Proposal for joint Psi-k – CECAM – CCP9 workshop

Title: "**Linear-scaling ab initio calculations: applications and future directions**"

Location: CECAM, Lyon, France.

Time: Between June and early September 2006. Preferably from Monday 3 September 2007 till Thursday 6 September 2007 (4 days).

Organisers

Dr Chris-Kriton Skylaris (cks@soton.ac.uk)
School of Chemistry, University of Southampton, Highfield, Southampton SO17 1BJ, UK
Tel. ++44 2380 599381

Dr Peter Haynes (pdh1001@cam.ac.uk)
Theory of Condensed Matter group, Cavendish Laboratory, J J Thomson Avenue, Cambridge CB3 0HE, UK
Tel. ++44 1223 337005

Dr Jean-Luc Fattebert (fattebert1@llnl.gov)
Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, Livermore, CA, USA
Tel. ++1 925 4245296

Dr David Bowler (david.bowler@ucl.ac.uk)
Department of Physics & Astronomy, University College London, Gower St, London, WC1E 6BT, UK
Tel:++44 20 76797229

Professor Mike Gillan (m.gillan@ucl.ac.uk)
Department of Physics & Astronomy, University College London, Gower St, London, WC1E 6BT, UK
Tel: ++44 20 76797049

Abstract

The ongoing development of linear-scaling methods for ground-state density functional theory (DFT) calculations on systems with a gap (e.g. molecules, semiconductors and insulators) is now approaching a state of maturity. The particular focus of this workshop is therefore to look forward at what might be achieved in the next five years, both in terms of applications with these methods and in terms of extending linear-scaling to methods for metals, excited states and theories beyond DFT.

Scientific summary

This workshop will be the main activity of the Psi-k Working Group on linear scaling and local orbitals for 2007 and is intended to be a continuation of previous highly successful workshops in the area of linear-scaling (O(N)) ab initio methods.

While physically motivated, ab initio methods where the computational cost increases only linearly with the number of atoms have proved particularly hard to develop as they require the introduction of highly non-trivial localisation constraints. Especially in terms of reaching the high accuracy of conventional cubic-scaling density functional theory (DFT) calculations, progress has been slower than originally predicted. Nevertheless, many major obstacles have been overcome and a number of O(N) methods for ground-state DFT calculations (e.g. SIESTA, CONQUEST, ONETEP, etc.) are now available and have reached a state of maturity that allows their use in applications on "real" materials. These methods are now beginning to make an impact in areas such as nanotechnology and biochemistry where traditionally DFT calculations were not applicable due to the large number (thousands) of atoms involved. We believe that a critical review of these applications will be timely as it will provide an understanding of the capabilities of current linear-scaling methods though addressing the following questions: What are the major applications so far of O(N) DFT (e.g. what types of nanostructures, biomolecules, surfaces, etc.)? How many atoms are typically involved in these applications? What level of accuracy is achieved (e.g. has the plane-wave accuracy of traditional cubic-scaling methods been achieved in the applications reported so far)? What are the future applications going to be, both in terms of numbers of atoms and in terms of kinds of materials studied? What is the overhead associated with O(N) algorithms? For what system size do O(N) algorithms become advantageous over traditional approaches and how does this size varies with the atom-density and 3D structure of the material we want to study?

