



## Quantum Dynamics E-CAM modules IV

E-CAM Deliverable 3.5

Deliverable Type: Other

Delivered in December, 2019



E-CAM

The European Centre of Excellence for  
Software, Training and Consultancy  
in Simulation and Modelling



Funded by the European Union under grant agreement 676531

### Project and Deliverable Information

Project Title	E-CAM: An e-infrastructure for software, training and discussion in simulation and modelling
Project Ref.	Grant Agreement 676531
Project Website	<a href="https://www.e-cam2020.eu">https://www.e-cam2020.eu</a>
EC Project Officer	Juan Pelegrín
Deliverable ID	D3.5
Deliverable Nature	Other
Dissemination Level	Public
Contractual Date of Delivery	Project Month 50(30 <sup>th</sup> November, 2019)
Actual Date of Delivery	20 <sup>th</sup> December, 2019
Deliverable Description	6 software modules delivered to the E-CAM repository in the area of quantum dynamics based on user requests and their documentation.

### Document Control Information

Document	Title:	Quantum Dynamics E-CAM modules IV
	ID:	D3.5
	Version:	As of 20 <sup>th</sup> December, 2019
	Status:	Accepted by WP leader
	Available at:	<a href="https://www.e-cam2020.eu/deliverables">https://www.e-cam2020.eu/deliverables</a>
Review	Document history:	<a href="#">Internal Project Management Link</a>
Review	Review Status:	Reviewed
Authorship	Written by:	Ahai Chen(CEA)
	Contributors:	S. Bonella (EPFL), G. Christopoulou (UCL), S. Gómez (University of Vienna), E.Mangaud (Sorbonne University), E. Marsili (Durham University), T. Plé (Sorbonne University), C. Sanz (Autonomous University of Madrid), A. Schild (ETH Zürich)
	Reviewed by:	Sara Bonella (EPFL)
	Approved by:	Sara Bonella (EPFL)

### Document Keywords

Keywords:	E-CAM, Quantum Dynamics, Module, Potential Library, Surface Hopping, Exact Factorization, Interface, CECAM
-----------	--

20<sup>th</sup> December, 2019

**Disclaimer:** This deliverable has been prepared by the responsible Work Package of the Project in accordance with the Consortium Agreement and the Grant Agreement. It solely reflects the opinion of the parties to such agreements on a collective basis in the context of the Project and to the extent foreseen in such agreements.

**Copyright notices:** This deliverable was co-ordinated by Ahai Chen<sup>1</sup> (CEA) on behalf of the E-CAM consortium with contributions from S. Bonella (EPFL), G. Christopoulou (UCL), S. Gómez (University of Vienna), E.Mangaud (Sorbonne University), E. Marsili (Durham University), T. Plé (Sorbonne University), C. Sanz (Autonomous University of Madrid), A. Schild (ETH Zürich).

This work is licensed under the Creative Commons Attribution 4.0 International License. To view a copy of this license, visit <http://creativecommons.org/licenses/by/4.0>.



<sup>1</sup>[ahai.chen@cea.fr](mailto:ahai.chen@cea.fr)

# Contents

<b>Executive Summary</b>	<b>1</b>
<b>1 Introduction</b>	<b>2</b>
1.1 Overall scope of the module set . . . . .	2
1.2 General applications and possible exploitation of the codes . . . . .	3
<b>2 Modules</b>	<b>4</b>
2.1 Exact Factorization Analysis Code (EFAC) . . . . .	4
2.1.1 Scientific context . . . . .	4
2.1.2 Practical application and exploitation of the code . . . . .	4
2.2 CLstunfti . . . . .	5
2.2.1 Practical application and exploitation of the code . . . . .	5
2.3 PIM_QTB . . . . .	5
2.3.1 Practical application and exploitation of the code . . . . .	5
2.4 PerGauss . . . . .	6
2.4.1 Practical application and exploitation of the code . . . . .	6
2.5 Direct Dynamics Database . . . . .	6
2.5.1 Practical application and exploitation of the code . . . . .	6
2.6 GuessSOC . . . . .	7
2.6.1 Practical application and exploitation of the code . . . . .	7
<b>3 Conclusion and Outlook</b>	<b>8</b>
<b>References</b>	<b>9</b>

