Quantum Dynamics E-CAM modules III

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Executive Summary

In this report for Deliverable 3.4 of E-CAM, 6 software modules in quantum dynamics are presented. All modules stem from the activities initiated during the ESDW held by E-CAM at University College Dublin in July 2017 and further developed at ESDW: Quantum Dynamics, held at the Maison de la Simulation (Orsay) in June 2018. The modules originate from the input of E-CAM's academic user base. They have been developed by E-CAM post-docs (Momir Mališ and Donal MacKernan) and established collaborators of the project (David Lauvergnat, Université Paris Sud) as well as by new contributors (Federica Agostini, Université Paris Sud; Cristina Sanz-Sanz, CSIC; Johannes Ehrmaier, TU München).

Following the order of presentation, the 6 modules are named: `CTMQC`, `Single Path Surface Hopping Code`, `Zagreb Surface Hopping Code`, `QQ-Interface`, `PaPIM-CP2K Interface`, `Quantum Model Library`. In this report, a short description is written for each module, followed by a link to the respective Merge-Request on the GitLab service of E-CAM. These merge requests contain detailed information about the code development, testing and documentation of the modules.

1 Introduction

Work Package 3 (WP3) of E-CAM provides a means for academic and industrial users of addressing computational questions that involve quantum dynamics, in particular, by developing scalable, open source software with verified quality standards, appropriate documentation and testing. E-CAM's activities in this area can be divided in two, connected, main pillars: the production of modules solicited by our user base (academic and industrial) and the creation of an environment to foster the transition from in-house software to high performing and reliable community packages with long-term sustainability. Within the scope of this deliverable and based on the plan of activities outlined in deliverable D3.2: Identification/Selection of E-CAM Quantum Dynamics Codes for Development [1], we have:

- Developed modules implementing different Quantum-Classical dynamics methods;
- Constructed interfaces between quantum dynamics codes within WP3 and external electronic structure codes to obtain potential and forces necessary for dynamics calculations;

Out of the 6 modules, 4 module developments are done on the E-CAM's `GitLab` server, while two were recently moved from `CPPForge` to an external `GitLab` server fully accessible to E-CAM and authorized users. These servers allows full control of software development, including, for example, the private hosting of the code.

To describe each module, a module documentation repository is created in an E-CAM GitLab repository which automatically updates documentation for the E-CAM Quantum Dynamics Module Documentation on Read the Docs. To submit a module, a developer can fork the GitLab repository and create his own feature branch in which s/he documents the latest progress about module development, source code link/patch file, new feature commit, etc. Developers can submit a merge request of their branch into the E-CAM master branch via an established `Merge-Request` procedure. The E-CAM software manager and developers then run the module through the project's acceptance criteria (coding style and structure, source code documentation and module testing). The software manager then accepts the merge or rejects it providing at the same time feedback and, when necessary, assistance to overcome the reasons for the rejection. The documentation will only appear as part of the Work Package 3 Software Modules on ReadTheDocs.org once the `Merge-Request` is accepted.

In the next section, a short description is provided for each reported module, followed by a link to the `Merge-Request` on the GitLab service of E-CAM. More detailed information about code development, testing and documentation can be found there.

1.1 Overall scope of the module set

This modules set expands the scope of E-CAM's production of software in the area of quantum dynamics via two new main venues identified in the overall development plan described in deliverable D3.2.[1] The first set of modules implements in the E-CAM library two approximate methods in the area of mixed quantum-classical dynamics with particular focus on nonadiabatic processes, the second enables PaPIM and QUANTICS (E-CAM's main codes in WP3) and other similar software to interface efficiently with codes for electronic structure calculations.

