Electronic structure E-CAM modules V

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The European Centre of Excellence for
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Contents

Executive Summary

In this report for Deliverable 2.6 of E-CAM, 9 software modules for electronic structure computations —Work Package 2 (WP2)—are presented.

The modules in this report are part of larger software packages and are intended to extend their features and functionalities. In particular, four of the modules presented here are part of the QMCPack package [4], an open source Quantum Monte Carlo (QMC) package for ab initio electronic structure calculations. QMC methods are a class of ab initio, stochastic techniques for the study of quantum systems. While QMC simulations are computationally expensive, they have the advantage of being accurate, fully ab initio and scalable to a large number of core with limited memory requirements. These features make QMC methods a valuable tool to assess the accuracy of Density Functional Theory (DFT) computations, which are widely used in the fields of condensed matter physics, quantum chemistry and material science. We present in this document four modules that are interfaces between QMCPack and a software commonly used in electronic structure computations, Quantum Espresso. These are `QMCQEPack`, `ESInterfaceBase`, `ESHDF5Interface` and `ESPWSCFInterface`. Such interfaces can be used to establish an automated, black box workflow to benchmark and validate the results of DFT simulations involving physical systems of interest which can have applications for industry, e.g. in the study of metal-ion or water-carbon interfaces.

Three of the modules presented here were written as part of the Electronic-Structure Library (ESL) project. Electronic structure simulations are a fundamental tool in the study of a large array of problems in condensed matter and quantum chemistry, which have a large range of applications in several fields of research, from condensed matter physics and material science to quantum chemistry to biology and nanomedicine. Theoretical studies in electronic structure are mostly performed independently by separate research groups, employing a wide array of different methods (such as but not limited to DFT classical, quantum Monte Carlo and various quantum chemistry methods), each implemented in different software's and employing different data standards. The goal of the ESL initiative is to provide a library of standard, high quality software for electronic structure computations, to facilitate sharing of data, results and ultimately knowledge between different research group, and to allow scientists to focus more on their research topics than coding and software engineering. Herein we present three software modules from the ESL produced during the *ESDW: Integration of ESL modules into electronic-structure codes* held at CECAM Headquarters in Lausanne on 17-28 February 2020. These are `Integration of ELSI-RCI in DFTB+`, `Integration of Libxc in FHI-AiMS` and `PSolver in SIESTA and Octopus`.

Finally, the MaZe code is presented in this deliverable. MaZe stands for the Mass-Zero constrained molecular dynamics approach discussed in Ref. [1]. This method enforces, at each time step, the Born-Oppenheimer condition that the system relaxes instantaneously to the ground state through the formalism of massless constraints. The adiabatic separation between the degrees of freedom is enforced rigorously, and the algorithm is symplectic and time-reversible in both physical and additional set of degrees of freedom. The code is intended for condensed matter physicists and for material scientists and it can be used for various purposes related to the subject. The main goal of the software is to produce particles trajectories to be analyzed in post-production by means of external software. Three modules are presented here for the MaZe code: the `MaZe for OF-DFT`, the `MaZe for OF-DFT (HPC version)` and the `NLCG for OF-DFT`.

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.

As this deliverable is the last one of its series, a section on the overall impact of the results achieved within the Workpackage Electronic Structure was also included, with an overview of the results achieved so far, how these have been disseminated in scientific publications, the industrial impact of the software developed, the training given in the WP which lead to many of the software outputs, and the societal impact of the WP.

1 Introduction

Work Package 2 (WP2) of E-CAM focuses on software for the study of electronic structure; understanding the behaviour of electron systems is fundamental to evaluate and predict the properties of physical systems of interest in condensed matter physics and quantum chemistry, which have a great range of applications e.g. in material science, biology and nano-medicine.

There are several methods for the theoretical study of electronic structure systems, such as Density Functional Theory (DFT), Quantum Monte Carlo (QMC), mean field and quantum chemical methods, as well as more recent techniques based on artificial intelligence and neural networks. All these techniques rely on computer simulations, and the aim of the WP2 of E-CAM is to provide high quality, standard codes and interfaces that can be used in these studies.

1.1 Overall scope of the module set

Four of the modules presented in this report are part of a larger software package, QMCPack [4], an open source package for QMC simulations. These modules are interfaces between QMCPack and Quantum Espresso, a commonly used package for electronic structure computations. We also present three modules that are part of the ESL initiative [8], and that are libraries that improve larger software packages for Electronic Structure Simulations. Finally, two of the modules presented here are part of the MaZe code [1], that uses the Mass-Zero constrained molecular dynamics approach for Orbital Free Density Functional Theory. One of these modules constitutes the HPC version of the MaZe code.

