

September 25th-27th 2017 Idris Paris-Saclay, Université Paris-Saclay (France)

This school will focus on quantum dynamics, i.e. on the time evolution of quantum systems and more precisely on the **Multi Configuration Time Dependent Hartree (MCTDH)** approach, one of the most successful methods to propagate multidimensional wavepackets. It will cover a collection of important topics where **chemistry and physics** strongly overlap. **MCTDH** has been applied to very different fields: heterogeneous catalysis, reactive or non-reactive collisions, infrared spectroscopy, ultraviolet spectroscopy involving, or not, non-Born-Oppenheimer processes, photochemistry, processes guided by laser pulses and optimal control. Additionally, its new variants **MCTDHB** and **MCTDHF** open the possibility to simulate the dynamics of Bosonic and Fermionic systems, for instance, for the time evolution of cold atoms or the simulation of attosecond experiments.

The school will be part of a four-weeks program (25 September – 20 October) devoted to the **future of MCTDH**. It is conceived for students, postdocs or any researchers interested in using the MCTDH approach. Lab sessions will be organized at the Institute for Development and Resources in Intensive Scientific Computing (IDRIS). We will offer also courses and lab sessions on MCTDHB and MCTDHF. We support students and young researchers to attend the school and other parts of the program in order to start concrete research projects with more experienced scientists.

Teaching program:

Courses:

- Introduction to quantum dynamics, Roberto Marquardt, Strasbourg France (6 hours)
- Introduction to MCTDH, Hans-Dieter Meyer, Heidelberg, Germany (3 hours)
- Introduction to MCTDHF (dynamics of electrons, attospectroscopy), Daniel Haxton, Berkeley, USA (3 hours)
- Introduction to MCTDHB (dynamics of ultra-cold atoms), Sven Krönke, Munich, Germany (3 hours)

Lab sessions:

- MCTDH (coordinated by Hans-Dieter Meyer): Infrared spectroscopy, photodissociation, bimolecular reactions, non-adiabatic processes, control of molecular processes with laser pulses. (12 hours)
- MCTDHF (coordinated by Daniel Haxton): attosecond dynamics of electrons (4 hours)
- MCTDHB (coordinated by Alexej I. Streltsov, Kassel/Heidelberg, Germany): quantum many-body dynamics on trapped ultra-cold bosons (4 hours)

Scientific coordinators:

Fabien Gatti, Institut des Sciences Moléculaires d'Orsay (ISMO), Université Paris-Saclay.

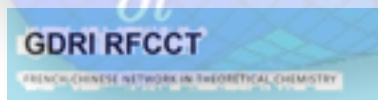
Daniel Peláez-Ruiz, Laboratoire de Physique des Lasers, Atomes et Molécules (PhLAM), Université Lille 1.

Hans-Dieter Meyer, Institute of Physical Chemistry, Universität Heidelberg (Germany).

Graham Worth, Department of Chemistry, University College London (UK).



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