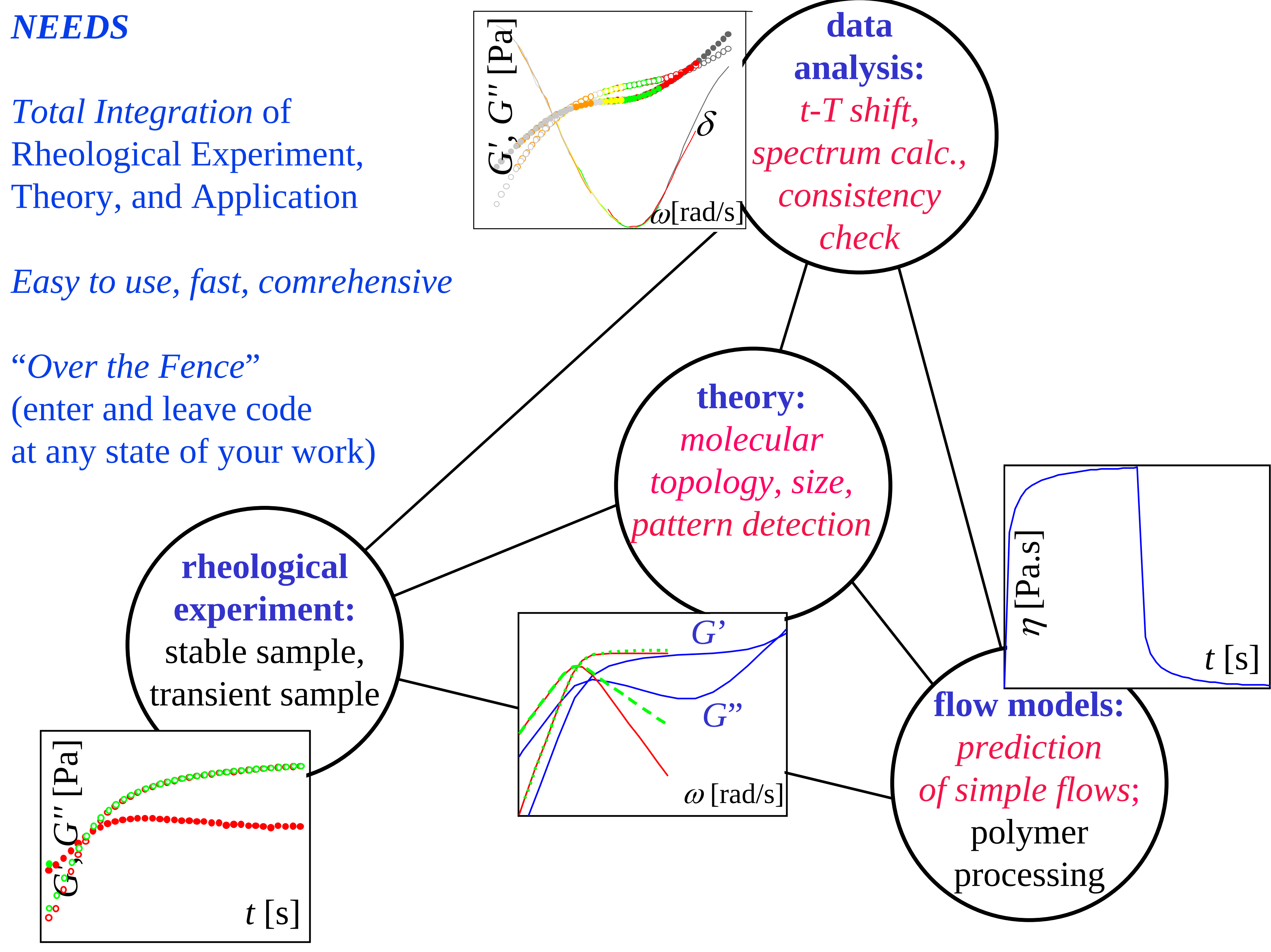
The IRIS Platform for Visualizing Experimental Data and Theoretical Predictions in Rheology

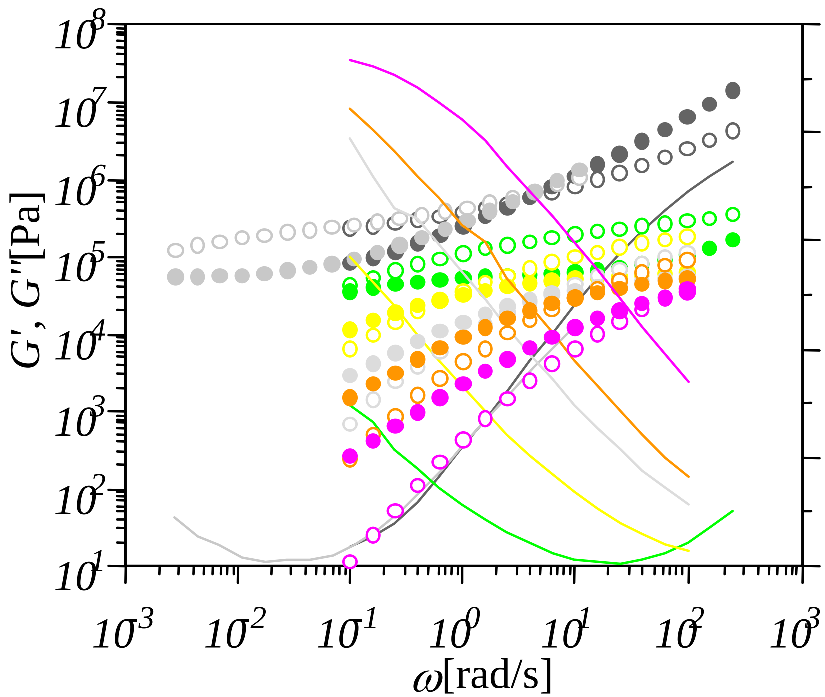
H. Henning Winter *UMass Amherst, USA;* **winter@ecs.umass.edu**
and *Marian Mours*, Weisenheim am Sand, Germany
in collaboration with Manfred Wagner, Richard Blackwell, and Yuichi Masubuchi

