



The Abdus Salam
International Centre for Theoretical Physics



Latin American School on
Computational Materials Science

19 - 30 January 2009

Santiago, Chile



The School is being jointly organized by:

- the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy
- Universidad Andrés Bello (UNAB), Santiago, Chile
- Project Anillo ACT/24/2006 - Universidad de Chile "Computer Simulation Lab in Nanobio Systems"

STRUCTURE OF THE SCHOOL

- A. Introduction to high-performance computing
- B. Advanced talks covering recent developments
- C. Hands-on tutorial, using the Quantum-Espresso distribution

Electronic structure methods are becoming a fundamental tool of investigation in condensed matter physics, materials science, biology and nanoscience. These methods are based on the solution of the Schrödinger equation for the electrons, without any empirical input, and allow for the description of the mechanical, vibrational, electrical, magnetic and several other properties of solids with "chemical" accuracy. This is a rapidly evolving field which also offers people in developing countries the opportunity to carry out cutting-edge theoretical research with relatively low financial investment in equipment. The purpose of this school is to strengthen the scientific base of junior scientists (PhD students and junior postdocs) by exposing them to a selection of international high-level lectures combined with a week-long session of computational laboratories aimed at training students to the independent use of the codes for their own research.

SUMMARY OF TOPICS

Part A

- Basics of high performance computing (HPC)
- Tools for scientific HPC on Linux
- Parallel approach to scientific computations
- How to set up and use efficiently Linux clusters for parallel scientific computing

Part B

- Applications to
Condensed matter physics
Nanoscience
Biology
Materials Science
Geophysics

Part C

- Electronic structure theory
- Energy bands
- Total energy and its derivatives
- Density functional theory and functionals
- Plane waves
- Pseudopotentials
- *ab-initio* molecular dynamics
- Advanced sampling methods NEB
- Phonons
- Magnetism

PARTICIPATION

Scientists and students from all countries which are members of the United Nations, UNESCO or IAEA may attend the School. Given the regional character of the initiative, applications from Latin American countries will be privileged. The school will be conducted in English. Participants are required to have a basic knowledge of Linux. As a rule, travel and subsistence expenses of the participants should be borne by the home institution. Every effort should be made by candidates to secure support for their fare (or at least half-fare). However, limited funds are available for some participants, who are nationals of, and working in, a developing country, and who are not more than 45 years old. There is no registration fee.

The **Application Form** is obtainable from the ICTP Website
http://cdsagenda5.ictp.trieste.it/full_display.php?smr=0&ida=a08192

For applicants from Chile (.doc or .pdf file or paper): to Professor Eduardo Menéndez Proupin, Universidad de Chile, Facultad de Ciencias, Departamento de Física, Casilla 653, Santiago, Chile emenendez@uchile.cl. Moreover a Curriculum Vitae, Research Abstract and a separate letter of recommendation (junior scientists) should be sent, these will be refereed by a Scientific Selection Committee together with their application. - Deadline 10 November 2008.

For applicants from all other countries (on-line):

Interested applicants should fill in and submit the Online Application Form. Applicants are also requested to upload on the online form a Curriculum Vitae and Research Abstract. A separate signed letter of recommendation (junior scientists) in PDF format should be sent to smr2071@ictp.it, which will be refereed by a Scientific Selection Committee together with the application. Deadline 15 October 2008.

Contact Information

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Activity Web pages:

http://cdsagenda5.ictp.trieste.it/full_display.php?smr=0&ida=a08192

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<http://www.gnm.cl>

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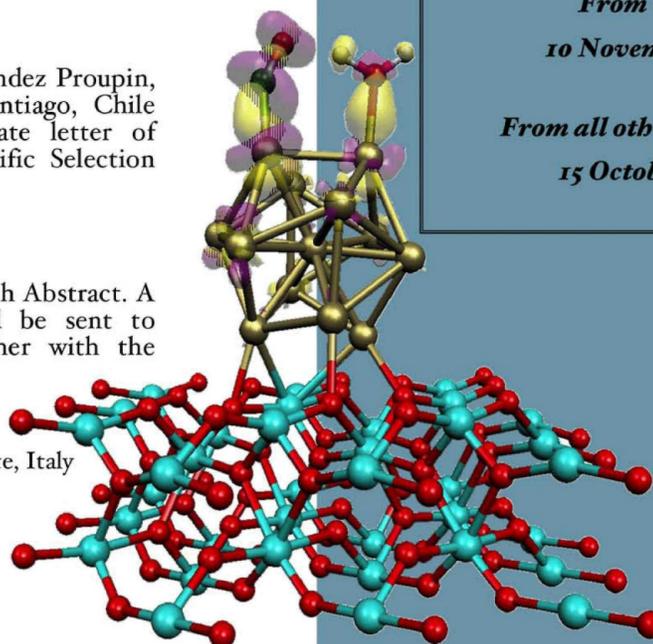
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DEADLINE FOR REQUESTING
PARTICIPATION

From Chile:
10 November 2008

From all other countries:
15 October 2008



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