The challenge of creating a European domain on Theoretical Chemistry and Computational Modeling.

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Building up a Joint Doctorate at the European level is always a challenge, because you need to harmonize very different approaches and very administrative constrains.

But in the domain of the Computational Chemistry is even more complicated, simply because this domain is enormous, going from extremely small systems, as in astrochemistry, to huge compounds, like proteins, in biochemistry.

The problem is that the methodology to treat very small molecular systems is totally different from the one needed to describe macromolecules like polymers, enzymes or proteins. In practice is unrealistic trying to have experts able to cover the whole domain.
What to do?

Trying to give a practical answer to such a simple and, at the same time extremely complicated question we have launched an Erasmus Mundus (now Erasmus+) European Master on Theoretical Chemistry and Computational Modelling (TCCM) and Joint Doctoral Program on TCCM.
http://www.emtccm.org/

The problem is complicated, but the motivations are very clear:

★Crucial role of Computational Chemistry and Modelling on the development of modern chemistry, physics, biochemistry, pharmacy and material science.
(J.A. Pople and Walter Kohn. Nobel Prize in Chemistry 1998. M. Karplus, M. Levitt, A. Warshel. Nobel Prize in Chemistry 2013).
"Quantum chemistry is today used within all branches of chemistry and molecular physics [and] affords deeper understanding of molecular processes that cannot be obtained from experiments alone."

★Need to create a European offering in this important area

★Need of having a minimum critical mass

★Need of making a rational offering in a strong interdisciplinary field (from astrochemistry to biochemistry) IMPOSSIBLE to cover not only by a single institution but even by a reduced number of them.

To be honest, in our efforts to put together a coherent offer at the Doctorate level, our previous experience at the Master level was crucially important.

Challenges

How to offer a European Integrated Doctorate Programme based on PhD Thesis done in co-tutelle between two Universities ?

But ensuring at the same time a minimum homogeneity of the level reached and a substantial mobility within the Consortium.

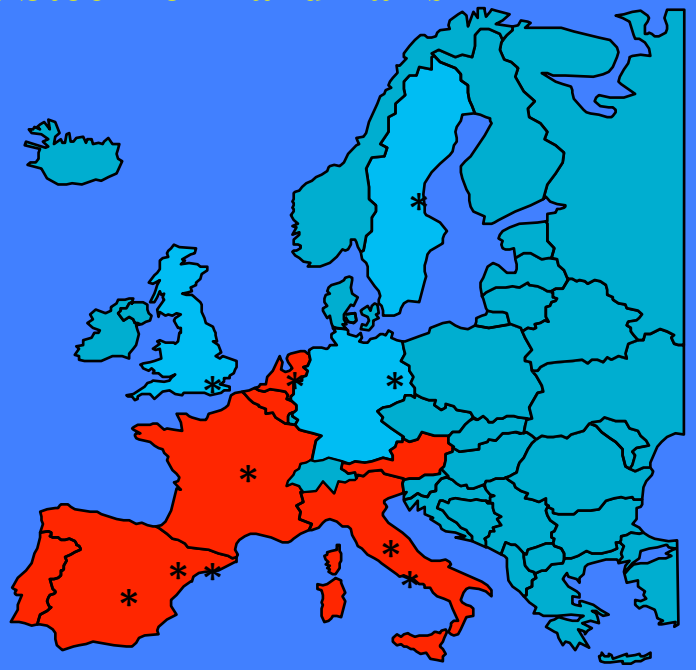
Going beyond the conventional scheme of a Doctorate through a well defined program of common activities; but not training courses (already done at the Master level). i.e., What does our proposal offer that makes it different from existing offers?

What is its "European flavor"?

The Consortium

We do not start from scratch. Previous experience in an Erasmus Mundus Master on TCCM with Eurolabel of ECTNA

Consortium: 12 European Universities from 7 countries and 14 associate entities, mainly from the private sector, including two supercomputing centers, BSC and CINECA and two Universities: Stockholm and Paris-Saclay.



Main Objetives

★ **Working in an truly European atmosphere. The ESRs will develop their research in at least *three different* environments.**

★ **The possibility of carrying out a multi-scale research, impossible to be attained working only in one center.**

★ **A multicultural and multilingual experience**

★ **An important mobility inside and outside Europe (Minimum of two presentations in International Symposia).**

★ **Regular Quality control not only of the ESR, but of the supervisors together with a critical evaluation of the research project and its development**

Besides the scientific research associated with the PhD Thesis we provide :

- **Training in reporting**
- **Supervision skills (of master students)**
- **Teaching in hands-on activities**
- **Project management**
- **Language training**
- **Young Researcher Forum**
- **Communication to the general public and non-technical audiences**
- **Communication with students and young scientists**
- **Events Organization**

Very important: All the details matter, even when they look insignificant matter. It is not enough to be "Very good" It has to be "Excellent", if one is not above 95/100 it is out and to get 5/5 in the different sections is almost mission impossible! 4.7 out of 5 is already excellent or close.