## Executive Summary

In this report for Deliverable 3.5 of E-CAM, 6 software modules in quantum dynamics are presented. All modules stem from the activities initiated during the [E-CAM State-of-the-Art Workshop \(SAW\)](#) held at Lyon (France) in June 2019 and the workshop [Extended Software Development Workshop \(ESDW\): Quantum Dynamics](#), held at Durham University (UK) in July 2019. The modules originate from the input of E-CAM's academic user base. They have been developed by members of the project (S. Bonella EPF-L), established collaborators (G. Worth University College London, S. Gomez University of Vienna, C. Sanz University of Madrid, D. Lauvergnat Univeristy of Paris Sud) and new contributors to the E-CAM repository (E. Agostini University of Paris Sud, Basile Curchod University of Durham, A. Schild ETH Zurich, S. Hupper and T. Plé Sorbonne University, G. Christopoulou University College London). The presence of new contributors indicates the interest of the community in our efforts. Furthermore, the contributors to modules in WP3 continue to be at different stages of their careers (in particular, Thomas Plé and G. Christopoulou are PhD students) highlighting the training value of our activities.

Following the order of presentation, the 6 modules are named: CLstunfti, PIM\_QTB, PerGauss, Direct Dynamics Database, Exact Factorization Analysis Code (EFAC), GuessSOC. In this report, a short description is written for each module, followed by a link to the respective Merge-Request document 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 into 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, with particular reference to nonadiabatic phenomena;
- Constructed interfaces between quantum dynamics codes within WP3 and external electronic structure codes to obtain potential and forces necessary for dynamics calculations;
- Expanded the functionalities and the efficiency of E-CAM WP3 flagship codes, PaPIM and QUANTICS.

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 section 2, a short description is provided for each reported module, followed by a link to the Merge-Request on the GitLab service of E-CAM, where more detailed information about code development, testing and documentation can be found. A section dedicated to the practical application and exploitation of the code is also presented for each module.

## 1.1 Overall scope of the module set

This module set further 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 (`CLstunfti`, `Exact Factorization Analysis Code`) implements in the E-CAM library approximate methods in the area of mixed quantum-classical dynamics with particular focus on non-adiabatic processes; the second set of modules (`PIM_QTB`, `PerGauss`, `Direct Dynamics Database`, `GuessSOC`) make further extension and improvement of the [PaPIM](#) and [QUANTICS](#) (E-CAM's main codes in WP3) and continue to provide useful tools for an efficient and easy accessibility crossing the interface between quantum dynamics simulations and electronic structure calculations.

As mentioned in the previous deliverable, nonadiabatic processes (i.e. phenomena in which nuclear motion, external probes, or environmental effects cause transitions between the quantum electronic states of a system) are becoming increasingly relevant in areas ranging from the manipulation of materials via photochemical or photophysical processes (e.g. conversion of light to electricity in solar cells, mimicking photosynthetic processes in new devices, reactions in fuel cells), to health (e.g. in studying the radiation induced damage to DNA that eventually lead to skin cancer), or in 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, based on D3.2[1] and D3.3[2], implement state-of-the-art algorithms in the domain and extend, by recruiting new codes and methods, the scope of the E-CAM repository. `Exact Factorization Analysis Code` (see section 2.1) provides a post processing tool to transform the result of a molecular quantum dynamics simulation from the Born-Huang representation to the one of the Exact Factorization. It enables easy access to the time-dependent potential energy surface and vector potential of the Exact Factorization from the results of quantum dynamics simulations. `CLstunfti` (see section 2.2) implements the simulation of electron scattering in liquids and amorphous solids, with a relevant range of potential applications.

The second set of modules provide further improvements and extensions to two E-CAM codes, [PaPIM](#) and [Quantics](#) [3]. In particular, `PIM_QTB` enables the generation of trajectories that can be exploited directly or used to sample initial conditions for linearized semiclassical initial value representation (LSC-IVR) calculations within the general framework of the PaPIM. `PerGauss` implements the periodic boundary conditions for Gaussian bases for Quantics, while `Direct Dynamics Database`, included in Quantics, is an improved, more efficient version of the database used to provide the potential energy surfaces in the Direct Dynamics variational multi-configuration Gaussian (DD-vMCG) method [4, 5]. `GuessSOC` provides a tool for smoothing the off-diagonal values of an electronic structure calculation to remove the sudden changes in the off-diagonal elements (spin-orbit couplings). While developed in association with specific codes, some of these modules can in fact be used stand alone, thus enabling adoption in a wider community.

## 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.

## 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 Exact Factorization Analysis Code (EFAC)

The Exact Factorization Analysis Code (EFAC) provides a post processing tool to transform the result of a molecular quantum dynamics simulation from the Born-Huang representation to the one of the Exact Factorization. Using the output provided by the grid-based quantum dynamics ElVibRot code [6], this module calculates the two key quantities of the Exact Factorization – the *time-dependent potential energy surface* and *time-dependent vector potential* – that have been used to offer new perspectives on numerous nonadiabatic processes (see Refs [7, 8, 9, 10, 11]).

