computers", *International Journal of Theoretical Physics* **21**, 6 (1982).

[4] A. Aspuru-Guzik, A. D. Dutoi, P. J. Love, and M. Head-Gordon, "Simulated quantum computation of molecular energies", *Science* **309**, 1704 (2005).

[5] G. S. Engel, et al. "Evidence for wavelike energy transfer through quantum coherence in photosynthetic complexes." *Nature* **446**, 782, (2007).

amongst others to whom I apologize in advance if I inadvertently did not mention them. Another important biological process that has received attention from the quantum information community is that of the avian compass.[6] Many biophysicists, including Klaus Schulten, postulated that a radical ion-pair mechanism is responsible for the ability of birds to sense the earth's magnetic field. Quantum information scientists such as Iannis Kominis, Hans Briegel and Vlatko Vedral have followed up with a number of preprints. The secrets of how birds can migrate has become the domain of those same scientists whose shared goal is that of building a quantum computer.

These developments led Matt Goodman at DARPA to call for a workshop on Quantum Biological Effects (QuBE) in November of 2008. The gathering turned out to be quite fruitful as many of the questions posed by quantum optician John Dowling at that meeting have proven to be influential. Masoud Mohseni and Yasser Omar recently organized the Quantum Effects in Biological Systems 2009 (QuEBS 2009) conference this summer in Lisbon. At QuEBS, physical chemists who are experts in theoretical and experimental energy transfer met with quantum information scientists to help the development of a new pidgin language for this young and exciting trading zone: the relatively new creole of quantum information for biology.

***Alán Aspuru-Guzik** is beginning his fourth year as an assistant professor in the Department of Chemistry and Chemical Biology at Harvard University. He obtained his Ph.D. and carried out postdoctoral research in theoretical chemistry at the University of California, Berkeley. His research group works at the intersection of quantum information and theoretical physical chemistry. His work in quantum information is supported by the Army Research Office, and he was recently selected as a DARPA Young Faculty Award recipient, a Camille Henry Dreyfus Teacher-Scholar and a Sloan Research Fellow to work on the pursuit of new directions for practical quantum simulation of chemical systems.*

The Editor's Desk

If you did not notice sweeping changes with this issue of *The Quantum Times*, you are either a new reader or you might want to watch out for pick pockets. The story of the redesign is simple enough: a crashed computer hard drive. Besides, change is good once in awhile. Perhaps the changes will be enough impetus to garner a few letters to the editor. While I cannot force

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Editorial Board

Contributions

Contributions from readers for any and all portions of the newsletter are welcome and encouraged. We are particularly keen to receive

- **op-ed pieces and letters** (the APS is *strongly* encouraging inclusion of such items in unit newsletters)
- **books reviews**
- **review articles**
- **articles describing individual research** that are aimed at a broad audience
- **humor** of a nature appropriate for this publication

Submissions are accepted at any time. They must be in electronic format and may be sent to the editor at idurham@anselm.edu. Acceptable forms for electronic files (other than images) include LaTeX, Word, Pages (iWork), RTF, PDF, and plain text.

Editorial policy

All opinions expressed in *The Quantum Times* are those of the individual authors and do not represent those of the Topical Group on Quantum Information or the American Physical Society in general.

[6] See, for example, S. Johnsen and K.J. Lohmann, "Magnetoreception in Animals," *Physics Today* **61**, 29-35 (2008).

anyone to write in, I would like to remind readers that the APS has instituted a policy that *strongly* encourages the inclusion of op-ed pieces and letters to to the editor. This is a very important part of APS' mission to foster meaningful dialogue among its members.

In addition we are always interested in articles on individual research as well as book reviews or anything else that might seem appropriate. If you think you might be interested in serving on the Editorial Board, please do not hesitate to contact me (see the masthead on the previous page for further details). In this issue I am very pleased to have received an excellent article from Alán Aspuru-Guzik of Harvard University (who graciously dealt with my pestering) on the intersection of quantum information with chemistry and biology.

The interdisciplinary nature of our field is one of the things that I like the most about it. We can legitimately include physicists (obviously), mathematicians, computer scientists, engineers (of varying stripes), chemists, biologists, philosophers, historians of science, and perhaps others we may be unaware of in our menagerie of minds. This is particularly interesting to me since I teach at a college dedicated to the liberal arts tradition, where a well-rounded education is taken quite seriously.

With that said, please enjoy the rest of your summer (or winter for those of you below the Equator) as well as the rest of this issue!

