i-Rheo-Tempo (Python App)

Model-Free, Quadrature-Free Reconstruction of the Shear Relaxation Modulus from Complex Viscosity

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1. Overview

i-Rheo-Tempo is a Python-based graphical application for the model-free, quadrature-free reconstruction of the shear relaxation modulus $G(t)$ from experimentally measured dynamic viscoelastic spectra.

The method operates in the complex-viscosity domain and implements the interval-slope formulation derived from the exact second-derivative representation of the inverse Fourier transform presented in:

> Ramírez, J. & Tassieri, M., *i-Rheo-Tempo: A model-free, quadrature-free reconstruction of the shear relaxation modulus from complex viscosity*, 2026.

Unlike conventional numerical Fourier inversion, recursive quadrature schemes, or generalized-Maxwell fitting, *i-Rheo-Tempo*:

- avoids numerical quadrature,
- does not impose a predefined relaxation spectrum,
- reconstructs $G(t)$ analytically from the local slopes of the complex-viscosity spectrum,
- incorporates explicit low- and high-frequency conditioning to reduce boundary artefacts,
- reports the reconstructed relaxation modulus only within the experimentally supported reciprocal time window.

The application is implemented in Python as a desktop graphical interface built with `PySide6`. It uses embedded `Matplotlib` figures for visualisation, while numerical processing is carried out with `NumPy`, `SciPy`, and `csaps`. The main program (`iRheoTempo.py`) provides a complete interactive workflow from input dynamic moduli to reconstructed time-domain relaxation behaviour, together with diagnostic plots, optional comparison with experimental stress-relaxation data, and export of the reconstructed results.

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2. Theoretical Basis

For viscoelastic fluids, the complex modulus

$$G^*(\omega) = G'(\omega) + iG''(\omega)$$

is converted into the complex viscosity

$$\eta^*(\omega) = \frac{G^*(\omega)}{i\omega} = \eta'(\omega) - i\eta''(\omega),$$

with

$$\eta'(\omega) = \frac{G''(\omega)}{\omega}, \qquad \eta''(\omega) = \frac{G'(\omega)}{\omega}.$$

The shear relaxation modulus can then be written equivalently as

$$G(t) = \frac{2}{\pi}\int_0^\infty \eta'(\omega)\cos(\omega t)\,d\omega, \tag{1}$$

$$G(t) = \frac{2}{\pi}\int_0^\infty \eta''(\omega)\sin(\omega t)\,d\omega. \tag{2}$$

In *i-Rheo-Tempo*, these relations are reformulated through two integrations by parts, yielding a second-derivative representation in which the inverse transform depends on the curvature of the viscosity functions rather than on the functions themselves. When the spectrum is represented piecewise linearly between neighbouring frequency points, the second derivative becomes a sum of Dirac delta contributions at the slope discontinuities. This leads to a compact interval-slope reconstruction formula in which each spectral interval contributes analytically through differences of neighbouring sine or cosine kernels.

In practical form, the two reconstructed branches are evaluated as

$$G_{\eta'}(t) = \frac{2}{\pi t^2}\sum_{k=1}^{N-1} a_k^{(1)}\left[\cos(\omega_{k+1}t) - \cos(\omega_k t)\right], \tag{3}$$

$$G_{\eta''}(t) = \frac{2}{\pi}\left[\frac{\eta''(0)}{t} + \frac{1}{t^2}\sum_{k=1}^{N-1} a_k^{(2)}\left[\sin(\omega_{k+1}t) - \sin(\omega_k t)\right]\right], \tag{4}$$

where $a_k^{(1)}$ and $a_k^{(2)}$ are the interval slopes of $\eta'(\omega)$ and $\eta''(\omega)$, respectively.