The available methods contain highly sophisticated algorithms that allow for the practical utilisation of the "Nearsightedness" principle of Walter Kohn to achieve O(N) cost. We can roughly distinguish two stages in the calculation which are common in all O(N) approaches: (1) the construction of the Hamiltonian and (2) the solution of the Hamiltonian. The construction of the Hamiltonian (which involves details such as techniques for maintaining localisation and the most suitable types of basis sets) has been investigated exhaustively in previous workshops and has led to a good understanding in the community of the strengths and weaknesses of the various approaches. On the other hand, the solution of the Hamiltonian which requires techniques that avoid the cubic-scaling step of diagonalisation has not been covered in any detail in previous workshops. A number of such "linear-scaling functional" approaches have been reported in the literature (e.g. the Kim-Mauri-Galli-Car, Palser-Manolopoulos, Li-Nunes-Vanderbilt and Haynes-Payne functionals, etc.). Existing methods often use combinations of these approaches which have been evolved and fine-tuned through years of extensive experimentation. At present there is no general consensus as to their relative advantages and disadvantages in practical applications, their "optimum" implementation (including sparse storage methods for matrices and performance on parallel computers) or their combinations - that have been adopted in each code in a somewhat evolutionary fashion. As these important details are often not reported in papers, we feel that there is a strong need to cover this crucial topic in this workshop in order to address questions such as: What are the practical details of implementation of the various linear-scaling functionals and why some currently available methods have chosen to use combinations of more than one functional? Does the implementation of these functionals within the framework of direct energy minimisation offer any advantages as compared to a density mixing framework? What are their relevant strengths and weaknesses in terms of robustness, parallel performance, speed of convergence, accuracy, general applicability? Is there room for development of significantly better linear-scaling functionals?

Taking into account the above-mentioned current status of O(N) ground state DFT we feel that now the time is ripe to look into the future: What has been done and what can be done in terms of accurate ab initio O(N) methods for metals and methods beyond ground-state DFT calculations (e.g. excited states or correlated wavefunction methods)? Clearly we have a long way to go here as methods for these kinds of applications are considered "non-standard" even without any modifications for O(N) cost. We would like to examine the current state-of-the-art in such methods and investigate ways to reformulate them into O(N) frameworks. In the case of the methods for metals we hope to focus around the following questions: What are currently the most well-established DFT methods for metals? At what stage of development are the current efforts for linear-scaling (or at least reduced-scaling) approaches for metals? What developments are needed to develop robust and accurate O(N) methods for metals? How much of the available O(N) technology for insulators can we re-use to develop such methods, and are particular approaches more suitable than others? Will we be obliged to always use specific constraints (e.g. finite electronic temperature) and if so how are these going to affect the accuracy and applicability of our calculations?

Finally, in the area of O(N) methods beyond ground-state DFT calculations we would like to focus around the following questions: What is the current state of progress in the development of O(N) methods beyond ground state DFT (e.g. quantum Monte Carlo, wavefunction correlation methods such as many-body perturbation theory or variants of configuration interaction)? Do these methods achieve the same high accuracy as their traditional approaches – or even traditional DFT – and do they offer the same advantages (e.g. reliable estimation of dispersion interactions)? How far are we from having these methods in a robust form suitable for applications? Are they ever likely to overtake O(N) DFT in terms of the system sizes that can be studied?

Strong emphasis during the workshop will be given to discussion in order to promote the exchange of ideas between different communities (Physics, Chemistry, Materials Science, Biochemistry) which are all interested in large-scale applications with ab initio accuracy but are approaching them from different perspectives. We are also hoping that it will stimulate significant new methodological developments by bringing together the developers of metal and wavefunction-based methods with the developers of O(N) DFT methods.

Meeting Programme

This workshop is intended to be a forum for discussion and exchange of points of view, in order to stimulate knowledge transfer that will play a pivotal role in tackling important scientific issues that our (diverse) communities will have to face in the next few years. All these issues are shared by the people who will attend, but from quite different perspectives. Therefore, we want the format of the workshop to consist of short talks (about 40 minutes), focusing on clear presentation of results and techniques. From these presentations ideas for addressing the questions raised in the scientific summary will emerge, during the ample time for discussion which we will devote both after each talk and at special discussion sessions. These will be introduced and led by one of the organisers.