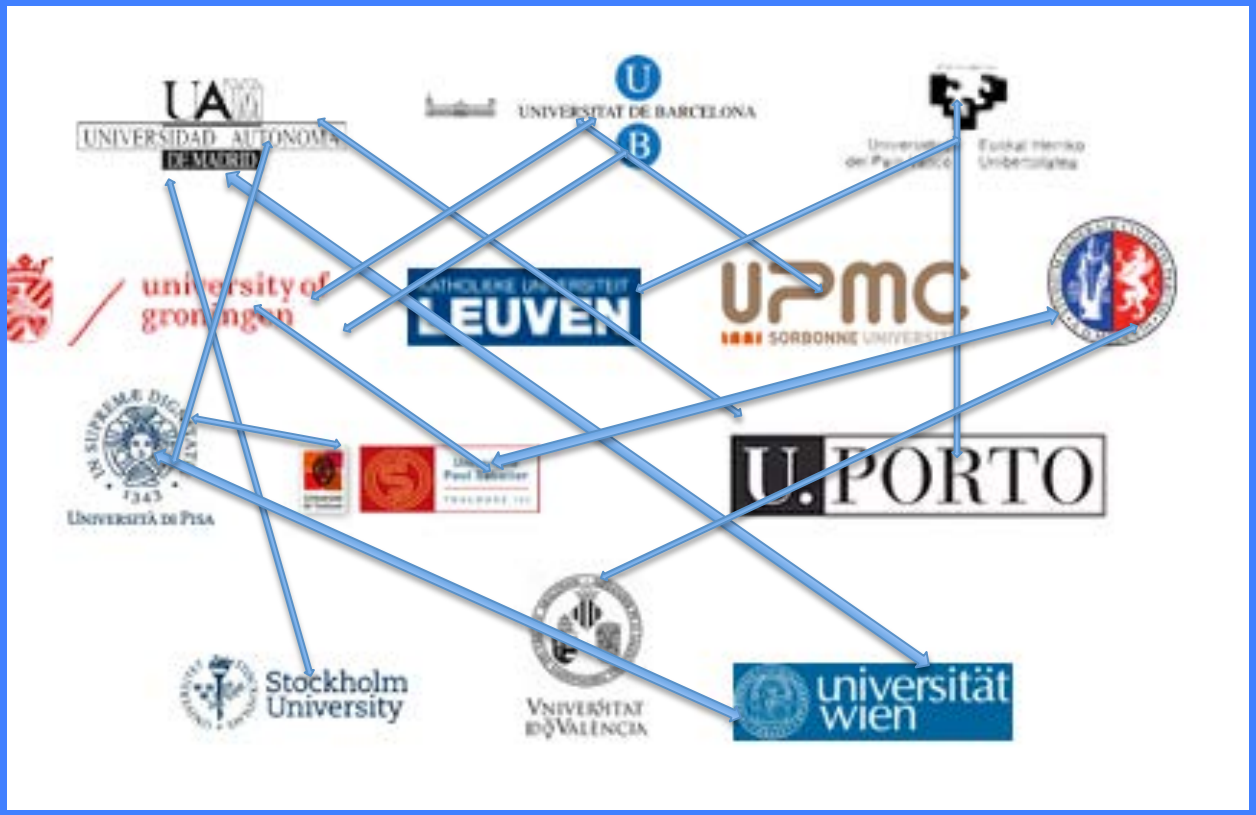
Corollary: It is not enough to have a scientifically excellent project !!!
The help of a competent and experienced scientific manager can be crucial.

In my experience: to have both, a very solid scientific together with a good management (including administration, coordination, etc.) are fundamental.

Joint Doctorate

A more complicated structure. Has to be established on the basis of cotutelle agreements involving two Universities (very rarely more than two).

The great variety of possible research topics requires larger consortia:



It provides:

★ Participation in a Europe-wide training environment

★ Fully coordinated follow-up of the training and the research activity of the doctoral candidates

★ Contact with non-academic Associated Partners (supercomputing centers and industries in which modelling is a fundamental activity)

★ A unique research environment. A multi-scale approach

★ A multicultural and multilingual training.

★ A significant mobility (perhaps too much)

The challenge:

How it can be offered an integrated Doctorate program including students who work in PhD Thesis carried out in co-tutelle by two partners?

The program must contain common activities, but they should not be regular teaching activities (supposed to be covered at the Master level).

