The Maison de la Simulation (MdS) and the Institut du développement et des ressources en informatique scientifique (IDRIS) are now hiring a scientific programmer for 2 years.

This position is associated with the EINFRA-5 E-CAM centre of excellence, as described in the E-CAM Grant Agreement N° 676531 and associated annexes, and in particular the role described there of the CNRS partner and of the FR-IDF CECAM Node. The researcher will report to the chief E-CAM scientific contact person at MdS/IDRIS, in connection with the E-CAM software manager in Jülich (Germany). **He will be located at IDRIS, Orsay, France**.

This role offers candidates the opportunity to work on scientific as well as real industrial problems in an environment that promotes individual initiative and active professional development and that conforms to the standards of the European Charter for Researchers. He/she will benefit from the favourable HPC environment at IDRIS and MdS.

The goals of E-CAM will be achieved through the:
1. Development, testing, maintenance, and dissemination of software targeted at end-user needs;
2. Training of current and future academic and industrial researchers through Extended Software Development Workshops;
3. Consultancy to support both large multinationals and SMEs in their use of simulation and modelling.

Principal Duties and Responsibilities

The post holder will be required to support E-CAM’s activities and collaborate with its teams in the:
- Development, testing and documentation of E-CAM software and its deployment on massively parallel computation platforms (through testing and optimization of association modules).
- To fully participate in and occasionally lead the E-CAM Extended Software Development Workshops and follow up activities.
- Support the production of E-CAM deliverables and reporting in the form and timing agreed with the European Commission.

Applications will be assessed on the basis of the following selection criteria:

- Master (MSc) or equivalent in Computational Science or Informatics or PhD in a relevant discipline in Chemistry, Physics, Mathematics or Engineering.
- Proven excellent skills in software architecture including high-level scientific programming, the implementation of algorithms in Fortran, C or C++, and their deployment on massively parallel computational platforms with OpenMP and/or MPI.
- Excellent communication skills – written and verbal
- Ability to work in an international collaborative environment and travel when required

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1 www.idris.fr
E-CAM Centre of Excellence Summary

E-CAM will create, develop and sustain a European infrastructure for computational science applied to simulation and modelling of materials and of biological processes of industrial and societal interest. Building on the already significant network of 15 CECAM\(^2\) centres across Europe and the PRACE\(^3\) initiative, it will create a distributed centre for simulation and modelling across the electronic, molecular and continuum length scales. It will build on the considerable European expertise and capability in this area of significant industrial and scientific relevance. E-CAM has the potential to make a very strong impact on the European economy through the development of a key industrial capability in the rapidly developing area of technological innovation through computer modelling.

The ambitious goals of E-CAM will be achieved through three complementary instruments: the development, testing, maintenance, and dissemination of software targeted at end-user needs; the advanced training of current and future academic and industrial researchers to exploit this software; and the multidisciplinary, applied consultancy to support industrial end-users (both large multinationals and SMEs) in their use of simulation and modelling. The creation and development of this infrastructure will also impact academic research by creating a training opportunity for young researchers in aspects of computational science that will enhance their domain expertise. It will also provide an environment for the long-term optimisation and maintenance of academic codes and will help to ensure that, in future, these codes are properly exploited by industry.

Based on requests and in discussions with its end-users, E-CAM will deliver new software in the area of the simulation and modelling of atoms and molecules in condensed phases to be applied to practical and immediate problems. E-CAM will create over 120 new, robust software modules in the areas of: electronic structure calculations; classical molecular dynamics; quantum dynamics; mesoscale and multi-scale modelling. These modules will be interfaced with and will significantly extend existing standard packages in this arena. The modules will be written to run with maximum efficiency on hardware with different architectures, available at four PRACE centres and at the Hartree Centre for HPC in Industry. The modules will form the core of a software library (the E-CAM library) that will continue to grow and provide benefit well beyond the EINFRA-5 funding period. E-CAM will be sustainable beyond the life of the EC funding period and it will eventually become an independent, well-established European network for simulation and modelling.

\(^2\) CECAM (Centre Européen de Calcul Atomique et Moléculaire, see www.cecam.org) was founded in Paris in 1969 by Dr. Carl Moser and is devoted to the promotion of fundamental research on advanced computational methods and to their application to important problems in frontier areas of science and technology. Today CECAM is structured as 18 trans European nodes (plus one node in Israel) with its headquarters in Lausanne.

\(^3\) PRACE (see www.prace-ri.eu) is established as an international not-for-profit association. It has 25 member countries whose representative organizations create a pan-European supercomputing infrastructure, providing access to computing and data management resources and services for large-scale scientific and engineering applications at the highest performance level.