Extended software development workshop (WP3: quantum dynamics): quantum mechanics and electronic structure
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1. State of the art

Simulating the exact quantum dynamics of multi-component systems of electrons and nuclei is a task currently out of reach, except for the simplest molecules with a few degrees of freedom due to the exponential scaling of exact methods. Available approximate algorithms can be broadly classified as follows: exact quantum calculations (applicable to low dimensional systems), wave-function based methods (where the wave-functions are expanded in convenient truncated basis, variationally optimized during the evolution), trajectory-based and trajectory–guided methods (in which the properties of the quantum system are mimicked via averages over ensembles of generalized, interfering, classical trajectories), semi-classical dynamics (based on second order approximations of the path integral representation of the quantum propagator), and path integral methods (employing exact methods to sample the quantum thermal density to tackle the time-domain). The main challenge for all these schemes is to maintain the balance between efficiency and accuracy, i.e. to keep the computational costs manageable while preserving the ability to predict and interpret experiments. Due to this variety of methods, none of which has clearly outperformed the others, software development in quantum dynamics has so far been less systematic than in other fields of modelling, such as classical molecular dynamics or electronic structure. Thus, one of E-CAM WP3's goals is to provide an environment to stimulate the transition from in-house codes, often developed and used by single groups, to the development of modular, community-based, packages capable of multiple functionalities and adopting common benchmarks.

The approach pursued in the ESDW is in direct connection with the outcomes of the E-CAM state-of-the-art workshop (SAW) "Different routes to molecular quantum dynamics", CECAM-HQ Lausanne June 6-10 2016. In that workshop, the importance of defining well-established benchmarks and potential libraries to provide a fair comparison ground for alternative methods was stressed. This task was initiated in the ESDW (see below). The need to encourage discussion among the developers of existing packages and promote modular programming was also stressed in the SAW. A scientific report from this workshop can be found in the E-CAM website here.

In this ESDW, three codes dedicated to quantum dynamics (QUANTICS, PAPIM, AND TNUM) were compared and common future work to homogenize their development and avoid overlap of capability was planned. Two more codes (CPMD and CP2K) were also discussed in the framework of combining approximate quantum methods with first principle evaluation of the forces. The need to systematically promote these discussions and explore alternative means of generating potentials was also indicated as urgent in the SAW outcomes.

2. Training provided

10 students and 6 tutors, including Dr. Ivano Tavernelli representing the industrial partner of the WP, IBM, participated to the ESDW. The key scientific topics discussed were:

1. Quantum Computing (of interest to the IBM industrial partner);
2. Exact quantum propagation methods for low dimensional systems to be used to provide benchmarks for approximate schemes (of interest to the IBM industrial partner);
3. Single and multi-surface potentials for benchmark systems (of interest to the IBM industrial partner);
4. Calculation of approximate quantum time correlation functions (Linearized methods and the Quantum Thermal Bath approach);
5. Coupling of approximate methods with first principle force calculations.

Training on software development included the following items: The on-line E-CAM tools for software development, the E-CAM Git repository, tools for the documentation (Doxygen) and performance analysis. Instruction occurred via tutorials and hands-on practice.

Interactions with experts on software and hardware development working at La Maison de la Simulation were also integral part of the training activities. These experts gave talks on hardware architectures and programming paradigms and the use of advanced visualization tools such as the Image wall hosted by the Maison de la Simulation

3. List of the software development projects

The modules developed or initiated in the ESDW (see also E-CAM deliverable 3.1) are:

1. **SodLib:** exact wavefunction propagation using the second-order differencing integrator scheme to solve the time-dependent Schoedinger equation. This routine has been implemented and tested as an added functionality within the Quantics quantum dynamics package.
2. **ChebLib:** Chebyshev integration scheme for exact wave function propagation on the grid. This routine has been implemented and tested as an added functionality within the Quantics quantum dynamics package.
3. **SpoLib**: solver for the time dependent Schroedinger equation using the Split Operator Fourier Transform method.
4. **InpTnum**: two main subroutines to read input data and set up information into two fortran derived types: zmatrix (coordinates definition) and Tnum (information to compute the numerical kinetic energy operator).
5. **PhysConst**: enables the use of physical constants and the correct isotopic masses.
6. **PotMod**: a library in which users can store new potentials. Potentials currently available in the module are: harmonic and Morse potentials; empirical potential, based on high level electronic structure calculations, of the ground state of CH_5^+.
7. **AuxMod**: a set of subroutines which enables any user to construct easily a Fortran input parser. It also contains a library of adapted MPI subroutines for easier programming of Fortran MPI parallel codes.

8. **ClassMC**: Metropolis Monte Carlo sampling of the classical Boltzmann distribution function and calculation of classical time correlation functions from the sampled initial conditions.
9. **PIM**: exact sampling of the Wigner density. It provides quantum initial conditions for the approximate calculation of the time correlation functions.
10. **ClassMd**: a solver for the Hamilton evolution of the and computing autocorrelation functions. This subroutine outputs the Kubo autocorrelation of the dipole moment.
11. **CoorTrans**: set of subroutines enabling transformations between coordinates and a subroutine which transform the gradient and the hessian from Cartesian to curvilinear components for exact wave function propagation.

Modules 1,2,4,5,7,8 have been uploaded in the E-CAM repository for WP3 and are documented in deliverable D3.1. Work on the other modules is on-going. Although not directly originating them, IBM is interested, in particular, in the development of the modules for exact quantum dynamics (1,2,3) and for approximate time-correlation functions (8,9) in view of future applications to modelling of open quantum system for quantum computing.