For viscoelastic fluids, the default physical condition is

$$\eta''(0) = 0.$$

3. Key Features

- Import experimental dynamic moduli $G'(\omega)$ and $G''(\omega)$
- Automatic conversion to complex viscosity $\eta^*(\omega)$
- Explicit low-frequency conditioning through insertion of the zero-frequency node
- Polynomial estimation of $\eta'(0)$ from the low-frequency spectrum
- Optional enforcement or manual specification of $\eta''(0)$

- Optional single-mode Maxwell terminal reference
- Modest high-frequency spectral completion for numerical regularisation
- Interpolation options: PCHIP, SPLINE, CSAPS
- Logarithmic resampling for numerical stability
- Interval-slope inversion of the second-derivative formulation
- Independent reconstruction from both viscosity branches:

$$G_{\eta'}(t), \qquad G_{\eta''}(t)$$

- Long-time robustness diagnostics based on the first low-frequency interval
- Slope-jump diagnostic plots
- Optional comparison with experimental $G(t)$, if supplied
- Interactive zooming and panning in all plots
- Export of reconstructed relaxation spectra

4. Input Data Formats

4.1. Dynamic Moduli (mandatory)

A text file (`.txt`, `.dat`, `.csv`, `.tsv`, `.tts`) containing three columns:

Column	Quantity	Units
1	Frequency	Hz or rad/s
2	Storage modulus $G'(\omega)$	Pa
3	Loss modulus $G''(\omega)$	Pa

Notes

- Frequencies must be strictly positive.
- Duplicate frequency points are removed automatically.
- At least 5 valid data points are required.
- If frequencies are supplied in Hz, the app automatically converts them to angular frequency using $\omega = 2\pi f$.

4.2. Experimental Relaxation Modulus (optional)

A text file (`.txt`, `.dat`, `.csv`, `.tsv`, `.gt`) containing two columns:

Column	Quantity	Units
1	Time t	s
2	Relaxation modulus $G(t)$	Pa

This dataset is used only for comparison, visual validation, and error diagnostics. It does not enter the inversion itself.

5. Workflow Summary

The workflow implemented in *i-Rheo-Tempo* is:

1. Load experimental dynamic moduli $G'(\omega)$ and $G''(\omega)$
2. Convert them into $\eta'(\omega)$ and $\eta''(\omega)$
3. Estimate and insert the explicit zero-frequency point:

$$\big(0,\ \eta'(0),\ \eta''(0)\big)$$

4. Optionally fit a single Maxwell terminal mode
5. Apply a modest high-frequency completion
6. Interpolate the extended spectrum in linear ω
7. Resample the interpolated spectrum on a logarithmically spaced grid
8. Compute the interval slopes of the resampled viscosity branches
9. Reconstruct $G(t)$ analytically from the interval-slope formulation
10. Report the result only in the experimentally supported reciprocal window

$$t \in \left[\frac{1}{\omega_{\max}^{\exp}},\ \frac{1}{\omega_{\min}^{\exp}}\right]$$

6. Boundary Conditioning

Because experimental spectra are finite in bandwidth, accurate inversion requires careful treatment of the spectral boundaries.

6.1. Low-Frequency Conditioning

The low-frequency limit is handled explicitly by inserting a zero-frequency node before interpolation:

- $\eta'(0)$ is estimated from a local polynomial fit to the low-frequency portion of $\eta'(\omega)$, or
- alternatively inferred from an optional single-mode Maxwell fit.

For viscoelastic fluids, the natural default condition is

$$\eta''(0) = 0.$$

This can either be enforced automatically or replaced with a user-specified value.

6.2. Maxwell Terminal Reference

Optionally, the low-frequency regime may be approximated by a single Maxwell mode:

$$G'(\omega) = G_0 \frac{(\omega\tau)^2}{1 + (\omega\tau)^2}, \tag{5}$$

$$G''(\omega) = G_0 \frac{\omega\tau}{1 + (\omega\tau)^2}, \tag{6}$$

which implies

$$\eta'(0) = G_0\tau, \qquad \eta''(0) = 0.$$

This option is useful as a physically constrained terminal reference and can help stabilise the long-time behaviour.

6.3. High-Frequency Completion

A modest high-frequency extension is constructed from local polynomial fits near the upper end of the measured spectrum. This extension is used only to regularise interpolation and reduce spurious curvature at the upper boundary. It is not intended to assign physical meaning to the unmeasured region.

7. User-Controlled Parameters

7.1. Frequency Units

- Hz or rad/s
- automatic conversion through $\omega = 2\pi f$ when Hz is selected

7.2. Low-Frequency Conditioning

- Low Freq Order: polynomial order for estimating $\eta'(0)$.
- Low Freq Fit Dec: spectral range (number of decades) used for the low-frequency fit.
- Low Freq Vis Dec: extra range (number of decades) shown in the plot for visual guidance.