A Common *Core Course* mandatory for all the PhD students and focused on transferable skills:

i) Communication in scientific research, including both scientific writing and oral presentations
ii) formulation of a research work plan, definition of objectives, timing, testing hypotheses
iii) Literature and searching of scientific information and patent review
iv) group working,
v) preparation and delivering of (written and oral) progress reports
vi) Entrepreneurship.

Three Annual International workshops mandatory for all the PhD students

Three Annual International Schools on High Performance Computing

Three Annual Tutorials, devoted to acquire basic knowledge on the use of important codes on the field, and other focused on hot topics closely related to the research lines offered by the network

Quality control

Annually, through the reports of the external experts invited to the annual workshop.

Participation of at least one International Congress or Symposium per year, presenting one communication or poster.

Mandatory publication of at least two papers in peer-reviewed journals along the three-years period.

Before the thesis can be deposited at the Universities in which it is going to be defended, it is mandatory: i) a report of each of the supervisors ,ii) a report of a responsible of the Institution or company in which the Secondment was carried out, iii) the text of the Thesis and iv) at least the report of one external (to the consortium) expert on the thesis. This material will be then examined by the Supervisory Board and if approved, the Thesis could be deposited to start the administrative steps for its defense.

Core Course Goals **(*https://emtccm.qui.uam.es/?page_id=1583*)**

Two weeks:

i) School on Sustainable Entrepreneurship, directed by Porf. A. Laganà

ii) Supercomputing. Drs. A. Luna and P. Sanz

iii) Tutorial on Scientific Publication. Rob Van Daalen from Elsevier

iv) Workshop on Communication in Science (two sections including a practical work done by the ESRs. **Scientific information Unit UAM**

v) Doctorate Scientific Workshop. Two plenary lectures and 34 oral communications by PhD students from 13 European Universities of nine different countries

School on High Performance Computing-1

Organized by the University of Barcelona and the Barcelona Supercomputing Center. Focused on parallel computing (the two most important programming strategies: MPI for the distributed-memory environments, and OpenMP for the shared-memory architectures were analyzed) Organized through a combination of formal lectures and practical/programming sessions designed to reinforce the most important concepts.

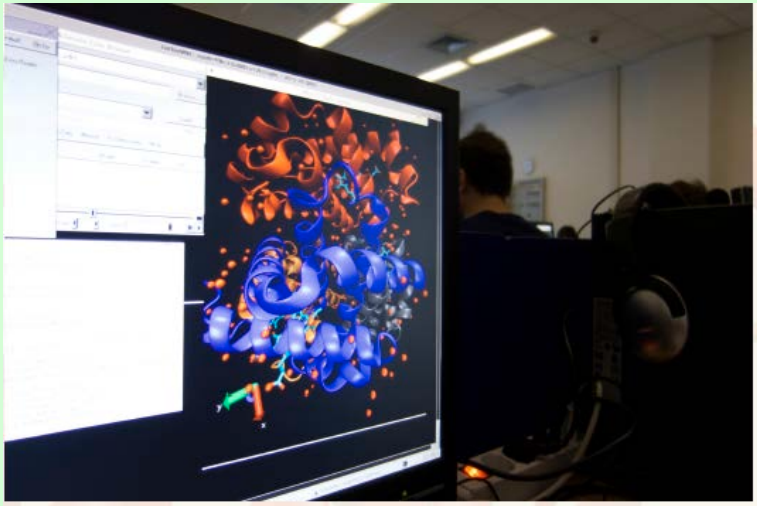
Delivered by the staff of the BSC and members of the Polytechnic University of Catalonia. Included a guided visit to the installations of the Barcelona Supercomputing Center.

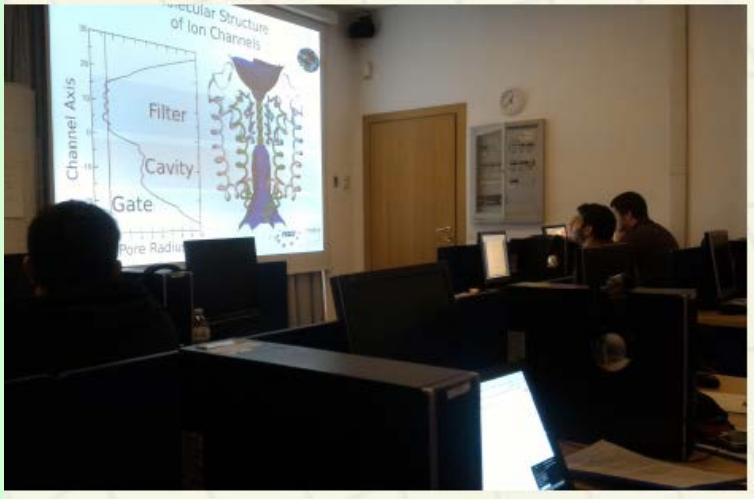
School of scientific visualization

took place at the Cineca venue in Rome.

