

## **Title**

Advances in continuum quantum Monte Carlo methods

## **Venue**

CECAM, Lyon

## **Dates**

3-7 September 2007, 1 week

## **Organisers**

Claudia Filippi

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Universiteit Leiden  
Leiden, The Netherlands  
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## **Abstract**

The workshop will focus on advances in continuum quantum Monte Carlo (QMC) approaches, in particular recent methodological developments and efforts to push the frontier of applications to ever more complex systems. The aim of the workshop is to bring together QMC experts and new additions to the field, and to involve a larger community of electronic structure researchers with an interest in these techniques.

## Summary

The proposed workshop serves multiple purposes:

- The workshop is part of the activities of the quantum Monte Carlo working group WG2 of the ESF Psi-k Programme.
- The workshop will focus on the latest developments and applications of quantum Monte Carlo techniques for continuum systems. The current state of the art and prospects of these approaches will be reviewed and discussed, and several outstanding issues such as ionic forces, transition metals, fermionic sign problem, etc. will be covered.
- The workshop will reach out to researchers doing quantum Monte Carlo in smaller or isolated groups, and to researchers who have recently started to use quantum Monte Carlo techniques. The Summer School on Many-body Theory organized in San Sebastian in July 2007 will be complementary and introduce some of the more junior researchers to the basics of the theory; our workshop will then provide the necessary background and context, highlighting the most challenging problems and the topics of current interest.

## Scientific Program

An important area of research within electronic structure theory is the development of alternatives to density functional (DFT) methods. Despite the successes of DFT in describing the electronic structure of complex molecules and solids, the treatment of electronic correlation within DFT is only approximate, sometimes leading to incorrect results for both strongly and weakly correlated systems.

Quantum Monte Carlo (QMC) methods are among the most successful of the post-DFT approaches, and have yielded highly accurate results for the correlated properties of large molecules and solids where conventional quantum chemistry methods are extremely difficult to apply. Consequently, it is now realized by many DFT practitioners that QMC methods are likely to become the method of choice for such accurate post-DFT calculations.

The focus of the workshop will be on the current methodological developments in continuum QMC methods, including efforts to incorporate molecular dynamics and improve geometry optimisation schemes, to find more efficient ways of optimising trial wave functions, and to develop new algorithms alternative to the fixed-node diffusion Monte Carlo method. Speakers involved in pushing the frontier of applications to ever more complex systems will also be invited.

Since the number of researchers in the field is still relatively small, we feel that it is important to bring together QMC experts and new additions to the field. Therefore, we intend to involve several researchers who are coming from the quantum chemistry or the density functional theory communities and have embraced quantum Monte Carlo approaches in recent years.

We list below the main topics covered in the workshop, each followed by a partial list of key speakers:

- Geometry optimisation and incorporation of molecular dynamics in QMC.  
Assaraf, Pierleoni, Ceperley, Moroni.
- General and robust ways to obtain variational many-body wave functions.  
Sorella, Toulouse, Filippi, Umrigar.
- New accurate forms of many-body wave functions.  
Mitas, Needs, Sorella.
- New algorithms alternative to the fixed-node diffusion Monte Carlo method.  
Kalos, Zhang.
- Pseudopotential in many-body calculations.  
Dolg, Mitas, Drummond, Casula, Aspuru-Guzik.
- Applications to large realistic systems (nano-clusters, transition metals, ...).  
Alfé, Lopez-Rios, Henning, Guidoni, Luchöw, Towler, Gaudoin, Hine.

## Participants

We expect of the order of 40 participants, including the invited speakers and the 3 organisers. We are expecting of the order of 15 student/postdocs.

## Outreach and tutorial element

We want to reach out to researchers doing quantum Monte Carlo in smaller groups as well as researchers who have just entered or are interested in entering the field. In this respect, our workshop will complement the 2007 Summer School on Many-body Theory in San Sebastian, introducing new participants to the research frontier.

To encourage the participation of younger researchers, we plan to allocate a substantial amount of the budget to pay their travel expenses in addition to lodging.

The number of talks will be limited to 6 per day and ample time will be given to discussion, stimulating active participation from students and postdocs. We will also organise a poster session where young participants will be encouraged to present their work.

It is hoped that the meeting will help to create a stronger and broader quantum Monte Carlo community.

## Tentative list of speakers

Among the invited speakers, we plan to have leading experts as well as several junior promising researchers in the field. The number of talks will be limited to 6 per day and ample time will be given to discussions.

Depending on the available funding, we may or may not be able to invite all the people listed below.

