DMP du projet "ERC PTEROSOR"

Plan de gestion de données créé à l'aide de DMP OPIDoR, basé sur le modèle "ERC DMP" fourni par Conseil européen de la recherche (European Research Council, ERC).

Plan Details

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Project Details

Project title	ERC PTEROSOR
Abstract	Catalysis and solar cell technologies are underpinned by a fundamental process: that of exciting systems to a higher energy level than the ground state. Defining an effective method to achieve this that also provides accurate energies of the excited states is often a challenge. The EU-funded PTEROSOR project will tackle this fundamental problem using mathematical techniques. The researchers' novel approach for measuring the energies of excited states and defining wave functions in molecular systems will hinge on the use of a general class of Hamiltonians with parity-time (PT) symmetry. The gateway between ground and excited states will be provided by exceptional points which lie at the boundary between broken and unbroken PT-symmetric regions.
Funding	• Conseil européen de la recherche (European Research Council, ERC) : 863481

Produits de recherche :

1. Quantum Package (Logiciel)
2. QuAcK (Logiciel)
3. Notebooks (Resource interactive)
4. Publications (Texte)

Contributeurs

Nom	Affiliation	Rôles
Pierre-Francois Loos		• Coordinateur du projet • Personne contact pour les données (QP, Quack, Publications, Notebooks)
Scemama Anthony		• Responsable du plan

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Summary

QuAcK

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QuAcK is a small quantum chemistry package written in Fortran by the coordinator of the project. It is mostly used for prototyping.
The size of the archive containing the source code is around 4MiB, and is composed of Fortran source files, Python and Bash scripts, and Makefiles.

Quantum Package

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Quantum Package is an open-source quantum chemistry package for performing selected configuration interaction calculations. It is developed on three sites : Toulouse (LCPQ), Paris (LCT) and Argonne (USA).
The code is under the AGPL v3 license and is hosted on GitHub (https://github.com/QuantumPackage/qp2), with a mirror on the Git repository of the institute of the coordinator of the project (https://git.irsamc.ups-tlse.fr/LCPQ/qp2).
The latest version was uploaded on Zenodo (10.5281/zenodo.3677565), and the GitHub repository is set up to automatically upload on Zenodo every new release. For each publication requiring a modification of Quantum Package, a release will be made and the zenodo DOI will be cited.

Notebooks

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All along the project, Mathematica / Jupyter / Org-mode notebooks will be produced. All this data will be versioned in the Git repository of the institute of the coordinator, publicly accessible. All the notebooks will be archived on Zenodo, and the DOI will be provided in publications.

Publications

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Question sans réponse.

FAIR data and resources

QuAcK is hosted on GitHub (https://github.com/pfloos/quack), with a mirror on the Git repository of the institute of the coordinator of the project (https://git.irsamc.ups-tlse.fr/scemama/quack).
The latest version was uploaded on Zenodo (http://doi.org/10.5281/zenodo.3745928), and the GitHub repository is now set up to automatically upload on Zenodo every new release. For each publication requiring a modification of QuAcK, a release will be made and the zenodo DOI will be cited.

QuAcK is open-source under the GPL v3 license. The project doesn't require any part of the code to be closed.
The latest version was uploaded on Zenodo (http://doi.org/10.5281/zenodo.3745928), and the GitHub repository is now set up to automatically upload on Zenodo every new release. For each publication requiring a modification of QuAcK, a release will be made and the zenodo DOI will be cited.

QuAcK operates internally with text files.
Standard 'xyz' format is used for atomic coordinates and GAMESS/US format for atomic basis sets is used. The Basis Set Exchange (BSE) website provides data in this format.

QuAcK is open-source under the GPL v3 license. The project doesn't require any part of the code to be closed. Along the project, the code will be structured in independent inter-operating components to make easier the extraction of a particular feature of the package.
Continuous integration will be set up to guarantee that the package is functional in the main branch. Developments will be made in a secondary development branch.

The mirroring of the GitHub repository in the institute of the coordinator provides a backup.
The automatic upload of new releases on Zenodo provides secure storage and long-term preservation of the source code.
We also plan to upload the code in the Software Heritage digital archive.