



The Abdus Salam  
**International Centre  
for Theoretical Physics**

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## "Advanced Quantum ESPRESSO Developers' Training"

19 - 30 January 2015

Trieste, Italy

In collaboration with the Quantum ESPRESSO Foundation and CECAM, the Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy, is organizing an **Advanced Quantum-ESPRESSO Developers' Training Workshop** to be held in Trieste from 19 to 30 January 2015.

The rapid development of computer technologies, combined with the current state of 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. On the other hand, 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 activities organized in 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 contiguous 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 features,
- 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, small group of scientists with relevant experience in scientific code development. Prior to the event, all the selected participants are requested to follow 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 the participants working closely with world-class experts with the final goal of implementing an additional, new feature into the official distribution of Quantum ESPRESSO. The organizers target at a successful event whose advances 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 attend the Workshop. Upon evaluation of the application forms and related questionnaire, the Organizers will select a limited number of participants.

Potential candidates will have experience on DFT theory, and 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.

As a rule, travel and subsistence expenses of the participants should be borne by their home institutions. Every effort should be made by candidates to secure support for their fare (or at least half-fare). Limited funds are available for some participants, who are nationals of, and working in, a developing country. There is no registration fee.

**How to apply for participation:** until 30 October 2014, candidates can access the [Online Application](http://indico.ictp.it/event/a14257) at the activity website: <http://indico.ictp.it/event/a14257>. 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.

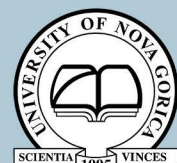
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Trieste, September 2014



### Organizers:

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(SISSA)

**Paolo Giannozzi**  
(University of Udine)

**Emine Kucukbenli**  
(EPFL)

**Layla Martin-Samos Colomer**  
(University of Nova Gorica)

**Ari Paavo Seitsonen**  
(Ecole Normale Supérieure)

### Local Organizer:

**Ivan Giroto**  
(ICTP)

### Instructors:

**Alexander David Hernandez-Nieves**  
(Bariloche Atomic Center, Argentina)

**Javier Daniel Fuhr**  
(Bariloche Atomic Center, Argentina)

**DEADLINE**  
**30 October 2014**

**Workshop Webpage:**

<http://indico.ictp.it/event/a14257>