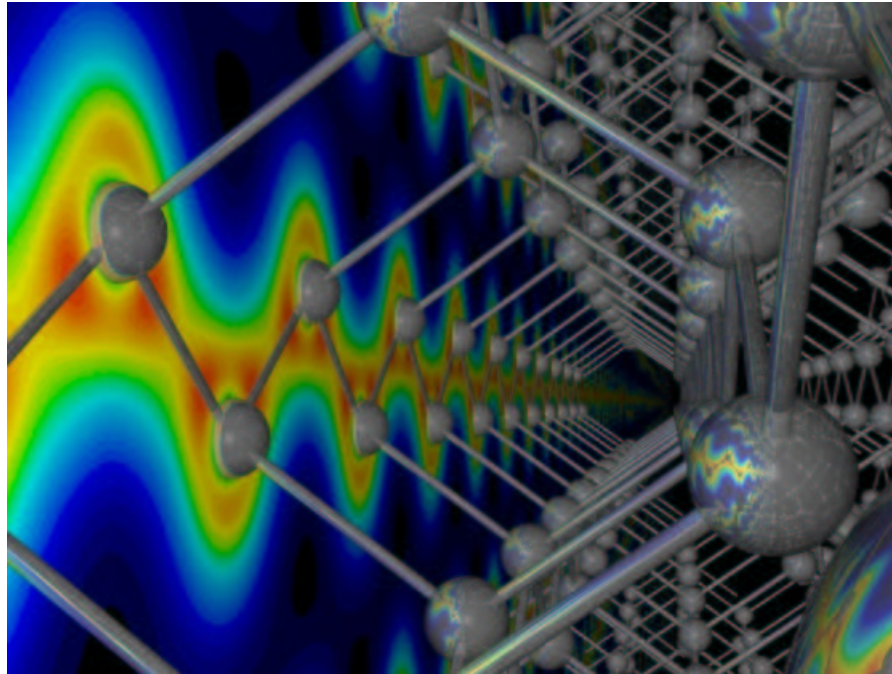


Experiments abroad

Introducing QMC to Japan and Australia, and vice versa



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Theory of Condensed Matter Group
Cavendish Laboratory
University of Cambridge

My trip



Questions and Plans

How is CASINO used around the world, and how can we make it better? Is it easy to understand and use? What do people find difficult about it? How can we get more people using it?

Japan

- Make contacts within the group where Ryo Maezono works and use his supercomputer access to finish the QMC NiO project.



- Check Ryo's recent work and encourage future directions.
- Learn something about Japanese culture..

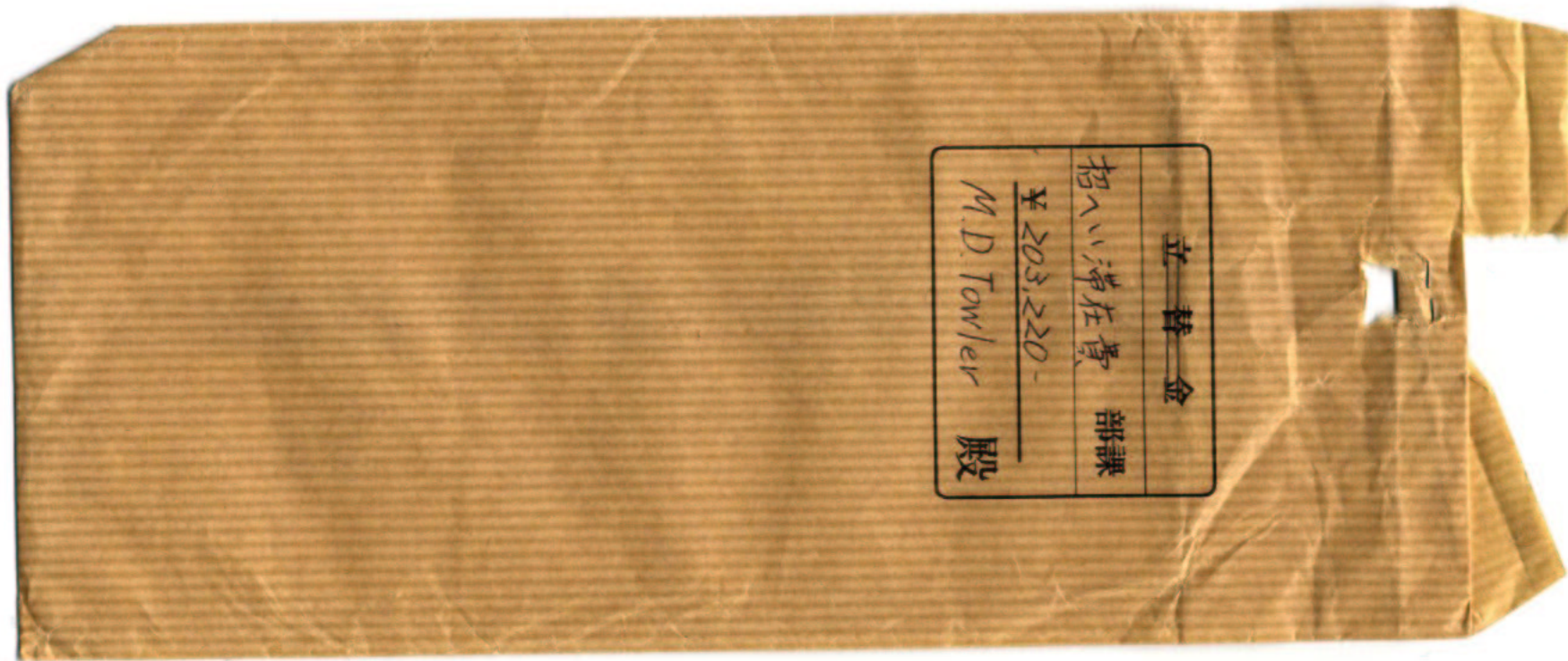
Australia

- Dr. Towler's quantum Monte Carlo workshop.
- Observe new group (15+ people) and their reaction to CASINO.
- Start collaborations and encourage people to work on applications of CASINO (not enough people do this currently!).