1.1.1 QMCPack Interfaces for Electronic Structure Computations

QMC methods are a class of ab initio, stochastic techniques for the study of quantum systems. While QMC simulations are computationally expensive, they have the advantage of being accurate, fully ab initio and scalable to a large number of cores with limited memory requirements.

These features make QMC methods a valuable tool to assess the accuracy of DFT computations, which are widely used in the fields of condensed matter physics, quantum chemistry and material science.

QMCPack [4] is an open source package for QMC simulations of electronic structure developed in several national labs in the US. This package is written in object oriented C++, offers great flexibility in the choice of systems, trial wave functions and QMC methods and supports massive parallelism and the usage of GPUs.

Trial wave functions for electronic QMC computations commonly require the use of single electron orbitals, typically computed by DFT. The aim of the E-CAM pilot project developed at the Maison de la Simulation in France, was to build interfaces between QMCPack and other software for electronic structure computations, e.g. the DFT code Quantum Espresso.

These interfaces are used to manage the orbital reading or their DFT generation within QMCPack, to establish an automated, black box workflow for QMC computations. QMC simulation can for example be used in the benchmark and validation of DFT calculations: such a procedure can be employed in the study of several physical systems of interest in condensed matter physics, chemistry or material science, with application in industry, e.g. in the study of metal-ion or water-carbon interfaces.

The following modules have been built as part of this pilot project and are presented in this report:

- QMCQEPack, that provides the files to download and properly patch Quantum Espresso 5.3 to build the `libpwinterface.so` library; this library is required to use the module `ESPWSCFInterface` to generate single particle orbitals during a QMCPack computation using Quantum Espresso.
- `ESInterfaceBase` that provides a base class for a general interface to generate single particle orbitals to be used in QMC simulations in QMCPack; implementations of specific interfaces as derived classes of `ESInterfaceBase` are available as the separate modules as follows:
  - `ESHDF5Interface`
  - `ESPWSCFInterface`

The documentation about interfaces in QMCPack can be seen in the QMCPack user manual at this location.

1.1.2 Extending the functionalities of the Electronic-Structure Library

The ESL — The Electronic Structure Library — is a community-maintained library of software of use for electronic structure simulations. It is an extended library that can be employed by everyone for building their own packages

and projects. It consists of entries documenting functionalities, algorithms, interfaces, standards and pieces of code ranging from small routines for performing simple tasks, all the way up to complete libraries.

The ambition of the ESL is to segregate layers of functionality within modules which are general, standardised and efficient. In this way, new ideas, and new science, can be coded by scientists without needing to rewrite functionalities that are already well-established, and without needing to know more software engineering than science.

The background, vision and content of the ESL are described in a 2020 *J. Chem Phys.* featured article [8]. E-CAM is working closely with the ESL initiative for some years now, and four of our ESDWs have been dedicated to the ESL, which has helped foster the developments of this community initiative and, as evidenced by the featured article, can have a great impact on the community.

The following three modules were developed as part of the ESL ESDW *Integration of ESL modules into electronic-structure codes* that took place on February 17-28 2020 at the Centre Européen de Calcul Atomique et Moléculaire (CECAM) Headquarters in Lausanne:

- integration of ELSI-RCI in DFTB+: ELSI-RCI provides and enhances open-source software packages (such as DFTB+ which solve mathematical equations related to the simulation of materials and molecules at the atomic scale. ELSI is a library of numerical methods to deal with linear algebra problems, in particular to solve eigenvalue equations in electronic structure simulations. Scalability and portability were the main design pillars of ELSI: this library can efficiently run on a wide array of machines, going from laptops to High Performance Computing (HPC) supercomputers, both on CPUs and GPUs. See the ELSI documentation here.
- Integration of Libxc in FHI-AiMS: Libxc provides hundreds of well-tested approaches to calculate interactions between electrons at the atomic scale. Implementing them individually is long and tedious. With this integration, FHI-AIMS has undergone a paradigm shift and greatly expanded its capabilities in this domain.
- integration of PSolver in SIESTA and Octopus: A Poisson solver is an efficient tool to determine electromagnetic fields produced by an electric charge distributed in space. The integration of PSolver into SIESTA and Octopus has opened the way for these software programs to access more complex physical systems.

1.2 Mass-Zero Constrained Dynamics for Orbital Free Density Functional Theory

MaZe stands for the Mass-Zero constrained molecular dynamics approach discussed in ref. [1]. This method enforces, at each time step, the Born-Oppenheimer condition that the system relaxes instantaneously to the ground state through the formalism of massless constraints. The adiabatic separation between the degrees of freedom is enforced rigorously, and the algorithm is symplectic and time-reversible in both physical and additional set of degrees of freedom.

