Workshop on Advanced Techniques for Scientific Programming and Management of Open Source Software Packages

10 - 21 March 2014

followed by

LAMMPS Users and Developers Workshop & Symposium

24 - 28 March 2014

Trieste, Italy
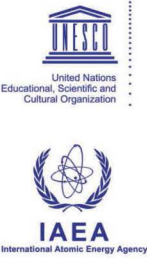
The Abdus Salam International Centre for Theoretical Physics is organizing a *Workshop on Advanced Techniques for Scientific Programming and Management of Open Source Software Packages*, to be held at ICTP (Trieste, Italy) from 10 to 21 March 2014, followed by a one-week *LAMMPS Users and Developers Worskhop and Symposium.*

Modern scientific research work involves using computers for simulation, modeling, data processing and visualization. The growing complexity of those calculations favors using software packages that provide an abstract interface to computations through scripting language interfaces, modular software design, and code reuse. Such design patterns also facilitate transparent optimizations for modern multi-core architectures or accelerators, and specialization of contributors to subsets of a package program. Software package developers therefore need to learn how to work effectively in a collaborative environment.

This Hands-on Workshop focuses on disseminating best practices and building fundamental skills in creating, extending and collaborating on modular and reusable software frameworks with a scripting language interface. The curriculum also covers using modern collaborative software management tools, testing frameworks, and embedding structured documentation into software packages.

The *optional* **LAMMPS** *Users and Developers Workshop and Symposium* during the third week takes the LAMMPS Molecular Dynamics package as an example and provides specialized training for computational scientists that already are or want to become LAMMPS developers. The training will consist of lectures on the LAMMPS software overall design and implementation details as well as hands-on tutorial sessions by LAMMPS experts and developers.

PARTICIPATION

Applicants from countries which are members of the UN, UNESCO or IAEA may attend. The Workshop will be conducted in English, so participants should have an adequate knowledge of that language. **Other essential requirements are a strong knowledge of the Linux command line environment, as well as a good knowledge of one of the following programming languages: FORTRAN, C, or C++.**

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 graduate students and post-doctoral scientists from developed countries are also welcome to attend. **For organizational reasons, we will be able to accept only a limited number of participants**.

As a rule, travel and subsistence expenses of the participants should be borne by their 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 to be selected by the Organizers, 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 (10 - 21 March). Applications for the second part of the activity only (24 - 28 March) are accepted as well, with no financial support. There is no registration fee.**

How to apply for participation: until 1 December 2013, the online application form can be accessed at the activity website: *http://agenda.ictp.it/smr.php?2574*. Once in the website, comprehensive instructions will guide you step-by-step, on how to fill out and submit the application form. **The application process includes** a brief questionnaire **to be filled in and uploaded. Applications without the completed questionnaire will not be considered.**

Participant selection criteria: due to the advanced nature of the workshop, only sufficiently qualified applicants are selected for participation based on the submitted application materials. **Preference** will be given to applicants that can document their involvement in package software development or being an experienced user with the intent or need to actively participate in development. Participation at the LAMMPS workshop in addition requires documented knowledge in molecular dynamics simulations, since the workshop will focus on technical aspects only.

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DEADLINE
for submitting applications:

1 December 2013

For further information, please see the

Workshop website:

http://agenda.ictp.it/smr.php?2574