

Proposal for Tutorial on use of the $\mathcal{O}(N)$ *ab initio* code CONQUEST

Location: CECAM, Lyon, France

Time: Two days between June and September 2007, preferably September 7th and 8th

Organisers:

Dr David Bowler (david.bowler@ucl.ac.uk)

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1 Abstract

Linear scaling electronic structure techniques are becoming mature, as shown by recent CECAM/PsiK workshops (and a proposed workshop in 2007). The CONQUEST code is ready for release, and a tutorial in the use and application of the code would both broaden the user base and enable widespread use of the code. This tutorial will be aimed at researchers who are familiar with standard electronic structure codes.

2 Scientific Summary

The use of *ab initio* electronic structure calculations has become ubiquitous in physics, chemistry, materials science and biology over the last twenty years. These techniques are immensely important scientifically, and have been supported strongly by the ESF Psi-K network and, more recently, by CECAM workshops. However, the standard techniques all require a computer effort which scales with the cube of the number of atoms in the system, placing a limit of around 1,000 atoms on the size of system which can be considered. Despite this, there are good scientific reasons which show that a computer effort which scales *linearly* with system size can be achieved. A little over ten years ago the first proposals for realistic linear scaling methods were made, and codes which put these proposals into practice have been in development ever since. The CONQUEST code has been one of the leading codes, and is now at the stage of beta release (with full public release under the Gnu GPL anticipated by late 2006 or early 2007). A tutorial on the use of the code is both timely and important. There are other proposals related to this one: first, a workshop on $\mathcal{O}(N)$ techniques (organised by Skylaris, Haynes, Fattebert, Bowler and Gillan); second, a tutorial for the SIESTA code (organised by Garcia and Junquera). We will aim to link loosely with the first. After discussion with the organisers of the second, we have concluded that the target audiences are too different, and we require separate tutorials.

3 Meeting Programme

- Day 1
 - Basic introduction to linear scaling methods
 - Overview of Conquest formalism: support functions and density matrices
 - Basics of input: choice of basis, pseudopotentials, solver, simple options

- Practical calculations
- Day 2
 - Details of basis sets: advantages & disadvantages of PAOs; blips
 - Details of solvers: $O(N)$ and ranges; use of the diagonaliser and scalapack
 - Self-consistency and Harris-Foulkes techniques
 - Practical calculations
- Other topics to be covered briefly
 - Organisation of code
 - Contributing to the project, terms of use
 - Roadmap for Conquest development

The facilities at CECAM will be used to provide the appropriate environment for a tutorial. As the meeting is designed to be a tutorial, we cannot provide a list of participants at this stage. The three organisers will give the talks and run the practical sessions.

4 Budget

We assume thirty participants, and normal CECAM rules (so organisers and non-EU participants can receive a contribution to travel).

- Travel for organisers: 3×250 euros
- Assume five non-EU attendees; travel: 5×250 euros
- Subsistence for organisers and participants: $2 \times 80 \times 30$ euros
- Total of approximately 6800 euros: we will request 3500 from PsiK, 3500 from CECAM

5 CVs of Organisers

5.1 David Robert BOWLER

Date of birth : 12th August 1970

Place of birth : Oxford, England

Nationality : British

Present position : Reader in Physics, University College London and Royal Society University Research Fellow

Address : Department of Physics and Astronomy, University College London, WC1E 6BT, UK

Education :

1. B.A. in Natural Science, Cambridge University, 1991
2. D. Phil., Materials Science, Oxford University, 1997

Employment :

1. April 1997–July 1998 Department of Physics, Keele University.
2. July 1998–present: Department of Physics of Astronomy, UCL.
3. September 2004–June 2005: Senior Research Fellow, International Centre for Young Scientists, National Institute for Materials Science, Tsukuba, Japan

Research activity : Within the field of theoretical condensed matter, I concentrate on electronic structure calculations, both developing new techniques and modelling systems. Specific interests:

1. Development of linear-scaling *ab initio* techniques, particularly the CONQUEST code
2. Development of techniques for modelling correlated electron-ion dynamics (e.g. current-induced heating)
3. Modelling of growth of semiconductors using *ab initio* and semi-empirical techniques
4. Modelling of nanowire systems on semiconductor surfaces using *ab initio* and semi-empirical techniques

Five selected publications :

1. D. R. Bowler, R. Choudhury, M. J. Gillan and T. Miyazaki, 'Recent progress with large-scale *ab initio* calculations: the CONQUEST code', *phys. stat. sol.*, 243, 989 - 1000 (2006).
2. D.R.Bowler, A.P.Horsfield, C.Sanchez and T.N.Todorov, *J. Phys.:Condens. Matter* 17, 3985 (2005).
3. T. Miyazaki, D. R. Bowler, R. Choudhury and M. J. Gillan, *J. Chem. Phys.*, 121, 6186 (2004).
4. A.P.Horsfield, D.R.Bowler and A.J.Fisher, *Journal of Physics: Condensed Matter* 16 (7), L65 (2004).
5. D. R. Bowler, T. Miyazaki and M. J. Gillan, *J. Phys. Condens. Matter*, 14, 2781 (2002).