The code is intended for condensed matter physicists and for material scientists and it can be used for various purposes related to the subject. Even though some analysis tools are included in the package, the main goal of the software is to produce particles trajectories to be analyzed in post-production by means of external software. Three modules are presented here for the MaZe code:

- MaZe for OF-DFT: Orbital-Free Density Functional Theory Molecular Dynamics (OF-DFT-MD) using the Mass-Zero (MaZe) constrained molecular dynamics approach described in [1];
- MaZe for OF-DFT (HPC version), is the optimized version of the MaZe for OF-DFT. The proposed optimisations allow a reduction of the execution time by roughly 50% compared to the original version of the code;
- NLCG for OF-DFT: Nonlinear Conjugate Gradient for OF-DFT, uses the Born-Oppenheimer approach to perform Orbital-Free Density Functional Theory Molecular Dynamics (OF-DFT-MD).

1.3 How to read this report

For each module, we give a short overview, followed by links to the module `Documentation` and the `Merge-Request` on the GitLab service of E-CAM, which shows detailed information about code development, testing and documentation. The different sections contain information on the practical applications of the codes developed, and their possible exploitation.

As this deliverable is the last one of its series, a section on the overall impact of the results achieved within the WP on Electronic Structure was also included, with an overview of the results achieved so far, how these have been disseminated in scientific publications, the industrial impact of the software developed, the training given in the WP which lead to many of the software outputs, and the societal impact of the WP.

2 QMCPack Interfaces for Electronic Structure Computations

The following four modules are interfaces between the QMCPack package and the DFT code Quantum Espresso.

2.1 ESInterfaceBase

2.1.1 Module description

Quantum Monte Carlo simulations of systems in the ground state require accurate trial wave functions to be able to give meaningful results. Such wave functions in electronic systems are given by a Jastrow term describing electronic correlations and a Slater determinant of single particle orbitals, to ensure that the trial wave function has the proper Fermi anti-symmetry. Usually Jastrow terms are defined in term of suitable pseudopotentials, which are then variationally optimized, while the particle orbitals in the determinant part are generated with a DFT computation. The ESInterface module consists in a base class to create interfaces for the generation and management of such single particle orbitals in QMCPack. Implementations of specific interfaces as derived classes of ESInterfaceBase are available as separate modules, which is the case of modules ESHDF5Interface and ESPWSCFInterface described below.

Direct Documentation Link	readme.rst of the ESInterfaceBase
Merge-Request Link	Merge-Request for the ESInterfaceBase Module

2.2 ESHDF5Interface

2.2.1 Module description

This module consists in a class, derived from ESInterfaceBase above, to create and manage interfaces for single particle orbitals written in suitable HDF5 files.

Direct Documentation Link	readme.rst of the ESHDF5Interface Module
Merge-Request Link	Merge-Request for the ESHDF5Interface Module

2.3 ESPWSCFInterface

2.3.1 Module description

This module consists in a class, derived from ESInterfaceBase above, to create and manage interfaces for single particle orbitals for QMCPack generated on the fly calling the Quantum Espresso software.

Direct Documentation Link	readme.rst of the ESPWSCFInterface Module
Merge-Request Link	Merge-Request for the ESPWSCFInterface Module

2.4 QMCQEPack_qepatch

2.4.1 Module description

This module provides the files to download and properly patch Quantum Espresso 5.3 to build the libpwinterface.so library; this library is required to use the module ESPWSCFInterface above, to generate single particle orbitals during a QMCPack computation using Quantum Espresso.

Direct Documentation Link	readme.rst of the QMCQEPack_qepatch Module
Merge-Request Link	Merge-Request for the QMCQEPack_qepatch Module

2.5 Motivation and exploitation of the QMCPack based modules data set

The aim of of the modules based on the QMCPack package that are presented here is to build interfaces with other software's commonly used in electronic structure computations, and specifically in this case the DFT code Quantum Espresso. These interfaces are used to manage the orbital reading or their DFT generation within QMCPack, to establish an automated, black box workflow for QMC computations. QMC simulations can, for example, be used in the benchmark and validation of DFT calculations: such a procedure can be employed in the study of several physical systems of interest in condensed matter physics, chemistry or material science, with applications in industry, e.g. in the study of metal-ion or water-carbon interfaces. Furthermore, QMC simulations are scalable to a large number of cores with limited memory requirements.

This work was done in connection to our pilot project on *QMCPack Interfaces for Electronic Structure Computations*.

3 Modules developed in collaboration with the ESL

The following three modules are developed in collaboration with the ESL initiative. Their aim is to expand the use of the ESL software library into other electronic structure codes. This contributes to fulfilling an important milestone for the ESL: proving the stability and applicability of libraries into real-world electronic structure codes.

