hermes-rheo: An open-source Python package for rheological data analysis

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Software

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Summary

Scientific research produces significant volumes of structured and hi-fidelity data which require expert-guided processing prior to the generation of insight through visualization and modeling. Data scientists with relevant physical science domain knowledge are key to making the connection between subject matter experts and emerging technologies with potential to improve their workflows. However, in many cases there are gaps in applications between generalized 'big data' approaches that seek to identify and establish qualitative 'trends' and the specific quantitative needs of measurement science. The *piblin* (Mills et al., 2024) Python package developed at 3M aims to address these needs by providing a fundamental conceptual framework for reading, visualizing, processing, and writing analytical data, along with a concrete, accessible implementation.

To specifically address the needs of the rheology community, we have developed the *hermes-rheo* (Perego et al., 2024) Python package to complement and extend the piblin library. *hermes-rheo* offers a set of specialized transforms tailored for advanced rheological analysis within the piblin framework. These transforms can enhance data analysis workflows in rheological datasets, bridging the gap between general data-rich methodologies and the specialized research and development requirements of measurement science.

Statement of Need

The analysis of rheological datasets presents several technical challenges that hinder efficient data processing and the integration of novel analytical methodologies. Current workflows are predominantly dependent on proprietary software, which imposes significant limitations in customizing analysis pipelines and implementing emerging techniques such as Optimally Windowed Chirp (Geri et al., 2018), Gaborheometry (John Rathinaraj & McKinley, 2023), and Recovery Rheology (Lee et al., 2019). Moreover, the frequent development of new rheological models requires adaptable tools capable of accommodating evolving analytical frameworks, a flexibility often lacking in existing solutions. The increasing volume of experimental data further exacerbates the complexity of managing and processing large datasets efficiently. Additionally, the integration of multi-instrument and multi-technique data formats remains a critical bottleneck, complicating data interoperability and standardization across different measurement platforms.

The *hermes-rheo* Python package addresses these limitations by providing an open-source, extensible framework designed to facilitate the analysis, visualization, and processing of rheological data with enhanced flexibility, scalability, and reproducibility.

Installation

hermes-rheo is available on the Python Package Index (PyPI). It can be installed or updated using the following commands:

```
pip install hermes-rheo
pip install hermes-rheo --upgrade
```

Documentation

The package documentation is publicly available at hermes-rheo.readthedocs.io.

Features

The hermes-rheo package provides a series of powerful transforms designed to handle rheological data analysis,

Key transforms include:

```
from hermes_rheo.transforms.rheo_analysis import RheoAnalysis
from hermes_rheo.transforms.automated_mastercurve import AutomatedMastercurve
from hermes_rheo.transforms.mutation_number import MutationNumber
from hermes_rheo.transforms.owchirp_generation import OWChirpGeneration
```

- The `RheoAnalysis` transform is the core tool in *hermes-rheo*, offering a fast and efficient analysis of viscoelastic properties from datasets collected in both the frequency and time domains. It supports standard rheological tests, including frequency and temperature sweeps, creep, stress-relaxation, and flow and temperature ramps. Additionally, it can analyze time-resolved mechanical spectroscopy measurements obtained via Optimally Windowed Chirp, accommodating data from both stress- and strain-controlled rheometers.
- The `AutomatedMasterCurve` transform automatically generates master curve datasets (e.g., time-temperature superposition) through a data-driven machine learning algorithm developed by (Lennon et al., 2023). The method employs Gaussian process regression and maximum a posteriori estimation to automatically superimpose datasets.
- The `MutationNumber` transform returns the mutation number, M_u, using the following definition:(Jamali & McKinley, 2022)

$$M_u = \frac{T}{\lambda_\mu}$$

where $\lambda_\mu(t)$ is:

$$\lambda_\mu(t) = \left(\frac{d\ln g}{dt}\right)^{-1} \approx \frac{t_2 - t_1}{\ln\left(\frac{g_{t_2}}{g_{t_1}}\right)}$$

where g can be any viscoelastic property of interest (e.g. G*, G', G'').

- The `OWChirpGeneration` transform helps users design Optimally Windowed Chirp signals for use in their rheometers. Currently, it is specifically optimized for experiments conducted with TA TRIOS software.

The *hermes-rheo* project is under continuous development, and new transforms are regularly introduced to expand its functionality. If you have ideas or suggestions for additional transforms, please open a new issue on the GitHub Issues page. Contributions and feedback from the community help shape the future of **hermes-rheo** and ensure its capabilities stay aligned with user needs.

Tutorials

The software repository contain a `tutorial_notebooks` folder with a comprehensive set of Jupyter notebooks demonstrating the diverse capabilities of *hermes-rheo*.

Available File Readers

The `file_readers` directory contains an example file reader for rheological data collected using `TA TRIOS software`.

This reader was specifically designed to handle `.txt` files generated via the "Export to LIMS" command in TRIOS.
With the release of TRIOS V5, a new export format, `.json`, has been introduced (see new features here).
A reader for this format is currently in development. Additionally, a reader for Anton Paar CSV files is actively being developed and is expected to be released soon.

For other data formats or instruments, users can develop custom readers while leveraging the `hermes-rheo` package's data transforms for analysis. Requests for additional file formats can be raised as an issue in the hermes-rheo GitHub repository.

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References

Geri, M., Keshavarz, B., Divoux, T., Clasen, C., Curtis, D. J., & McKinley, G. H. (2018). Time-resolved mechanical spectroscopy of soft materials via optimally windowed chirps. *Phys. Rev. X*, *8*, 041042. https://doi.org/10.1103/PhysRevX.8.041042

Jamali, S., & McKinley, G. H. (2022). The mnemosyne number and the rheology of remembrance. *Journal of Rheology*, *66*(5), 1027–1039. https://doi.org/10.1122/8.0000432

John Rathinaraj, J. D., & McKinley, G. H. (2023). Gaborheometry: Applications of the discrete gabor transform for time resolved oscillatory rheometry. *Journal of Rheology*, *67*(2), 479–497. https://doi.org/10.1122/8.0000549

Lee, J. C.-W., Weigandt, K. M., Kelley, E. G., & Rogers, S. A. (2019). Structure-property relationships via recovery rheology in viscoelastic materials. *Phys. Rev. Lett.*, *122*, 248003. https://doi.org/10.1103/PhysRevLett.122.248003

Lennon, K. R., McKinley, G. H., & Swan, J. W. (2023). A data-driven method for automated data superposition with applications in soft matter science. *Data-Centric Engineering*, *4*, e13. https://doi.org/10.1017/dce.2023.3

Mills, M. J. L., Williams, B., Perego, Alessandro, & Alex, B. (2024). *3mcloud/piblin: Release of initial public package (v0.0.0a1)*. Zenodo. https://doi.org/10.5281/zenodo.13946933

Perego, A., Mills, M. J. L., & Vadillo, D. C. (2024). *Hermes-rheo (1.2.0)*. Zenodo. https://doi.org/10.5281/zenodo.14453081