The purpose of EFAC is to familiarize the user with the framework of the Exact Factorization and to connect it with the more commonly used quantum dynamics methods. Hence, the central purpose of this module is to make the Exact Factorization of the electron-nuclear wavefunction easily accessible to the broad quantum dynamics community.

The two time-dependent potentials of the Exact Factorization can be easily recovered by expressing them in a diabatic or adiabatic basis. This connection offers a bridge between quantum dynamics simulation conducted in the Born-Huang representation and the Exact Factorization; a bridge exploited in this module.

In the framework of the Exact Factorization, the nuclear and electronic wavefunctions are unique up to gauge transformation. While this gauge can in principle be chosen arbitrarily, the current implementation enforces two specific gauges that have proved useful in previous studies (see references above). For one-dimensional simulations, the gauge is fixed by making the time-dependent vector potential equal to zero. While being convenient, this gauge cannot be generalized to higher dimensions. As such, the tool uses a different gauge for problems in higher dimensions where the phase of the nuclear wavefunction is zero, i.e., the nuclear wavefunction will be real and non-negative at all times.

The module uses the result of a grid-based quantum dynamics calculation – (time-dependent) nuclear wavefunctions in a diabatic basis and corresponding diagonal and off-diagonal potential surfaces – to construct the time-dependent potential energy surface (TDPES). The TDPES can be split into three components, two gauge-independent and one gauge-dependent. It outputs separately the two gauge-independent contributions as well as the gauge-dependent one. Additionally, the time dependent vector potential is obtained.

#### 2.1.1 Scientific context

This module is an analysis tool to be employed for excited-state, nonadiabatic dynamics simulations. The physical situation to be studied is, for instance, the sub-picosecond response of a molecule to an UV/visible ultrashort laser pulse, that excites the molecule electronically. The photo-excited molecule can relax via, so-called, radiationless channels, i.e., internal conversion processes, towards the electronic ground state. To describe such ultrafast processes, it is essential to account for (i) electronic transitions, thus changes of electronic states, that are induced by nuclear motion, and (ii) the quantum mechanical nature of the nuclei. Various numerical approaches exist nowadays to perform simulations of nonadiabatic processes, based on the – standard, and thus widely used – Born-Huang representation, and on the Exact Factorization. The ultimate goal here is to provide the quantum dynamics community with an easy-to-use analysis tool able to make the link between Born-Huang and Exact Factorization.

#### 2.1.2 Practical application and exploitation of the code

This code is intended to provide an easy access to the time-dependent potential energy surface and vector potential of the Exact Factorization from the result of a quantum dynamics simulation in any arbitrary number of dimensions and electronic states. This allows the user to study simple nonadiabatic model systems in low dimensions, but also the more complex nonadiabatic dynamics of molecules through conical intersections.

Merge Request	<a href="#">Merge-Request of EFAC module.</a>
Direct Documentation Link	<a href="#">readme.rst of EFAC module.</a>

## 2.2 CLstunfti

CLstunfti is a Python package for the simulation of electron scattering in liquids and amorphous solids. It is designed to be lightweight and easily extendable while being able to perform computations with reasonable efficiency. While the main code is written in Python, speed-critical parts were translated to Fortran. Its basic functionality is to calculate electron trajectories of a certain electron kinetic energy ( $eKE$ ) from a given photoelectron angular distribution (PAD) for ionization, a given differential scattering cross section (DSCS), and given values of the elastic mean free path (EMFP) and inelastic mean free path (IMFP) at the selected  $eKE$ . A continuum model is employed to describe scattering in the medium, where both elastic and inelastic collisions happen according to an exponential distribution for the probability of scattering.

As CLstunfti has a potentially wide range of users, it was decided to make it available to the public. In the E-CAM module, a documentation was written and examples were designed to guide new users through the essential features. The examples include relevant possible applications of CLstunfti like the determination of the effective attenuation length as well as the photoelectron angular distribution of photoelectrons ionized in the medium and detected outside.

### 2.2.1 Practical application and exploitation of the code

CLstunfti was used to simulate two experiments [12]: a measurement of the effective attenuation length (EAL) of photoelectrons in liquid water [13] and a measurement of the PAD of photoelectrons in liquid water [14]. These simulations were performed to determine the two central theoretical parameters of every simulation of electron scattering in liquids: the EMFP and the IMFP, which are both experimentally rather inaccessible.

The values of the EMFP and IMFP are needed for a simulation of an attosecond spectroscopy experiment of liquid water. For this purpose, a program based on CLstunfti was developed which can describe certain effects of electron scattering in liquids in the presence of laser fields. Results of the simulations are currently prepared for publication.