3.1 Integration of ELSI-RCI in DFTB+

3.1.1 Module description

This module integrates the library ELSI into the electronic structure code DFTB+. ELSI is a library of numerical methods to deal with linear algebra problems. In particular ELSI allows solving the Kohn–Sham eigenvalue problem, which is often the bottleneck when performing large scale calculations during electronic structure simulations. ELSI acts as a unified software interface to access different algorithms, thus allowing an optimal use of different strategies. In addition, ELSI was designed to be scalable and portable and the resulting module can efficiently run on a wide array of machines, going from laptops to HPC supercomputers, both on CPUs and GPUs.

3.1.2 Motivation and exploitation

ELSI-RCI provides and enhances open-source software packages which solve mathematical equations related to the simulation of materials and molecules at the atomic scale. In essence, ELSI will allow an electronic structure code to run its eigenvalue and/or density matrix solutions through a single interface, leaving the details of handling the different libraries that are actually used to solve the problem to ELSI.

Direct Documentation Link	readme.rst of the module
Merge-Request Link	Merge-Request for the module

3.2 Integration of Libxc in FHI-AiMS

3.2.1 Module description

Libxc provides hundreds of well-tested approaches to calculate interactions between electrons at the atomic scale. Implementing them individually is long and tedious. By integrating Libxc with FHI-AIMS, this module allows for a paradigm shift and greatly expands FHI-AIMS capabilities in this domain.

3.2.2 Motivation and exploitation

The motivation for this module is twofold:

1. Implementation of a unified Libxc interface in FHI-aims
2. Enabling the use of Libxc functionals with the corresponding, properly generated minimal basis functions for GGA and meta-GGA functionals. This interfaces the scalar- relativistic atomic solver of FHI-aims (default version) with Libxc.

Libxc in FHI-aims is not only used for DFT calculations, but is needed for DFPT and the calculation of magnetic and optical response properties. After full integration of Libxc, it will form an essential part of each simulation and will be used by most of the FHI-aims users. In the long term, we hope that Libxc can extend and finally replace the internal FHI-aims XC library helping to move FHI-aims from a monolithic to a more modular software architecture. At the same time, we expect that the Libxc project will benefit from the increase of usability and visibility.

Direct Documentation Link	readme.rst of the module
Merge-Request Link	Merge-Request for the module

3.3 Integration of PSolver in SIESTA and Octopus

3.3.1 Module description

A Poisson solver is an efficient tool to determine electromagnetic fields produced by an electric charge distributed in space. The PSolver library allows solving the Poisson equation in much more general ways than using Fourier Transform. By integrating PSolver into SIESTA and Octopus, this module has opened the way for these electronic structure calculation tools to access more complex physical systems.

The PSolver library solves the Poisson equation using wavelets. With this approximation one can more easily take into account certain boundary conditions such as molecules (no boundaries), wires (periodic along 1 direction) and slabs (periodic along 2 directions). This is in contrast to Fourier transforms which assumes periodic boundary conditions

along all lattice vectors. Additionally it allows cavities for different dielectric constants. This implementation integrates the PSolver library into the DFT codes SIESTA and Octopus in such a way, that they may be used for end-users who require the functionalities.

3.3.2 Motivation and exploitation

Users of the SIESTA code have always been using the Fourier transforms for solving the Poisson equation. However, a great deal of users are dealing with, in particular, slab systems given the advent of graphene, 2D materials and surface calculations. This integration allows users to control the boundaries in a very strict way without any approximations, and opens the way for these electronic structure calculation codes to access more complex physical systems.

Direct Documentation Link	readme.rst of the module
Merge-Request Link	Merge-Request for the module

3.4 General application and exploitation of the ESL modules

The goal of the ESL is to provide a repository of tested, common software for electronic structure computations that can work as a tool box of utilities used by many electronic structure codes, that is simple to use by non-experts in a wide range of fields and applications (material science, chemistry, biology, ...). This allows researchers from both industry and academia to focus more on research in their specialised field rather than in software design or matters relating to the installation and compilation of their codes. The aim of the ESL modules set presented in this deliverable is to expand the use of the ESL software library into other electronic structure codes. This contributes to fulfilling an important milestone for the ESL: proving the stability and applicability of libraries into real-world electronic structure codes.

4 Modules for the code MaZe

4.1 MaZe for OF-DFT

4.1.1 Module description

The present module represents the main MaZe program. MaZe performs orbital-free density functional theory molecular dynamics (OF-DFT-MD) using the Mass-Zero (MaZe) constrained molecular dynamics approach as discussed in [1]. This method enforces, at each time step, the Born-Oppenheimer condition that the system relaxes instantaneously to the ground state through the formalism of massless constraints. The adiabatic separation between the degrees of freedom is enforced rigorously, and the algorithm is symplectic and time-reversible in both physical and additional set of degrees of freedom.