We plan to structure the workshop around 4 sessions, according to the 4 topics in the scientific summary above. Although a detailed schedule of the talks will not be possible until the list of confirmed people is complete, the tentative structure of the talks will be as follows:

1) Applications to nanostructures and biomolecules

Emilio Artacho - (bio applications with SIESTA)
Tsuyoshi Miyazaki - (Ge huts on Si with Conquest)
Arash Mostofi - (bio and nano applications with ONETEP)
Joost VandeVondele - (bio applications with QuickSTEP)
Takeo Fujiwara - (nano applications)
Jerzy Bernholc - (nano transport applications)

2) Energy minimisation functionals and algorithms

Jose Soler - (KMGC & Harris functionals in SIESTA)
Mark Tuckerman - (DVR method)
Luis Seijo - (MOSAICO method)
Taisuke Ozaki - (O(N) functionals)

Weitao Yang - (O(N) functionals / Divide and Conquer approach)
David Bowler - (Palser-Manolopoulos purification scheme in Conquest)
Peter Haynes/Chris-Kriton Skylaris - (Li-Nunes-Vanderbilt / penalty scheme in ONETEP)
Stefan Goedecker - (O(N) functionals implemented in the BigDFT ABINIT project)
Jean-Luc Fattebert - (Finite Differences and adaptive localization regions)

3) Progress in linear-scaling methods for metals

Emily Carter - (orbital-free DFT for metals)
Florian Krajewski - (stochastic O(N) for metals)
Marcella Iannuzzi - (reciprocal space localisation for metals)
John Pask - (DFT-based methods for metals)
Nicola Marzari - (ensemble DFT method for metals)
Emil Prodan - (nearsightedness and DFT theories for metals)
Andrew Williamson - (O(N) QMC for metals)

4) Linear-scaling methods beyond DFT and ground state properties

Martin Head-Gordon – (wavefunction-based correlation models with O(N) cost)
Fred Manby - (O(N) MP2 approaches)
Pablo Ordejon - (transport properties with the TRANSIESTA code)
Matt Challacombe - (O(N) linear response in the MondoSCF code)
Dario Alfe - (O(N) QMC)
Aiichiro Nakano - (O(N) methods for large MD and applications)
Eiji Tsuchida - (O(N) methods for large MD and applications)
GuanHua Chen - (O(N) TDDFT)
Ursula Roethlisberger - (TDDFT and dispersion from atom-centred potentials)

We expect that the contributions of the workshop will be of outstanding quality. There will certainly be strong interest to collect these authoritative accounts by world-leading researchers in a form suitable for dissemination well beyond the participants of the workshop. We will therefore produce a compilation of articles based on the workshop talks as a special issue of an international peer-reviewed journal. The Journal of Physics: Condensed Matter has already agreed to publish such an issue, as confirmed by Dr David Bowler who is a member of the editorial board of the Journal.

Budget

As discussed above, our proposal contains 33 participants (see also list of participants below), of whom a fairly large proportion (17 speakers) are from overseas (12 from the US, 4 from Japan and 1 from China), and whose participation is essential to achieve the goals of the workshop. Of the 33, already 27 have replied to an informal invitation and have expressed strong support and have agreed to participate if the workshop is funded. Even though it is inevitable that a small number of the proposed participants will not be able to attend the workshop in the end, we are certain (also from the experience of previous workshops in this area) that there will be strong interest on the topics we will cover and we expect that several new participants beneficial to the workshop goals will be added to the list. We estimate that we will eventually have about 35 participants. The following budget is therefore for a four day workshop at CECAM with 35 participants.

Assuming that most participants will arrive on Sunday and depart on Friday morning, we would like to cover 5 days of subsistence at the CECAM rate of 80 EURO per day. We would also like to organise one working dinner with all participants, at the CECAM rate of 45

EURO per participant. For the travel expenses we would like to offer a contribution of 300 EURO per participant. Therefore:

Estimated cost per participant: 5(days) x 80(EURO per day) + 300(EURO for travel) + 45 (EURO for working dinner) = 745 EURO

Estimated total cost: 35(participants) x 745(EURO per participant) = 26075 EURO

We are therefore requesting:

9110 EURO from ESF(Psi-k)
12665 EURO from CECAM
4300 EURO from CCP9

26075 EURO in total

As CECAM is able to make a travel costs contribution of 300 EURO per overseas participant (but no travel costs contribution for Europeans), the requested CECAM funding will be used to cover the costs of the overseas participants [17(participants) x 745 (EURO per participant) = 12665 EURO]. Still, the travel costs of the overseas participants will be significantly higher than 300 EURO, so for the participants from the US we shall also seek further travel support from the NSF.