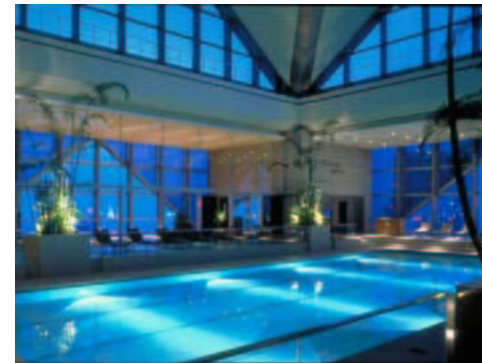
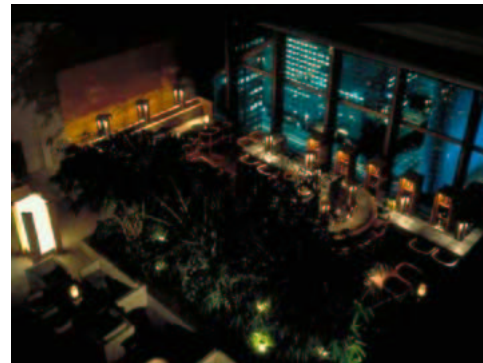
Tsukuba



Tsukuba



The Tokyo Park Hyatt



Haiku



*Northerner,
returning to Oz,
rests atop a skyscraper.*

*Skyscraper window,
up here a pretty good view
of the next building.*

*Tokyo dawn,
Mount Fuji refracted
through my bedroom window.*

Melbourne, Australia



RMIT University



Computational physics group



Ian Snook



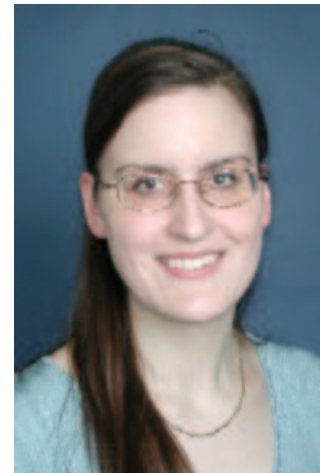
Irene Yarovsky



Salvy Russo



Peter Davies



Michelle Spencer

What happened in Oz

Workshop and Seminar Announcement



Dr. Mike Towler from the Cavendish Laboratory, Cambridge University, UK will be visiting the Atomic Simulation of Matter Group of the Applied Physics Department between 31 March and 16 April 2003. The visit is supported by an RMIT Foundation International Fellowship.

Dr. Towler is a Royal Society research fellow in the Condensed Matter Theory Group and previously held a Lloyd's fellowship in the same laboratory. He also holds a College Lecturer position at Emmanuel College, Cambridge.

Dr. Towler's research interests are

- Electronic structure theory and its use in the first principles simulation of matter
- Development of the theory of the quantum Monte Carlo method and its implementation
- The relationship between quantum chemistry and theoretical physics
- The physics of strongly correlated systems
- Fundamental problems in density functional theory
- The interpretation of quantum mechanics

Dr. Towler's program includes

- A **workshop** on the Quantum Monte Carlo Method, consisting of three one-hour lectures. These lectures will take place on 2-4 April and will start at 10.30 am in room 14.6.27 (Building 14, Applied Physics Department, RMIT City Campus). They will be followed by hands-on learning sessions using the QMC CASINO code under his guidance the following week (7-11 April).
- A **seminar** "The Quantum Monte Carlo (QMC) Method as Applied to Electronic Structure Calculation", on 10 April 2003 at 12.30 pm in the Applied Physics conference room, 14.4.37.

For more information, contact Professor Ian Snook, Department of Applied Physics, RMIT University, phone (03) 9925 2143, or e-mail ian.snook@rmit.edu.au.

- Test calculations get started on the helium dimer, aluminium slabs, van der Waal's interactions in graphite, and um.. phenylphosphonic acid dimer (33 atom cluster with P/O/C/H).

Jenny and Alexi



Wombat



Conclusions

- CASINO is really hard to use. People never read the manual. People are not prepared to look inside scripts, programs or Makefiles if something goes wrong, and I shouldn't assume they are.
- Don't document your life to the extent that you never do anything worth documenting.
- I don't like pseudopotentials.
- It really is nice to be able to go outside your laboratory and be confronted by an huge choice of lovely coffee houses, bars, and places to eat, rather than being placed at the mercy of miserable canteen people with a monopoly who don't care what other people eat, so long as they make money.
- Animal facts : wombats should be accidentally allowed to escape from a zoo in England, so that they can establish a colony like the wallabies in Derbyshire. Kangaroo scrotums are really handy for keeping money in.
- Travel reminds you of a host of untried possibilities lurking beneath the surface of an apparently undesirable, apparently eternal existence. Remember to travel occasionally.