United Nations
Educational, Scientific and
Cultural Organization

ICTP - East African Institute
for Fundamental Research
under the auspices of UNESCO

Collaborative Research
in
Atomistic/Molecular Modeling

Announcement:
Invitation for Collaborative Research
September 08, 2021

Background

The ICTP Trieste Italy in collaboration with CINECA is providing computational resources to ICTP-EAIFR researchers and their affiliates for research which require state-of-the-art HPC technology and which is capable of using a Tier-0 parallel infrastructure for scientific computing, efficiently. Resources are made available on the Marconi-100, where 90% of the compute capability is given by Volta NVIDIA GPUs and, therefore, priority is attributed to projects that can really benefit from these. To this end, researchers in Africa with matching interests who wish to collaborate with scientists at ICTP-EAIFR are invited for online collaborative research.

Who should apply?

Lecturers/researchers at the University of Rwanda, Institutions/agencies in Rwanda, and other African countries who carry out research in atomistic/molecular modeling. These include those who use electronic structure methods (DFT, HF, etc.) or sampling methods such as Monte Carlo and Molecular Dynamics in different fields: Condensed Matter Physics, Materials Science, Computational/Quantum Chemistry, Computational Drug Design and others areas. Postdoctoral fellows and advanced post-graduate students at the masters or doctoral levels working in Africa can also apply. The application is for collaborative research which requires large amounts of computational resources. Resources are provided by the ICTP Trieste Italy in collaboration with CINECA. Selection of successful collaborators will be based upon mutual interests at EAIFR, availability of resources, and broad scope of the work for which computer time is needed. Preference will be given to applicants whose research require state-of-the-art HPC technology and capable of efficiently using a Tier-0 parallel infrastructure for scientific computing. This includes, but is not limited to research that apply the following codes: CP2K, Quantum Espresso, GROMACS, AMBER, LAMMPS, i-PI, MCTDH, SIESTA, YAMBO.

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How to apply:

To apply, **fill out the Google form at https://forms.gle/yAzAjLJLx75RGB9u6** In addition, please send an uploaded copy of your CV and a one-page pre-proposal to cramm@eaifr.org. The pre-proposal should include responses to the following questions:

1. What is the scientific problem you are trying to solve?
2. How is the problem related to atomistic/molecular modeling?
3. How will you use high performance computational resources to solve the scientific problem? (For example, which calculations will you perform, with what codes?)
4. Describe your previous experience with computer simulations with a particular focus on the scientific problem described in your proposal
5. On which computers are you currently carrying out your computation? Where were you carrying them out in the past?
6. Estimate of the compute time (core-hours) needed on the facility/facilities mentioned in (5) above
7. Which scientist at EAIFR do you plan to collaborate with?

The **first deadline is 18/September/2021** after which applications will be considered on a first-come, first-served rolling basis.

For further information contact: cramm@eaifr.org