# Molecular Dynamics

## Angers, Feb. 19th - 23rd., 2024

## Université d'Angers

### Bât I - Salle 001
### UFR de Sciences de l'université d'Angers
### Bd. Lavoisier - Angers.

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**Location**:
Laboratoire angevin de recherche mathématique (Larema)
Faculté des Sciences, Bât. I - Salles 001
2 Boulevard Lavoisier
Campus de Belle-Beille
49045 Angers cedex 01

**How to come from downtown ?**
Bus Line 2 direction Beaucouzé-Hauteroche, stop IUT.
Tram B or C, direction Belle-Beille Campus, last stop
Maps and more information on:
`https://math.univ-angers.fr/nous-visiter/`

**Organisers:**
Rémi Carles (`Remi.Carles@math.cnrs.fr`)
Clotilde Fermanian Kammerer (`clotilde.fermanian@univ-angers.fr`)
Caroline Lasser (`classer@ma.tum.de`)
Nicolas Raymond (`nicolas.raymond@univ-angers.fr`)

# Program

| Lundi | Mardi | Mercredi | Jeudi | Vendredi |
|---|---|---|---|---|
| | | | | |
| | 9h30 - 10h15 Irene Burghardt | 9h30 -10h15 Erwan Faou | 9h30 - 10h15 Selina Burkhard | 9h30 - 10h15 Benjamin Lasorne |
| | 10h30 -11h15 Nicolas Raymond | 10h30 -11h15 Loic Joubert-Doriol | 10h30 -11h15 Jiri Vanicek | 10h30 -11h15 Lysianne Hari |
| | 11h15 - 12h Discussions | 11h15 - 12h Discussions | 11h15 - 12h Discussions | 11h15 - 12h Discussions |
| | | | | |
| 14h | 14h - 15h Séminaire 2PMA | 14h30 - 15h15 Antonia Freibert | 14h30 - 15h15 Thomas Cauchy | |
| Discussions for those | Christian Lubich | 15h30 - 16h15 Yohnann le Henaff | 15h30 - 16h15 Martin Averseng | |
| who will be arrived | 15h45 Discussions | Discussions | Discussions | |
| | | | | |
| Diner 19h 30 | | | | |

# Abstracts

— **Erwan Faou and Yohann Le Henaff - A modulation algorithm for the nonlinear Schrödinger equation**

**Abstract** : In this talk, a recently proposed modulation algorithm will be presented. It is based on the idea of 'Bubbles', and consists in plugging a parametrized ansatz into the Schrödinger equation and then choosing the correct evolution for the parameters. The linear part of the Schrödinger equation is recovered exactly (theoretically as well as numerically), and the nonlinear part can be approximated numerically. The method is completely grid-free and scales well with dimension. This talk will focus on the numerical aspects of the method and compare it to the classical variational gaussian wavepackets, while E. Faou will focus on more theoretical aspects.

Travail en collaboration avec Olivier Bourget et Amal Taarabt de l'Université Catholique de Santiago du Chili.

— **Antonia Freibert - A Quantum Dynamics Approach for Resonant Inelastic X-ray Scattering**

**Abstract** : Recent developments of short-pulse X-ray sources have enabled the extension of ultrafast pump-probe techniques into the X-ray domain allowing to measure not only equilibrium X-ray spectra but also to track dynamical processes in transient species. The combination of element-specific core-level probing with unprecedented femtosecond time resolution revolutionized the ability to observe photoinduced electronic and structural changes. Due to the complex nature of detecting structural dynamics on ultrafast time scales, detailed theoretical studies are required to link the spectroscopic observables to the underlying dynamics and thereby access the high information content contained in ultrafast X-ray spectra.

In this context, a substantial influence of nuclear dynamics is expected in nonlinear spectroscopy, demanding a time-dependent framework capable of describing non-adiabatic phenomena. I will present a full time domain approach for calculating resonant inelastic X-ray scattering (RIXS) using time-dependent perturbation theory. Our modification of the standard approach will yield an expression illustrating the impact of pulsed incident X-ray radiation, providing a foundation for state-of-the-art time-resolved experiments with pulsed coherent light sources.

To exemplify this approach, I will showcase RIXS simulations of pyrazine at the nitrogen K-edge, incorporating wavepacket dynamics in both valence- and core-excited state manifolds. The validity of the widely used short-time (or Lorentzian limit) approximation which neglects the nuclear dynamics following the X-ray interrogation will be discussed. Furthermore, the impact of an explicit description of the external electric field will be demonstrated.

— **Christian Lubich - Time integration of three tensor networks.**
**Abstract** : TBA

## Participants

Martin Averseng
Lino Benedetto
Irene Burghardt
Selina Burkhard
Rémi Carles
Thomas Cauchy
Erwan Faou
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Christian Lubich
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