Saverio Moroni	Universita' di Roma La Sapienza, Italy
Leonardo Guidoni	Universita' di Roma La Sapienza, Italy
Carlo Pierleoni	Universita' del L'Aquila, Italy
Sandro Sorella	SISSA, Trieste, Italy
Paolo Umari	SISSA, Trieste, Italy
Roland Assaraf	University of Paris, Jussieu, France
Julien Toulouse	University of Paris, Jussieu, France
Dario Alfé	University College London, UK
Nick Hine	Imperial College London, UK
Neil Drummond	University of Cambridge, UK
Pablo Lopez-Rios	University of Cambridge, UK
Mike Towler	University of Cambridge, UK
Arne Luchow	University of Dusseldorf, Germany
Michael Dolg	University of Koln, Germany
René Gaudoin	San Sebastian, Spain
Alan Aspuru-Guzik	Harvard University, USA
Michele Casula	University of Illinois, USA
David Ceperley	University of Illinois, USA
Richard Hennig	Cornell University, USA
Mal Kalos	Lawrence Livermore National Laboratory, USA
Lubos Mitas	North Carolina State University, USA
Cyrus Umrigar	Cornell University, USA
Shiwei Zhang	College of William and Mary, Williamsburg, USA

## Budget

We would like to pay the lodging expenses of all participants. We expect that most European participants will pay their own travel expenses, but will encourage the participation of younger researchers by contributing to their travel costs where possible. We will also contribute to the travel expenses of the invited scientists from the USA.

Lodging	40 participants × 5 days × 70 euro	=	14000 euro
Travel	20 participants × 140 euros	=	2800 euro
Travel	8 speakers from USA × 400 euros	=	3200 euro
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Total		=	20000 euro

The request for the ESF Psi-k Programme is 10000 euro.

## Additional funding

We are currently applying for funding from CECAM, which we hope will provide the remaining 10000 euro.

## Curriculum Vitae of Scientific Organisers

### Dr. Claudia Filippi

Universiteit Leiden  
 Instituut-Lorentz for Theoretical Physics  
 Niels Bohrweg 2, NL-2333 CA, Leiden  
 The Netherlands

#### Employment History

2001-        Senior Research Scientist (FOM Springplanker)  
               Instituut Lorentz, Universiteit Leiden, The Netherlands

1998-2001    Lecturer  
               National University of Ireland, Cork

1996-1998    Postdoctoral Research Associate  
               University of Illinois at Urbana-Champaign

1991-1992    INFM (National Institute of Condensed Matter Physics) Fellow  
               University of Trento, Italy

#### Education

1996    Ph.D.    Physics    Cornell University, USA  
 1991    B.S.     Physics    University of Trento, Italy

#### Selected Professional Activities

- Member of the Steering Committee of the European Science Foundation Network “Towards Atomistic Materials Design” (Psi-k, 2003-2008).

- Co-organizer with M. Foulkes and S. Zhang of the Workshop “Electronic Structure Beyond Density Functional Theory”, Lorentz Center, Leiden, 12-16 July 2004.
- Co-organizer with R. Needs and M. Towler of the Workshop “The Diffusion Monte Carlo Method”, CECAM, Lyon, 19-21 September 2002.

Five most relevant publications during the last five years

1. *Energy and variance optimization of many body wave functions*, C. J. Umrigar and C. Filippi, Phys. Rev. Lett. **94**, 150201 (2005).
2. *Diffusion Monte Carlo method with lattice regularization*, M. Casula, C. Filippi and S. Sorella, Phys. Rev. Lett. **95**, 100201 (2005).
3. *Excitations in photoactive molecules from quantum Monte Carlo*, F. Schautz, F. Buda, and C. Filippi, J. Chem. Phys. **121**, 5836 (2004).
4. *Optimized Jastrow-Slater wave functions for ground and excited states*, F. Schautz and C. Filippi, J. Chem. Phys. **120**, 10931 (2004).
5. *Quantum Monte Carlo calculations of H<sub>2</sub> dissociation on Si(001)*, C. Filippi, S. B. Healy, P. Kratzer, E. Pehlke and M. Scheffler, Phys. Rev. Lett. **89**, 166102 (2002).