5.2 Michael John GILLAN

Date of birth : 3rd January 1944

Place of birth : Birmingham, England

Nationality : British

Present position : Professor of Physics, University College London

Address : Department of Physics and Astronomy, University College London, WC1E 6BT, UK

Education :

1. B.A. 1st class, Physics, Oxford University, 1965
2. D. Phil., theoretical physics, Oxford University, 1968

Membership of professional societies : Fellow of Institute of Physics

Employment :

1. Sept 1968 Aug.–1970: post-doc with Dr. J. Woods Halley, Dept. of Physics and Astronomy, Univ. of Minnesota, Minneapolis, MN, USA
2. Sept. 1970–April 1991: Statistical Physics Group, Theoretical Physics Division, AERE Harwell. (May 1988 April 1991 part-time.)
3. Sept 1985–Dec. 1985: Section de Recherches de Metallurgie Physique, Centre d'Études Nucleaires de Saclay, Gif-sur-Yvette, France
4. May 1988–June 1998: Physics Department, Keele University
5. July 1998–present: Physics and Astronomy Department, University College London.

Research activity : General field is theory and computational modelling of condensed matter. More specific interests over past 10 years include:

1. Development and application of linear-scaling methods for the ab initio modelling of large systems containing many thousands of atoms. The CONQUEST code.
2. Quantum Monte Carlo techniques for the energetics of condensed matter, with particular attention to minerals.
3. Ab initio thermodynamics, with particular attention to the calculation of free energies and chemical potentials.
4. Ab initio modelling of the water-mineral interface.
5. Ab initio modelling of geological materials, with particular attention to the materials of the Earth's core. Use of ab initio methods in combination with seismic data to place constraints on the temperature and chemical composition of the Earth's core.

Awards : UK Institute of Physics Dirac medal and prize 2006. Citation reads: For his contributions to the development of atomic-scale computer simulations, which have greatly extended their power and effectiveness over an immense range of applications.

Five selected publications :

1. D. R. Bowler, R. Choudhury, M. J. Gillan and T. Miyazaki, 'Recent progress with large-scale ab initio calculations: the CONQUEST code', *phys. stat. sol.*, 243, 989 - 1000 (2006). DOI 10.1002.
2. D. Alfe and M. J. Gillan, 'An efficient localised basis set for quantum Monte Carlo calculations on condensed matter', *Phys. Rev. B*, 70, 161101(R) (2004).
3. T. Miyazaki, D. R. Bowler, R. Choudhury and M. J. Gillan, 'Atomic force algorithms in DFT electronic structure techniques based on local orbitals', *J. Chem. Phys.*, 121, 6186 (2004).
4. D. Alfe and M. J. Gillan, 'Linear-scaling quantum Monte Carlo with non-orthogonal localized orbitals', *J. Phys.: Condens. Matter*, 16, L305 (2004).
5. D. R. Bowler, T. Miyazaki and M. J. Gillan, 'Recent progress in linear scaling ab initio electronic structure techniques', *J. Phys. Condens. Matter*, 14, 2781 (2002).

5.3 Tsuyoshi MIYAZAKI

Date of birth : 10th June 1966

Place of birth : Nagoya, Japan

Nationality : Japanese

Present position : Senior Researcher, National Institute for Materials Science (Japan)

Address : Computational Materials Science Center, National Institute for Materials Science 1-2-1 Sengen Tsukuba, Ibaraki 305-0047, Japan

Education :

1. B.Sc., Physics, Science and Engineering, Waseda University, 1990
2. Master Sc., Physics, Science, University of Tokyo, 1992
3. Ph. D., Physics, Science, University of Tokyo, 1995

Membership of professional societies : Member of Japanese Physics Society

Employment :

1. Feb. 1995–Dec. 1995: Agency of Industrial Science and Technology (Joint Research Center for Atom Technology)
2. Jan. 1996–Mar. 1996: JSPS Fellow (Physics, University of Tokyo)
3. Apr. 1996–Mar. 2001: Researcher, National Institute for Metals
4. Oct. 1999–Sep. 2000: Honorary Research Fellow, Physics and Astronomy Department, University College London
5. Apr. 2001–Mar. 2003: Researcher, National Institute for Materials Science.
6. Apr. 2003–present : Senior Researcher, National Institute for Materials Science.

Research activity : Electronic structure calculations based on the density functional theory.

Publications :

1. D. R. Bowler, T. Miyazaki and M. J. Gillan, Parallel Sparse Matrix Multiplication for Linear Scaling Electronic Structure Calculations, *Comp. Phys. Commun.* 137, 255(2001)
2. D. R. Bowler, T. Miyazaki and M. J. Gillan, Recent Progress in Linear Scaling Ab Initio Electronic Structure Techniques, *J. Phys.: Condens. Matter*, vol. 14, p2781-2798 (2002)
3. T. Miyazaki, D. R. Bowler, R. Choudhury, M. J. Gillan, Atomic force algorithms in density functional theory electronic-structure techniques based on local orbitals, *J. Chem. Phys.*, Vol.121, p6186-6194 (2004)
4. T. Miyazaki, R. Choudhury, D.R. Bowler and M.J. Gillan, Large-scale ab-initio calculations, *Proc. of 3rd Int. Conf. on Comput. Model. and Simul. of Materials*, ed. P. Vincenzini. (Techna Group, Faenza, Italy, 2005)
5. D. R. Bowler, R. Choudhury, M. J. Gillan, T. Miyazaki, Recent progress with large-scale ab initio calculations: the CONQUEST code, *physica status solidi (b)*, 243, p.989-1000 (2006).