Workshop on Computer Programming and Advanced Tools for Scientific Research Work

(11 – 22 March 2013)

& Quantum ESPRESSO Developer Training

(25 - 28 March 2013)

(Miramare - Trieste, Italy)

The Abdus Salam International Centre for Theoretical Physics is organizing a *Workshop on Computer Programming and Advanced Tools for Scientific Research Work* to be held at ICTP, Trieste, Italy from 11 to 22 March 2013 followed by a Quantum ESPRESSO Developer Training.

Modern scientific research work involves the use of computers for simulation, modeling, data processing and visualization. The complexity of those calculations favors using tools, packages or frameworks that provide domain specific scripting, modular software design and code reuse. Often large parts of the work can be implemented in a script language, with time critical operations offloaded to external libraries or modules written in Fortran, C, or C++. In step with this, modern multi-core architectures or accelerators like GPUs may be needed.
In all of these cases, a good understanding of performance issues like when to use scripting and when compiled code or what kind of algorithm to choose (for good performance and memory scaling with problem size) is required. Similarly, knowledge of effective multi-core parallel programming and a clean memory management has to be acquired and applied.
This hands-on workshop focuses on sharing best practices and building fundamental skills in creating and enhancing modular, reusable and extensible software along with training in selecting and using adequate high level tools for scientific research work. Emphasis is also given to using modern collaborative software management tools and including facilities for validation and embedded documentation of newly written or added software.

Topics of the working sessions:
- Scripting for scientific computing (e.g. Python)
- Writing modular, extensible, and reusable code
- Computer architecture and memory hierarchy of multi-core systems.
- Design of scientific software for clean memory management, efficient I/O, effective data structures and well scaling algorithms
- Multithread and SIMD programming (OpenMP, OpenCL)
- How to build complex software packages using multiple programming languages
- Debugging and profiling serial and multithreading software
- Use of scientific libraries for linear algebra operations and signal processing
- Effective use of source code management systems
- Building unit and regression tests suites
- Use of tools for extracting embedded documentation
- Usage of data processing and visualization tools for scientific research

Requirements: strong knowledge of Linux command line environment and good knowledge of one of the following programming languages: FORTRAN, C, or C++.

The *optional* Quantum ESPRESSO training *during the third week of the activity* is mainly aimed at scientific developers interested in the Quantum ESPRESSO distribution.
The topics presented and directly applied will be:

1) Fundamentals of the Quantum ESPRESSO suite of codes
    a) Source code management system
    b) Configuration and Packaging
    c) Development methodology

2) Computational aspects and general structure of the software package

3) Best practices for developing with Quantum ESPRESSO and integrating external packages

Further information will be available through the ICTP Network system and the Quantum ESPRESSO website (www.quantum-espresso.org)

Co-organized by

QUANTUM ESPRESSO FOUNDATION
foundation.quantum-espresso.org

Organizers

S. de Gironcoli
(SISSA Trieste, Italy)

P. Giannozzi
(University of Udine, Italy)

I. Girotto
(ICTP Trieste, Italy)

D. Grellscheid
(University of Durham, UK)

A. Kohlmeyer
(ICTP Trieste, Italy)

C. Onime
(ICTP Trieste, Italy)

U. Singe
(ICTP Trieste, Italy)

P. Umari
(University of Padova, Italy)

Participation
Applicants from all countries that are members of the United Nations, UNESCO or IAEA may attend. As it will be conducted in English, participants should have an adequate working knowledge of this language. Although the main purpose of the Centre is to help research workers from developing countries through a programme of training activities within a framework of international cooperation, a limited number of students and scientists from developed countries are also welcome to attend.
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). However, limited funds are available for some participants, who are nationals of, and working in, a developing country. Such support is available only to those attending at least the entire first part of the activity (March 11th to 22nd). Application for only the second part of the activity (March 25th to 28th) are accepted as well. *There is no registration fee.*

HOW TO APPLY FOR PARTICIPATION
The Online Application can be accessed at the activity website: http://agenda.ictp.it/smr.php?2503. 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

6 January 2013