



## Quantum Dynamics E-CAM modules I

E-CAM Deliverable 3.1

Deliverable Type: Report

Delivered in Month 14– November2016



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 PELEGRIN
Deliverable ID	D3.1
Deliverable Nature	Report
Dissemination Level	Public
Contractual Date of Delivery	Project Month 14(November2016)
Resubmission Date	04.09.2017
Deliverable Description	6 Software modules delivered to the E-CAM repository in the areas of:(1) approximate methods for computing quantum time correlation functions; (2) exact integrators for the Schrödinger equation; (3) model potentials of increasing complexity for benchmarking

### Document Control Information

Document	Title:	Quantum Dynamics E-CAM modules I
	ID:	D3.1
	Version:	As of September 4, 2017
	Status:	Accepted by Technical Manager
	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
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### Document Keywords

Keywords:	E-CAM, Quantum Dynamics, Module, Exact Integrators, Time Correlation Functions, Potentials, <a href="#">CECAM</a>
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September 4, 2017

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## Executive Summary

In this report for Deliverable 3.1 of E-CAM, 6 software modules in quantum dynamics, which are related to the Extended Software Development Workshop ([ESDW](#)) held by E-CAM at Maison de la Simulation, Saclay, in July 2016, are presented.

The 6 modules are respectively named: `SodLib`, `ChebLib`, `PhysConst`, `PotLib`, `AuxMod`, `ClassMC`. They include codes for exact integrators of quantum dynamics for low dimensional systems, potentials, calculation of quantum time correlation functions, and their documentation. 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 open source software with verified quality standards, appropriate documentation and testing. 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, E-CAM WP3 will also 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.

With these goals, software development in the first year of E-CAM activity has focused on launching the following areas:

- Numerically exact solution of the time-dependent Schrödinger equation (SE):
- Creation of a library of empirical potentials to be used in benchmark or realistic calculations:
- Approximate methods for computing quantum time correlation functions:

The module developments are done either on E-CAM's [GitLab](#) server (for 4 of the 6 modules) or on [CPPForge](#) (for the modules for exact numerical integration of the SE). Both the GitLab and Forge use powerful version control system service for software development, but E-CAM's own GitLab Server allows more control of software development, for example, the private hosting of the code.

In order to describe each module, a [module documentation repository](#) is created in an [E-CAM GitLab repository dedicated to Quantum Dynamics](#) 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 he documents his latest progress about module development, source code link/patch file, new feature commit, etc. The developer can ask to merge their branch into the E-CAM master branch, which is called a Merge-Request. The E-CAM software manager and developers can then run the module through its acceptance criteria (coding style and structure, source code documentation and module testing). 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 module created, 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

Quantum mechanics describes matter at typical atomic length and energy scales. As our ability to design drugs and new materials reaches these scales, quantum mechanics may enable exciting technological and societal benefits. For example, a quantum treatment is necessary to control the interaction of matter with light to engineer more efficient photovoltaic materials and fully harvest solar power as a sustainable energy source. Skin cancer drugs may be developed by understanding and preventing or counteracting the damage caused by the same power to our DNA. Hydrogen, the most common element in the universe and a key player, for example, in the quest to replace oil as a sustainable energy carrier for our cars, is a quantum element. Quantum computers may one day increase exponentially our computational power and change informatics as we know it today.

The applications above still represent very difficult challenges for simulation and modelling. The complexity of exact numerical solutions of the evolution equations for quantum systems, in fact, is exponential, making it impossible to solve the problem except for very simple systems. E-CAM is engaged in overcoming this challenge by translating the most advanced, and computationally affordable, approximate method for quantum dynamics into verified and validated code with optimal scalability.

## 1.2 General applications and possible exploitation of the codes

The modules developed so far within WP3 represent the initial effort towards the creation of modular packages with the ambition to become standard community codes. They are the first building block of the two main workflows described in this deliverable.

### Quantics modules

**Quantics** is a package to study chemical reactions of molecules whose main developer (G. Worth, University College London) is a member of E-CAM's WP3. It incorporates a variety of quantum dynamical methods joined by the fact that the state system is usually described via wavefunctions (containing the quantum analogue of the information given by positions and velocities for classical atoms). It is increasingly used by the computational chemistry community for scientific applications (there are presently 50 people signed up on the CCPForge repository as developers and users). Work is on-going in E-CAM to improve its scalability (see E-CAM deliverable D7.2<sup>2</sup>) and add new functionalities in view of applications to study materials and light harvesting complexes. The modules added in this first year focused on including exact solution methods for small quantum systems to be used to test approximations. The need for these modules was identified, in particular, in the E-CAM State of the Art workshop on quantum dynamics (see E-CAM deliverable D8.1<sup>3</sup>).