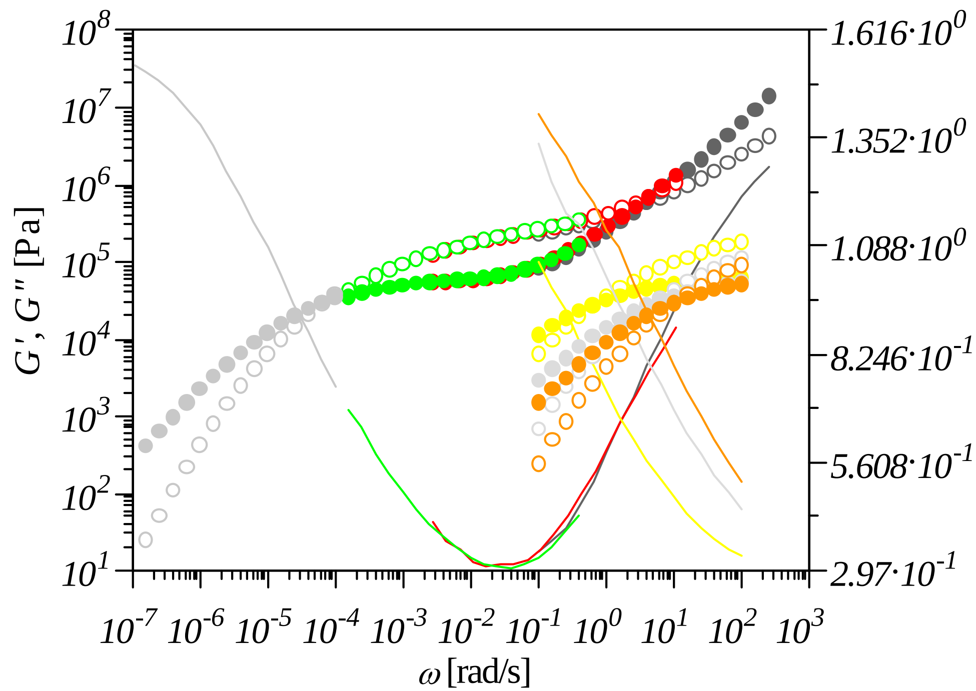

NEEDS
Total Integration of
Rheological Experiment,
Theory, and Application
Easy to use, fast, comrehensive
“Over the Fence”
(enter and leave code
at any state of your work)
G', G'' [Pa]
δ
ω[rad/s]
data analysis:
t-T shift,
spectrum calc.,
consistency check
theory:
molecular topology, size,
pattern detection
η [Pa.s]
t [s]
rheological experiment:
stable sample,
transient sample
G’
G”
ω [rad/s]
flow models:
prediction of simple flows;
polymer processing
G', G'' [Pa]
t [s]

Time–Temperature-Superposition
(Manual Shifting or Automated Shifting)

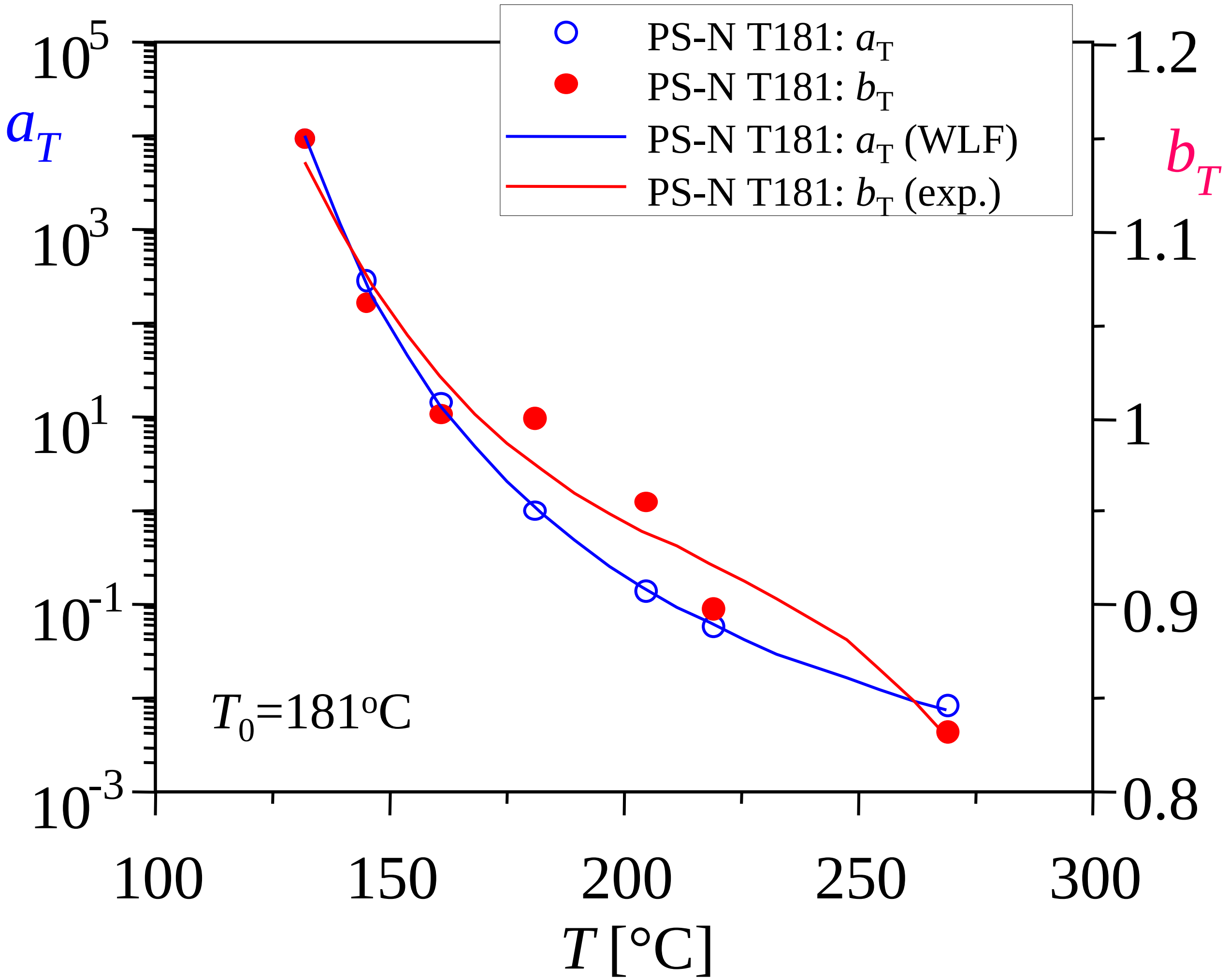
We would like to answer questions such as