Ian T. Durham *is Associate Professor and Chair of the Department of Physics, Director of the Computational Physical Sciences Program, and occasional lecturer in the Department of Mathematics at Saint Anselm College in Manchester, New Hampshire. He drinks four liters of Moxie per week and recently bought a new splitting axe for his woodpile that has been causally linked to seven stitches appearing in his leg.*

Bits, BYTES, and Qubits

QUANTUM NEWS & NOTES

Ultracold atoms behave like theorists

...that is, they have a tendency to walk rather randomly. A group led by Artur Widera at the University of Bonn in Germany have realized an idea originally suggested by Richard Feynman: the quantum random walk. We are likely all familiar with the classical version of a random walk in which a path is essentially dictated by a 'coin flip' (robotic vacuums and lawnmowers as well as de-mining robots are among the many applications of this principle). Feynman proposed a quantum version wherein a particle simultaneously took both paths (options) presented to it (it's amazing how many things you can make 'quantum' just by allowing for superpositions).

In the Widera experiment, a single, cold cesium atom is trapped in two optical lattices that initially overlap. A laser pulse is used to prepare the atom in a superposition of two internal states. The lattices are then moved in opposite directions which causes the atom to simultaneously move with each lattice putting it in a superposition of locations. Repeating this process causes the superposition to remain in place for another step. However, the 'middle' position (i.e. the original which ends up being a bit like the average) then contains two parts of the atom that interfere with one another.

The Widera experiment involved ten such steps, after which a high-resolution microscope was used to

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THE LIGHTER SIDE

THE MATHEMATICS OF ZOMBIES

While not strictly quantum, the following item came to my attention recently and I know there are a number of quantum information people who are fans of zombies and/or zombie flicks. A group of Canadian researchers led by the curiously – but legally – named statistician 'Robert J. Smith?' (Ottawa) has published a research paper analyzing the mathematics behind a zombie attack on civilization. Not only does the paper appear in a compilation alongside serious articles, but it has led to serious debate over such jargon-laden topics as Reed-Frost kinetics. One anonymous online commenter went so far as to complain that the paper was *too* mundane, dressing up a legitimate problem in zombie-like clothing. For those interested in judging for themselves, you may download a copy of the paper at:

http://www.mathstat.uottawa.ca/~rsmith/Zombies.pdf detect the atom's fluorescence, causing it to settle in a single position. Repeating the experiment a number of times produced results consistent with computer models of quantum walks. In other words, the probability distribution of the final locations matched the expected asymmetry of the theoretical model. Destroying the superposition at every step, however, produces a distribution that is symmetric and thus matches the classical case. The research recently appeared in the journal *Science*.

Playing with single photons

The group led by Prof. Gerhard Rempe, Director of the Max Planck Institüt für Quanten Optik (MPQ), is well-known for their work controlling single photons. In the past they have controlled their shape, frequency, and polarization. Now, for the first time, the group has successfully controlled the phase of these photons.

The group's requirements for reliable generation of single photons on demand led them to the use of a single rubidium atom trapped in an optical micro resonator that, when repeatedly excited by finely tuned laser pulses, emitted single photons, one after another. Two such photons are then engineered to simultaneously impinge on the two 'input ports' of a beam splitter producing the standard quantum interference. In the Rempe experiment, after the first photon is detected, the user may introduce a particular phase shift that automatically ends up determining the path of the second photon, even if they initially impinge simultaneously. The group even discovered that it is possible to guide the photons to two different output ports, something normally only achievable by fermions (photons are bosons).

The results not only demonstrate the ability to control phase, but also that phase is as inherent to the characterization of a single photon as amplitude, frequency, and polarization. The work appeared in a recent issue of *Nature Photonics*.

Scaling up: sometimes bigger *is* better

A team at NIST-Boulder led by Dave Wineland has successfully carried out *multiple* computing operations on a group of qubits. The NIST group's qubits are beryllium ions held in an ion trap. While individual operations on qubits are largely ubiquitous (even some primarily undergraduate institutions (PUIs) have systems that perform single operations), this is the first time that certain critical steps have been strung together. These steps include state preparation (getting qubits into specific states), performing a logical operation on qubits, transferring that information within the given hardware (a transport operation), and reading out any results. In addition it is important to be able to perform a string of operations, something the group was able to demonstrate.