Invited Talks at International Conferences

1. 11<sup>th</sup> Nanoquanta Workshop on Electronic Excitations, Houffalize, Belgium (2006)
2. Progress in Ab-initio Modeling of Biomolecules: Methods and Applications, Lorentz Center, Leiden, The Netherlands (2006)
3. Spring School 2006: Computational Methods in Condensed Matter Physics, Forschungszentrum Juelich, Germany (2006)
4. Psi-k 2005 Conference Toward atomistic materials design, Schwäbisch Gmünd, Germany (2005)
5. Summer School on Fundamental Problems in Statistical Physics XI, Leuven, Belgium (2005)
6. Symposium of the Deutsche Forschungsgemeinschaft Programme “Modern and Universal First-principles Methods for Many-electron Systems in Chemistry and Physics”, Bonn, Germany (2005)
7. XII Workshop on Computational Material Science: Total Energy and Force Methods, Trieste, Italy (2005)
8. Conference on Computational Physics 2004, Genova, Italy (2004)
9. 16<sup>th</sup> Workshop on “Recent Developments in Electronic Structure Methods”, Rutgers University, New Jersey, USA (2004)
10. School on Continuum Quantum Monte Carlo Methods, Trieste, Italy (2004)
11. American Chemical Society National Meeting, New York, USA (2003)

12. Workshop on “Ab-initio Many-Body Theory for Correlated Electron Systems”, Trieste, Italy (2003)
13. Physics School “Modeling and Simulation in Micro-Nano Technologies and Material Engineering”, Toulouse, France (2003)
14. March Meeting of the American Physical Society, Austin, Texas, USA (2003)
15. 43<sup>rd</sup> Sanibel Symposium, St. Augustine, Florida, USA (2003)
16. European Physical Society, CMMP 2002, Brighton, England (2002)
17. European Materials Research Society, Spring Meeting 2002, Strasbourg, France (2002)
18. March Meeting of the American Physical Society, Seattle, WA, USA (2001)
19. X Workshop on Computational Material Science: Total Energy and Force Methods, Trieste, Italy (2001)
20. Pacifichem 2000, IV International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, USA (2000)
21. Psi-k 2000 Conference on Ab Initio Calculations of Complex Processes in Materials, Schwäbisch Gmünd, Germany (2000)
22. XII Workshop on Recent Developments in Electronic Structure Methods, Georgia Institute of Technology, Atlanta, Georgia, USA (2000)
23. Workshop on Physics of Insulators, Aspen Center for Physics, Aspen, CO, USA (1998)
24. Workshop on Numerical Methods for Strongly Interacting Quantum Systems, Institute for Nuclear Theory, University of Washington, Seattle, WA, USA (1997)
25. IX Workshop on Recent Developments in Electronic Structure Methods, Cornell University, Ithaca, NY, USA (1997)
26. Workshop on Real atoms and solids, core and valence electrons, Università di Roma “La Sapienza”, Italy (1997)

## Prof. Matthew M.C. Foulkes

Department of Physics  
Imperial College London  
Prince Consort Road  
London SW7 2BW  
United Kingdom

Employment History

2004- Professor of Physics  
 Physics Department, Imperial College London

1999-2004 Reader in Physics (US equivalent: Associate Professor)  
 Physics Department, Imperial College London

1993-1999 Lecturer in Physics (US equivalent: Assistant Professor)  
 Physics Department, Imperial College London

1990-1993 Probationary Lecturer in Physics  
 Physics Department, Imperial College London

1988-1990 Post-Doctoral Member of Technical Staff  
 AT&T Bell Laboratories, Murray Hill, NJ

1986-1998 Drapers' Research Fellow, Pembroke College, University of Cambridge

#### Education

1987 Ph.D. Physics University of Cambridge, United Kingdom

1983 B.S. Physics University of Cambridge, United Kingdom

#### Selected Professional Activities

- Member and Chair of the High Performance Computing Users' Forum of the UK Engineering and Physical Sciences Research Council (EPSRC).
- Member of EPSRC High Performance Computing Steering Committee, EPSRC CCP9 Steering Committee, Imperial/UCL Condensed Matter Physics Merger Panel, Imperial College High-Performance Computing Committee, Imperial College Physics Graduate Studies Committee, Imperial College Physics Teaching Committee.

#### Five most relevant publications during the last five years

1. *Accurate and Efficient Method for the Treatment of Exchange in a Plane-Wave Basis*, A. Sorouri, W.M.C. Foulkes and N.D.M. Hine, *J. Chem. Phys.* **124**, 064105 (2006).
2. *Coulomb Finite-Size Effects in Quasi-Two-Dimensional Systems*, B. Wood, W.M.C. Foulkes, M.D. Towler and N.D. Drummond, *J. Phys.: Condens. Matter* **16**, 891 (2004).
3. *Ab Initio Calculations of Bulk Moduli and Comparison with Experiment*, R. Gaudoin and W.M.C. Foulkes, *Phys. Rev. B* **66**, 0521041 (2002)
4. *Quantum Monte Carlo Analysis of Exchange and Correlation in the Strongly Inhomogeneous Electron Gas*, M. Nekovee, W.M.C. Foulkes and R.J. Needs, *Phys. Rev. Lett.* **87**, 0364011 (2001)
5. *Quantum Monte Carlo Simulations of Solids*, W.M.C. Foulkes, L. Mitas, R.J. Needs and G. Rajagopal, *Rev. Mod. Phys.* **73**, 33 (2001).