- does time-temperature superposition apply to our material ?
- if it applies, what are the shift factor values ?
- does the horizontal shift follow WLF behavior ?





data analysis with IRIS



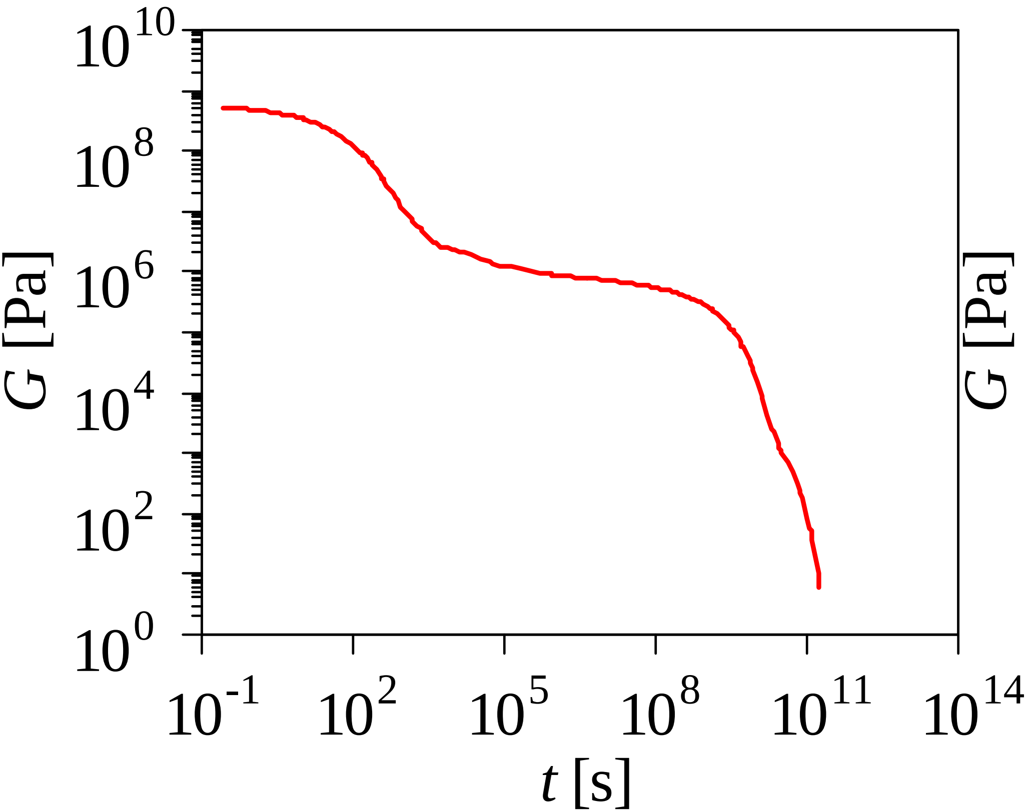
temperature shift factors

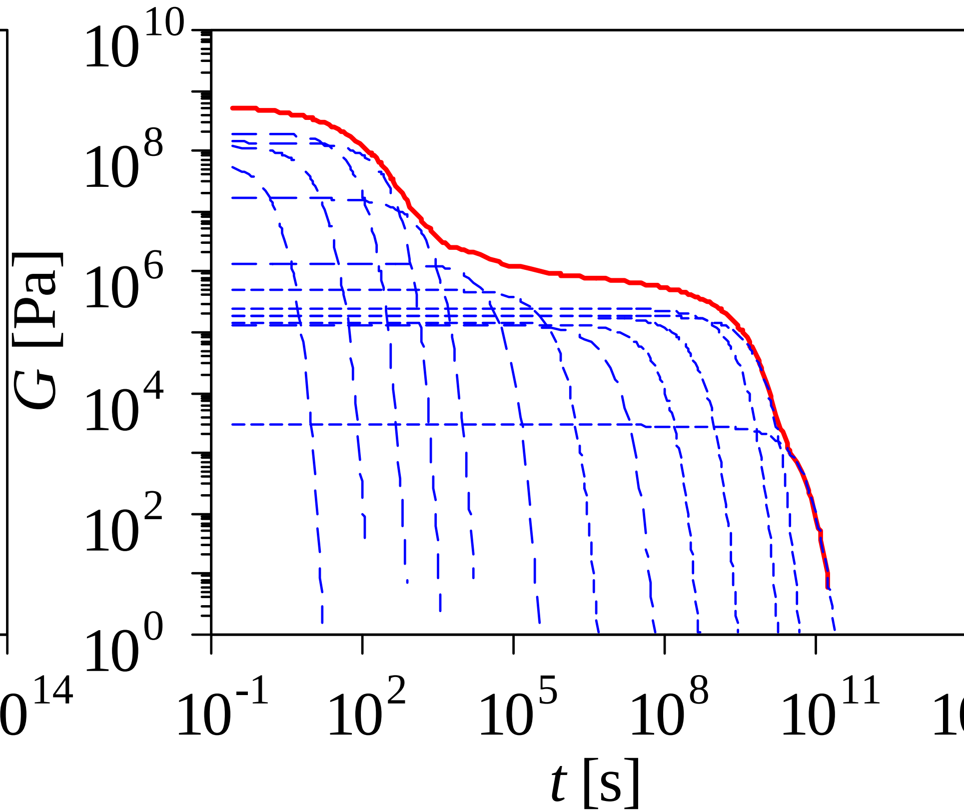
$$a_T(T;T_o) = \frac{\lambda_i(T)}{\lambda_i(T_0)}$$

