Joint *DEMOCRITOS* - ICTP School on
Continuum Quantum Monte Carlo Methods

12 - 23 January 2004
Miramare - Trieste, Italy

An international course on quantum Monte Carlo simulations will be held at the Abdus Salam International Centre for Theoretical Physics (ICTP), from 12 to 23 January 2004, with the co-sponsorship of the INFM *DEMOCRITOS* National Simulation Centre.

This School aims at a general introduction to quantum Monte Carlo methods for continuum systems, both at zero and finite temperature. The focus will be on the physical principles and numerical algorithms which underlie the implementation of state-of-the-art computer codes.

For each of the methods presented, a series of elementary lectures will introduce the basic formalism, and hands-on computer sessions using simple codes for simple systems will help familiarizing with concepts and algorithms. At a later stage, advanced topics will be covered, full-fledged codes will be discussed, and a series of tutorials will be held to illustrate their usage with a number of physically significant applications.

Topics Covered:

- Monte Carlo integration; Random walks; Metropolis method; Statistical analysis of data.
- Variational Monte Carlo; Correlated trial functions; Atomic and molecular systems; Forces.
- Diffusion Monte Carlo; Electron gas; Pseudopotential electronic structure calculations for solids.
- Reptation Monte Carlo; Response functions; Excited states.
- Auxiliary field Monte Carlo; Pseudopotential electronic structure calculations for molecules.
- Path Integral Monte Carlo: Superfluidity and Bose condensation; Exchange in quantum crystals.

Participation:

This School is intended for strongly motivated graduate students and young post-doctoral scientists. Prior specific training in Monte Carlo simulations is not required. However, participants are expected to have a good working knowledge of elementary quantum mechanics.   Some knowledge of FORTRAN and UNIX is a prerequisite. As the School will be conducted in English, participants should have an adequate working knowledge of that language.

There is no registration fee. As a rule, travel, lodging and subsistence expenses of the participants are borne by their home institutions. However, limited funds are available for some applicants, to be selected by the Organizers Such financial support is available only for those attending the entire School.

The **Application Form** is obtainable from the ICTP WWW server: **http://www.ictp.trieste.it/** and by clicking on the Scientific Calendar 2004 (which will be constantly up-dated) or from the activity Secretariat (smr1595@ictp.trieste.it). It should be completed and returned **before 30 September 2003** (if requesting financial support or requiring a visa) and **31 October 2003** (if not requesting financial support or not requiring a visa) to:

the Abdus Salam International Centre for Theoretical Physics
"School on Continuum Quantum Monte Carlo Methods" (smr1595)
Strada Costiera 11,   I-34014 Trieste, Italy

or

smr1595@ictp.trieste.it
(Please save and send file attachments in RTF format)

 The decision of the Organizers will be communicated to all candidates as soon as possible thereafter.

Telephone: +39-040-2240305   Telefax: +39-040-224531   E-mail: smr1595@ictp.trieste.it
ICTP Home Page: **http://www.ictp.trieste.it/**

Trieste, revised August 2003

Co-sponsors*:*

**INFM *DEMOCRITOS*
National Simulation Centre**

ESF/Psi-K Network

UIUC MCC (Materials Computation Center of the University of Illinois of Urbana, Champaign)

Organizers:

D. M. Ceperley
(UIUC/NCSA, Urbana, Illinois)
S. Moroni
(INFM/SMC, Rome)
S. Baroni   (Local organizer,
(SISSA/DEMOCRITOS, Trieste)

Lecturers:

D.M. Ceperley (Urbana, USA)

C. Filippi (Leiden, NL)

S. Moroni (Rome, I)

C. Pierleoni (L.Aquila, I)

M. Towler (Cambridge, UK)

Z. Zhang (Williamsburg, VA, USA)*

* to be confirmed

Application Deadlines

30 September 2003
(if requesting financial support)

31 October 2003
(if no financial support requested and no visa required)