The cost of the UK participants is 5960 EURO [8(participants) x 745(EURO per participant)] of which 4300 EURO will be covered from the requested CCP9 funding and the remainder from the requested ESF(Psi-k) funding which will also cover the entire costs of the non-UK European participants.

Provisional list of proposed invited speakers/participants

Speakers with a "*" next to their name have already replied to an informal invitation (provided our workshop proposal is accepted) and have expressed strong support for our proposal and have agreed to participate. Speakers without a "*" have not yet replied.

Dario	Alfe	(UK)
*Emilio	Artacho	(UK)
*Jerzy	Bernholc	(USA)
*David	Bowler	(UK)
*Emily	Carter	(USA)
*Matt	Challacombe	(USA)
*GuanHua	Chen	(China)
*Jean-Luc	Fattebert	(USA)
*Takeo	Fujiwara	(Japan)
*Mike	Gillan	(UK)
*Stefan	Goedecker	(Switzerland)
*Peter	Haynes	(UK)
*Martin	Head-Gordon	(USA)
*Marcella	Iannuzzi	(Switzerland)
Florian	Krajewski	(Switzerland)
*Fred	Manby	(UK)
Nicola	Marzari	(USA)
*Tsuyoshi	Miyazaki	(Japan)
*Arash	Mostofi	(UK)

*Aiichiro	Nakano	(USA)
*Pablo	Ordejon	(Spain)
*Taisuke	Ozaki	(Japan)
*John	Pask	(USA)
*Emil	Prodan	(USA)
Ursula	Roethlisberger	(Switzerland)
*Luis	Seijo	(Spain)
*Chris-Kriton	Skylaris	(UK)
*Jose	Soler	(Spain)
*Eiji	Tsuchida	(Japan)
*Mark	Tuckerman	(USA)
Joost	VandeVondele	(Switzerland)
Andrew	Williamson	(USA)
*Weitao	Yang	(USA)

CVs of scientific organisers including list of five most relevant publications during the last five years

CHRIS-KRITON SKYLARIS

PERSONAL DETAILS

Date of birth: 17 June 1973
Nationality: Greek

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University of Southampton
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Southampton SO17 1BJ
UK
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++ 44 (0)7952 650563 (mobile)
E-mail: cks@soton.ac.uk
Homepage: http://www.chem.soton.ac.uk/skylaris.htm

EMPLOYMENT

Jun. 2006 – to date
School of Chemistry, University of Southampton
Lecturer in Structural and Materials Chemistry and Royal Society University Research Fellow.

Oct. 2004 – May 2006
Physical & Theoretical Chemistry Laboratory, University of Oxford
Royal Society University Research Fellow.

Mar. 2003 – Sep. 2004
Physics Department (Cavendish Laboratory), University of Cambridge
Postdoctoral research associate with Professor Mike C. Payne.

Jan. 2002 – Mar. 2003
Greek Army, Greece
Compulsory national service. Ordnance Corps.

Jan. 2000 – Dec. 2001
Physics Department (Cavendish Laboratory), University of Cambridge
Postdoctoral research associate with Professor Mike C. Payne.

Sept 1999 – Dec. 1999
CINECA supercomputing centre, Bologna, Italy
Visiting fellow funded by the EU ICARUS programme.

EDUCATION

Apr. 1996 – Aug.1999
Chemistry Department, University of Cambridge
Ph.D. in Quantum Chemistry. Supervisor: Professor N. C. Handy F.R.S. Thesis: “The computational modelling of heavy atom chemistry”

Sep. 1991 – Mar. 1996
Chemistry Department, University of Athens
B.Sc. in Chemistry. Overall mark 85% “άριστα” (=“distinction”, the highest mark).
EU ERASMUS scholarship for spending academic year 1993-1994 at the University of Liverpool. Degree research project supervisor: Professor B. T. Heaton F.R.S.C. Dissertation: “Rhodium (I) complexes of N-acetyl-3-butanoyl tetramic acid”.