Nonadiabatic processes (i.e. phenomena in which nuclear motion, external probes, or environmental effects cause transitions between the quantum electronic states of a system) play a key role in several cases of high potential technological impact. In fact, manipulation of materials via photochemical or photophysical processes often involve nonadiabatic dynamics in areas ranging from clean energy production (e.g. conversion of light to electricity in solar cells, mimicking photosynthetic processes in new devices, reactions in fuel cells), health (e.g. in studying the radiation induced damage to DNA that eventually lead to skin cancer), optimizing and guiding chemical reactions towards desired products via laser pulses. Brute force methods for these problems, however, are numerically too expensive to be of practical use, leading to the development of several approximate methods as described in detail in D3.2: Identification/Selection of E-CAM Quantum Dynamics Codes for Development [1]. The modules presented here are the first steps to include such approximate methods in the E-CAM library. In particular, CTMQC (see section 2.1) implements the evolution of a system in the framework of the so-called exact factorization schemes, while the Single Path Surface Hopping Code (sec. 2.2) implements the Wigner-Liouville formalism. The third module in this set, Zagreb Surface Hopping, stems from a new collaboration linking E-CAM and researchers from the CSIC and the group of Dr. Nadja Doslic (Rudjer Boskovic Institute), and provides an interface to link to the E-CAM QUANTICS code to a code for nonadiabatic dynamics based on Tully's surface hopping scheme. More details on these methods can be found in the following and in their description in D3.2: Identification/Selection of E-CAM Quantum Dynamics Codes for Development [1].

The second set of modules enable to provide key input information (such as potential energies, forces, and - for nonadiabatic processes - couplings between electronic states) to quantum dynamics codes either by employing interesting empirical models taken from the literature or, perhaps more importantly, using efficient electronic structure codes as

external engines to perform the necessary calculations. The modules are aimed at the two E-CAM codes, QUANTICS and PaPIM, and to ElVibRot, a code which is being restructured and optimized within this project in collaboration with Prof. David Lauvergnat, Université Paris Sud. These modules have, however, been structured so that they can easily be used by other codes, providing templates for future developments. Coupling quantum dynamics codes with electronic structure calculations is a fundamental step to extend the range of phenomena accessible to include, in particular, chemical reactions and situations in which empirical models of the interactions are not sufficiently accurate. This is also an interesting computational challenge, since the cost of both the electronic structure and the (approximate) quantum dynamics is considerable. Thus an optimal implementation of these modules requires appropriate parallelization structures and strategies to fully exploit HPC environments.

1.2 General applications and possible exploitation of the codes

The modules presented are aimed principally at the academic user base in E-CAM. This is in itself an important target because, due to the novelty and complexity of the area of nonadiabatic dynamics, no well established community software exists and E-CAM is playing an important role in creating a reference library and a set of well maintained training and research tools for the growing community of users in this area. Furthermore, the codes developed have the potential to enable applications in domains of societal impact and technological interest. In addition to the ones listed in the previous section, we recall that nonadiabatic quantum dynamics is also key in quantum computing (see for example E-CAM's collaboration with IBM). [2] In particular, the mixed quantum classical methods presented here can be used to study not only isolated qubits, but also to model the effect of their interaction with realistic environments.

2 Modules

In this section, a short description is written for each module, followed by a link to the `Merge-Request` on GitLab service of E-CAM, which shows detailed information about code development, testing and documentation.

2.1 CTMQC

`CTMQC` is a module for excited-state nonadiabatic dynamics. It is used to simulate the coupled dynamics of electrons and nuclei (ideally in gas phase molecular systems) in response to, for instance, an initial electronic excitation. The CTMQC module is based on the coupled-trajectory mixed quantum classical (CT-MQC) algorithm [3, 4] that has been derived starting from the evolution equations in the framework the exact factorization of the electron-nuclear wavefunction [5, 6, 7]. Within this scheme, trajectories are used to mimic the evolution of the nuclear degrees of freedom and are coupled to electronic dynamics involving excited states. The evolution employs the adiabatic basis to represent the electronic states, enabling to couple the method with most current electronic structure packages. Ground-state and excited-state electronic properties, i.e., potential energy surfaces and nonadiabatic couplings, are represented on a grid in the adiabatic basis, and read as input. The number of electronic states to be included is not limited, and can also be specified as input. The CTMQC algorithm belongs to the family of quantum-classical methods, as the time evolution of the nuclear degrees of freedom is treated within the classical approximation, whereas electronic dynamics is treated fully quantum mechanically. Initial conditions for the nuclei are obtained via sampling of the Wigner density as provided either directly (for wave functions properties), or by PaPIM (for thermal properties). In its current implementation (used in Refs. [8, 9]), the module can treat up to 3-dimensional problems, but it will be extended to higher dimensional systems in future activities.