CLstunfti has potentially a wide range of users as it can be used to determine scattering properties of electrons in any liquid and to simulate the scattering processes themselves. However, by design a good understanding of the way how the module works is necessary, as for most applications CLstunfti provides a basis for further developments. To introduce new users to the program, example scripts were developed that illustrate how the parts of CLstunfti can be used. These examples contain simplified versions of the scripts used to calculate the results of [12], in particular the determination of the effective attenuation length and of the photoelectron angular distribution of photoelectrons as well as the determination of EMFP and IMFP given certain constraints.

Merge Request	<a href="#">Merge-Request of CLstunfti module.</a>
Direct Documentation Link	<a href="#">readme.rst of CLstunfti module.</a>

## 2.3 PIM\_QTB

PIM\_QTB module implements different molecular dynamics methods based on the Langevin equation. It generates trajectories that can be exploited directly or used to sample initial conditions for LSC-IVR calculations within the general framework of the PaPIM code. The methods implemented are: the classical Langevin dynamics, the Quantum Thermal Bath (QTB) [15] and two flavors of adaptive QTB (adQTB-r and adQTB-f) [16].

### 2.3.1 Practical application and exploitation of the code

The QTB method is based on a generalized Langevin equation with a colored random force. It allows approximating zero-point energy contributions to equilibrium properties with a very limited computational overhead with respect to classical Langevin simulations [15]. Despite its simplicity, the method has so far found relatively few applications, mainly due to the difficulty to assess its general accuracy. In particular, it suffers from zero-point energy leakage (ZPEL), which can significantly affect the results. The recently proposed adaptive QTB [16] method uses the quantum fluctuation-dissipation theorem to quantify the ZPEL and compensate for it in a systematic way. This improves the reliability of the QTB and opens the way to a wider use of this simulation framework. The contents of the module have been used in the PhD thesis project of T. Plé and in the post-doctoral research work of E. Managaud (Sorbonne University).

Merge Request	<a href="#">Merge-Request of PIM_QTB module.</a>
Direct Documentation Link	<a href="#">readme.rst of PIM_QTB module.</a>



## 2.4 PerGauss

PerGauss (**P**eriodic **G**aussians) consists on an implementation of periodic boundary conditions for Gaussian bases for the Quantics program package [3]. In quantum dynamics, the choice of coordinates is crucial to obtain meaningful results. While xyz or normal mode coordinates are linear and do not need a periodical treatment, particular angles, such as dihedrals, must be included to describe accurately the (photo-)chemistry of the system under consideration. In these cases, periodicity can be taken into account, since the value of the wave function and Hamiltonian repeats itself after certain intervals.

This feature is already implemented for grid basis functions such as exponential-DVR and FFT to use in the framework of the Multiconfiguration Time-Dependent Hartree (MCTDH) method [17], within the Quantics package. Using as wave function ansatz a linear combination of Gaussians, following the original idea of Heller [18], has enormous advantages: First, a Gaussian that follows a classical trajectory is the exact solution of the quantum harmonic oscillator and harmonic oscillators are generally the first step into approximating potential energy surfaces. This also allows a smooth transition to dynamics methods based on classical trajectories such as Ab-Initio Multiple Spawning (AIMS) [19] and Surface Hopping [20]. Second, one can easily take advantage of the locality of Gaussians and move towards on-the-fly methods, where the potential is calculated as the basis functions span the conformational space.

In the case of methods that use Gaussian basis functions, such as G-MCTDH, variational multi-configuration Gaussian (vMCG) and its on-the-fly version DD-vMCG within the Quantics set of programs, no implementation of periodic boundary conditions has been made until this contribution.

### 2.4.1 Practical application and exploitation of the code

The module is expected to provide the quantum dynamics community with a more efficient way of treating large systems whose excited state driving forces involve periodic coordinates. When used on precomputed potentials (in G-MCTDH and vMCG), the model can improve the convergence since smaller grid sizes are needed. Used on-the-fly, it reduces considerably the amount of electronic structure computations needed compared to Cartesian coordinates, since conformations that seemed far in the spanned space may be closer after applying a periodic transformation.

Merge Request	<a href="#">Merge-Request of PerGauss module.</a>
Direct Documentation Link	<a href="#">readme.rst of PerGauss module.</a>

## 2.5 Direct Dynamics Database

The Direct Dynamics Database module is an improved, more efficient version of the database used to provide the potential energy surfaces in the DD-vMCG method [4, 5] which is included in the powerful and flexible Quantics package program [21].

