

# ISCD Summer School 2018

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

Organisers: Eric Cancès, Yvon Maday, Jean Philip Piquemal

July 16th – August 10th, 2018, Roscoff - France





Science at the interfaces

A multidisciplinary way of learning

Improve your curriculum

Discover the challenges of tomorrow

## Welcome to ISCD 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 our Summer Schools Programme at:

[iscd.upmc.fr/training/summer-school](http://iscd.upmc.fr/training/summer-school)

## ISCD Commitment to Teaching

For talented undergraduate and graduate students who wish to broaden their experience, our unique four-week 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, ISCD Summer School

## A stimulating experience

ISCD invites motivated undergraduate and graduate 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/projects and seminars by worldwide speakers are scheduled.

## Eligibility

The Summer School is for advanced Bachelor’s and Master’s degree (L3 to 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, and accommodation in Roscoff.

## Language requirements

Students from all over the world are encouraged to apply.

All courses are taught in 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 found on the ISCD web site:

[iscd.upmc.fr/training/summer-school/applications/](https://iscd.upmc.fr/training/summer-school/applications/) and must be uploaded on the web site.

Contact : [training\\_iscd@upmc.fr](mailto:training_iscd@upmc.fr)

# 2018 Summer School Program

Mathematics – Chemistry – High Performance Computing

**The purpose of these 4 weeks of training is to introduce the mathematical and numerical formalisms together with 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 thanks to nowadays computer power available on desktops, computer clusters and High Performance Computing (HPC) platforms. Numerical simulation provides better understanding of the complex mechanisms that occur at the atomic scale, where quantum mechanics (QM) comes into play. There is a phenomenal increase of applications both in academic and industrial research centers, ranging from the prediction of the properties of new materials and nano-objects, to drug design. There is thus a pressing need for trained scientists able to act at different levels: mathematical modelling, numerical methods, computer implementation, post-processing and analysis of the simulation results.

**This advance training is open to young, brilliant students (Master (M1 or M2), first years of PhD, excellent L3 students). No specific prior knowledge besides a solid undergraduate scientific background is required. This multidisciplinary program aims at attracting students from different fields (mathematics, chemistry, physics, mechanics).**

To benefit from this program, students need to have a strong desire to learn and understand new topics. There will be ample time for filling some gaps in the different disciplines. Instructors will be happy to give further explanations, either in face-to-face discussions or during the tutorial sessions.

The four-week training will introduce the basic equations of mathematical modelling in quantum chemistry, the different approaches to simplify these equations and the various assumptions and theoretical foundations

underlying them. Even after simplifications, these equations are very complex and their explicit solutions are unknown. To deal with them, the only approach is to make numerical simulations on computers. The process to derive the right numerical schemes for these equations is complex and requires some expertise in numerical linear algebra and optimization. Simulating a large molecular system such as a protein complex in solution at the quantum level is completely out of reach. This can only be done using classical molecular dynamics (or molecular mechanics), or multi-scale models such as hybrid QM/MM approaches.

**The main areas that will be covered include:**

- Basic Linear Algebra and Optimization Techniques
- Mathematical Models and Numerical Methods for Quantum Chemistry: Hartree-Fock, Density Functional Theory (DFT), Valence Bond
- Molecular Dynamics and Force Fields
- Molecular Modelling of Biological Systems
- Multi-scale Modelling: QM/MM hybrid methods
- Molecular visualisation and intermolecular forces
- Introduction to parallel computing: use of a computer clusters

**Keynote Speakers and Supervisors**

**Felix Aviat, PhD student at Sorbonne Université**  
**Benoit Braida, Associate Professor at Sorbonne Université**  
**Eric Cancès, Professor at Ecole des Ponts-ParisTech**  
**Julia Contreras-Garcia, Researcher at Sorbonne Université**  
**Geneviève Dusson, Research Associate at the University of Warwick**  
**Emanuel Giner, Researcher at Sorbonne Université**  
**Nohad Gresh, Researcher at Sorbonne Université**  
**Laura Grigori, Researcher at INRIA**  
**Louis Lagardere, Researcher at Sorbonne Université**  
**Tony Lelièvre, Professor at Ecole des Ponts-ParisTech**  
**Eleonora Luppi, Researcher at Sorbonne Université**  
**Yvon Maday, Professor at Sorbonne Université**  
**Pierre Monmarché, Associate Professor at Sorbonne Université**  
**Jean Philip Piquemal, Professor at Sorbonne Université**  
**Peter Reinhardt, Professor at Sorbonne Université**



## Plenary lectures

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

Full details about the lecturers and speakers will appear in the daily timetable emailed after registration.

## Hands-on simulations

The 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 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.



## Institute for Computing and Data Sciences

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