Jun. 1991
Athens, Greece.
Graduated from Lyceum and succeeded in the national examinations for admission to the University of Athens for a B.Sc. Degree in Chemistry.

RESEARCH ACTIVITY

- Development of new linear-scaling methods for performing large scale first-principles quantum mechanical simulations. Author of the ONETEP linear-scaling plane-wave DFT code for parallel computers which is the current flagship project of the Accelrys Inc Nanotechnology consortium and is licensed for commercial distribution from October 2007. Founding member of the ONETEP Developers' Group (ODG).
- Modelling of biological systems using linear-scaling first-principles and classical techniques.
- Modelling of nanostructures using linear-scaling first-principles techniques.
- Development of efficient, highly-scalable, algorithms for parallel computers.

FIVE SELECTED RECENT PUBLICATIONS

1. "The Nonorthogonal Generalised Wannier Function pseudopotential plane-wave method". C.-K. Skylaris, A. A. Mostofi, P. D. Haynes, O. Dièguez and M. C. Payne. **Phys. Rev. B <u>66</u> (2002) 035119.**
2. "Introducing ONETEP: Linear-scaling density functional simulations on parallel computers". C.-K. Skylaris, P. D. Haynes, A. A. Mostofi and M. C. Payne. **J. Chem. Phys. <u>122</u> (2005) 084119**.
3. "Using ONETEP for accurate and efficient O(N) density functional calculations". C.-K. Skylaris, P. D. Haynes, A. A. Mostofi and M. C. Payne. **J. Phys.: Condens. Matter <u>17</u> (2005) 5757**.
4. "Implementation of linear-scaling plane wave density functional theory on parallel computers". C.-K. Skylaris, P. D. Haynes, A. A. Mostofi and M. C. Payne. **Phys. Stat. Solidi B**. **<u>243</u> (2006) 973.**
5. "Novel Structural Features of CDK Inhibition Revealed by an ab Initio Computational Method Combined with Dynamic Simulations". L. Heady, M. Fernandez-Serra, R. L. Mancera, S. Joyce, A. R. Venkitaraman, E. Artacho, C.-K. Skylaris, L. Colombi-Ciacchi, and M. C. Payne. **J. Med. Chem. <u>49</u> (2006) 5141.**

Peter David Haynes

Royal Society University Research Fellow		Telephone:	+44 (0)1223 3 37005
Cavendish Laboratory, University of Cambridge			+44 (0)1223 3 38855
J. J. Thomson Avenue		Fax:	+44 (0)1223 3 37356
Cambridge CB3 0HE		E-mail:	pdh1001@cam.ac.uk
Date of birth:	26 February 1974	Nationality:	British
Place of birth:	Abingdon, Oxon	Status:	Married

I am a computational physicist and holder of a Royal Society University Research Fellowship in the Theory of Condensed Matter group at the Cavendish Laboratory in the University of Cambridge. My research is focussed on the development of new linear-scaling methods for performing large-scale first-principles quantum-mechanical simulations, and their application to biological systems, materials science and nanotechnology. I have a broad range of teaching experience including lecturing and supervising both undergraduates and graduates.

Employment

Oct 2005–	**Cavendish Laboratory, University of Cambridge** Royal Society University Research Fellow in Physics.
Oct 2002– Sep 2005	**Sidney Sussex College, Cambridge** Ramon Jenkins Senior Research Fellow in Physics.
Oct 1999– Sep 2002	**Magdalene College, Cambridge** Thomas Nevile Research Fellow in Physics.
Oct 1998– Sep 1999	**Cavendish Laboratory, University of Cambridge** Post-doctoral Research Associate in the Theory of Condensed Matter.
Jul–Aug 1995	**Chemistry Department, University College London** Theoretical research into the dynamic response of gas sensors (under Prof. D. E. Williams).
Jul–Sep 1994	**Physics Department, University of California at Santa Barbara** Experimental research into light-emitting conjugated polymers (under Prof. A. J. Heeger, winner of the Nobel Prize in Chemistry, 2000).
Jul–Aug 1993	**Capteur Sensors and Analysers, Milton, Oxon** Testing gas sensors and characterising new materials.
Jul–Aug 1992	**Harwell Laboratory, AEA Technology, Oxon** Research into the use of sols in ink-jet printers and diesel exhaust catalysis (under Prof. A. Atkinson).