$$b_T(T;T_0) = \frac{\rho_0 T_0}{\rho\, T}$$

Relaxation Modulus *G*(*t*) and Relaxation Time Spectrum *H*(*λ*),

$$G(t) = G_e + \int_0^{\infty} H(\lambda)\, e^{-t/\lambda}\, \frac{d\lambda}{\lambda}$$



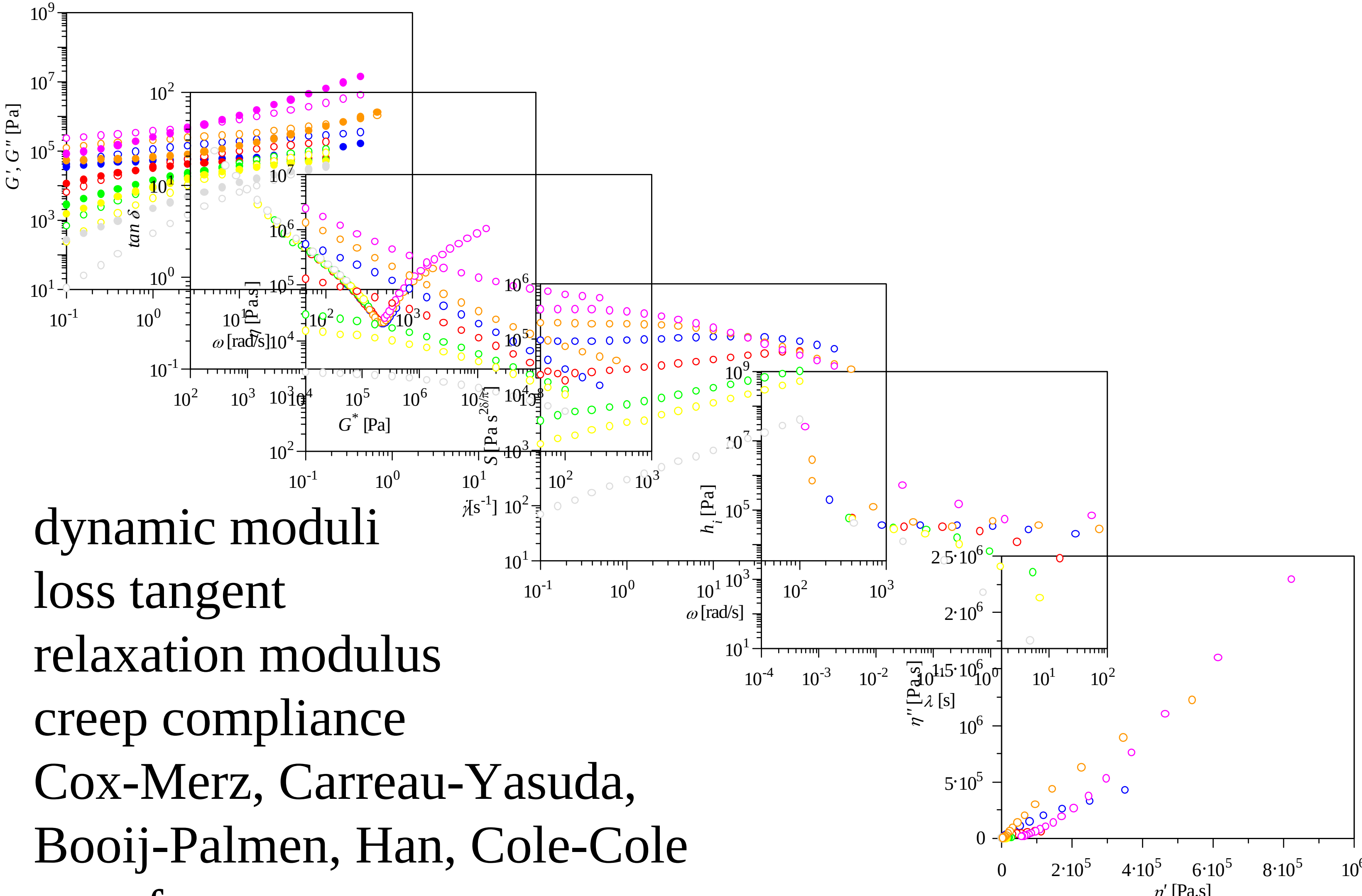


spectral decomposition

$$G(t) = \sum_{i=1}^{\infty} g_i e^{-t/\lambda_i}$$

data analysis with IRIS

Rheological Material Functions: generate your favorite plot



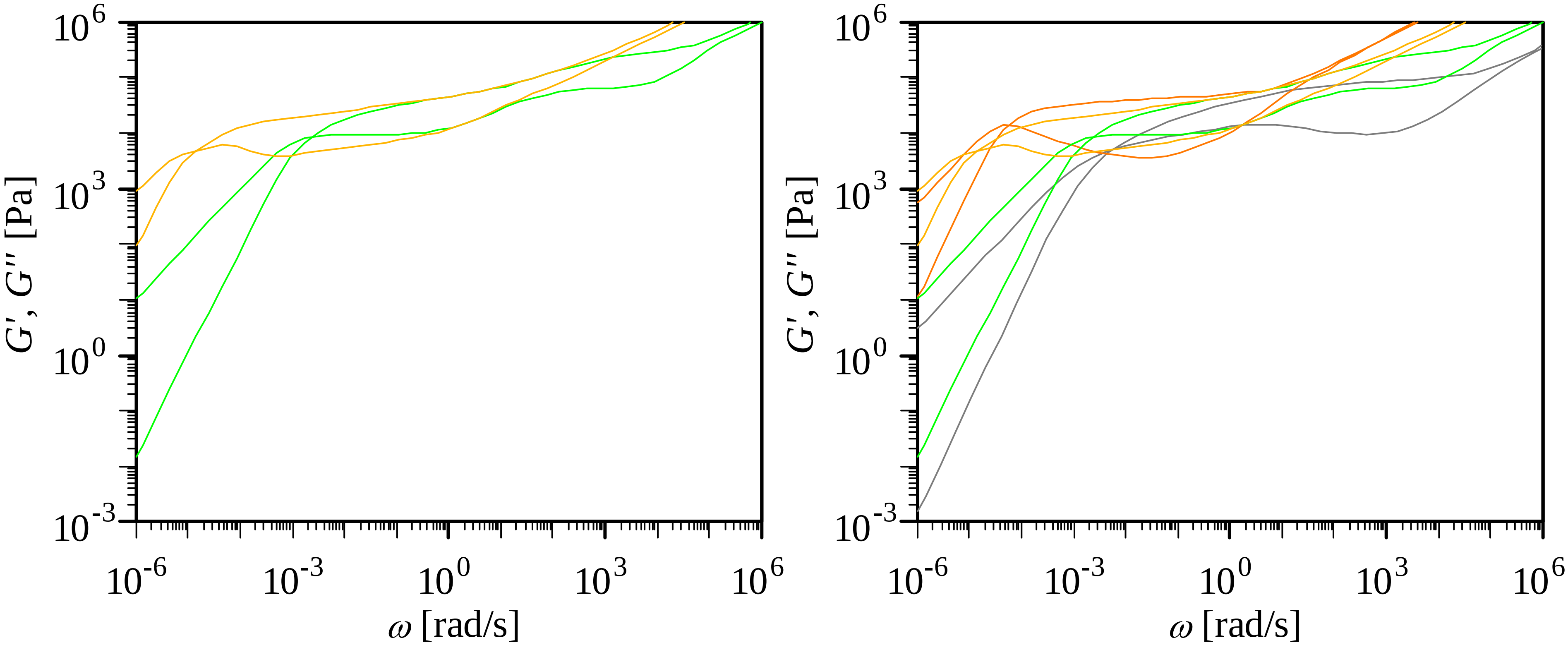
dynamic moduli
loss tangent
relaxation modulus
creep compliance
Cox-Merz, Carreau-Yasuda,
Booij-Palmen, Han, Cole-Cole
waveform
etc., etc.

calculated with IRIS module

Emulsion of Two Viscoelastic Phases (**Palierne Model)**

G'G"-data of

component A (linear polymer) and
component B (star polymer)
50/50 blend of A in B (Palierne model)
50/50 blend of B in A (Palierne model)