2.1.1 Practical application and exploitation of the code

The module is designed to apply the CTMQC procedure to one-, two-, and three-dimensional model systems where an arbitrary number of electronic states are coupled via the nuclear dynamics. The purpose of the module is to familiarize the user with a new simulation technique, i.e., the CTMQC method, for treating problems where electronic excited states are populated during the molecular dynamics. Tully model systems [10] are within the class of problems that can be treated by the module, as well as a wide class of multidimensional problems involving, for instance, ultrafast radiationless relaxation of photo-excited molecules through conical intersections [11]. These photo-activated ultrafast processes are typical situations in which an approach like CTMQC can be used to predict molecular properties, like structures, quantum yields, or quantum coherence.

CTMQC has been analyzed and benchmarked against exact propagation results on typical low-dimensional model systems [3, 4, 8, 9], and applied for the simulation of the photoinitiated ring-opening process of Oxirane [12]. For this study, CTMQC has been implemented in a developer version of the CPMD electronic structure package based on time-dependent density functional theory.

Merge Request	Merge-Request of `CTMQC` module.
Direct Documentation Link	readme.rst of `CTMQC` module.

2.2 Single Path Surface Hopping Code

This module is the first realization of a highly scalable, advanced, implementation of the Wigner-Liouville scheme [13]. The developed software is based on a Trotter-based scheme for simulating quantum-classical Liouville dynamics in terms of an ensemble of surface-hopping trajectories.[14] The focus of this module is on refactoring the original, in-house, serial code so that it can be used efficiently on massively parallel machines. This module implements, in particular, effective tools to circumvent the convergence problems of the method with respect to the strength of the nonadiabatic coupling. An OpenMP and a MPI parallelized versions of the module were developed and their scaling performance analyzed by the developers.

2.2.1 Practical application and exploitation of the code

Potential applications of Wigner-Liouville dynamics include, among others, nonadiabatic chemical rate processes involving electronic, vibrational or other degrees of freedom, decoherence in open quantum systems and quantum

transport processes (see also previous module). The development and testing of the module was conducted in collaboration with undergraduate students at University College Dublin within a specific research and training program in the Physics Department.

2.2.2 Single Path Surface Hopping Code performance analysis

The code's scaling tests were performed on the Kay supercomputer from ICHEC. Kay is composed of nodes, where each node has 40 cores (2 x 20 cores CPU). The parallel efficiency of the OpenMP and MPI versions of the code was tested via benchmarking on 20 - 200 cores (1 - 5 nodes). The results shown in the figures below for a typical benchmark system (high dimensional spin-boson problem with two electronic states and varying sizes of the bath representing the environment) indicate almost perfect scaling of the MPI version of the code that will then be used in further developments. In particular, the development of an interface to couple this module with PaPIM to obtain appropriate sets of initial conditions from a thermal Wigner density will be considered.

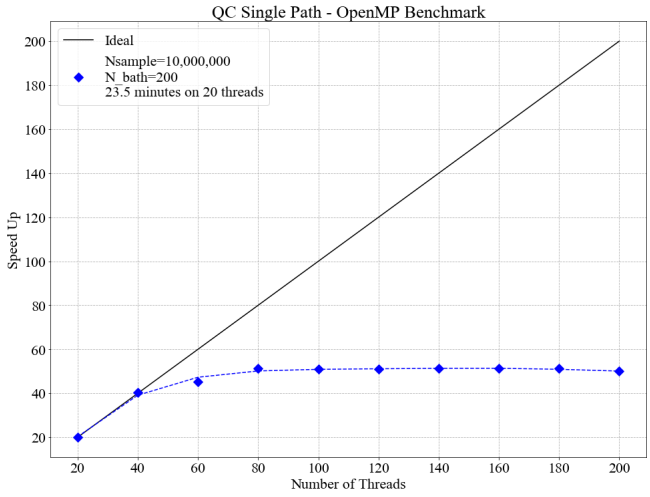

Figure 1: Scaling test for the OpenMP parallelized version of the Single Path Surface Hopping Code. The OpenMP version was run for 10,000,000 samples and for a bath size of 200. As can be seen in the lower left part of the graph OpenMP scales well on a single node (i.e. 40 cores), but increasing the number of threads beyond the cores available provides no significant benefit.