Education

1995–98 **Cavendish Laboratory, University of Cambridge**

Ph.D. research degree under the supervision of Prof. M. C. Payne in the Theory of Condensed Matter group at the Cavendish Laboratory (Department of Physics in the University of Cambridge). Dissertation entitled:
Linear-scaling methods in ab initio *quantum-mechanical calculations*.

Awards Bachelor Scholarship from Christ's College, Cambridge (1995–98).
Ph.D. degree conferred: 14 November 1998.

1992–95 **Christ's College, University of Cambridge**

1995 B.A. (Hons.) in Physical Natural Sciences Tripos.
Part II (First Class) in Experimental & Theoretical Physics (91% overall mark).
1994 Part IB (First Class) in Advanced Physics (85%) and Mathematics (95%).
1993 Part IA (First Class) in Chemistry (81%), Crystalline Materials (85%), Physics (88%) and Mathematics (95%).
Highest overall mark in the University for Part IA Natural Sciences.

Awards University Smith System Engineering Prize for Physics (1993).
College Scholarship (1993–95).
College Darwin Prize for Part II Natural Sciences (1995).
College S. W. Greig Prize for Part I Natural Sciences (1993 & 94).
College Fay Prize for Part IA Natural Sciences (1993).
B.A. degree conferred: 30 June 1995.
M.A. degree conferred: 20 March 1999.

1985–92 **Abingdon School, Oxfordshire**

1992 'A'- and 'S'-level Physics (A1) and Chemistry (A1).
'A'-level Further Mathematics (A) and 'AS'-level German (A).
1991 'A'- and 'S'-level Mathematics (A1).
1990 Additional (formerly 'A/O') level Mathematics (A).
G.C.S.E. English (A1), English Literature (A), Latin (A), German (A), Religious Studies (A), Physics (A), Chemistry (A), Biology (A) and Geography (A).
1989 G.C.S.E. French (A) and Mathematics (A).

Awards Foundation Scholarship (1987–92).
Gold medal, Theory Prize and overall winner of the British Physics Olympiad – a competition supported by the Royal Society and Institute of Physics (1992).
Silver medal at the International Physics Olympiad in Helsinki (1992).
St. Catherine's College (Oxford) Prize for Intellectual Initiative (1992).
Bennett Prize for Academic Achievement (1991).
Ingham Prize for Physics (1991 & 92).
Birnbirg Prize for German and Mathematics Prize (1992).
Music Exhibition for trombone (1989–92).
Middle School House Prize (1988) and Lower School Prize (1986).

Selected Publications

1. Elimination of basis set superposition error in linear-scaling density-functional calculations with local orbitals optimised *in situ*
P. D. Haynes, C.-K. Skylaris, A. A. Mostofi & M. C. Payne, *Chem. Phys. Lett.* **422**, 345–9 (2006).

2. ONETEP: linear-scaling density-functional theory with local orbitals and plane waves
P. D. Haynes, C.-K. Skylaris, A. A. Mostofi & M. C. Payne, *phys. stat. sol. (b)* **243** 2489–99 (2006).

3. Using ONETEP for accurate and efficient *O(N)* density functional calculations
C.-K. Skylaris, P. D. Haynes, A. A. Mostofi & M. C. Payne, *J. Phys.: Condens. Matter* **17**, 5757–69 (2005).

4. Preconditioned iterative minimisation for linear-scaling electronic structure calculations
A. A. Mostofi, P. D. Haynes, C.-K. Skylaris & M. C. Payne, *J. Chem. Phys.* **119**, 8842–8 (2003).