7.3. High-Frequency Conditioning

- High Freq Order: polynomial degree for the high-frequency fit.
- High Freq Fit Dec: fitting range (in number of decades) below ω_{max}^{exp}.
- High Freq Vis Dec: extra range (number of decades) used to extend the spectrum beyond the maximum experimental frequency.

7.4. Interpolation and Resampling

- Method: PCHIP, SPLINE, or CSAPS
- CSAPS smoothing parameter: $p \in [0, 1]$ ($p = 1$ is equivalent to SPLINE)
- Resample points: number of logarithmically spaced points used in the inversion

7.5. Boundary Conditions

- Enforce $\eta''(0) = 0$: default for viscoelastic fluids
- User-defined $\eta''(0)$: optional override when enforcement is disabled
- Fitting of $\eta'(0)$
  - Polynomial: use the low-frequency fit to estimate $\eta'(0)$
  - Maxwell: use the overlaid Maxwell tail to estimate $\eta'(0)$ (when the Overlay Maxwell tail option is enabled).

7.6. Optional Features

- Overlay Maxwell tail: superimposes

  $$G(t) = G_0 e^{-t/\tau}$$

  as a terminal reference
- Show threshold: displays the constant robustness threshold marking the onset of long-time fragility

8. Outputs

8.1. Numeric Outputs

The GUI reports the following read-only quantities:

- fitted $\eta'(0)$
- Maxwell-based $\eta'(0) = G_0\tau$ when the terminal fit is enabled
- Maxwell parameters G_0, τ, and crossover frequency
- long-time robustness threshold
- mean relative absolute error (MRAE) versus experimental $G(t)$, when available

8.2. Plots

The app provides four main diagnostic plots:

- viscoelastic moduli $G'(\omega)$ and $G''(\omega)$
- complex viscosity spectrum, including experimental, interpolated, and resampled data
- reconstructed relaxation modulus $G(t)$ from both branches
- slope-jump spectrum, highlighting the spectral curvature structure

9. Long-Time Robustness and Interpretation

At long times, the reconstruction becomes increasingly sensitive to the lowest-frequency intervals of the viscosity spectrum. In practice, once

$$t \sim \frac{1}{\omega_{\min}^{\exp}},$$

the inversion becomes numerically fragile, and the reconstructed tail may exhibit amplified fluctuations.

To help identify this regime, *i-Rheo-Tempo* reports a constant robustness threshold derived from the first low-frequency interval. This threshold is a practical indicator of the onset of long-time unreliability. It should not be interpreted as a physical modulus level.

Accordingly:

- the long-time tail should be interpreted with caution near the upper end of the reciprocal experimental window,
- high- and low-frequency completions should be regarded as numerical stabilisation tools only,
- the reported relaxation modulus should be interpreted only within the experimentally supported time range.

10. Saving Results

The `Save G(t)` button exports a tab-delimited text file containing:

Column	Description
`t_s`	Time t in seconds
`G_from_eta1`	Reconstructed $G(t)$ from the cosine branch, i.e. from $\eta'(\omega)$
`G_from_eta2`	Reconstructed $G(t)$ from the sine branch, i.e. from $\eta''(\omega)$

11. Python Requirements

- Python 3.10 or later (recommended)
- NumPy 1.24 or later
- SciPy 1.10 or later
- Matplotlib 3.7 or later
- PySide6 6.5 or later
- CSaps 1.1 or later (required for `csaps`)

The requirements are listed in `pyproject.toml`. If Python 3.10 or later is installed, the application and its dependencies can be installed by running `pip install .` in the folder containing the Python source files and `pyproject.toml`.

12. Limitations and Notes

- The method is designed for linear viscoelastic spectra.
- The default formulation is tailored to viscoelastic fluids, for which $\eta''(0) = 0$.
- The long-time tail becomes progressively more ill-conditioned as $t \to 1/\omega_{\rm min}^{\rm exp}$.
- The high-frequency completion is purely numerical and should not be over-interpreted physically.
- The reconstructed $G(t)$ is reported only over the experimentally supported reciprocal time window.
- Agreement between the two reconstructed branches, $G_{\eta'}(t)$ and $G_{\eta''}(t)$, provides a useful internal consistency check.

13. Citation

If you use this software in academic work, please cite:

> J. Ramírez and M. Tassieri,
> *i-Rheo-Tempo: A model-free, quadrature-free reconstruction of the shear relaxation modulus from complex viscosity*, 2026.