Direct Dynamics is a branch of molecular dynamics simulations that solves the time-dependent Schrödinger equation by allowing the calculation of potential energy surfaces *on-the-fly*. This enables the analysis of the influence of the quantum effects on chemical reactivity. During every direct dynamics propagation step the calculated energies, gradients and Hessian matrix are stored in a database. One important challenge is the time needed to continually reread, sort and analyse this database which makes the calculation of a large system very expensive. To this end, this module enables the use of a dynamic and smaller version of the database with selected points only relevant to each basis function each time the program needs to use stored data points so it is feasible to treat large molecules.

### 2.5.1 Practical application and exploitation of the code

The Quantics package grew out of the Heidelberg MCTDH method [22]. Quantics has many features and various algorithms are available, depending on the system of interest and the accuracy required. For example, different studies such as photodissociation [23], spectra simulations [24], and nonadiabatic direct dynamics [25] are also possible. The focus of this module is the G-MCTDH algorithm and the DD-vMCG method. This module will enable studying the nonadiabatic excited state dynamics of large sized molecules, considerably extending the system sizes treatable until now with the DD-vMCG.

Merge Request	<a href="#">Merge-Request of Direct Dynamics Database module.</a>
Direct Documentation Link	<a href="#">readme.rst of Direct Dynamics Database module.</a>

## 2.6 GuessSOC

GuessSOC is a standalone program that allows smoothing the off-diagonal values (this program is created for spin-orbit couplings) of an electronic structure calculation. The purpose of the module is to remove the sudden changes in the off-diagonal elements (spin-orbit couplings) due to the swap between near states and sign changes that electronic structure calculation programs produce along one of the coordinates (internuclear distance in the test example). The way to remove the discontinuities is based on the idea that after the diagonalisation of the matrix, the eigenvalues are the spin-orbit states that are obtained from the electronic structure calculation. So the (spin-orbit) coupling elements can be optimised (using conjugate gradient in this program) so that after the diagonalisation using the optimised value the eigenvalue is as near as possible as the one obtained from the electronic structure calculation. We ensure the continuity using the couplings of a point near to the point that we want to optimise. Further details can be found in [26].

### 2.6.1 Practical application and exploitation of the code

The module is particularly thought for computational chemists that need to fit the spin-orbit couplings to use them in quantum and/or classical dynamics simulations. It is a very practical code that saves time to scientists that need to remove discontinuities in the off-diagonal values of the (spin-orbit) couplings. It is particularly useful for matrices bigger 3x3 or 4x4 where the number of couplings makes it difficult to smooth manually.

The applicability of the code is general for all types of dynamical simulations that require the (spin-orbit) couplings as an analytical function or requires the derivatives of the (spin-orbit) couplings. The code has been already used for the control of the photodissociation of IBr system, where the total number of the states for the simulations is 36, producing a total number of (spin-orbit) couplings equal to 1260. All the couplings needed to be fit to use them in a wavepacket propagation [26].

Merge Request	<a href="#">Merge-Request of GuessSOC module.</a>
Direct Documentation Link	<a href="#">readme.rst of GuessSOC module.</a>

### 3 Conclusion and Outlook

The report of Deliverable 3.5 of E-CAM describes 6 Software modules in quantum dynamics related to the [E-CAM State-of-the-Art Workshop](#) held at Lyon (France) in June 2019 and to the workshop [ESDW: Quantum Dynamics](#), held at Durham University (UK) in July 2019. The modules include codes for mixed quantum-classical nonadiabatic dynamics, and interfaces between codes of interest in WP3 and electronic structure codes. All the modules have been accepted into the E-CAM software library at [this location](#). Work for further modules has been initiated during the [ESDW: Quantum Dynamics](#), held at Durham University and a follow-up meeting is planned for early spring 2020 in Durham to plan delivery of the next six modules in 2020.

Further plans for module development were made during the [ESDW: Quantum Dynamics](#) held at Durham University (UK) in July 2019.

## References

### Acronyms Used

<b>CECAM</b>	Centre Européen de Calcul Atomique et Moléculaire
<b>WP</b>	Work-package
<b>ESDW</b>	Extended Software Development Workshop
<b>SAW</b>	E-CAM State-of-the-Art Workshop
<b>MCTDH</b>	Multi-Configuration Time-Dependent Hartree
<b>eKE</b>	electron kinetic energy
<b>PAD</b>	photoelectron angular distribution
<b>DSCS</b>	differential scattering cross section
<b>IMFP</b>	inelastic mean free path
<b>EMFP</b>	elastic mean free path
<b>EAL</b>	effective attenuation length
<b>vMCG</b>	variational multi-configuration Gaussian
<b>DD-vMCG</b>	Direct Dynamics variational multi-configuration Gaussian
<b>MCTDH</b>	Multiconfiguration Time-Dependent Hartree
<b>EFAC</b>	Exact Factorization Analysis Code
<b>TD PES</b>	time-dependent potential energy surface
<b>QTB</b>	Quantum Thermal Bath
<b>ZPEL</b>	zero-point energy leakage
<b>AIMS</b>	Ab-Initio Multiple Spawning
<b>LSC-IVR</b>	linearized semiclassical initial value representation

