ICS Summer School 2015

Scientific Trends at the Interfaces
Mathematics – Chemistry – High Performance Computing

Organisers: Eric Cancès, Yvon Maday, Jean Philip Piquemal

July 15th – August 14th, 2015, Roscoff - France

Science at the interfaces

A multidisciplinary way of learning

Improve your curriculum

Discover the challenges of tomorrow

Welcome to ICS Summer School

Experience a multidisciplinary way of learning, explore areas outside your major and enjoy international campus life at the UPMC Marine Station in Roscoff.

Ideally located on the Northern Brittany coast, the renowned research and training centre is jointly operated by the French National Centre for Scientific Research (CNRS) and the Pierre & Marie Curie University (UPMC).

Read more on the Summer Schools at :

ics.sorbonne-universite.fr/formations/ecole-dete.html

ICS Commitment to Teaching

For talented undergraduate students who wish to broaden their experience, our unique four weeks summer program offers challenging opportunities.

We are committed to provide the best level of teaching and academic environment in view of creating a community beyond the classroom and build life lasting friendships.

Full sponsorship may be provided thanks to French state funds awarded to CALSIMLAB under the *Investissements d'Avenir* programme, reference ANR-11-IDEX-0004-02

Students working on an educational task with YASARA software (Wikimedia Commons)

''Interdisciplinary programmes are a unique opportunity to achieve scientific breakthroughs in numerical simulations''

Pascal Frey,
Programme Director, ICS Summer School

A stimulating experience

ICS invites motivated undergraduate and recent graduated students to apply.

We select students with excellent academic results and who wish to experience a different style of learning with world-class faculty.

The Summer School Programme allows students to enlarge their curriculum and explore areas at the interfaces between disciplines that are making extensive use of scientific computing and simulation.

Morning classes, afternoon tutorials and seminars by worldwide speakers are scheduled.

Eligibility

The Summer School is for advanced Bachelor's and Master's degree (L3-M2 levels). To apply, students should have completed at least three years of university studies.

Scholarships

A limited number of full/partial scholarships is available. A full scholarship covers tuition fees, accommodation in Roscoff.

Language requirements

Students from all over the world are encouraged to apply.

All courses are taught in French or English, depending on the audience. Applicants are expected to be fluent in either language in order to follow the lectures and participate to classrooms discussions.

Accommodation

All Summer School students have the opportunity to live on campus hotel. Breakfast, lunch and evening meals (except on Saturdays and Sundays) are included.

Application and registration

To secure your participation, we advise you to apply as soon as possible.
Application form can be filled online from the ICS web site:
http://ics.sorbonne-universites.fr/formations/ecole-dete/inscriptions.html

2015 Summer School Programme

The purpose of these 4 weeks of training is to introduce the mathematical, numerical formalisms and the pre-requisites in chemistry and physics that are necessary to understand the basics of simulation in computational chemistry.

Computational chemistry is a booming area. With nowadays computer power available on desktops, computer clusters and High Performance Computing (HPC) platforms, it is fully sensible to bring in numerical simulation to better understand the complex mechanisms that occur at a quantum mechanical (QM) level of matter. There is a phenomenal increase of applications both in academic research and at industrial centres to improve the design of products such as new materials and new medical drugs. There is thus a pressing need for trained scientists able to act at different levels.

This advance training is open to young and brilliant scientist students (Master, L3, M1 or M2) and does not specifically require prior knowledge other than a solid 3-years scientific university background.

To benefit from this formation, students need to have a strong desire to learn and understand new elements. There will be ample time for filling some gaps in understanding. Instructors will be happy to explain, either in face-to-face discussions or during the tutorial sessions.

The four weeks training will introduce the basic equations of mathematical modelling in quantum chemistry, the different formalisms to simplify these equations and the various assumptions and theoretical foundations that guide them. Once simplified, these equations are very complex and their solutions are still unknown. To deal with them, the only approach is to make numerical simulations on computers. The process to derive the right numerical scheme from the equations is complex and requires much expertise. This process will be explained with emphasis on what is known in terms of matrix algebra and optimisation techniques. As, in the near future, no simulation of any component can be completed at the only quantum level, thus justifying the formalism of multi-scale coupling. It includes methods ranging from classical force fields (or molecular mechanics) to hybrid QM/MM approaches.

The main areas that will be covered include:

- Basic Linear Algebra
- Mathematical Models and numerical methods for Chemistry
- Molecular Dynamics and Force Fields
- Molecular Modelling of Biological Systems
- Advanced Mathematical Models for Dynamical Systems
- Multi-scale Modelling: QM/MM hybrid methods, molecular visualisation and intermolecular forces
- Electronic Structure and Electronic Correlation: Hartree-Fock, Density Functional Theory (DFT), Valence Bond
- Introduction to Quantum Modelling: use of a computer clusters
- Control Theory

Keynote Speakers and Supervisors

Roberto Alvarez-Boto, *PhD student at UPMC*
Roland Assaraf, *Researcher at UPMC*
Eric Cancès, *Professor at CERMICS, Ecole des Ponts-ParisTech*
Emanuele Coccia, *Post-doctoral fellow at UPMC*
Julia Contreras-Garcia, *Researcher at UPMC*
Jérémy Dalphin, *Post-doctoral fellow at UPMC*
Geneviève Dusson, *PhD researcher at UPMC*
Hélène Gérard, *Professor at UPMC*
Nohad Gresh, *Researcher at UPMC*
Tony Lelièvre, *Researcher at CERMICS, Ecole des Ponts-ParisTech*
Antoine Levitt, *Post-doctoral fellow at UPMC*
Yvon Maday, *Professor at UPMC*
Jean Philip Piquemal, *Professor at UPMC*
Peter Reinhardt, *Professor at UPMC*
Julien Reygner, *Post-doctoral fellow at ENS Lyon*
Julien Toulouse, *Professor at UPMC*

Plenary lectures

Plenary lectures are held every morning on weekday and will propose talks on a wide range of topics of importance for Computational Chemistry: from basic linear algebra, numerical methods, mathematical chemistry models to advanced multi-scale modelling and high performance computing techniques.

Full details about the lecturers and speakers will appear in the daily timetable you receive upon registration.

Hands-on simulations

These afternoon sessions are meant to be interactive, educational and, possibly fun.

They will provide various insights and concrete experiences with educational software packages.

Students will be encouraged to develop their intuition and skills by interacting with experienced users in a user-friendly environment. Under the guidance of experts, participants will play and learn by doing.

Students are encouraged to assist and participate actively.

Evening lectures

During the sessions, a few topic-related lectures will take place on evenings, given by invited speakers and faculty members.

These sessions are aimed to enhance your understanding and enjoyment of the programme. Speakers are experts in their field: senior figures from within and beyond the University, Course Directors, and Guest Lecturers from industrial research centres.

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