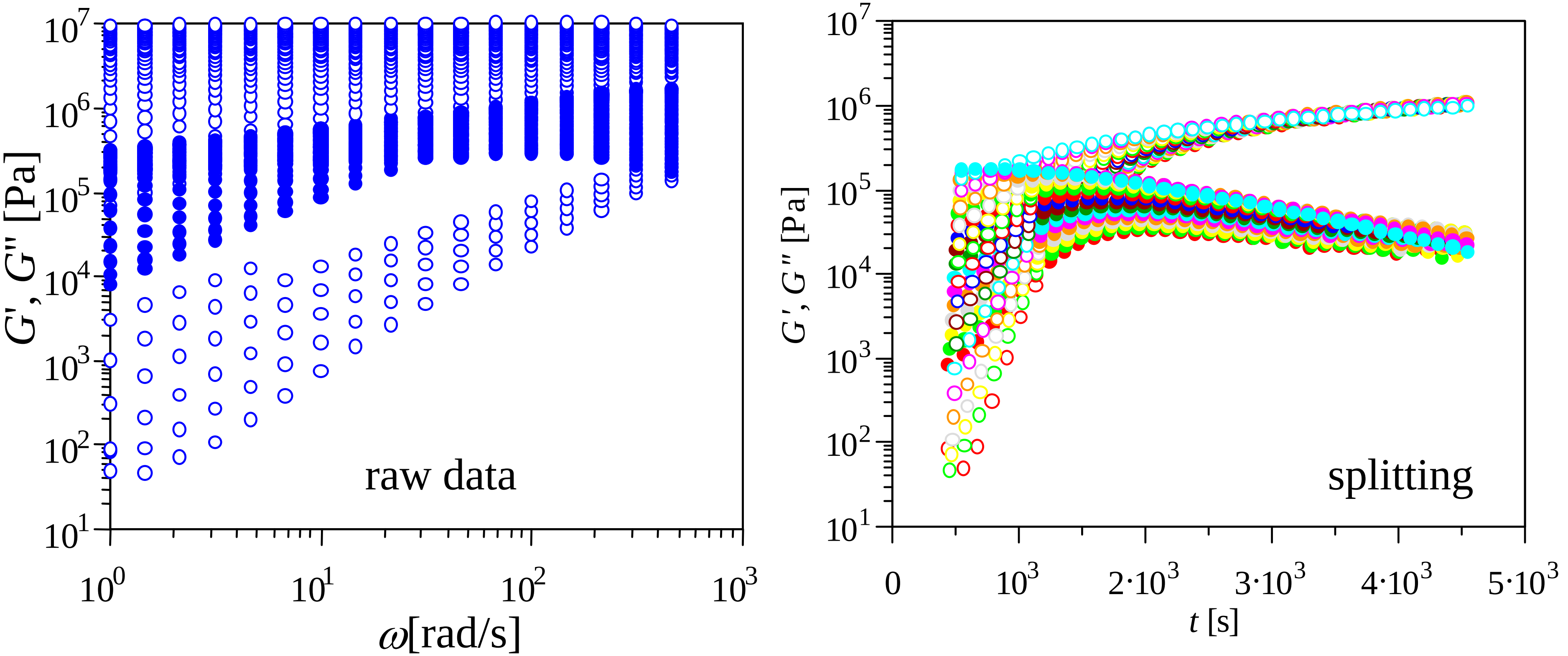


calculated with IRIS module

Time Resolved Mechanical Spectroscopy (TRMS)

Application for time-dependent matrial structure:

- gelation
- degradation
- crystallization
- melting