Wineland's group successfully performed five quantum logic operations and ten transport operations in series without degradation of the states of the ions that were acting as qubits. This last part, of course, is one of the trickier aspects of practical quantum manipulation as most anyone involved in quantum information knows. In the NIST case the problem is due to the fact that the ions heat up when an operation is performed on them since the operations are performed by lasers. So, for instance, in order to, say, perform a bit flip operation on a given ion, lasers would impinge on the ion, flipping its logical value, often encoded in the ion's spin. The problem is obvious in that the lasers heat up the ion making it more difficult to hold its state. Thus the group added cold magnesium ions to chill the beryllium ions. The magnesium ions are used solely as a heat sink and not for computation.

Another persistent problem the group was able to overcome was the interference of outside magnetic fields that also led to state degradation. However, it turns out there are specific energy levels in which the ions remain temporarily unaffected by such fields. By putting the ions in these energy levels the group was able to maintain qubit states for up to fifteen seconds giving them plenty of time to perform a string of millisecond-long operations. The work was reported in a recent issue of *Science*.

Probing the quantum-classical divide

Klemens Hammerer of the Universität Innsbruck, in conjunction with colleagues at Ludwig-Maximilians-Universität München, NIST-Boulder, and Caltech has suggested an experiment to see just how macroscopic a quantum mechanical effect can get. Hammerer's colleagues and co-authors who are experimentalists (Hammerer is a theorist) are attempting to carry out the experiment described.

Usually scaling up a quantum effect involves either entanglement or the coupling of something quantum to something macroscopic. One problem with the former is that recent work by M. Hossein Partovi (Cal State-Sacramento) has demonstrated the possibility of macroscopic entanglement. The problem with the latter is that there is such an enormous difference in mass between the quantum object and the macroscopic object.

Hammerer and his colleagues have taken a slightly different approach. They have suggested the possibility of using an optical trap containing a single atom that sits next to a thin membrane of crystal with a high refractive index. The membrane would act as the macroscopic object in the setup. Any change in the atom's quantum state would theoretically shift the membrane which would change the resonance of the cavity thus forcing the membrane and the atom to move even more, i.e. the system should display resonance. Any amplified movement would then be

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observed either by shining a separate laser on the atom or by monitoring the amount of light leaving the cavity revealing the membrane's state. Hammerer's colleagues have reported some initial progress in realizing the proposed experiment.

Quantum errors *do* compute

It turns out that quantum computers may be more fault tolerant and thus stable than previously thought. Tom Stace and Andrew Doherty of the University of Queensland and Sean Barrett of Macquarie University have concluded that certain quantum computers, at least theoretically, can tolerate a complete loss of up to half of the machine's physical qubits or can suffer an error in up to ten percent of the internal states of the its qubits. In particular, the group's analysis was carried out on surface codes developed by Alexei Kitaev at CalTech and included a local and uncorrelated error model.

Their work is of particular importance to the future design and manufacture of realistic quantum computers (i.e. quantum engineering) since it dictates just how precise engineers need to be in actually creating these devices. The work is slated to appear in an upcoming issue of *Physical Review Letters*.

Theorists gather; no one injured

A relatively new society, dedicated to theoretical and computational physicists at primarily undergraduate institutions (PUIs), held its first workshop recently at Amherst College in central Massachusetts. The Anacapa Society grew out of discussions among several KITP Scholars at the Kavli Institute for Theoretical Physics at the University of California, Santa Barbara. The society's mission is to promotes "research in all areas of theoretical and computational physics at primarily undergraduate institutions. The Society facilitates professional contacts and collaboration, and supports the distinctive role theorists at undergraduate institutions can play in physics, the intellectual community, and the broader world."

While not strictly devoted to quantum information or quantum foundations, roughly one-third of workshop participants have, in some way, worked in these or related areas. Participants included Bill Wootters (Williams), Lea Dos Santos (Yeshiva), Elizabeth Behrman (Wichita State), Peter Love (Haverford), Ian Durham (Saint Anselm), Don Spector (Hobart & William Smith), and the effervescent Herb Bernstein (Hampshire), among others.

Despite the sweltering heat, the workshop was a definite success, particularly considering no one got seriously lost and no one blew anything up (a local experimentalist was on hand to make sure participants didn't randomly press any buttons). Further information on the society may be found at its website, http://anacapasociety.org/.

-ITD

Center for Quantum Information and Control (CQuIC)

The Center for Quantum Information and Control (CQuIC) is a new research center, established under the auspices of a grant from the National Science Foundation's Physics at the Information Frontier (PIF) program. The PIs on the NSF grant are Carlton Caves and Ivan Deutsch of the University of New Mexico (UNM) and Poul Jessen of the Univesity of Arizona (UA). CQuIC is based at the UNM and has research nodes at UNM and at the College of Optical Sciences at UA. The Center's Director is Carlton Caves.