The computation of the electronic density is carried out in reciprocal space through a plane-waves expansion so that the mass-zero degrees of freedom are associated to the Fourier coefficients of the electronic density field. The evolution of the ions is performed using Velocity-Verlet algorithm, while the SHAKE algorithm is used for computation of the additional degrees of freedom. The code can sample the NVE and the NVT ensemble, the latter through a Langevin thermostat.

The code was optimised to run on HPC machines, effort that we describe in Section 4.2.

Direct Documentation Link	readme.rst of the module
Merge-Request Link	Merge-Request for the module

4.2 MaZe for OF-DFT (HPC version)

4.2.1 Module description

This version of the MaZe program has been optimized by the Istituto Italiano di Tecnologia (IIT) in Genova through the following steps:

- Improved FFTW usage: use FFTW patient planning;
- Async FFT/iFFT execution via pthread threadpool (C-Thread-Pool);
- ComputeForcesFromStructureFactor / ComputeStructureFactor loops parallelization through OpenMP.

The proposed optimizations on the FFT/iFFT routines allow a reduction of the execution time on all the GGA test cases by roughly 50% compared to the original version of the code.

Direct Documentation Link	readme.rst of the module
Merge-Request Link	Merge-Request for the module

4.3 NLCG for OF-DFT

4.3.1 Module description

This program performs Orbital-Free Density Functional Theory Molecular Dynamics (OF-DFT-MD) using the Born-Oppenheimer approach. The condition that the system relaxes instantaneously to the ground state is enforced, at each time step, finding the minimum of the energy for a given nuclear configuration using a nonlinear conjugate gradient method. The results of these simulations are used as benchmarks in [1].

Direct Documentation Link	readme.rst of the module
Merge-Request Link	Merge-Request for the module

4.4 Motivation and exploitation of the MaZe modules data set

The code is intended for condensed matter physicists and for material scientists and it can be used for various purposes related to the subject. Even though some analysis tools are included in the package, the main goal of the software is to produce particles trajectories to be analysed in post-production by means of external software.

MaZe implements the orbital-free formulation of density functional theory, in which the optimisation of the energy functional is performed directly in terms of the electronic density without use of Kohn-Sham orbitals. This feature avoids the need for satisfying the orthonormality constraint among orbitals and allows the computational complexity of the code to scale linearly with the dimensionality of the system. The accuracy of the simulation relies on the choice of the kinetic energy functional, which has to be provided in terms of the electronic density alone.

5 Overall impact of the results achieved within the Work-package

5.1 Overview of the results achieved so far

E-CAM's WP2 Electronic Structure focuses on the development of software that can help understand the behaviour of electron systems, fundamental to evaluating and predicting the properties of physical systems of interest in condensed matter physics and quantum chemistry, which have a great range of applications e.g. in material science, biology and nano-medicine. So far within this WP, **54** software modules have been developed which were certified according to the E-CAM guidelines [2]. The modules developed are:

- **Modules that are contributions to the ESL initiative**. E-CAM is working closely with the ESL — The Electronic Structure Library[8] initiative for some years now, and four of our ESDWs have been dedicated to the ESL and to supporting this community initiative. The goal of the ESL is to provide a repository of tested, common software for electronic structure computations that can work as a tool box of utilities used by many electronic structure codes, and that is simple to use by non-experts in a wide range of fields and applications. In this way, new ideas, and new science, can be coded by scientists without needing to rewrite functionalities that are already well-established, and without needing to know more software engineering than science. In other words, the goal is to separate the coding effort for cutting-edge research from the software infrastructure it rests on top of, which needs maintaining and rewriting at every step of the hardware race. The impact of the ESL can be therefore quite significant for the electronic structure community.

  For instance, the ESL Demonstrator is an atomic-scale simulation software illustrating how to use and bring together the various available components of the ESL. ESL-Demo is part of the ESL and is already used by newcomers to the electronic-structure field who want to learn how to perform electronic-structure calculations. In the same way, the ESL Bundle is a collection of libraries and utilities broadly used in electronic structure calculations, put together by the ESL to make their use easier by researchers and scientific software developers.

  The modules contributed by the ESL to E-CAM's software library are listed here.

- **Modules that extend the Wannier90 software package**. Wannier90[7] is a program that, for a given system, generates the Wannier functions with minimum spatial spreads, known as Maximally Localised Wannier Functions (MLWFs), among the class of all possible Wannier functions (WFs). The locality of MLWFs can be exploited to compute, among other things, band-structure, density of states and Fermi surfaces at modest computational cost. Wannier functions are an important class of functions which enable to obtain a real-space picture of the electronic structure of a system. They provide an insightful chemical analysis of the nature of bonding, and chemical reaction in condensed-matter physics, similar to the role played by localized molecular orbitals in chemistry. They are also a powerful tool in the study of dielectric properties via the modern theory of polarisation. The modules built in the context of E-CAM originate from one Wannier90 dedicated Extended Software Development Workshop (ESDW) and one pilot project (see next point), and they meet the desire of the electronic-structure community to extend the use of WFs, and in particular of MLWFs, to a broader class of physical and chemical problems by adding new functionalities to the Wannier90 code.

