README – i-Rheo Tempo Data Repository

DOI: 10.5525/gla.researchdata.2230

Version: 1.0

Date: April 2026

Title:

Data supporting "i-Rheo Tempo: A Model-Free, Quadrature-Free Reconstruction of the Shear Relaxation Modulus from Complex Viscosity"

Authors:

Manlio Tassieri (University of Glasgow)

Jorge Ramírez (Universidad Politécnica de Madrid)

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1. DESCRIPTION

This repository contains all datasets used in the manuscript describing the i-Rheo Tempo method, a model-free analytical framework for reconstructing the time-domain relaxation modulus G(t) from frequency-domain measurements.

The datasets span a range of systems used for validation, including:

- Synthetic viscoelastic models
- Industrial elastomers (SBR)
- Monodisperse polymer melts (polybutadiene)
- Model comb polymers
- Broadband microrheology (DWS)

These data are used to demonstrate the accuracy, robustness, and general applicability of the method across different materials and experimental conditions.

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2. FILE LIST AND CONTENT

DWS_Compliance

- Creep compliance derived from DWS microrheology measurements
- Used to benchmark broadband inversion performance

DWS_iRheo_Moduli

- Dynamic moduli G'(ω), G''(ω) obtained from DWS data
- Input dataset for i-Rheo Tempo reconstruction (Fig. 7)

lc3c50

- Dynamic moduli and/or relaxation data for the model comb polymer (Kapnistos & Vlassopoulos)
- Used for hierarchical relaxation validation (Fig. 6)

Moduli_Burgers

- Synthetic dynamic moduli generated from a two-mode Burgers model
- Used for analytical benchmarking and validation of reversibility

Moduli_Burgers_HighModuli

- Variant of Burgers model with extended terminal regime
- Used to assess robustness at long times

PB1.txt

PB2.txt

PB3.txt

- Dynamic moduli G'(ω), G''(ω) for three monodisperse polybutadiene melts

- Molecular weights:

  PB1: Mw ≈ 7.09 × 10^4 g/mol

  PB2: Mw ≈ 3.55 × 10^5 g/mol

  PB3: Mw ≈ 9.25 × 10^5 g/mol

- PB3 includes experimental G(t) for validation (Fig. 5)

PI_130k_Tminus30_tts

- Time–temperature superposition (TTS) dataset for monodisperse polyisoprene melt

- Used to reconstruct G(t) from frequency-domain data (Fig. 4)

SBR

- Step-strain dataset for industrial styrene–butadiene rubber

- Used to compare reconstructed G(t) with σ(t)/γ(t) (Fig. 3)

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3. DATA FORMAT

All datasets are provided as plain text files (.txt) or structured ASCII files.

Typical format:

- Column 1: angular frequency ω [rad/s] or time t [s]

- Column 2: storage modulus G'(ω) or stress/response

- Column 3: loss modulus G''(ω) (if applicable)

Units:

- Frequency: rad/s

- Time: s

- Moduli: Pa

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4. USAGE

These datasets can be directly used as input for:

- i-Rheo Tempo (MATLAB and Python implementations)

- Other viscoelastic analysis tools

The reconstruction workflow is described in detail in the manuscript (see Sections II–III).

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5. NOTES ON DATA INTERPRETATION

- All datasets correspond to linear viscoelastic measurements.

- The reconstructed relaxation modulus G(t) is physically meaningful within the time window:

$$t \in [1/\omega_{max}, 1/\omega_{min}]$$

- Apparent oscillations at long times originate from finite spectral bandwidth and do not carry additional physical information (see manuscript discussion).

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6. SOFTWARE

MATLAB and Python implementations of i-Rheo Tempo are available.

These tools enable direct reconstruction of G(t) from frequency-domain data using the interval-slope formulation described in the manuscript.

(Repository link or access details can be provided upon request.)

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7. LICENCE AND ACCESS

This dataset is provided for academic and research use.

Please cite the associated publication when using these data.

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8. CONTACT

Dr Manlio Tassieri

University of Glasgow

Email: manlio.tassieri@glasgow.ac.uk

Dr Jorge Ramírez

Universidad Politécnica de Madrid

Email: jorge.ramirez@upm.es

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9. RELATED PUBLICATION

See the accompanying manuscript for full methodological details and analysis:

i-Rheo Tempo: A Model-Free, Quadrature-Free Reconstruction of the Shear Relaxation Modulus from Complex Viscosity