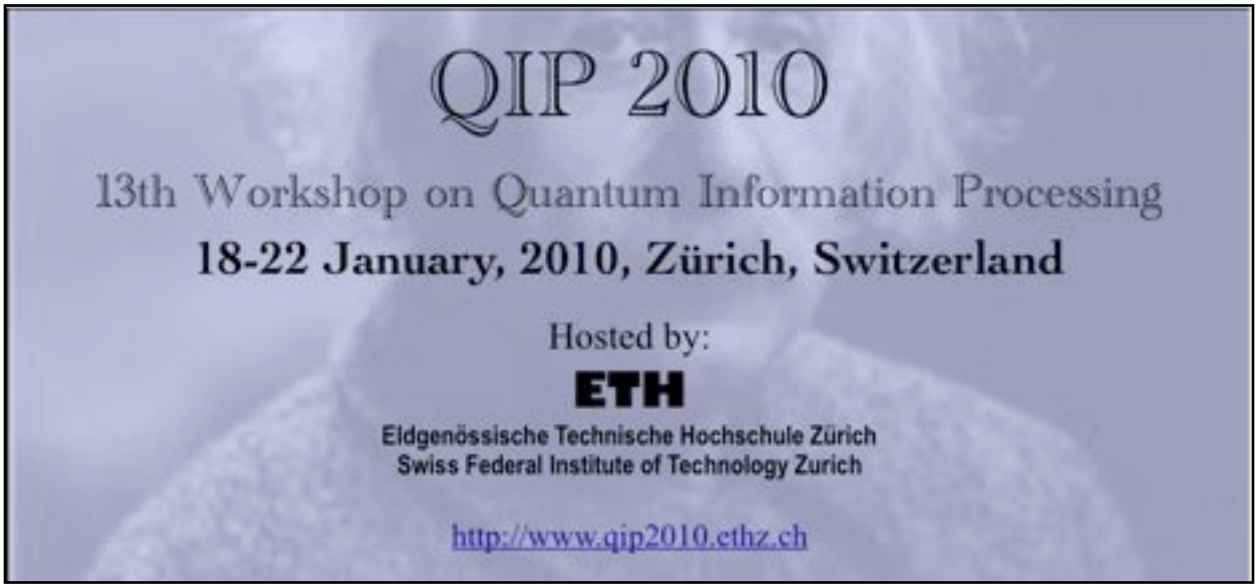
Research at CQuIC is focused on quantum information, quantum control, quantum metrology, and quantum optics. Theoretical research at UNM encompasses topics in all these areas. The experimental program at UA seeks to implement ideas from quantum information and quantum control in laser-cooled neutral-atom systems.

CQuIC has funds to support undergraduate and graduate students and postdoctoral fellows; to bring short- and long-term visitors to UNM and UA; and to support the activities of the Southwest Quantum Information and Technology (SQuInT) Network.

CQuIC is currently seeking to hire at least three postdoctoral fellows over the next year. CQuIC postdocs are expected to take an active interest in both theoretical and experimental projects at the Center.

A successful postdoc applicant must have a PhD in physics, optical sciences, or a related discipline. *Applicants should submit applications to cquic@unm.edu; the applicant should state whether he/she is applying for a theoretical postdoc at UNM or an experimental postdoc at UA.* Applications should include a curriculum vitae and a statement of research accomplishments and plans, and the applicant should arrange to have three letters of recommendation submitted to the same e-mail address.

Applications will be processed as they are received. For full consideration in the first round of hiring, a complete application should be received by October 31, 2009. Applications will continue to be reviewed till all positions are filled.



Dear Colleagues,

This is the first announcement of the Tenth International Conference on Quantum Communication, Measurement and Computing (QCMC), which will be held at the University of Queensland, Brisbane, Australia, on July 19 to 23, 2010.