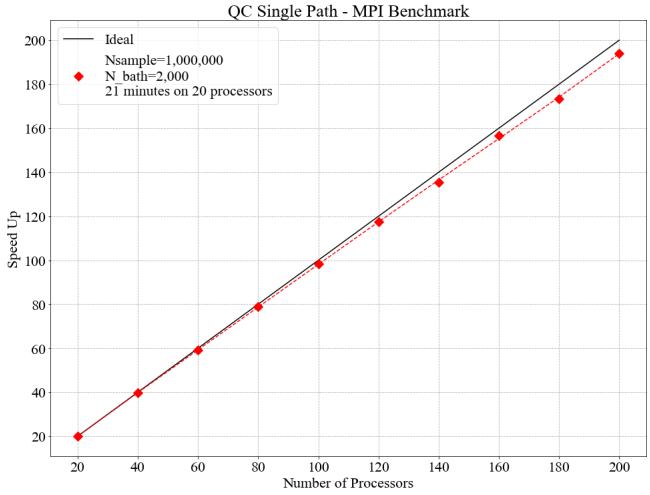

Figure 2: Scaling test for the MPI parallelized version of the Single Path Surface Hopping Code. The MPI version was run for 1,000,000 samples and for a bath size of 2,000. MPI version scales very well over the entire benchmark (up to 200 cores), with an average efficiency of 96.3%.

Merge Request	Merge-Request of `Single Path Surface Hopping Code.`
Direct Documentation Link	readme.rst of `Single Path Surface Hopping Code.`

2.3 Zagreb Surface Hoping

The `Zagreb Surface Hoping` module is an interface between QUANTICS package and Tully's surface hopping algorithm [10]. Users can study the quantum/classical molecular dynamics in several electronic states, within the surface hopping approximation. The full set of quantum and classical methods implemented in QUANTICS package can be used within this approximation and viceversa thus extending considerably the functionalities of both codes.

2.3.1 Practical application and exploitation of the code

The QUANTICS set of programs can study classical dynamics as well as quantum dynamics using exact wavepackets, MCTDH wavepackets, Gaussian wavepackets, etc. using different types of propagation methods and representations of the system (basis set and/or grids). QUANTICS was released in 2015 as an update to the G-MCTDH (Gaussian-MCTDH) package,[15], which also include direct dynamics and classical trajectories. The QUANTICS package has been used in studies of photodissociation,[16] spectra simulations,[17] nonadiabatic direct dynamics,[18] etc. The surface hopping code implemented by the group of Dr. Nadja Doslic implements the nonadiabatic effects in the study of the dynamics using the surface hopping approximation given by Tully. The code has been used in several thesis and articles.[19, 20, 21, 22, 23]

Merge Request	Merge-Request of `Zagreb Surface Hoping Code.`
Direct Documentation Link	readme.rst of `Zagreb Surface Hoping Code.`

2.4 QQ-Interface (QUANTICS–Q-Chem-Interface)

The `QQ-Interface` module connects the full quantum nonadiabatic wavefunction propagation code QUANTICS to the time dependent density functional (TDDFT) module of the electronic structure program Q-Chem. Q-Chem provides analytic gradients, hessians and derivative couplings at the TDDFT level. With this module it is possible to use the Q-Chem TDDFT module for excited state direct dynamics calculations. QUANTICS will start Q-Chem calculations whenever needed, prepare the input file from a template and will read the output of Q-Chem. The Q-Chem results are stored in the QUANTICS database and can be used in dynamics simulations. Due to the modular design of QUANTICS the TDDFT module of Q-Chem can be used for all dynamics simulations, e.g. direct-dynamics with variational multi-configurational Gaussians (dd-vMCG) or surface hopping simulations.

2.4.1 Practical application and exploitation of the code

The module will be used to examine the nonadiabatic excited state dynamics of small to medium sized molecules. The TDDFT module of Q-Chem allows to treat systems that are too large for efficient CASSCF calculations. Until today photoinduced dynamics simulations of such molecules were only possible using trajectory based algorithms. With QUANTICS a full quantum-mechanical description of the nuclear motion is possible.