### URLs referenced

#### Page ii

<https://www.e-cam2020.eu> ... <https://www.e-cam2020.eu>  
<https://www.e-cam2020.eu/deliverables> ... <https://www.e-cam2020.eu/deliverables>  
 Internal Project Management Link ... <https://redmine.e-cam2020.eu/issues/145>  
[ahai.chen@cea.fr](mailto:ahai.chen@cea.fr) ... <mailto:ahai.chen@cea.fr>  
<http://creativecommons.org/licenses/by/4.0> ... <http://creativecommons.org/licenses/by/4.0>

#### Page 1

SAW ... <https://www.cecama.org/workshop1774/>  
 ESDW: Quantum Dynamics ... <https://www.cecama.org/workshop1697/>

#### Page 2

E-CAM GitLab repository ... <https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/tree/master/Quantum-Dynamics-modules>  
 E-CAM Quantum Dynamics Module Documentation ... <http://e-cam.readthedocs.io/en/latest/Quantum-Dynamics-modules/>  
 Read the Docs ... <https://readthedocs.org/>  
 Work Package 3 Software Modules ... <http://e-cam.readthedocs.io/en/latest/Quantum-Dynamics-Modules/ReadTheDocs.org> ... <http://readthedocs.org>  
 PaPIM ... <https://e-cam.readthedocs.io/en/latest/Quantum-Dynamics-Modules/modules/PaPIM/readme.html>  
 QUANTICS ... <http://chemb125.chem.ucl.ac.uk/worthgrp/quantics/doc/index.html>

**Page 3**

PaPIM... <https://www2.chem.ucl.ac.uk/worthgrp/quantics/doc/index.html>

Quantics ... <https://www2.chem.ucl.ac.uk/worthgrp/quantics/doc/index.html>

**Page 4**

GitLab service of E-CAM... <https://gitlab.e-cam2020.eu/>

Merge-Request of EFAC module. ... [https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/merge\\_requests/217](https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/merge_requests/217)

readme.rst of EFAC module. ... [https://gitlab.e-cam2020.eu/marsili/E-CAM-Library/blob/master/Quantum-Dynamics-Modules/modules/EF\\_module/EF\\_analysis\\_report.tex](https://gitlab.e-cam2020.eu/marsili/E-CAM-Library/blob/master/Quantum-Dynamics-Modules/modules/EF_module/EF_analysis_report.tex)

**Page 5**

Merge-Request of CLstunfti module. ... [https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/merge\\_requests/196](https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/merge_requests/196)

readme.rst of CLstunfti module. ... <https://gitlab.e-cam2020.eu/axelschild/E-CAM-Library/blob/CLstunfti/Quantum-Dynamics-Modules/modules/CLstunfti/readme.rst>

PaPIM... <https://e-cam.readthedocs.io/en/latest/Quantum-Dynamics-Modules/modules/PaPIM/readme.html>

Merge-Request of PIM\_QTB module. ... [https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/merge\\_requests/216](https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/merge_requests/216)

readme.rst of PIM\_QTB module. ... [https://gitlab.e-cam2020.eu/thomas.ple/E-CAM-Library/blob/master/Quantum-Dynamics-Modules/modules/PIM\\_qtb/readme.rst](https://gitlab.e-cam2020.eu/thomas.ple/E-CAM-Library/blob/master/Quantum-Dynamics-Modules/modules/PIM_qtb/readme.rst)

**Page 6**

Merge-Request of PerGauss module. ... [https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/merge\\_requests/46](https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/merge_requests/46)

readme.rst of PerGauss module. ... <https://gitlab.e-cam2020.eu/sandra.gomez/E-CAM-Library/blob/pergauss1/Quantum-Dynamics-Modules/modules/Pergauss/readme.rst>

Merge-Request of Direct Dynamics Database module. ... [https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/merge\\_requests/200](https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/merge_requests/200)

readme.rst of Direct Dynamics Database module. ... [https://gitlab.e-cam2020.eu/gechri8/E-CAM-Library/blob/Direct\\_Dynamics\\_Database/Quantum-Dynamics-Modules/modules/Direct\\_Dynamics\\_Database/readme.rst](https://gitlab.e-cam2020.eu/gechri8/E-CAM-Library/blob/Direct_Dynamics_Database/Quantum-Dynamics-Modules/modules/Direct_Dynamics_Database/readme.rst)