The scope of the conference will be similar to that of previous meetings in the series and include the following topics:

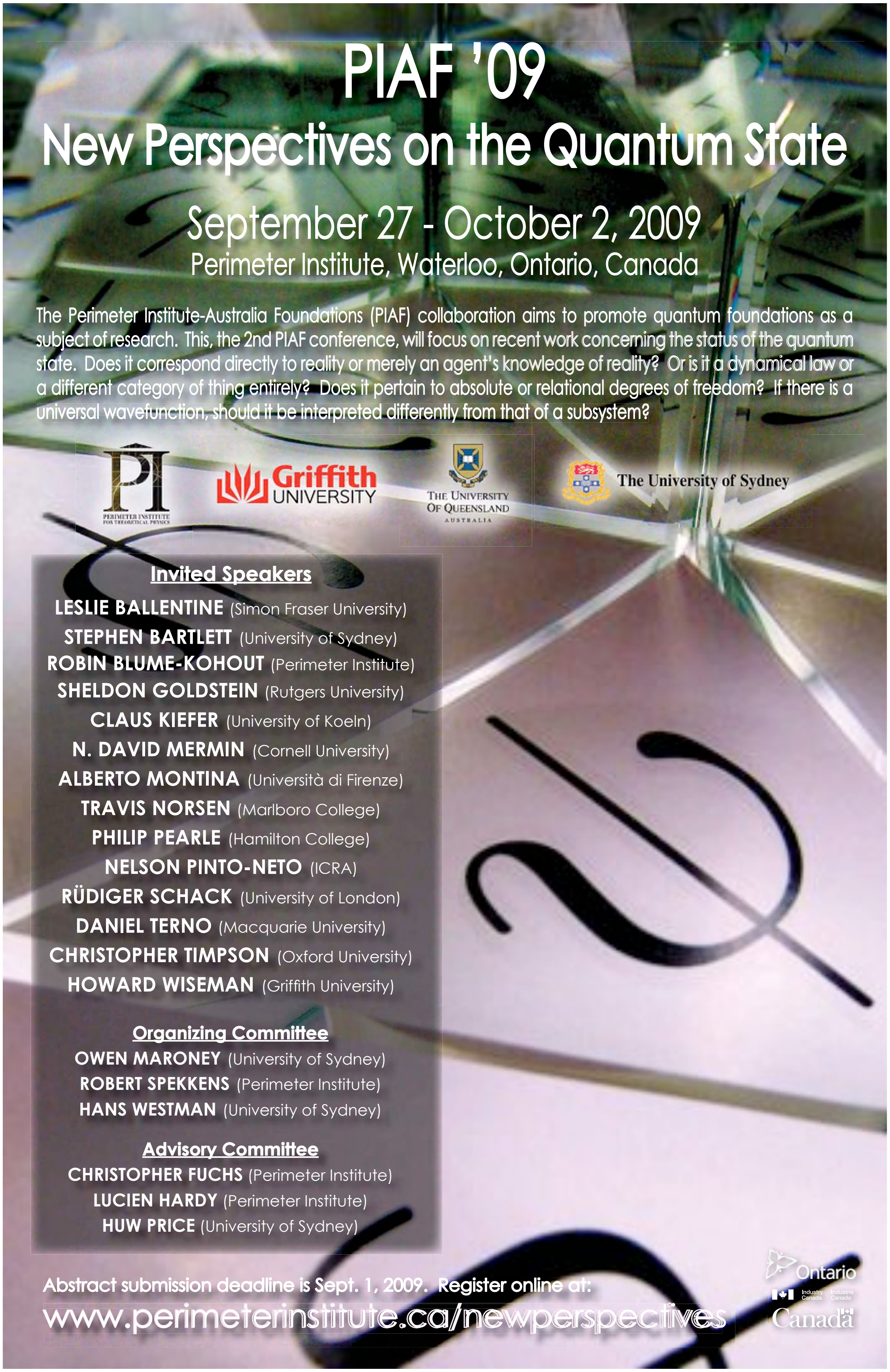
- Quantum Cryptography and Quantum Communications
- Quantum Measurement and Quantum Metrology
- Quantum Computing and Quantum Information Theory
- Implementations of Quantum Information Processing
- Quantum Control

The abstract submission deadline for contributed papers is March 31, 2010, and the early registration deadline is May 31, 2010. Further details about the meeting can be found in the attached flyer and on the website http://qcmc2010.org

We look forward to seeing you in Brisbane in July 2010.

On behalf of the organizing committees,

Tim Ralph,
Ping Koy Lam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The Perimeter Institute-Australia Foundations (PIAF) collaboration aims to promote quantum foundations as a subject of research. This, the 2nd PIAF conference, will focus on recent work concerning the status of the quantum state. Does it correspond directly to reality or merely an agent's knowledge of reality? Or is it a dynamical law or a different category of thing entirely? Does it pertain to absolute or relational degrees of freedom? If there is a universal wavefunction, should it be interpreted differently from that of a subsystem?
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