Merge Request	Merge-Request of `QQ-Interface` module.
Direct Documentation Link	readme.rst of `QQ-Interface` module.

2.5 PaPIM-CP2K Interface

This module couples the PaPIM code with the CP2K program package using the latter for calculation of system electronic structure properties in PaPIM trajectories. The module links CP2K directly as a library for potential energy calculations to the PaPIM code thus avoiding the significantly slower exchange of information between the two codes that would arise by communication via reading and writing to an external file. The module enables to exploit the MPI split communicator approach so that CP2K subroutines can be executed on multiple cores for each PaPIM trajectory, implementing a parallel calculation of system potential energy and gradient values. To fully exploit the coupling with CP2K, the PaPIM code has also been upgraded with periodic boundary conditions to enable simulations of solid and liquid state systems.

2.5.1 Practical application and exploitation of the code

The CP2K program package provides a general framework for different modeling methods such as DFT using the mixed Gaussian and plane waves approaches, semi-empirical methods and classical force fields. Accessing forces from this package then paves the way for using PaPIM in calculation of time-dependent correlation functions for very general systems, without depending on the availability of analytical potentials. This considerably extends the range of potential applications of PaPIM compared to the past. The first application of this module will be conducted in collaboration with Dr. Ari Seitsonen (ENS Paris) to study *ab initio* diffusion processes and infrared spectra in water.

Merge Request	Merge-Request of `PaPIM-CP2K Interface` module.
Direct Documentation Link	readme.rst of `PaPIM-CP2K Interface` module.

2.6 Quantum Model Library

The `Quantum Model Library` enables to incorporate energy surfaces extracted from the literature in quantum dynamics codes. The module implements in particular the following potentials:

- Buckingham potential [24]
- Morse potential (Parameters for HF) [25]
- Linear H-bond potential [26]
- Hénon-Heiles potential [27]
- Tully potentials [10]
- Phenol potential [28]

The module allows users to select the number of degrees of freedom and of electronic states of the system, and for each electronic state provides the energy, gradient, and hessian in the adiabatic or in the diabatic representation. The gradient and the hessian can be computed analytically (even in the adiabatic representations) or numerically (with finite differences).

2.6.1 Practical application and exploitation of the code

This module can currently be interfaced with the E-CAM codes PaPIM and QUANTICS and with the exact propagation code ElRotVib, developed by Prof. David Lauvergnat (Université Paris Sud), but it can be easily included in other Fortran based codes. It is the first realization (and template for future expansions) of a library of empirical potentials for systematic benchmarking of quantum dynamic methods.

Merge Request	Merge-Request of `Quantum Model Library` module.
Direct Documentation Link	readme.rst of `Quantum Model Library` module.

3 Conclusion and Outlook

The report of Deliverable 3.4 of E-CAM describes 6 Software modules in quantum dynamics related to the Extended Software Development Workshop (ESDW) held at University College Dublin in July 2017 (with a wrap-up event in March 2018) and to the workshop ESWD: Quantum Dynamics, held at the Maison de la Simulation (Orsay) in June 2018. The modules include codes for mixed quantum-classical nonadiabatic dynamics, and interfaces between codes of interest in Work-package (WP)3 and electronic structure codes. All the modules have been accepted into the E-CAM software library at this location.

New modules will also be developed in the upcoming period as discussed in deliverable D3.2: Identification/Selection of E-CAM Quantum Dynamics Codes for Development [1]. Further plans for module development were made during the ESDW: Quantum Dynamics held at Maison de la Simulation (Paris) in June 2018. These include modules for Wigner sampling using Langevin dynamics and quantum thermal bath for PaPIM, modules for generating bath modes of a system as well as implementing periodic boundary conditions with Gaussian basis in the QUANTICS program package, whose overall efficiency will be also improved by parallelizing portions of the code. A module based on generalized quantum master equation for efficient dynamical evolution of a small quantum subsystem embedded in a complex environment, a multi-path correlated sampling for the Trotter Based Quantum Classical Surface Hopping Propagator code and implementation of an efficient OpenMP Smolyak scheme for quantum dynamics in ElVibRot program are also expected.

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Acronyms Used

CECAM Centre Européen de Calcul Atomique et Moléculaire

WP Work-package

ESDW Extended Software Development Workshop

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