**Page 7**

Merge-Request of GuessSOC module. ... [https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/merge\\_requests/157](https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/merge_requests/157)

readme.rst of GuessSOC module. ... [https://gitlab.e-cam2020.eu/sanz/E-CAM-Library/blob/module\\_guessoc/Quantum-Dynamics-Modules/modules/guessoc/guessoc\\_readme.rst](https://gitlab.e-cam2020.eu/sanz/E-CAM-Library/blob/module_guessoc/Quantum-Dynamics-Modules/modules/guessoc/guessoc_readme.rst)

**Page 8**

E-CAM State-of-the-Art Workshop ... <https://www.cecarn.org/workshop1774/>

ESDW: Quantum Dynamics ... <https://www.cecarn.org/workshop1697/>

this location... <https://gitlab.e-cam2020.eu/e-cam/E-CAM-Library/tree/master/Quantum-Dynamics-Modules/modules>

ESDW: Quantum Dynamics ... <https://www.cecarn.org/workshop1697/>

ESDW: Quantum Dynamics ... <https://www.cecarn.org/workshop1697/>

## Citations

- [1] S. Bonella, M. Mališ, B. Courchod, and A. Seitsonen, "Identification/Selection of E-CAM Quantum Dynamics Codes for Development," Mar. 2018. [Online]. Available: <https://doi.org/10.5281/zenodo.1210416>
- [2] S. Bonella, M. Mališ, A. O'Caïs, and L. Liang, "Quantum Dynamics E-CAM modules III," Mar. 2018. [Online]. Available: <https://doi.org/10.5281/zenodo.1210077>
- [3] G. A. Worth, K. Giri, G. W. Richings, I. Burghardt, A. M. H. Beck, Jäckle, and H.-D. Meyer, *The QUANTICS Package, Version 1.1*. Birmingham, U.K.: University of Birmingham, 2015.
- [4] G. Worth, M. Robb, and B. Lasorne, "Solving the time-dependent schrödinger equation for nuclear motion in one step: direct dynamics of non-adiabatic systems," *Molecular Physics*, vol. 106, no. 16-18, pp. 2077–2091, 2008. [Online]. Available: <https://doi.org/10.1080/00268970802172503>