- phase separation

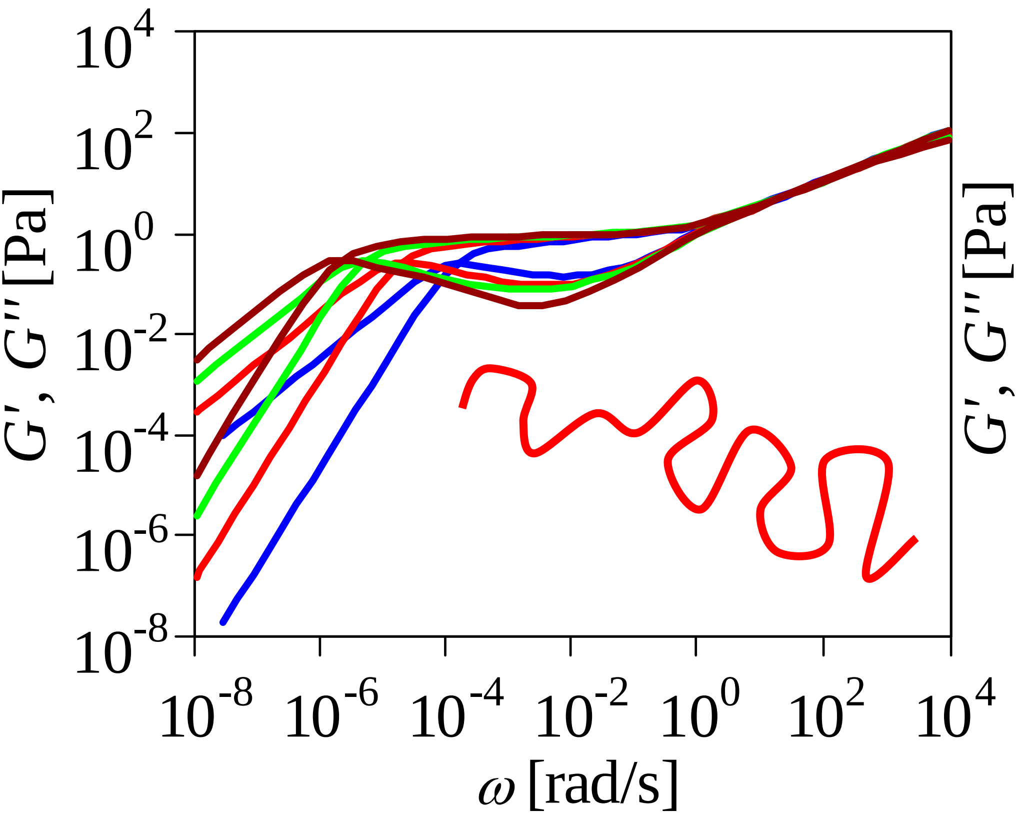


calculated with IRIS module

IRIS Module written by Richard J. Blackwell

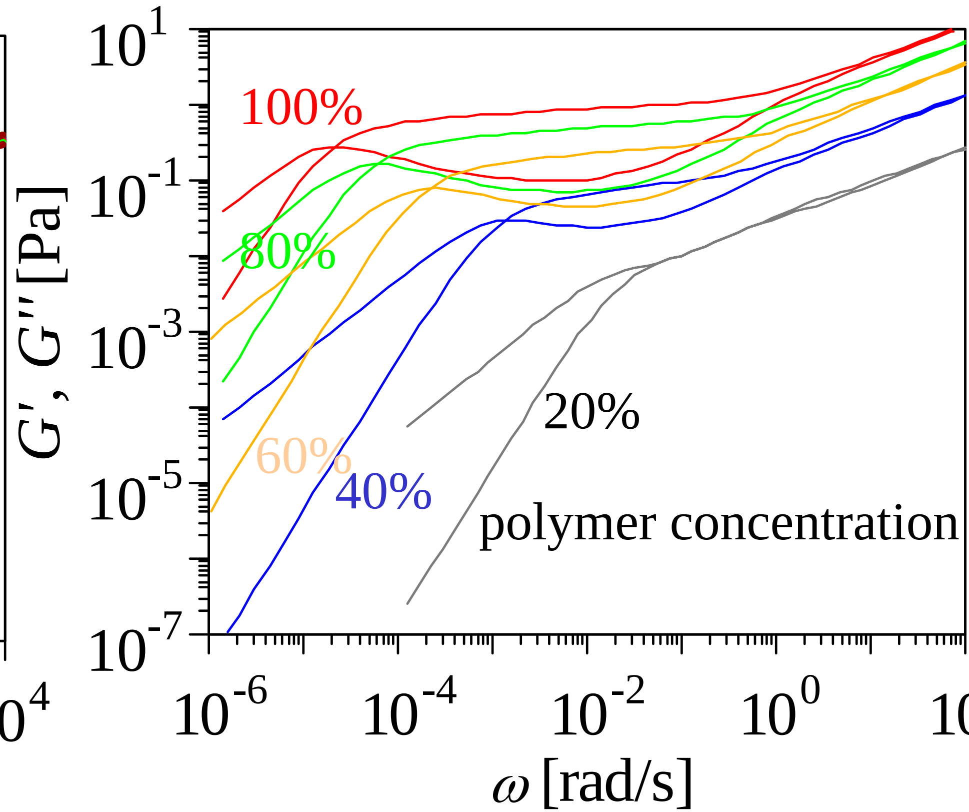
Tube Dilation Theories for Polymer Melt Rheology