  The modules contributed by the Wannier90 developers to E-CAM's software library are listed here.

- **Modules that build electronic structure functionalities for multi-thread workflows**. In the context of a pilot project at the University of Cambridge, E-CAM developed tools to improve, isolate and automatize the calculation of MLWFs, key quantities to analyze the nature of chemical bonding (and therefore of material's properties) and its evolution during, for example, chemical reactions [7]. In particular, researchers implemented the Selected Columns of Density Matrix (SCDM) method in the pw2wannier90 interface code between the Quantum Espresso software and the Wannier90 code. Then, they used this implementation as the basis for a complete computational workflow for obtaining MLWFs and electronic properties based on Wannier interpolation of the Brillouin zone, starting only from the specification of the initial crystal structure. The workflow was implemented within the AiiDA materials informatics platform, and used to perform a High Throughtput study on a dataset of 200 materials. This work was done in the context of a collaboration between E-CAM, the MaX Centre of Excellence and NCCR MARVEL, and it is described in detail in Ref. [9] and in a success story reported here.

- **Modules for the quantum mechanical parameterisation of metal ions in proteins**. In the context of the E-CAM Pilot Project on Quantum Mechanical Parameterisation of Metal Ions in Proteins in collaboration with the Small and medium-sized enterprise (SME) BiKi Technologies, we developed a new approach for the accurate parameterisation of the metal ion-protein interactions in water using machine learning techniques. One quarter to one third of all proteins require metals to function but the description of metal ions in standard force fields is still quite primitive. The training scheme combines classical simulation with electronic structure calculations to produce a force field comprising standard classical force fields with additional terms for the metal ion-water and metal ion-protein interactions. The approach allows simulations to run as fast as standard molecular dynamics codes, and is suitable for efficient massive parallelism scale-up.

The modules developed for this purpose are listed here. Furthermore, the metal-ion force field developed by E-CAM is freely available. A paper was published with this work [3], as well as a success story.

- **Modules that are interfaces between the QMCPack package and Quantum Espresso**. In the context of an E-CAM pilot project, we built interfaces between QMCPack and the commonly used software for electronic structure computations Quantum Espresso. Such interfaces can be used to establish an automated, black box workflow for QMC computations (see sec. 1.1.1 of this deliverable). The modules developed in the context of this pilot project are listed here.
- **Modules that are tools to easily manipulate molecular geometries**. A set of pre- and post-treatment Fortran codes that can be used to easily manipulate molecular geometries was created, allowing to minimize the average energy obtained for a range of internuclear distances for the dimers of each element, and decrease the computational cost of a DFT calculation. These modules were developed in the context of the Pilot Project on Calculations for Applications in Photovoltaic Devices, in collaboration with Merck. Then, E-CAM scientists have used electronic structure calculations to study how a key magnitude – the HOMO-LUMO band gap – changes with respect to the molecular disposition of the donor-acceptor molecule pair. The work was reported in a joint publication with Merck[5], and in this success story.
- **Neural network models of condensed matter systems with PANNA**. PANNA (Properties from Artificial Neural Network Architectures) is a Python package for the design, implementation and deployment of deep neural networks for the study of solid state, and especially for crystal systems. The tools provided in this package allow the user to input their own data to train and validate neural networks to model condensed matter systems; an interface with the TensorFlow package allows efficient and user friendly implementation and monitoring of the network. Computation of energies and forces are available, to perform structural optimisation, and an interface with the molecular dynamics software LAMMPS allows the network model to be used to build an effective interatomic potential. As an open source software PANNA aims to provide to users both in academia and in the industry a platform for realistic simulations in material science, for example for the prediction of the equilibrium geometry of a solid or a molecule, or the computation of optical spectra and electronic properties of crystals (band gaps, Debye temperatures or the density of states). The work is described in Ref. [6], and the list of software modules developed in the context of the work can be found in our software library.
- **Modules for Mass-Zero Constrained Dynamics for Orbital Free Density Functional Theory**. The Mass-Zero (MaZe) package implements the orbital-free formulation of density functional theory, in which the optimisation of the energy functional is performed directly in terms of the electronic density without use of Kohn-Sham orbitals. This feature avoids the need for satisfying the orthonormality constraint among orbitals and allows the computational complexity of the code to scale linearly with the dimensionality of the system. The main goal of the software is to produce particles trajectories to be analysed in post-production by means of external software. The MaZe modules are described in the present document, in sec. 4.