- [5] M. M. Law and A. Ernesti, *Molecular Potential Energy Surfaces in Many Dimensions*. CCP6, Daresbury Laboratory, 2009. [Online]. Available: <http://www.ccp6.ac.uk/publications.htm>
- [6] D. Lauvergnat, “Elvibrot: Quantum dynamics code,” 2015. [Online]. Available: <https://github.com/lauvergn/ElVibRot-TnumTana>
- [7] A. Abedi, N. T. Maitra, and E. K. U. Gross, “Exact factorization of the time-dependent electron-nuclear wave function,” *Phys. Rev. Lett.*, vol. 105, p. 123002, Sep 2010. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevLett.105.123002>
- [8] —, “Correlated electron-nuclear dynamics: Exact factorization of the molecular wavefunction,” *The Journal of Chemical Physics*, vol. 137, no. 22, p. 22A530, 2012. [Online]. Available: <https://doi.org/10.1063/1.4745836>
- [9] B. F. E. Curchod and F. Agostini, “On the dynamics through a conical intersection,” *The Journal of Physical Chemistry Letters*, vol. 8, no. 4, pp. 831–837, 2017, pMID: 28151670. [Online]. Available: <https://doi.org/10.1021/acs.jpcllett.7b00043>
- [10] F. Agostini, A. Abedi, Y. Suzuki, S. K. Min, N. T. Maitra, and E. K. U. Gross, “The exact forces on classical nuclei in non-adiabatic charge transfer,” *The Journal of Chemical Physics*, vol. 142, no. 8, p. 084303, 2015. [Online]. Available: <https://doi.org/10.1063/1.4908133>
- [11] F. Agostini, A. Abedi, Y. Suzuki, and E. Gross, “Mixed quantum-classical dynamics on the exact time-dependent potential energy surface: a fresh look at non-adiabatic processes,” *Molecular Physics*, vol. 111, no. 22-23, pp. 3625–3640, 2013. [Online]. Available: <https://doi.org/10.1080/00268976.2013.843731>
- [12] A. Schild, M. Peper, C. Perry, D. Rattenbacher, and H. J. Wörner, “An alternative approach for the determination of mean free paths of electron scattering in liquid water based on experimental data,” *Submitted*, 2019.
- [13] Y.-I. Suzuki, K. Nishizawa, N. Kurahashi, and T. Suzuki, “Effective attenuation length of an electron in liquid water between 10 and 600 eV,” *Phys. Rev. E*, vol. 90, p. 010302, Jul 2014. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevE.90.010302>
- [14] S. Thürmer, R. Seidel, M. Faubel, W. Eberhardt, J. C. Hemminger, S. E. Bradforth, and B. Winter, “Photoelectron angular distributions from liquid water: Effects of electron scattering,” *Phys. Rev. Lett.*, vol. 111, p. 173005, Oct 2013. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevLett.111.173005>
- [15] H. Dammak, Y. Chalopin, M. Laroche, M. Hayoun, and J.-J. Greffet, “Quantum thermal bath for molecular dynamics simulation,” *Phys. Rev. Lett.*, vol. 103, p. 190601, Nov 2009. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevLett.103.190601>
- [16] E. Mangaud, S. Huppert, T. Plé, P. Depondt, S. Bonella, and F. Finocchi, “The fluctuation–dissipation theorem as a diagnosis and cure for zero-point energy leakage in quantum thermal bath simulations,” *Journal of Chemical Theory and Computation*, vol. 15, no. 5, pp. 2863–2880, 2019, pMID: 30939002. [Online]. Available: <https://doi.org/10.1021/acs.jctc.8b01164>
- [17] M. Beck, A. Jäckle, G. Worth, and H.-D. Meyer, “The multiconfiguration time-dependent hartree (mctdh) method: a highly efficient algorithm for propagating wavepackets,” *Physics Reports*, vol. 324, no. 1, pp. 1 – 105, 2000. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/S0370157399000472>
- [18] E. J. Heller, “Frozen gaussians: A very simple semiclassical approximation,” *The Journal of Chemical Physics*, vol. 75, no. 6, pp. 2923–2931, 1981. [Online]. Available: <https://doi.org/10.1063/1.442382>
- [19] S. Yang, J. D. Coe, B. Kaduk, and T. J. Martínez, “An “optimal” spawning algorithm for adaptive basis set expansion in nonadiabatic dynamics,” *The Journal of Chemical Physics*, vol. 130, no. 13, p. 134113, 2009. [Online]. Available: <https://doi.org/10.1063/1.3103930>
- [20] J. C. Tully and R. K. Preston, “Trajectory surface hopping approach to nonadiabatic molecular collisions: The reaction of H<sup>+</sup> with D<sub>2</sub>,” *The Journal of Chemical Physics*, vol. 55, no. 2, pp. 562–572, 1971. [Online]. Available: <https://doi.org/10.1063/1.1675788>
- [21] G. W. R. I. B. M. H. B. A. J. G. A. Worth, K. Giri and H.-D. Meyer, “The quantics package, version 1.1,” 2015. [Online]. Available: <https://www2.chem.ucl.ac.uk/worthgrp/quantics/doc/index.html>
- [22] H.-D. Meyer, U. Manthe, and L. Cederbaum, “The multi-configurational time-dependent hartree approach,” *Chemical Physics Letters*, vol. 165, no. 1, pp. 73 – 78, 1990. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/000926149087014I>
- [23] S. P. Neville and G. A. Worth, “Conformer-resolved quantum dynamics study of the photodissociation of 3-pyrroline,” *The Journal of Physical Chemistry A*, vol. 118, no. 51, pp. 11975–11986, 2014, pMID: 25222081. [Online]. Available: <https://doi.org/10.1021/jp507075c>

- [24] M. Taylor and G. Worth, "Vibronic coupling model to calculate the photoelectron spectrum of phenol," *Chemical Physics*, vol. 515, pp. 719 – 727, 2018, ultrafast Photoinduced Processes in Polyatomic Molecules: Electronic Structure, Dynamics and Spectroscopy (Dedicated to Wolfgang Domcke on the occasion of his 70th birthday). [Online]. Available: <http://www.sciencedirect.com/science/article/pii/S0301010418305433>
- [25] G. W. Richings and G. A. Worth, "Multi-state non-adiabatic direct-dynamics on propagated diabatic potential energy surfaces," *Chemical Physics Letters*, vol. 683, pp. 606 – 612, 2017, ahmed Zewail (1946-2016) Commemoration Issue of Chemical Physics Letters. [Online]. Available: <http://www.sciencedirect.com/science/article/pii/S0009261417302488>
- [26] C. Sanz-Sanz and G. A. Worth, "Field modified spin-orbit potential curves of ibr. preliminary dynamical results," *Phys. Chem. Chem. Phys.*, vol. 21, pp. 14 429–14 439, 2019. [Online]. Available: <http://dx.doi.org/10.1039/C8CP07248E>