Extended software development workshop in quantum dynamics

Location: Durham University
Webpage: https://www.cecam.org/workshop-details/145
Dates: July 8, 2019 to July 19, 2019
Organizers: Federica Agostini, Basile Curchod, Graham A. Worth

1 State of the art

Quantum molecular dynamics simulations are pivotal to understanding and predicting the microscopic details of molecules, and strongly rely on a combined theoretical and computational effort. When considering molecular systems, the complexity of the underlying equations is such that approximations have to be devised, and the resulting theories need to be translated into algorithms and computer programs for numerical simulations. In the last decades, the joint effort of theoretical physicists and quantum chemists around the challenges of quantum dynamics made it possible to investigate the quantum dynamics of complex molecular systems, with applications ranging from energy conversion, energy storage, organic electronics, light-emitting devices, biofluorescent molecules, or photocatalysis, to name a few.

Two different strategies have been successfully applied to perform quantum molecular dynamics: wavepacket propagation or trajectories. The first family of methods includes all quantum nuclear effects, but their computational cost hampers the simulation of systems with more than 10-12 degrees of freedom. The second family of methods introduces the idea of trajectories as a support to sample the nuclear configuration space, and can be divided, in turn, into two families: the so-called “trajectory basis functions” methods (as the variational multiconfigurational Gaussian or multiple spawning), and the quantum-classical methods (as Ehrenfest or surface hopping).

A few weeks before the ESDW on Quantum Dynamics in Durham, an ECAM state-of-the-art workshop was held in Lyon (France). Some of the topics discussed in Lyon have been presented in more detail at the ESDW, in particular to highlight the relationship between the fundamental theory and the computational developments of the modules that will be presented by the end of 2019.

2 Training provided

Different sessions with scientific presentations were organized to offer the opportunity to a large number of participants to discuss their work, in relation to the software developments proposed at the ESDW. With this idea in mind, we assigned 60-minute presentations to senior participants and postdoctoral researchers, and 30-minute presentations to PhD students. These scientific presentations focused largely on applications of wavepacket propagation methods and trajectory-based techniques, for which training was provided by experts in the fields (see below).
Many successful applications of such methods were highlighted, but at the same time some limitations and the problems encountered by the developers discussed. Both presenters and audience were composed of people strongly engaged in theory and numerical developments, therefore interesting discussions on various points arose during and after the presentations.

Among others:

- Performing calculations based on the trajectory surface hopping algorithm accounting explicitly for a laser field;
- Inclusion of spin-orbit interactions in the exact factorization formalism and the quantumclassical algorithm derived from it;
- Development of model potential energy surfaces (including spin-orbit coupling) for laserdriven dissociation of IBr;
- Limitations of the trajectory surface hopping algorithm, with and without decoherence corrections, in various molecular processes.

Concerning the training part of the ESDW, various aspects were covered

1. Theory: wavepacket propagation and trajectory-based methods;
2. Code development: ANVIL for continuous integration, GitLab, CUDA for GPU programming;
3. HPC: parallel computing with MPI.

On average, about 20 people attended the training sessions.

3 List of software development projects

The modules discussed and developed during the ESDW are the following:
1. Quantics OpenMP (designed to perform HPC)

2. Exact factorization analysis
3. PaPIM QTB
4. ClStunfti
5. GuessSOC
6. Quantics DB OpenMP (designed to perform HPC)
7. PerGauss

These modules will be documented by the developers and finalized by November 2019 to be submitted as deliverables. For almost all modules, a merge request has been opened on the GitLab account of the E-CAM developers.

4 Funding

The follow-up meeting of the ESDW will be held at Durham University to discuss progress and prepare the following ESDW, most likely at the beginning of 2020. All modules only need to be finalized and are currently proposed by people who have been involved in the ECAM project already for a few years. Therefore, we believe that the deadline for the submission of the deliverables will be met without the need for an additional meeting.