#### Invited Talks at International Conferences

1. Quantum Monte Carlo in the Apuan Alps II, Italy (2006)

2. CECAM Workshop on Ab Initio Simulation Methods Beyond Density-Functional Theory, Lyon, France (2005).
3. Quantum Monte Carlo in the Apuan Alps I, Italy (2005)
4. University of Cardiff; Imperial College Departmental Colloquium (2003).
5. Kavli Institute for Theoretical Physics Program on Realistic Theories of Correlated Electron Materials, Santa Barbara, USA (2002)
6. CECAM Workshop on the Diffusion Monte Carlo Method, Lyon, France (2002)
7. March Meeting of the American Physical Society, Seattle, USA (2001)
8. ES2001,
9. The Thirteenth Annual Workshop on Recent Developments in Electronic Structure Algorithms, Princeton, USA (2010)
10. Workshop on Frontiers in Fermion Quantum Monte Carlo Methods, Seattle, USA (1999)
11. Newton Institute Workshop on Strongly Correlated Systems, Cambridge (1999)
12. High Performance Computing Conference, Manchester (1999)
13. Institute of Physics Condensed Matter and Materials Physics Meeting, Exeter (1999)
14. Quantum Monte Carlo Network Meeting on Core and Valence Electrons in Real Atoms and Solids, Rome, Italy (1997)
15. American Chemical Society General Meeting, San Francisco, USA (1997)
16. High Performance Computing Initiative Workshop on Long-Ranged Forces, Southampton (1996)
17. Quantum Monte Carlo Network Meeting, Cork, Ireland (1996)
18.  $\Psi_k$  Network Conference, Schwäbisch Gmünd, Germany (1996) CECAM Workshop on Order-N Methods in Density Functional Theory, Lyon, France (1995)
19. Europhysics Workshop on Numerical Simulation of Quantum Many-Body Systems, Elba, Italy (1994)
20.  $\Psi_k$  workshop on *Quantum Theory of Solids: Improved Density Functionals*, Aarhus, Denmark (1994)
21. *An Appraisal of Models for the Atomistic Simulation of Complex Systems*, Bad Honnef, Germany (1993)
22. NSERC-CAP Summer Institute in Theoretical Physics Workshop, (1992)
23. *Density Functional Theory — Methods and Applications*, Kingston, Ontario, Canada (1992)
24. Fifth International Workshop on Computational Condensed Matter Physics, SISSA, Trieste, Italy (1991)

25. Second International Electronic Structure Workshop, Columbus, Ohio, USA (1991)
26. Italian Solid State Physics Meeting, Modena, Italy (1988)
27. CECAM Workshop on Interatomic Forces in Solids, Orsay, France (1987)

## Prof. Richard J. Needs

TCM Group  
Cavendish Laboratory  
Cambridge  
United Kingdom

### Employment History

- |           |   |
|-----------|---|
| 2003-     | Professor in Theoretical and Computational Physics<br>University of Cambridge |
| 1999-2003 | Reader in Theoretical and Computational Physics<br>University of Cambridge    |
| 1988-1999 | Lecturer<br>University of Cambridge   |
| 1984-1987 | Demonstrator (Assistant Lecturer)<br>University of Cambridge                  |
| 1983-1984 | Visiting Scientist<br>Xerox Palo Alto Research Center, USA                    |

### Education

- |      |       |         |   |
|------|-------|---------|---|
| 1983 | Ph.D. | Physics | University of Cambridge, United Kingdom |
| 1980 | B.S.  | Physics | University of Bristol, United Kingdom   |

### Five most relevant publications during the last 5 years

1. *Quantum Monte Carlo, Density-Functional Theory, and Pair-Potential Studies of Solid Neon*, N. D. Drummond and R. J. Needs, Phys. Rev. B 73, 024107 (2006).
2. *Electron Emission from Diamondoids: A Diffusion Quantum Monte Carlo Study*, N. D. Drummond, A. J. Williamson, R. J. Needs, and G. Galli, Phys. Rev. Lett. 95, 096801 (2005).
3. *Diamond and  $\beta$ -tin structures of Si studied with quantum Monte Carlo calculations*, D. Alfè, M. J. Gillan, M. D. Towler, and R. J. Needs, Phys. Rev. B 70, 214102 (2004).
4. *Diffusion quantum Monte Carlo study of three-dimensional Wigner crystals*, N. D. Drummond, Z. Radnai, J. R. Trail, M. D. Towler, and R. J. Needs, Phys. Rev. B 69, 085116 (2004).