### PaPim modules

PaPim is a package to study the properties of quantum materials (in particular time correlation functions from which experimental observations can be rationalised) via the so-called mixed quantum classical methods. In these schemes, quantum evolution is approximated by appropriately combining a set of classical trajectories for the system. This combination is such that several quantum effects, for example the possibility to find atoms in classically forbidden regions (tunnelling), are reproduced at a manageable fraction of the cost of exact solutions. The E-CAM developments build on an in house code developed in the group of the leader of WP3 (S. Bonella, EPF-Lausanne), which has been completely restructured to make it modular, and thus ready to act as a skeleton to include several computational methods in this family, and to achieve very good scalability (see E-CAM deliverable D7.2<sup>2</sup>). This code was identified as a good target for E-CAM in the State of the Art workshop on quantum dynamics (see E-CAM deliverable D8.1<sup>3</sup>). Even though the first official release of the code has not been made yet (release is expected for November 2017), it is currently used in collaborations with several groups: N. English, University College Dublin, to study properties of H<sub>2</sub> molecules in clathrates (materials for capture and storage of hydrogen and CO<sub>2</sub> in energy applications); F. Finocchi, Université Pierre et Marie Curie, to study infrared characterisation of molecules, and from it understand the effect that the environment has on their chemical properties, in the atmosphere; R. Vuilleumier, Ecole Normale Supérieure Paris, to characterise hydrogen at extreme pressures in the context of geophysical applications; and D. Marx, University of Bochum) to test new potentials to efficiently characterise the chemical reactivity of small water clusters, again with possible applications on the physics of the atmosphere in reactions related to green house effect.

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<sup>2</sup>Public deliverable, but DOI not yet available. Document will soon be available in [www.e-cam2020.eu/deliverables/](http://www.e-cam2020.eu/deliverables/)

<sup>3</sup>Confidential deliverable, only available for members of the consortium (including the Commission Services)

## 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 SodLib

The SodLib module provides exact wavefunction propagation using the second-order differencing (SOD) integrator scheme to solve the time-dependent SE. This routine has been implemented and tested as an added functionality within the [Quantics](#) quantum dynamics package.

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

The module has been incorporated in Quantics. It has been used to provide benchmark results for new mixed quantum classical E-CAM modules developed during the internship of a student from the Ecole Normale Supérieure Paris-Saclay at EPFL. Furthermore, it is currently being used in a Phd thesis supervised by G. Worth, a member of E-CAM's WP3, at the University College London. The results of this application will provide benchmarks for a model describing proton-transfer in a condensed phase system.

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

### 2.2 ChebLib

The ChebLib module implements the Chebyshev integration scheme for exact wavefunction propagation on the grid. This routine has been implemented and tested as an added functionality within the [Quantics](#) quantum dynamics package.

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

See SodLib for application and exploitation.

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

### 2.3 PhysConst

PhysConst enables the use of physical constants and the correct isotopic masses.

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

This is a general purpose module that can be incorporated in different codes to ensure that the, often different, systems of units employed by different communities can be smoothly translated from one application to another. The module has been tested in the TNum package, a wavepacket based code for exact solution of low dimensional quantum systems (up to 20 degrees of freedom) developed by D. Lauvergnat, Université Paris Saclay, a collaborator in WP3. Its extension to other E-CAM codes, Quantics and PaPIM, is planned.

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

## 2.4 PotMod

PotMod is structured as a library in which users can store new potentials. Potentials currently available in the module are: harmonic and Morse potentials (for testing purposes, different molecular systems can be simulated depending on parameters input by the user); empirical potential, based on high level electronic structure calculations, of the ground state of  $CH_5^+$ .

### 2.4.1 Practical application and exploitation of the code

This module is a key ingredient currently incorporated in the PaPIM code to provide the necessary potentials and gradients of studied systems. It is build so as to be easily interfaceable with other quantum codes. It has been recently extended to include a potential energy subroutine for small water molecule clusters and an interface to the CP2K code has been used to access DFT and neural network based potentials. Together with PaPIM, the module has been exploited in a Master thesis project at EPFL (spectroscopy of the water dimer) and a PhD project at the Université Pierre et Marie Curie and Ecole Normale Supérieure in Paris (spectroscopy of  $CH_5^+$ ). It is also used in an on-going collaboration with the University of Bochum (neural network potentials for the water dimer).

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

## 2.5 AuxMod

AuxMod contains 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.

### 2.5.1 Practical application and exploitation of the code

The AuxMod module was included as the input parser for the PaPIM code, while its modified MPI commands were adopted to parallelize the PaPIM code and the ClassMC module. Following these example, the AuxMod provides a pre-constructed input reader and adapted MPI library for any future Fortran code development in WP3. See PotMod for information on exploitation.

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

## 2.6 ClassMC

ClassMC samples, via Metropolis Monte Carlo, the classical Boltzmann distribution function and calculates classical time correlation functions from the sampled initial conditions. This module provides a classical reference result to assess the relevance of quantum effects for a given system.

### 2.6.1 Practical application and exploitation of the code

The module was included in PaPIM to provide classical results to contrast to the quantum ones, so as to assess the relevance of quantum effects in the systems studied. It has been extensively used in the applications described for PotMod.

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



### 3 Outlook

The report of Deliverable 3.1 of E-CAM describes 6 Software modules in quantum dynamics related to the [ESDW](#) held at La Maison de la Simulation, Saclay in July 2016 (with a wrap-up event in December 2016). They include codes and documentations of numerically exact integrators of the time-dependent [SE](#), approximate calculations of quantum time correlation functions, and a library for potentials.

At the initial time of writing the modules were in the process of the acceptance workflow being established within E-CAM. Over the coming months the E-CAM acceptance criteria will be consistently applied across all modules and all work packages of E-CAM, and in particular those related to WP3.

## References

### Acronyms Used

**CECAM** Centre Européen de Calcul Atomique et Moléculaire

**DFT** Density Functional Theory

**WP** Work-package

**ESDW** Extended Software Development Workshop

**SE** Schrödinger equation

**DFT** Density Functional Theory

**MPI** Message Passing Interface

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