

## 0.1 Report on Workshop

# Quantum Monte Carlo and the CASINO program IV

International summer school

Sunday 2nd August - Sunday 9th August

The Apuan Alps Centre for Physics @ TTI, Vallico Sotto, Tuscany, Italy

[www.vallico.net/tti/tti.html](http://www.vallico.net/tti/tti.html)

Sponsors: Psi-k, CCP9

Organizer: Mike Towler

Conference web page: [www.vallico.net/tti/qmcatcp\\_09/summer\\_school.html](http://www.vallico.net/tti/qmcatcp_09/summer_school.html)

The fourth international quantum Monte Carlo Summer School to be held at the Apuan Alps Centre for Physics took place in early August 2009 . The event was organized and run by Mike Towler, who was ably assisted with the teaching by Neil Drummond and Pablo López Ríos. All three instructors are members of the TCM Group from Cambridge University's Cavendish Laboratory. The purpose of the school was to provide the student with a thorough working knowledge of the quantum Monte Carlo electronic structure method as currently used in quantum chemistry and condensed matter physics, and to show him or her how to use the latest version of the Cambridge-developed QMC program CASINO for serious scientific research. The course consisted of around 20 hours of lectures and a series of practical exercises in using the CASINO program led by its authors. No previous background other than a basic knowledge of quantum mechanics was assumed, though it was stressed beforehand that a knowledge of density functional theory and similar methods is normally thought to be useful. As is usual at this venue, formal lectures were restricted to the mornings, and participants were given the freedom and space to think and to contemplate and discuss the issues at hand. In addition to hands-on exercises, a programme of healthy recreational activities such as mountain climbing was organized in the afternoons, during which the students were encourage to discuss their own research and to look into potential collaborations.

Quote from student: *“The summer school is an excellent in my whole life and I have really got inspired. I think every one who attends the QMC school will go back to home with great spirits. My words fail to explain how much I have enjoyed the lectures and outing trips. Thanks a lot for everything.. I will really miss you.”*

# 1 Programme

The following lectures were given during the school:

## Mike Towler

- Quantum Monte Carlo: a practical solution to the correlation problem in electronic structure calculations (2.5 hours)
- The CASINO program: a basic introduction to functionality and input/output (1 hour)
- Three QMC scaling problems (2 hours)
- Forces and dynamics. Expectation values other than the energy (2 hours)
- Practical aspects when using pseudopotentials with CASINO (1 hour)

## Pablo López Ríos

- Statistical analysis for QMC (1 hour)
- Wave functions and nodes in QMC (2 hours)
- Pseudopotentials for QMC (1 hour)

## Neil Drummond

- Diffusion Monte Carlo (2 hours)
- Optimization of many-electron wave functions (2 hours)
- Ewald interactions and finite size errors (2 hours)
- Some recent applications of quantum Monte Carlo simulation (1.5 hours)

During the afternoons the students completed the following exercises:

- Distribution, setup and compilation of the CASINO program
- Basic use of the CASINO program - simple VMC, DMC calculations
- Wave function optimization with CASINO
- Trial wave function generation with other programs (CRYSTAL/PWSCF/CASTEP etc.)
- Advanced use of the CASINO program (over two days)
- General CASINO applications

After the final lecture, a discussion session was held. Each student was asked to state their particular interest in the quantum Monte Carlo method; in each case the instructors attempted to give suitable advice for the chosen applications and to stimulate a short discussion.

The school was concluded with an exam in order to ascertain who had been paying attention. Just for the record, the student with the highest mark was James Shepherd of Cambridge University.

## 2 List of participants

Twenty-five students from sixteen countries took part, accompanied by three family members, plus our nine staff. The names and institutions of the participants were:

Ariunbayasgalan Alyeksyey (Mongolian Academy of Sciences, Mongolia)

Mohaddeseh Abbasnejad (University of Tehran, Iran)

Grigor Aslanyan (University of California, San Diego, U.S.A.)

Alexandre Carvalho (University of Oporto, Portugal)

David Dell'Angelo (University of Rennes, France)

Andrea Droghetti (Trinity College, Dublin, Ireland)

Tim Green (University of Cambridge, U.K.)

Santosh KC (Tribhuvan University, Kathmandu, Nepal)

Duck Young Kim (University of Uppsala, Sweden)

Peter Larsson (University of Uppsala, Sweden)

Pablo Maldonado (University of Cordoba, Spain)

José Mira McWilliams (Universidad Politécnica de Madrid, Spain)

Miroslawa Nedyalkova (University of Sofia, Bulgaria)

Johan Pohl (University of Darmstadt, Germany)

José Roberto dos Santos Politi (University of Brasilia, Brazil)

Hannah Price (University of Cambridge, U.K.)

Narendra Revanuri (University of Goa, India)

Sergio Santos (University of Aveiro, Portugal)

Priyanka Seth (University of Cambridge, U.K.)

Vinit Sharma (Agrawal College, Jaipur, India)

James Shepherd (University of Cambridge, U.K.)

Stefano Spezia (University of Palermo, Italy)

Maria Velinova (University of Sofia, Bulgaria)

Márton Vörös (Budapest University, Hungary)

Arkadius Wojs (University of Cambridge, U.K.)