5. Nonorthogonal generalized Wannier function pseudopotential plane-wave method
C.-K. Skylaris, A. A. Mostofi, P. D. Haynes, O. Diéguez & M. C. Payne, *Phys. Rev. B* **66**, 035119 (2002).

Meetings

- Principal organiser of a workshop on "Local Orbitals and Linear-scaling *ab initio* Calculations" sponsored by the European Science Foundation and the European Centre for Atomic and Molecular Computations, held in Lyons, September 2001.
See: Report on the CECAM/ESF STRUC-Ψ_k Workshop on "Local Orbitals and Linear-scaling *ab initio* Calculations"
P. D. Haynes, D. R. Bowler and E. Artacho, Ψ_k Newsletter **48**, 36–66 (December 2001).

- Invited speaker at the workshop on "State-of-the-art, developments and perspectives of real-space electronic structure techniques in condensed matter and molecular physics" in Lyons, June 2005.

- Invited speaker at ES04: the 16th annual workshop on "Recent Developments in Electronic Structure Methods" at Rutgers, New Jersey, May 2004.

- Invited speaker at a workshop on "Linear Scaling Electronic Structure Methods" at the Institute for Pure and Applied Mathematics, University of California, Los Angeles, April 2002.

- Invited speaker at a symposium on "Methods for Addressing Time and Length Scale Problems in Molecular Simulation" at the American Chemical Society's National Meeting in San Diego, April 2001.

- Invited speaker at a workshop on "Local orbital methods for large scale atomistic simulations" in Lyons, July 1998.

Grants & Funding

- Joint Principal Investigator on a pending application to EPSRC entitled "Understanding the dopant effect on dislocation mobility in semiconductors with new linear-scaling methods for large-scale first-principles simulations".
- Nuffield Foundation Undergraduate Research Bursary to support a summer student for six weeks (2005).
- Royal Society University Research Fellowship (2005–10).
- Royal Society Research Grant of $10k for computing equipment (2002).
- Ramon Jenkins Senior Research Fellowship, Sidney Sussex College, Cambridge (2002–05).
- Thomas Nevile Research Fellowship, Magdalene College, Cambridge (1999–2002).

Teaching Experience

- Six lectures on Computational Physics for Part II Experimental & Theoretical Physics in the Natural Sciences Tripos (2001 & 2005).
- Head of Class for the Examples Classes and assessed project in Computational Physics, Part II Experimental & Theoretical Physics (2001–06).
- Eight lectures on Solid State Theory for graduate students at the Cavendish Laboratory (2002 & 2003)
- Demonstrator at Examples Classes for Part IB Mathematical Physics, Part II Theoretical Physics and Part II Solid State Physics (1995–98).
- Supervisions in Part IA Physics and Part IB Advanced Physics and Mathematics for Sidney Sussex, Magdalene, Christ's and Corpus Christi Colleges (1995–2006).

Administrative and Other Responsibilities

- Member of the ONETEP Developers' Group, an academic partner in the Accelrys Nanotechnology Consortium and author of the ONETEP code licensed to Accelrys Inc. for commercial distribution from October 2007 under an agreement made through Cambridge University Technical Services.
- Member of the Management Committee, Departmental Representative and Webmaster for the Cambridge-Cranfield High Performance Computing Facility.
- Graduate Mentor, member of the College Council, and Director of Studies for Part III Natural Sciences at Sidney Sussex College.
- Member of the EPSRC College (2003–05) and referee for several journals including the *Physical Review*.

CURRICULUM VITAE

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Citizenship: Switzerland

EDUCATION

1992-1997: Ph.D. in applied mathematics, Swiss Federal Institute of Technology in Lausanne (EPFL), Switzerland. Ph.D. advisor: Prof. J. Descloux.

1987-1992: Master in physics, Swiss Federal Institute of Technology in Lausanne (EPFL), Switzerland.

PROFESSIONAL EXPERIENCE

1999-2006: Center for Applied Scientific Computing, Lawrence Livermore National Laboratory, California, USA

- Postdoctoral researcher from November 1999 to April 2001
- Research scientist since May 2001

1997-1999: Physics Department, North Carolina State University, USA
Postdoctoral research.

