

The European Theoretical Spectroscopy Facility opens new doors to numeric simulations

At the core of the central node

This first success story has been written in collaboration with Xavier Gonze, Gian-Marco Rignanese and Jean-Christophe Charlier, three Professors of the “Université catholique de Louvain” in Belgium, where the central core node of a distributed e-research infrastructure has recently been created. They tell us the story of a new type of research infrastructure: an infrastructure spreading across 10 European research institutions and involving more than 120 scientists; an infrastructure connecting experimentalists and theoreticians alike; an infrastructure selected within the Research Infrastructure Activity of the Seventh Framework Programme.

A network of excellence creates an electronic distributed research infrastructure

The story began about 20 years ago by an incipient collaboration between European researchers in the field of Condensed Matter Theory : Rodolfo Del Sole in Italy, Lucia Reining in France, Rex Godby in the UK, Angel Rubio in Spain and the others, increased and extended their collaboration through European training network projects such as “Nanophase” of the Fifth Framework Programme and “Nanoquanta Network of Excellence” of the Sixth Framework Programme.

From its very beginning, in 2004, the Nanoquanta project aimed at a long-term, sustainable outcome. Two options were considered: (1) the introduction of a European Master and (2) the realisation of a virtual research infrastructure. After the first year of the project, the second option was selected.

Nanoquanta’s “final product” is a facility bringing to its users - experimentalists or industry researchers - frontier-of-knowledge spectroscopy simulation tools. This facility, called European Theoretical Spectroscopy Facility (ETSF), is fully operational since March 2008. It consists of 10 core nodes, the central one being based in Louvain-La-Neuve, Belgium.

The ETSF has been structured in a similar manner to a synchrotron (i.e. ESRF, Soleil, etc) with beamlines. Each beamline covers a field of application of theoretical spectroscopy such as optics, quantum transport, time-resolved and photo-emission spectroscopies. “The concept of beamline was familiar to Lucia Reining because her husband, an experimental physicist, used to work in big experimental research infrastructures” tells us Xavier Gonze.



UCL Picture, seen left to right: Xavier Gonze, Gian-Marco Rignanese and Jean-Christophe Charlier

Two ETSF calls for proposals have already been launched and an Executive Director plus a Project Manager will soon be recruited. In order to continue the development of the infrastructure and answer to users demands on a European scale, funding beyond the Nanoquanta project was necessary.

The submission of an e-research infrastructure proposal

Two people were working full-time on the administrative management of the Nanoquanta network: Tony Patman in the UK and Gaëlle Bruant in France. They were actively looking for opportunities in the Seventh Framework Programme and they proposed to submit a proposal under the Research Infrastructure Activity of the Seventh Framework Programme.

A meeting was organized between a delegation of Nanoquanta and European Commission representatives. Their reaction was really positive and it was thus decided to submit an e-RI proposal under the action line 1.2.2 e-Infrastructure for scientific communities published on December 22, 2006.

Rex Godby in York coordinated the submission which was prepared jointly thanks to modern communication tools. In particular "Google doc", a free web-based word processor and spreadsheet was used to work together online on a unique document and to vote via a spreadsheet system. In addition Skype was used for audio-conferences.

A research infrastructure at the service of its users

The selection of the proposal "European Theoretical Spectroscopy Facility I3" will allow the ETSF members to further develop software and to answer a maximum number of user's proposals.

About 40 proposals were received in the last ETSF call. A dozen of them have been selected for direct support, and a similar number for trainings. Xavier Gonze explains that in the first case, the numerical simulations are done for the users. For example, they had the request from a mineralogist, who asked under which pressure a specific mineral would change from insulator to conductor. Since the mineralogist is lacking the expertise to use the advanced ETSF software applications, a scientist from ETSF will use the software and will make the necessary calculations. In the second case, the goal is to help those interested to use CORRECTLY the developed software. It is extremely important, adds Jean-Christophe Charlier that users do not use software as a black box, but that they really learn how it works.

And for the future...

The ETSF members would like to continue to improve the services of the research infrastructure, to reach wider scientific communities and to establish ETSF as an independent legal entity.

Additional information

ETSF website: <http://www.etsf.eu>

Nanoquanta website: <http://www.nanoquanta.eu>

Physical Chemistry and Physics of Materials Laboratory of UCL: <http://www.pcpm.ucl.ac.be>

Prof. Xavier Gonze: <http://www.pcpm.ucl.ac.be/people/people.php?id=200>

Prof. Gian-Marco Rignanese : <http://www.pcpm.ucl.ac.be/people/people.php?id=4400>

Prof. Jean-Christophe Charlier : <http://www.pcpm.ucl.ac.be/people/people.php?id=1009>

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