"Advanced Quantum ESPRESSO Developer Training"

9-19 December 2013

(Miramare - Trieste, Italy)

QUANTUM ESPRESSO FOUNDATION
foundation.quantum-espresso.org

THEOS
THEORY AND SIMULATION OF MATERIALS

EPFL
ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

In collaboration with the Quantum ESPRESSO Foundation and the Theory and Simulation of Materials group, EPF Lausanne, the Abdus Salam International Centre for Theoretical Physics is organizing an Advanced Quantum ESPRESSO Developer Training to be held at ICTP, Trieste, Italy from 9 to 19 December 2013.

The rapid development of computer technologies, combined with advances in electronic-structure theory, is opening new horizons to computational material science. However, the implementation of groundbreaking ideas requires a significant effort, due to the complexity of the current electronic-structure software. Indeed, innovative developments are often hindered by the steep learning curve required to master the state of the art. Overcoming this learning curve is necessary to deliver unique contributions to the field, to fully benefit from the availability of open-source software, and to use these tools to their fullest extent with competence and precision.

Following-up on the previous development training organized in early 2013 at ICTP, this advanced training will strongly focus on lowering the barrier to learn how to program within the Quantum ESPRESSO distribution. Quantum ESPRESSO is recognized to be one of the most popular packages for electronic-structure calculations worldwide, and it has been under continuous development since many years, thanks to its open-source nature and great community support.

Objectives of the workshop are:
- Enabling participants to close the gap between the theory and the implementation of Kohn-Sham DFT.
- Understanding the fundamentals of the most common codes for electronic-structure calculations, such as the setup of simulation environment and potentials, self-consistent solvers and energy functionals.
- Analyzing existing post-processing extensions to acquire experience about most common strategies for achieving a modular, extensible and reusable new feature.
- Identifying the major components of the Quantum ESPRESSO distribution that are relevant while designing a post-processing extension, including the phase of integration to the existing code.
- Expanding and consolidating a community of researchers who are comfortable with the internal workings of a complex software for electronic-structure calculations.

The event is aimed to a selected group of developers. Participants are expected to follow the (on-line) pre-course material that will be provided to guarantee an adequate preparation to both theoretical and practical aspects of the workshop. Main part of the laboratory session will see participants working closely with world-class experts with the final goal of implementing two additional new features into the official distribution of Quantum ESPRESSO. The organizers target a successful event where the new development will be submitted for publication in a computational physics peer-reviewed journal, after the completion of the workshop.

Participation:
Applicants from all countries that are members of the United Nations, UNESCO or IAEA may apply. All participants are expected to cover their travel and living expenses, as free lodging will be provided in the ICTP guest house. The selection is restricted to people with experience on DFT theory that demonstrate to fulfill the following requirements: good knowledge of Linux shell environment, basic knowledge of the FORTRAN programming language, basic knowledge of the Quantum ESPRESSO package or similar packages for electronic structure calculation based on DFT. As it will be conducted in English, participants should have an adequate working knowledge of this language. There is no registration fee.

Secretariat:
e-mail: smr2643@ictp.it   Telephone: +39 040 2240 484 ICTP   Home Page: www.ictp.it

Directors:

Stefano de Gironcoli
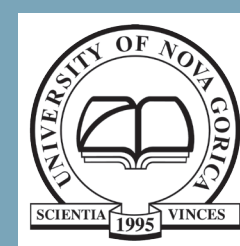(SISSA/DEMOCRITOS)

Paolo Giannozzi
(University of Udine)

Emine Kucukbenli
(EPFL)

Layla Martin-Samos Colomer
(University of Nova Gorica)

Internal Organizer:

Ivan Girotto
(ICTP)

In collaboration with:

SISSA
ma per seguir virtute e canoscenza

DEMOCRITOS
DEmocritos MOdeling Center for Research In aTOmistic Simulation
IOM

UNIVERSITAS STUDIORUM UTINENSIS

UNIVERSITY OF NOVA GORICA
SCIENTIA 1995 VINCES

How to apply for participation

The Online Application can be accessed at the activity website: http://agenda.ictp.it/smr2643. Comprehensive instructions will guide you step-by-step on how to fill out and submit the application form.
The Application includes a brief questionnaire to be filled in and uploaded. Applications without the completed questionnaire will not be considered.

DEADLINE
9 September 2013