1992-1997: Mathematics Department, Swiss Federal Institute of Technology in Lausanne (EPFL), Switzerland.
Research and teaching assistant

PROFESSIONNEL SOCIETIES

Member of:
SIAM (Society for Industrial and Applied Mathematics)
APS (American Physical Society)

RELEVANT RECENT SCIENTIFIC PUBLICATIONS

J.-L. Fattebert and F. Gygi, *Linear scaling first-principles molecular dynamics with plane-waves accuracy*, Phys. Rev. B, 73, (2006), 115124.

J.-L. Fattebert and F. Gygi, *Linear scaling first-principles molecular dynamics with controlled accuracy*, Comput. Phys. Comm., 162, no 1 (2004), pp. 24-36.

F. Gygi, J.-L. Fattebert and E. Schwegler, *Computation of Maximally Localized Wannier Functions using a Simultaneous Diagonalization Algorithm,* Comput. Phys. Comm., 155, no 1 (2003), pp. 1-6.

J.-L. Fattebert and M. Buongiorno Nardelli, *Finite difference methods for ab initio electronic structure and quantum transport calculations of nanostructures*, in *Handbook of Numerical Analysis*, eds Ph. Ciarlet and J.-L. Lions, Volume X: Special Volume: Computational Chemistry (2003).

M. Buongiorno Nardelli, J.-L. Fattebert and J. Bernholc, *O(N) real-space method for ab initio quantum transport calculations: Applications to carbon nanotube-metal contacts,* Phys. Rev. B 64, 245423 (2001).

David Bowler: Curriculum Vitae

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University College London	UCL
Gower Street	Gordon St
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WC1E 6BT	WC1H 0AH
Phone : +44 20 7679 7229	`david.bowler@ucl.ac.uk`
Fax : +44 20 7679 1360	`http://www.cmmp.ucl.ac.uk/~drb`
Date of Birth 12/8/1970. Present age 36 years.	

Education

1988-1991 B.A.(Hons. class: 2(i)) Natural Sciences, Cambridge University
1994-1997 D.Phil., Materials Department, Oxford University

Employment

Sept 1992-1994	Device Physicist with GaAsCode Ltd, Cambridge.
April 1997	UKCP Research Fellow in the Physics Department, Keele University.
July 1998	UKCP Research Fellow in the Department of Physics and Astronomy, University College London.
October 1999	EPSRC Postdoctoral Fellow in Theoretical Physics Department of Physics and Astronomy, University College London
October 2001–	Royal Society University Research Fellow Department of Physics and Astronomy, University College London
Sept 2004-2005	Senior Research Fellow (one year suspension of RSURF) ICYS, National Institute for Materials Science, Japan
October 2006–	Reader in Physics Department of Physics and Astronomy, University College London

Research Activity

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

Publications

Total Publications: 64 peer reviewed; 14 conference proceedings etc.

References

[1] A.P.Horsfield, D.R.Bowler, H.Ness, C.Sanchez, T.N.Todorov, and A.J.Fisher. The transfer of energy between electrons and ions in solids. *Rep. Prog. Phys.*, 69:1195–1234, 2006.

[2] 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. b*, 243:989–1000, 2006.

[3] D. R. Bowler, A. P. Horsfield, C. Sanchez, and T. N. Todorov. Correlated electron-ion dynamics with open boundaries: Formalism. *Journal of Physics: Condensed Matter*, 17:3985–3995, 2005.

[4] T. Miyazaki, D. R. Bowler, R. Choudhury, and M. J. Gillan. Atomic force algorithms in density functional theory electronic-structure techniques based on local orbitals. *Journal of Chemical Physics*, 121:6186–6194, 2004.

[5] K. Li, D. R. Bowler, and M. J. Gillan. Tight binding studies of strained Ge/Si(001) growth. *Surface Science*, 526:356–366, 2003.

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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'Etudes 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).