The full portfolio of modules developed under WP2 is accessible from the software library for WP2 at https://e-cam.readthedocs.io/en/latest/Electronic-Structure-Modules/index.html.

57% of the total number of modules developed under WP2 arise from external contributions (i.e. participants to our ESDWs and collaborations which are not directly supported by the project), and 43% arise from internal contributions (i.e. from Postdoctoral Research Associate (PDRA) contributions). The external contribution is notable and reveals the significant number of collaborations this WP has established. We have worked with different groups (e.g. the Max CoE, NCCR Marvel), community projects (e.g. the ESL), several packages (e.g. Quantum Espresso, QMCPack), and the events organized within this WP (ESDWs and State-of-the-art workshops (SAW)s) have helped catalyse new developments in the field. In general terms, the work performed in WP2 of E-CAM will have a significant impact in the community.

5.2 Dissemination and exploitation

8 scientific publications originated from the project in the area of Electronic Structure, and at least one is work in progress.

1. Quantum Monte Carlo determination of the principal Hugoniot of deuterium, Michele Ruggeri, Markus Holzmann, David M. Ceperley, and Carlo Pierleoni, *Phys. Rev. B* **2020**, 102, 144108.
   DOI: https://doi.org/10.1103/PhysRevB.102.144108.
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2. PANNA: Properties from Artificial Neural Network Architectures, Ruggero Lot, Franco Pellegrini, Yusuf Shaidu, Emine Küçükbenli, *Comput. Phys. Commun.* **2020**, 256, 107402.
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3. Automated high-throughput Wannierisation, Valerio Vitale, Giovanni Pizzi, Antimo Marrazzo, Jonathan R. Yates, Nicola Marzari and Arash A. Mostofi, *npj Comput Mater* **2020**, 6, 66.
DOI: https://doi.org/10.1038/s41524-020-0312-y.

4. The CECAM Electronic Structure Library and the modular software development paradigm, Micael J. T. Oliveira et al., J. Chem. Phys. 2020, 153, 024117.
DOI: https://doi.org/10.1063/5.0012901. Open access version here.

5. Gap variability upon packing in organic photovoltaics, D. López-Durán , Etienne Plésiat, Michal Krompiec and Emilio Artacho, *PLoS ONE* **2020**, 15(6): e0234115.
DOI: https://doi.org/10.1371/journal.pone.0234115.

6. Wannier90 as a community code: new features and applications, G. Pizzi, V. Vitale, N. Marzari, D. Vanderbilt, I. Souza, A. A Mostofi, J. R Yates, et al., J. Phys.: Condens. Matter 2020, 32 165902.
DOI: https://doi.org/10.1088/1361-648X/ab51ff.

7. Force Field Parametrization of Metal Ions from Statistical Learning Techniques, Francesco Fracchia, Gianluca Del Frate, Giordano Mancini, Walter Rocchia, and Vincenzo Barone, *J. Chem. Theory Comput.* **2018**, 14, 255-273.
DOI: https://doi.org/10.1021/acs.jctc.7b00779.
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8. ζ-Glycine: insight into the mechanism of a polymorphic phase transition, Craig L. Bull, Giles Flowitt-Hill, Stefano de Gironcoli, Emine Kuçukbenli, Simon Parsons, Cong Huy Pham, Helen Y. Playforda and Matthew G. Tucker, *IUCrJ* **2017**, 4, 569–574.
DOI: https://doi.org/10.1107/S205225251701096X

We would like to note, in particular, that the 4th article on this list relating to the ESL was deemed to be of sufficient importance for a highlight of the paper to be included in AIP Scilights.

The software produced within this Work Package (WP) was also disseminated via conferences (e.g. APS meetings) and workshops organized by the members of the WP; via the project website (e.g. in success stories, in the modules of the month category, on the newsletter, etc.) - for an overview of the news items on our website that are associated to this WP see here, and through six deliverables produced during the project lifetime and that are listed here (Number 2 deliverables).

The activities within this WP fostered several scientific collaborations and we highlight collaboration with researchers at the EPFL (S. Bonella, N. Marzari, G. Pizzi), SISSA (S. Gironcoli, E. Küçükbenli), SNS di Pisa (F. Fracchia, G. Mancini), IIT Genova (W. Rocchia), University of Cambridge (M. Payne, V. Vitale, E. Artacho), Imperial College London (A. Mostofi), ENS Paris (R.Vuilleumier), Maison de la Simulation - Université Paris-Saclay (C. Pierleoni, M. Ruggeri), CIC Nanogune (D. Lopez), Simune Atomistics (Y. Pouillon), MPSD Hamburg (M. Olivera).

