

ERC REGAL

Data Management Plan: Version 1

A. Laestadius

(Dated: August 10, 2023)

PROJECT DETAILS

Title	REGAL: Regularized Density Functional Analysis
Funder	European Research Council, ERC
Number	101041487
Principal Investigator	Andre Laestadius
ORCID iD	0000-0001-7391-0396
Affiliation	Oslo Metropolitan (OsloMet) University
Data Contact Person	Andre Laestadius

SUMMARY OF THE PROJECT

Density-functional theory (DFT), used together with the Kohn–Sham (KS) approach, is the most widely used method in quantum chemistry and its usefulness as a practical tool can hardly be overestimated. The central object is the universal density functional. However, this density functional is nondifferentiable, leaving many practical aspects of the theory unfounded. Nevertheless, extensive work has been done establishing exact conditions for the density functional, constituting one of the cornerstones of functional development. The aim of REGAL is to apply (generalizations of) the Moreau-Yosida regularization to DFT. This achieves not only differentiability, but also mitigates the problem of potential-representability and provides global solutions of the underlying variational problem. The project focuses on the mathematical understanding and development of approximate functionals, of particular use for the iterative KS scheme. The first objective is to establish the mathematical foundation of a regularized DFT, akin to the unregularized setting of standard DFT. Equipped with a regularized formulation, the aim of the second objective is to develop new and understand existing exact constraints for

the density functional. This intends to open up a whole new axis of method development for approximate functionals. Since the regularization transformation considered is lossless, REGAL opens up for a new theoretical bridge between formal DFT and density-functional approximations. The third objective is the study of the regularized KS iteration scheme.

RESEARCH OUTPUTS

1. Notebooks (Interactive Resource)
2. Textual data (Text)
3. Computer/source code (“proof-of-principle” codes in Python, Matlab, etc.)

I. DATA SUMMARY

- Purpose: The data generation is part of achieving and disseminating the objectives of REGAL.
- Types of data: The types of data generated by the project are the same as listed above as “Research outputs”.
- Origin and size of data: During the lifespan of the project, the team members of REGAL (researchers and PhD students) will produce Mathematica and/or Jupyter notebooks. The size of each notebook will be a few megabytes. Moreover, there will be a continuous production of publications, presentations, posters and reports, each a few megabytes. The size of these documents will be as small as possible. The size of the archive containing the generated data is projected at the moment to be around 10–100 megabytes.
- Data utility: The data generated within REGAL is (believed to be) useful to the greater community of this particular research field.

II. FAIR DATA

A. Making data findable

- A GitHub repository has been set up, <https://github.com/ERC-REGAL/REGAL>, which is publicly accessible. Possibly a Zenodo account will be created too. From the Github repository the source code can be updated automatically to Zenodo (if a DOI is needed).
- Important notebooks will be versioned in the GitHub repository. Such documents can be archived on Zenodo, so that the DOIs can be provided in publications (if applicable).
- Preprints will be made available on arXiv (and/or HAL) as early as possible and will be the main repository for preprints (links to arXiv will be posted in the GitHub repository). Publication will be posted in the Cristin repository (see below).
- Files of presentations, posters and reports will be made publicly accessible in the GitHub repository.
- A project web site will be created (using a OsloMet domain) that will help with the organization of the archived data (through links). Metadata in the HTML headers can be used to help the search engines reference this web site.

B. Making data openly accessible

- As mentioned above, the projects has a GitHub repository (<https://github.com/ERC-REGAL/REGAL>). This can if needed be set up to automatically upload on Zenodo for every new release of source code etc.
- The project doesn't require any part of the codes to be confidential. Nonetheless, the host institution (OsloMet) has decided that classification of data to be: Restricted (yellow).
- The Princial Investigator acknowledges that he must ensure open access to peer-reviewed scientific publications relating to the project's results. In particular, he

must ensure that:

- (i) At the latest at the time of publication, a machine-readable electronic copy of the published version or the final peer-reviewed manuscript accepted for publication, is deposited in a trusted repository for scientific publications (Cristin or arXiv).
 - (ii) Immediate open access is provided to the deposited publication via the repository, under the latest available version of the Creative Commons Attribution International Public Licence (CC BY) or a licence with equivalent rights; for monographs and other long-text formats, the licence may exclude commercial uses and derivative works (e.g. CC BY-NC, CC BY-ND).
 - (iii) Information is given via the repository about any research output (e.g., source code) or any other tools and instruments needed to validate the conclusions of the scientific publication.
- In conclusion: For publications, Creative Commons CC BY public license (Plan S compliant) will be used to permit the broadest form of re-use including for commercial purposes, provided that author attribution and integrity are maintained (<https://creativecommons.org/licenses/by/4.0/>)

C. Making data interoperable

- This will only be applicable if source code will be integrated into quantum chemistry software (or similar). This is not yet known whether this will be realized in the project's lifespan. However, e.g., the posting of relevant jupyter Notebooks on the project's GitHub allows for interoperability.

D. Increase data reuse

- Same remark as in Sec. II. C.

III. ALLOCATION OF RESOURCES

- The Principal Investigator will be responsible for making documents and data generated publicly available as outlined above.

IV. DATA SECURITY

- The GitHub repository provides backup. In addition, automatic upload of new releases on Zenodo provides secure storage and long-term preservation of the source code.

V. ETHICAL ASPECTS

- No ethics issues (identified) within this project.