Polymer Melt



path length: 20, 40 60, 80 * entanglement molecular weight

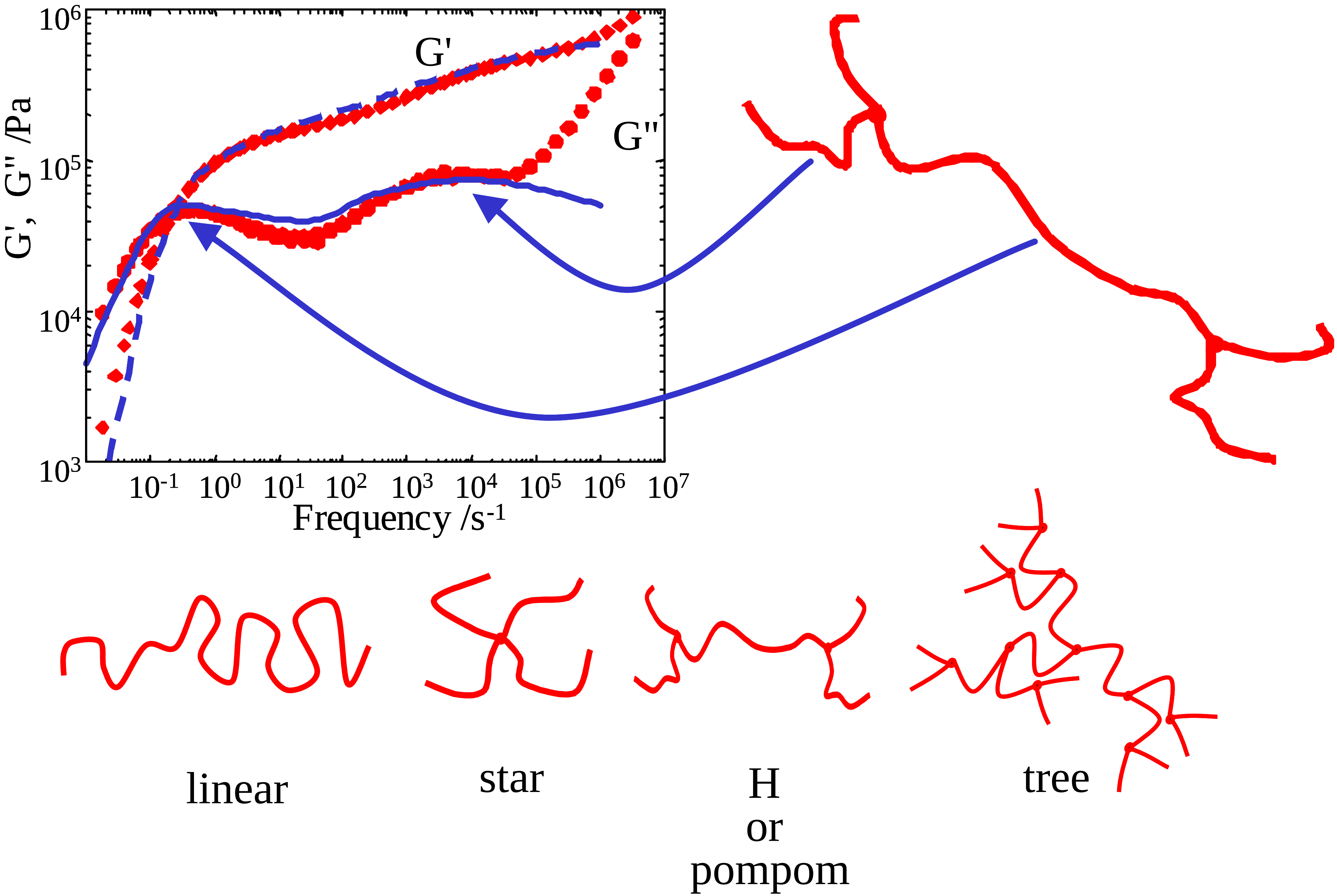
Dilution



40 * entanglement length, diluted

Calculated with IRIS, theory of Milner ST, McLeish TCB (1998)