5.3 Industrial impact

Industry connection within this WP happened through two pilot project in collaboration with industry:

- Calculations for Applications in Photovoltaic Devices, in collaboration with Merck. The objective of this work was to provide important insight into the fabrication of organic solar cells. The output of this work was documented in a scientific publication together with the industrial partners[3] and a success story here.
- Quantum Mechanical Parameterisation of Metal Ions in Proteins, in collaboration with BiKi Technologies. The objective of this work was to build-up a suitable parameterisation of metal ions in protein-water systems using machine learning techniques. The output of this work was documented in a scientific publication together with the industrial partners[5] and a success story here.

We have held three workshops in WP2 that dealt with topics of interest for industry:

1. State-of-the-Art Workshop in Electronic Structure, 12 - 14 September 2016, Cranage Hall, United Kingdom. See the workshop report;
2. State-of-the-Art Workshop: Improving the accuracy of ab-initio predictions for materials, 17 - 20 September 2018, CECAM-FR-MOSER, France. See the workshop report;
3. Scoping Workshop: From the Atom to the Material, 18 - 20 September 2017, CECAM-UK-JCMAXWELL, University of Cambridge, United Kingdom. See the workshop report.

The scoping workshop (number 3 on the list) had particular success among industry and was attended by 8 industrialists from 7 large companies.

5.4 Training

During the lifetime of the projects we organized four ESDWs in the area of Electronic Structure:

- Electronic Structure Library Coding - Solvers, 6 - 17 July 2016, CECAM-ES, The Zaragoza Scientific Center for Advanced Modeling, Zaragoza, Spain, Event website. Workshop report;
- Wannier90 Software Development Workshop, 12 - 16 September 2016, San Sebastian, Spain. Workshop report;
- Scaling Electronic Structure Applications, 7 - 18 January 2019, CECAM-IRL, University College Dublin, Ireland. Event website. Workshop report;
- Integration of ESL modules into electronic-structure codes, 17 - 28 February 2020, CECAM-HQ-EPFL, Lausanne, Switzerland. Event website.

In total, 83 people were trained at these events, against a target of 60. Lectures and other training material has been stored on our Online Training Portal here.

An ESDW postponed from the 2020 programme of events (due to the COVID-19 pandemics) will happen on the 11 - 22 November 2021 at the CECAM-HQ at EPFL. The website for the event "ESDW: Improving bundle libraries" is at https://www.cecam.org/workshop-details/23.

5.5 Societal impact

Developments in electronic structure theory have wide-reaching technological implications, by improving the understanding of materials, their properties, and help the discovery of new materials for a large range of applications. Specific classes of material directly addressed by E-CAM developments include, but are not limited to, photovoltaic materials, drug design, catalysts, novel superconductors, topological insulators, electronic devices. The methods developed can allow cheaper and more effective product development in a wide range of industries. This is supported by the work of the ESL as highlighted in sec. 5.1.

There is a significant level of academic/industrial interaction in the field of WP2; and studies point out that it is not unusual for industry to outsource their electronic structure work to research groups in academia. In a report from Goldbeck Consulting on "Industry interactions of the electronic structure research community in europe", results from a survey on more than 400 scientists from 33 different institutions in 12 European countries showed the significant number of collaborations (90% of the respondents) between academia and industry.

The workshops organized by E-CAM (sec. 5.3) and the results from the E-CAM pilot projects are key to promote collaborations and societal change in the field of WP2. In this regard, E-CAM has also produced a number of case studies that report on successful academic/industrial interactions, more specifically the following: Calculations for Applications in Photovoltaic Devices, Accelerating the design and discovery of materials with tailored properties using first principles high-throughput calculations and automated generation of Wannier functions, and The simulation of metal ions in protein-water systems using machine learning.

6 Outlook

The present deliverable contains nine software modules: three that are part of the ESL project; three that are the basis for the Mass-Zero (MaZe) package, and four that are interfaces between the QMCPack package for QMC simulations and the electronic structure package Quantum Espresso. All the modules have been accepted in the E–CAM software library.

As this deliverable is the last one of its series in E-CAM, a section on the overall impact of the results achieved within the Work-package was also included, with an overview of the results achieved , how these have been disseminated in scientific publications, the industrial impact of the software developed, the training given in the WP which lead to many of the software outputs and the societal impact of the WP.

References

Acronyms Used

CECAM Centre Européen de Calcul Atomique et Moléculaire
DFT Density Functional Theory
WFs Wannier functions
ESDW Extended Software Development Workshop
HPC High Performance Computing
MLWFs Maximally Localised Wannier Functions
QMC Quantum Monte Carlo
ESL Electronic-Structure Library
WP2 Work Package 2
WP Work Package
SME Small and medium-sized enterprise
PDRA Postdoctoral Research Associate
SAW State-of-the-art workshops

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