The aim of the school was to offer a general view of the available tools used for scientific data visualization and graphic representation.

professors and experts on scientific visualization and virtual reality showed, through theory and practical exercises, the use of various opensource software



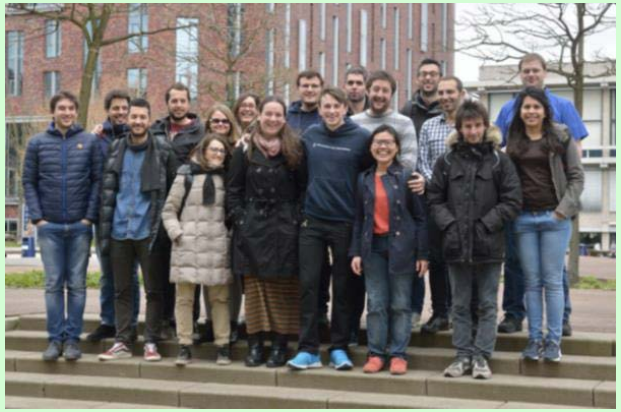


SCM Tutorial

Organized by SCM and the Univ. of Groningen.
Basic knowledge on the use of the modelling suite ADF (Amsterdam Density Functional) code.

Morning lectures on the different capabilities of ADF
Afternoon hands-on sessions, to see the real capabilities of the ADF code.

Members of the staff of ADF and leader scientists from the Vrije Universiteit Amsterdam as well as Rijksuniversiteit Groningen.
After the tutorial the ESRs acquired new knowledge on:
1. The fundamentals behind density functional theory (DFT) and its time-dependent version (TD-DFT)
2. How to deal with chemical reactivity based on DFT
3. How to treat relativistic effects within DFT



SHARC Tutorial

Aim: get familiarized with the SHARC code, which deals with multistate phenomena and non-adiabatic dynamics using surface-hopping.

Organized as a workshop around the general topic of "excited state dynamics", with emphasis on surface-hopping.

Morning; lectures given by the local organizers

Afternoon: practical exercises directly done by the ESRs

Friday, three renowned speakers gave extensive lectures on methods which go beyond the concept of surface hopping, adding more quantum effects, and interpretation of experiments.

Final round table with the ESRs and all lecturers about the future of the field, important questions to be solved, future challenges and interplay theory-experiment.

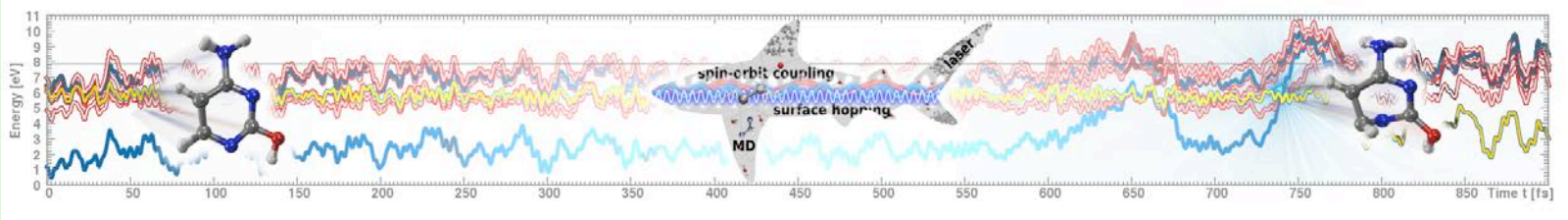
After the workshop the ESRs acquired new knowledge on:

1. important effects that take place when molecular systems are electronically excited

2. Available theories to model excited state dynamics

3. How theoretical results can be compared with experimental observables

THEORETICAL CHEMISTRY AND COMPUTATIONAL MODELLING



Outreach Activities. The week of Passion for Knowledge

Pictures of the students talking with the Nobel Laureate, Prof. Martin Karplus

Students with Dudley Hershbach (Nobel Prize in Chemistry 1986)

Some weak points

The mandatory activities are important as well as the mobility. However, both should be carefully harmonized. In our present implementation this was a weak point.
The scientific work requires a continuous attendance, in some aspects a kind of routine, that should not be broken very often as it happens in our implementation because we had ten mandatory activities.

What to do in future editions? We should not decrease the number of common and mandatory activities, neither the mobility, but it is possible to concentrate three of these mandatory activities in the same period organizing them in a sequential manner, though in different places. In this way the periods of scientific work without interruptions will be longer.