5. *Quantum Monte Carlo study of the optical and diffusive properties of the vacancy defect in diamond*, R. Q. Hood, P. R. C. Kent, R. J. Needs, and P. R. Briddon, *Phys. Rev. Lett.* 91, 076403 (2003).

#### Invited Talks at International Conferences

1. Workshop on Total Energy and Force Methods (Trieste, Italy, 1986)
2. EPS March meeting (Pisa, Italy, 1987)
3. Third International Workshop on Total Energy and Force Methods (Trieste, Italy, 1987)
4. MOSPOQ-88 Modulated structures polytypes and quasicrystals (Varanasi, India, 1988)
5. Workshop on Total Energy and Force Methods (Paris, France, 1990)
6. Supercomputers and Materials Science (London, UK, 1990)
7. APS March meeting (Los Angeles, USA, 1990)
8. 26th Yamada conference “Surface as a New Material” (Osaka, Japan, 1990)
9. Workshop on Total Energy and Force Methods (Schloss-Ringberg, Germany, 1992)
10. ERC conference on “Electronic structure of solids” (Cambridge, UK, 1992)
11. 40th International Field Emission Symposium (Nagoya, Japan, 1993)
12. Third Int. Conf. on Electrical Transport and Optical Properties of Inhomogeneous Media (Guanajuato, Mexico, 1993)
13. IOP Condensed Matter Conference (Leeds, UK, 1993)
14. Seventh International Workshop on Total Energy and Force Methods (Trieste, Italy, 1995)
15. WE-Heraeus seminar on “Continuum and atomistic aspects of morphological features of crystalline surfaces and small particles” (Bad Honnef, Germany, 1995)
16. Pacific Conference on Condensed Matter Theory: Complex Materials and Strongly Correlated Systems (Seoul, Korea, 1995)
17. Eighth Annual Conference on New Methods in Electronic Structure Calculations (Minneapolis, USA, 1996)
18. Meeting on “Stochastic Methods on Parallel Computers”, organised by the Edinburgh Parallel Computing Centre, (Cambridge, UK, 1997)
19. IOP Theory of Condensed Matter Group meeting (Birmingham, UK, 1999)
20. Workshop on Total Energy and Force Methods (Madrid, Spain, 2000)
21. 7th International Workshop on Computational Electronics (Glasgow, UK, 2000)
22. Ab Initio (from Electronic Structure) Calculations of Complex Processes in Materials (Schwäbisch Gmünd, Germany, 2000)

23. Electronic Structure: Prediction and Applications Conference (San Sebastian, Spain, 2000)
24. The International Chemical Congress of Pacific Basin Societies, Pacifichem 2000, (Honolulu, USA, 2000)
25. Workshop on “Computational Quantum Many-Body Physics” (Cambridge, UK, 2000)
26. Density Functional Theory for the study of complex oxides, (Royal Institution London, UK, 2001)
27. Recent Progress in Many-Body Theories, (Manchester, UK, 2001)
28. XXXIX European High Pressure Research Group Meeting, (Santander, Spain, 2001)
29. Total Energy Methods in Computational Condensed Matter, (Tenerife, Spain, 2002)
30. Workshop on “The Diffusion Quantum Monte Carlo Method”, (Lyon, France, 2002)
31. Euroconference on “Ab-Initio Many-Body Theory for Correlated Electron Systems”, (Trieste, Italy, 2003)
32. 226th American Chemical Society Meeting, (New York, USA, 2003)
33. International Workshop on Computational Physics and Materials Science: Progress in Ab Initio Computational Methods for Condensed Matter (Gif-sur-Yvette, France, 2004)
34. Electronic Structure beyond Density Functional Theory, (Leiden, Netherlands, 2004)
35. NAREGI workshop on “Electronic Transport, Excitation and Correlation in Nanoscience”, CRIS, Hokkaido University, (Sapporo, Japan, 2004)
36. KNAW conference on “Multi-scale modelling: Electons, Molecules and (Bio)Materials”, (Amsterdam, Netherlands, 2006)
37. Workshop on “New Developments in Quantum Monte Carlo” (Tempe, Arizona, USA, 2006)