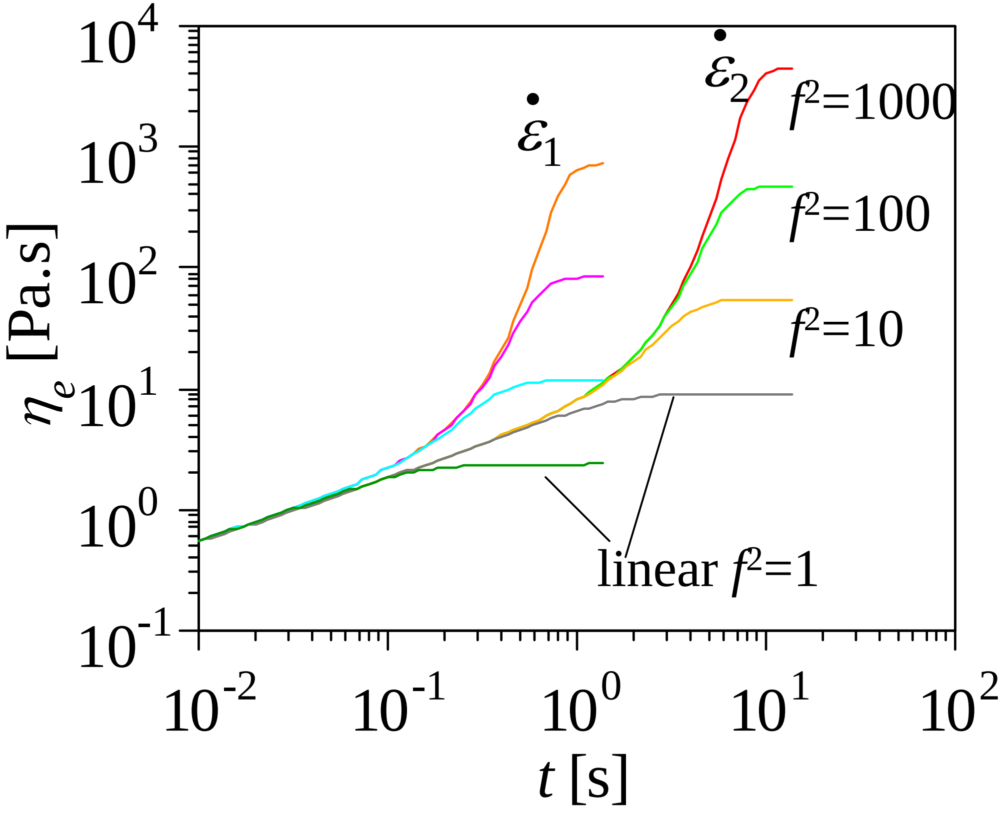
Expression of Macromolecular Architecture Through Rheology



Branching of Long Linear Flexible Chains of Uniform Length

Start with linear chains and
add more and more branches (increasing branching parameter f^2)

flow: start-up of uniaxial extension at rates $\dot{\varepsilon}_1 = 10 s^{-1}$ and $\dot{\varepsilon}_2 = 1 s^{-1}$



IRIS calculation with Molecular Stress Function Theory of M. Wagner

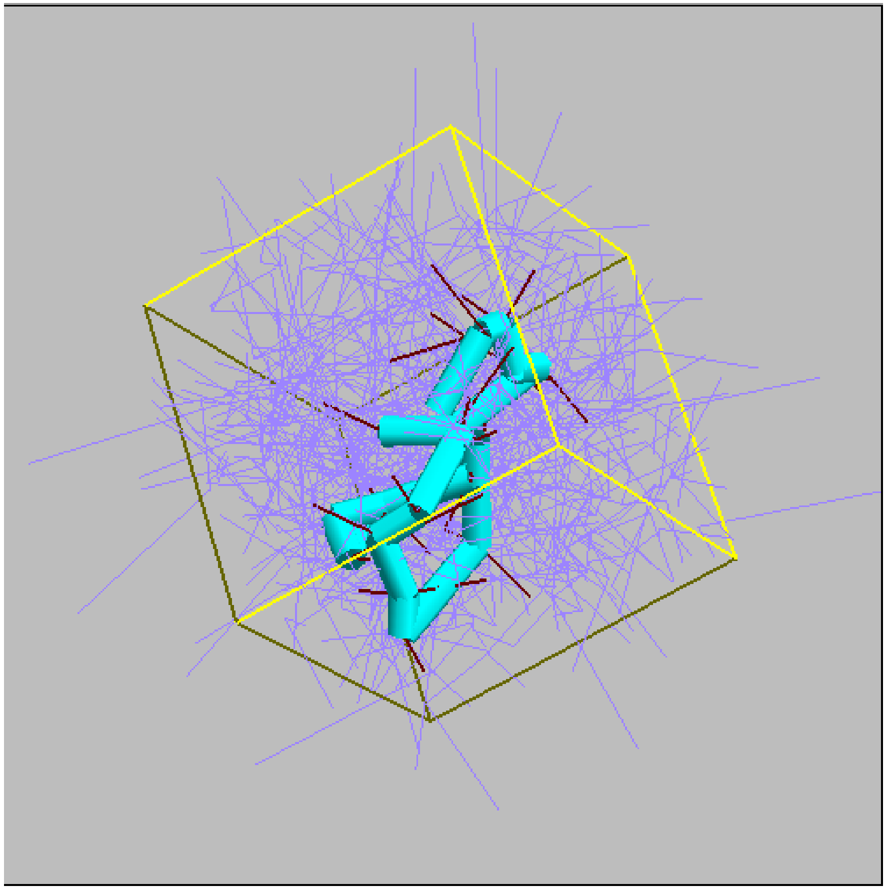
NAPLES Theory of Y. Masubuchi and Coworkers

Molecular Architecture and composition:

Linear, star, comb, H, homopolymer, blend, block copolymer

Parameters:

- Number of entanglement; $Z = M_w / M_e$
- Shape of the molecule (linear, star, comb…)
- Type of the flow (equilibrium, step shear,…)
- Plateau modulus; G_0 (stress shift factor)
- Characteristic time (time shift factor)



Masubuchi module in IRIS for NAPLES animation

SUMMARY

General Purposes of the IRIS

exploration of linear and non-linear viscoelasticity,
graphics tool for teaching rheology.

Specific Functions

1. data analysis of rheological experiments
   dynamic mechanical spectroscopy
   steady shear, step strain,
   transient shear, transient extension
2. theory predictions to relate molecular architecture with dynamics
   linear chains, stars, pom-pom, combs
3. search for patterns
4. prediction of some simple model flows
   start-up of shear or extension at constant rate

Information: http://rheology.tripod.com/ ; IRISrheo@yahoo.com